Model-Based Machine Learning

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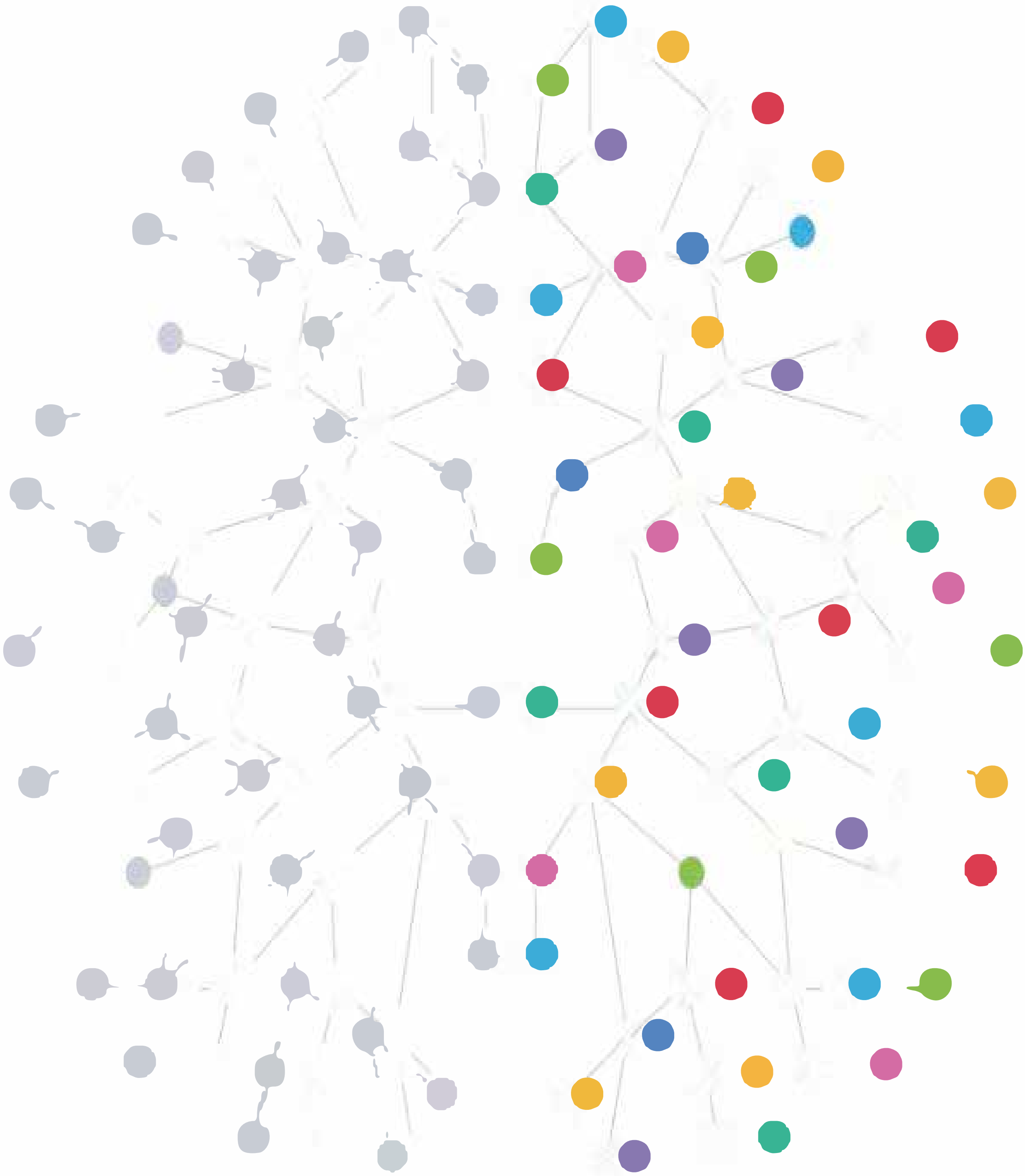

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with
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How can machine learning solve my problem?

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During the last few years, machine learning has moved to centre stage in the world of technology. Today, thousands of engineers and researchers are applying machine learning to an extraordinarily broad range of domains. However, making effective use of machine learning in practice can be daunting, especially for newcomers to the field. When someone is trying to solve a real-world problems using machine learning, they often encounter challenges:

> "I am overwhelmed by the choice of machine learning methods and techniques. There's too much to learn!"
>
> "I don't know which algorithm to use or why one would be better than another for my problem."
>
> "My problem doesn't seem to fit with any standard algorithm."

In this book we look at machine learning from a fresh perspective which we call **model-based machine learning**. Model-based machine learning helps to address all of these challenges, and makes the process of creating effective machine learning solutions much more transparent.

Machine learning can seem daunting to newcomers.

0.0.1 What is model-based machine learning?

Over the last five decades, researchers have created literally thousands of machine learning algorithms. Traditionally an engineer wanting to solve a problem using machine learning must choose one or more of these algorithms to try, or otherwise attempt to invent a new one. In practice, their choice of algorithm may be constrained by those algorithms they happen to be familiar with, or by the availability of specific software, and may not be the best choice for their problem.

By contrast the model-based approach seeks to create a bespoke solution tailored to each new application. Instead of having to transform your problem to fit some standard algorithm, in model-based machine learning you design the algorithm precisely to fit your problem.

The core idea at the heart of model-based machine learning is that all the *assumptions* about the problem domain are made explicit in the form of a **model**. In fact, a model is just made up of this set of assumptions, expressed in a precise mathematical form. These assumptions include the number and types of variables in the problem domain, which variables affect each other, and what the effect of changing one variable is on another variable. For example, in the next chapter we build a model to help us solve a simple murder mystery. The assumptions of the model include the list of suspected culprits, the possible murder weapons, and the tendency for particular weapons to be preferred by different suspects. This model is then used to create a model-specific algorithm to solve the specific machine learning problem. Model-based machine learning can be applied to pretty much any problem, and its general-purpose approach means you don't need to learn a huge number of machine learning algorithms and techniques.

So why do the assumptions of the model play such a key role? Well it turns out that machine learning cannot generate solutions purely from data alone. There are always assumptions built into any algorithm, although usually these assumptions are far from explicit. Different algorithms correspond to different sets of assumptions and, when the assumptions are implicit, the only way to decide which algorithm is likely to give the best results is to compare them empirically. This is time-consuming and inefficient, and it requires software implementations of all of the algorithms being compared. And if none of the algorithms tried gives good results, it is even harder to work out how to create a better algorithm.

Models versus algorithms

Let's look more closely at the relationship between models and algorithms. We can think of a standard machine learning algorithm as a monolithic box which takes in data and produces results. The algorithm must necessarily make assumptions since it is these assumptions that distinguish a particular algorithm from the thousands of others out there. However, in an algorithm those assumptions are implicit and opaque.

Now consider the model-based view. The model comprises the set of assumptions we are making about the problem domain. To get from the model to a set of predictions we need to take the data and compute those variables whose values we wish to know. This computational process we shall call *inference*. There are several techniques available for doing inference, as we shall discuss during the course of this book. The combination of the model and the inference procedure together define a machine learning algorithm, as illustrated in Figure 1.

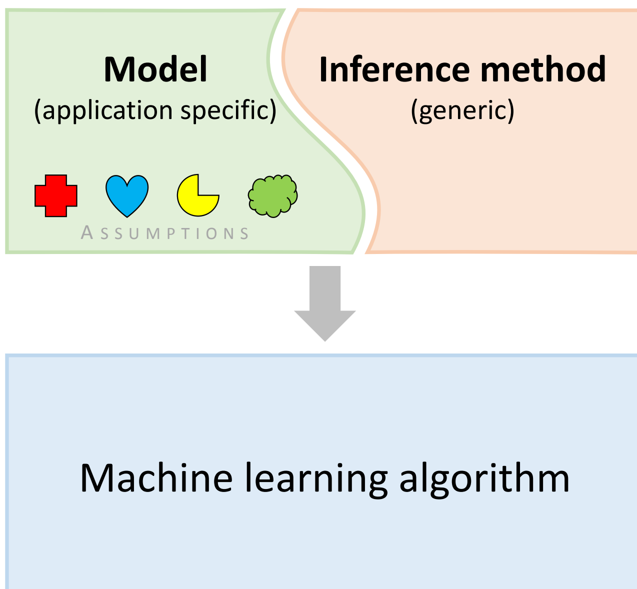


Figure 1: In the model-based view of machine learning, an algorithm arises from a particular combination of a model and an inference method. Here the coloured shapes within the model represent the assumptions comprising that specific model. Changes to the assumptions give rise to different machine learning algorithms, even when the inference method is kept fixed.

Although there are various choices for the inference method, by decoupling the model from the inference we are able to apply the same inference method to a wide variety of models. For example, most of the case studies discussed in this book are solved using just one inference method.

Model-based machine learning can be used to do any standard machine learning task, such as classification (chapter 4) or clustering (chapter 6), whilst providing additional insight and control over how these tasks are performed. Solving these tasks using model-based machine learning provides a way to handle extensions to the task or to improve accuracy, by making changes to the model – we will look at an example of this in chapter 4. Additionally, the assumptions you are making about the problem domain are laid out clearly in the model, so it is easier to work out why one model works better than another, to communicate to someone else what a model is doing, and to understand what's happening when things go wrong. Using models also makes it easier to share other people's solutions in order to adapt, extend, or combine them.

An example: predicting skills

Suppose you wish to track the changing skill of a player in an online gaming service (this is the problem we will explore in detail in chapter 3). A machine learning textbook might tell you that there is an algorithm called a 'Kalman filter' which can be used for these kinds of problems. Suppose you decide to try and make use of some Kalman filter software to predict how a player's skill evolves over time. First you will have to work out how to convert the skill prediction task into the form of a standard Kalman filter. Having done that, if you are lucky, the software might give a sufficiently good solution. However, the results from using an off-the-shelf algorithm often fail to reach the accuracy level required by real applications. How will you modify the algorithm, and the corresponding software, to achieve better results? It seems you will have to become an expert on the Kalman filter algorithm, and to delve into the software implementation, in order to make progress.

Contrast this with the model-based approach. You begin by listing the assumptions which your solution must satisfy. This defines your model. You then use this model to create the corresponding machine-learning algorithm, which is a mechanical process that can be automated. If your assumptions happen to correspond to those which are implicit in the Kalman filter, then your algorithm will correspond precisely to the Kalman filtering algorithm (and this will happen even if you have never heard of a Kalman filter). Perhaps, however, the model for your particular application has somewhat different assumptions. In this case, you will obtain a variant of the Kalman filter, appropriate to your application. Whether this variant already exists, or whether it is a novel algorithm, is irrelevant if your goal is to find the best solution to your problem. Suppose you try your model-based algorithm, and the results again fall short of your requirements. Now you have a framework for improving the results by examining and modifying the assumptions to produce a better model, along with the corresponding improved algorithm. As a domain expert it is far easier and more intuitive to understand and change the assumptions than it is to modify a machine learning algorithm directly. Even if your goal is simply to understand the Kalman filter, then starting with the model assumptions is by far the clearest and simplest way to derive the filtering algorithm, and to understand what Kalman filters are all about.

Tools for model-based machine learning

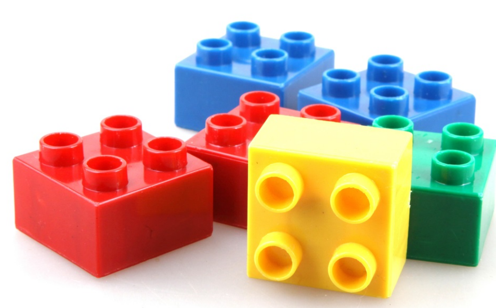
The decomposition of algorithms into a model and a separate inference method has another powerful consequence. It becomes possible to create a software framework which will generate the machine learning algorithm *automatically*, given only the definition of the model and a choice of inference method. This allows the applications developer to focus on the creation of the model, which is domain-specific, and frees them from the need to be an expert on the inner workings of the inference procedure.

For more than ten years we have been working on such a software framework at Microsoft Research, called **Infer.NET** [Minka et al., 2014]. Because a model consists simply of a set of assumptions it can be expressed in very compact code, which is relatively easy to understand and modify. The corresponding code for the algorithm, which is generally much more complex, is then produced automatically. All of the models in this book were created using Infer.NET, and the corresponding model source code is available online. However, these solutions could equally be implemented by hand or by using an alternative model-based framework – they are not specific to Infer.NET. Examples of alternative software frameworks that implement the model-based machine learning philosophy include BUGS [Lunn et al., 2000], Church, [Goodman et al., 2008], and Stan [Stan Development Team, 2014].

0.0.2 Who is this book for?

This book is rather unusual for a machine learning text book in that we do not review dozens of different algorithms. Instead we introduce all of the key ideas through a series of case studies involving real-world applications. Case studies play a central role because it is only in the context of applications that it makes sense to discuss modelling assumptions. Each chapter therefore introduces one case study which is drawn from a real-world application that has been solved using a model-based approach. The exception is the first chapter which explores a simple fictional problem involving a murder mystery.

Each chapter also serves to introduce a variety of machine learning concepts, not as abstract ideas, but as concrete techniques motivated by the needs of the application. You can think of these concepts as the building blocks for constructing models. Although you will need to invest some time to understand these concepts fully, you will soon discover that a huge variety of models can be constructed from a relatively small number of building blocks. By working through the case studies in this book you will learn how to use these components, and will hopefully gain a sufficient appreciation



Only a few building blocks are needed to construct an infinite variety of models.

of the power and flexibility of model-based
approach to allow *you* to solve *your* machine learning problem.

Inference deep-dive

This book is intended for any technical person who wants to use machine learning to solve a real-world problem – the focus of the book is on designing models to solve problems. However, some readers will also want to understand the mathematical details of how models are turned into inference algorithms. We have separated these parts of the book, which require more advanced mathematics, into inference deep-dive sections, which will be marked with panels like this one.

Deep-dive sections are *optional* – you can read the book without them. If you are planning on using a software framework like Infer.NET or just want to focus on modelling, you can skip these sections.

0.0.3 How to read this book

Sit back and relax, and we'll help you get to grips with machine learning.

Each case study in this book describes a journey from problem statement to solution. You probably do not want to follow this journey in a single sitting. To help with this, each case study is split into sections – we recommend reading a section at a time and pausing to digest what you have learned at the end of each section. To help with this, the machine learning concepts introduced in a section will be highlighted **like this** and will be reviewed at the end of each section (as you can see below). We aim to provide enough details of each concept to allow the case studies to be understood, along with links to external sources, such as Bishop [2006], where you can get more details if you are interested in a particular topic.

Now, on to the first case study!

Review of concepts introduced in this section

model-based machine learning An approach to machine learning where all the assumptions about the problem domain are made explicit in the form of a model. This model is then used to create a model-specific algorithm to learn or reason about the domain. The algorithm creation part of this process can be automated.

model A set of assumptions about a problem domain, expressed in a precise mathematical form, that is used to create a machine learning solution.

Infer.NET A software framework developed at Microsoft Research Cambridge which can do model-based machine learning automatically given a model definition. Available for download at the Infer.NET website.

Chapter 1

A Murder Mystery

As the clock strikes midnight in the Old Tudor Mansion, a raging storm rattles the shutters and fills the house with the sound of thunder. The dead body of Mr Black lies slumped on the floor of the library, blood still oozing from the fatal wound. Quick to arrive on the scene is the famous sleuth Dr Bayes, who observes that there were only two other people in the Mansion at the time of the murder. So who committed this dastardly crime? Was it the fine upstanding pillar of the establishment Major Grey? Or was it the mysterious and alluring femme fatale Miss Auburn?

We begin our study of model-based machine learning by investigating a murder. Although seemingly simple, this murder mystery will introduce many of the key concepts that we will use throughout the book.

The goal in tackling this mystery is to work out the identity of the murderer. Having only just discovered the body, we are very uncertain as to whether the murder was committed by Miss Auburn or Major Grey. Over the course of investigating the murder, we will use clues discovered at the crime scene to reduce this uncertainty as to who committed the murder.

Immediately we face our first challenge, which is that we have to be able to handle quantities whose values are uncertain. In fact the need to deal with uncertainty arises throughout our increasingly data-driven world. In most applications, we will start off in a state of considerable uncertainty and, as we get more data, become increasingly confident. In a murder mystery, we start off very uncertain who the murderer is and then slowly get more and more certain as we uncover more clues. Later in the book, we will see many more examples where we need to represent uncertainty: when two players play each other in Xbox live it is more likely that the stronger player will win, but this is not guaranteed; we can be fairly sure that a user will reply to a particular email but we can never be certain.

Consequently, we need a principled framework for quantifying uncertainty which will allow us to create applications and build solutions in ways that can represent and process uncertain values. Fortunately, there is a simple framework for manipulating uncertain quantities which uses **probability** to quantify the degree of uncertainty. Many people are familiar with the idea of probability as the frequency with which a particular event occurs. For example, we might say that the probability of a coin landing heads is 50% which means that in a long run of flips, the coin will land heads approximately 50% of the time. In this book we will be using probabilities in a much more general sense to quantify uncertainty, even for situations, such as a murder, which occur only once.

Let us apply the concept of probability to our murder mystery. The probability that Miss Auburn is the murderer can range from 0% to 100%, where 0% means we are certain that Miss Auburn is innocent, while 100% means we are certain that she committed the murder. We can equivalently express probabilities on a scale from 0 to 1, where 1 is equivalent to 100%. From what we know about our two characters, we might think it is unlikely that someone with the impeccable credentials of Major Grey could commit such a heinous crime, and therefore our suspicion is directed towards the enigmatic Miss Auburn. Therefore, we might assume that the probability that Miss Auburn committed the crime is 70%, or equivalently 0.7.

To express this assumption, we need to be precise about what this 70% probability is referring to. We can do this by representing the identity of the murderer with a **random variable** – this is a variable (a named quantity) whose value we are uncertain about. We can define a random variable called `murderer` which can take one of two values: it equals either `Auburn` or `Grey`. Given this definition of `murderer`, we can write our 70% assumption in the form

$$P(\texttt{murderer} = \texttt{Auburn}) = 0.7 \tag{1.1}$$

where the notation $P(\,)$ denotes the probability of the quantity contained inside the brackets. Thus equation (1.1) can be read as "the probability that the murderer was Miss Auburn is 70%". Our assumption of 70% for the probability that Auburn committed the murder may seem rather arbitrary – we will work with it for now, but in the next chapter we shall see how such probabilities can be *learned* from data.

We know that there are only two potential culprits and we are also assuming that only one of these two suspects actually committed the murder (in other words, they did not act together). Based on this assumption, the probability that Major Grey committed the crime must be 30%. This is because the two probabilities must add up to 100%, since one of the two suspects must be the murderer. We can write this probability in the same form as above:

$$P(\texttt{murderer} = \texttt{Grey}) = 0.3. \tag{1.2}$$

We can also express the fact that the two probabilities add up to 1.0:

$$P(\texttt{murderer} = \texttt{Grey}) + P(\texttt{murderer} = \texttt{Auburn}) = 1. \tag{1.3}$$

This is an example of the **normalization constraint** for probabilities, which states that the probabilities of all possible values of a random variable must add up to 1.

If we write down the probabilities for all possible values of our random variable `murderer`, we get:

$$\begin{aligned} P(\texttt{murderer} = \texttt{Grey}) &= 0.3 \\ P(\texttt{murderer} = \texttt{Auburn}) &= 0.7. \end{aligned} \tag{1.4}$$

Written together this is an example of a **probability distribution**, because it specifies the probability for every possible state of the random variable `murderer`. We use the notation $P(\texttt{murderer})$ to denote the distribution over the random variable `murderer`. This can be viewed as a shorthand notation for the combination of $P(\texttt{murderer} = \texttt{Auburn})$ and $P(\texttt{murderer} = \texttt{Grey})$. As an example of using this notation, we can write the general form of the normalization constraint:

$$\sum_{\texttt{murderer}} P(\texttt{murderer}) = 1 \tag{1.5}$$

where the symbol '$\sum$' means 'sum' and the subscript '`murderer`' indicates that the sum is over the states of the random variable `murderer`, i.e. `Auburn` and `Grey`. Using this notation, the states of a random variable do not need to be listed out – very useful if there are a lot of possible states!

At this point it is helpful to introduce a pictorial representation of a probability distribution that we can use to explain some of the later calculations. Figure 1.1 shows a square of area 1.0 which has been divided in proportion to the probabilities of our two suspects being the murderer. The square has a total area of 1.0 because of the normalization constraint, and is divided into two regions. The region on the left has an area of 0.3, corresponding to the probability that Major Grey is the murderer, while the region on the right has an area of 0.7, corresponding to the probability that Miss Auburn is the murderer. The diagram therefore provides a simple visualization of these probabilities. If we pick a point at random within the square, then the probability that it will land in the region corresponding to Major Grey is 0.3 (or equivalently 30%) and the probability that it will land in the region corresponding to Miss Auburn is 0.7 (or equivalently 70%). This process of picking a value for a random variable, such that the probability of picking a particular value is given by a certain distribution is known as **sampling**. Sampling can be very useful for understanding a probability distribution or for generating synthetic data sets – later in this book we will see examples of both of these.

The Bernoulli distribution

The technical term for this type of distribution over a two-state random variable is a **Bernoulli distribution**, which is usually defined over the two states `true`

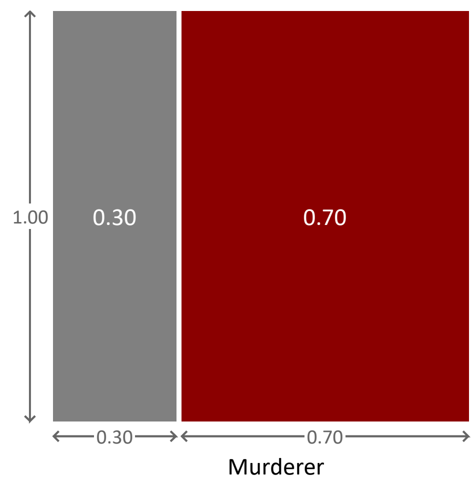


Figure 1.1: Representation of probabilities using areas. The grey area represents the probability that Major Grey is the murderer and the red area represents the probability that Miss Auburn is the murderer.

and `false`. For our murder mystery, we can use `true` to mean `Auburn` and `false` to mean `Grey`. Using these states, a Bernoulli distribution over the variable `murderer` with a 0.7 probability of `true` (`Auburn`) and a 0.3 probability of `false` (`Grey`) is written $Bernoulli(\texttt{murderer}; 0.7)$. More generally, if the probability of `murderer` being `true` is some number p, we can write the distribution of `murderer` as $Bernoulli(\texttt{murderer}; p)$.

Often when we are using probability distributions it will be unambiguous which variable the distribution applies to. In such situations we can simplify the notation and instead of writing $Bernoulli(\texttt{murderer}; p)$ we just write $Bernoulli(p)$. It is important to appreciate that is just a shorthand notation and does not represent a distribution over p. Since we will be referring to distributions frequently throughout this book, it is very useful to have this kind of shorthand, to keep notation clear and concise.

We can use the Bernoulli distribution with different values of the probability to represent different judgements or assessments of uncertainty, ranging from complete ignorance through to total certainty. For example, if we had absolutely no idea which of our suspects was guilty, we could assign $P(\texttt{murderer}) = Bernoulli(\texttt{murderer}; 0.5)$ or equivalently $P(\texttt{murderer}) = Bernoulli(0.5)$. In this case both states have probability 50%. This is an example of a **uniform distribution** in which all states are equally probable. At the other extreme, if we were absolutely certain that Auburn was the murderer, then we would set $P(\texttt{murderer}) = Bernoulli(1)$, or if we were certain that Grey was the murderer then we would have $P(\texttt{murderer}) = Bernoulli(0)$. These are examples of a **point mass**, which is a distribution where all of the probability is assigned to one value of the random variable. In other words, we are certain about the value of the random variable.

So, using this new terminology, we have chosen the probability distribution over `murderer` to be *Bernoulli*(0.7). Next, we will show how to relate different random variables together to start solving the murder.

Self assessment 1.0

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. To get familiar with thinking about probabilities, estimate the probability of the following events, expressing each probability as a percentage.
   (a) After visiting a product page on Amazon, a user chooses to buy the product.
   (b) After receiving an email, a user chooses to reply to it.
   (c) It will rain tomorrow where you live.
   (d) When a murder is committed, the murderer turns out to be a member of the victim's family.

   Given your estimates, what is the probability of these events not happening? (remember the normalization constraint). If you can, compare your estimates for these probabilities with someone else's and discuss where and why you disagree.

2. Write your answers to question 1 as Bernoulli distributions over suitably named random variables, using both the long and short forms.

3. Suppose I am certain that it will rain tomorrow where you live. What Bernoulli distribution represents my belief? What would the distribution be if instead I am certain that it will *not* rain tomorrow? What if I am completely unsure if it would rain or not?

4. For one of the events in question 1, write a program to print out 100 samples from a Bernoulli distribution with your estimated probability of the event happening (if you're not a programmer, you can use a spreadsheet instead). To sample from a *Bernoulli*(p) you first need a random number between 0 and 1 (RAND in Excel or random number functions in any programming language can give you this). To get one sample you then see if the random number is less than p in which case the sample is `true`, otherwise `false`. What proportion of the samples are `true`? You should find this is close to the parameter p. If you increase to 1,000 or 10,000 samples, you should find that the proportion gets closer and closer to p. We'll see why this happens later in the book.

Review of concepts introduced in this section

probability A measure of uncertainty which lies between 0 and 1, where 0 means impossible and 1 means certain. Probabilities are often expressed as a percentages (such as 0%, 50% and 100%).

random variable A variable (a named quantity) whose value is uncertain.

normalization constraint The constraint that the probabilities given by a probability distribution must add up to 1 over all possible values of the random variable. For example, for a $Bernoulli(p)$ distribution the probability of `true` is p and so the probability of the only other state `false` must be $1 - p$.

probability distribution A function which gives the probability for every possible value of a random variable. Written as $P(\mathtt{A})$ for a random variable `A`.

sampling Randomly choosing a value such that the probability of picking any particular value is given by a probability distribution. This is known as sampling from the distribution. For example, here are 10 samples from a $Bernoulli(0.7)$ distribution: `false`, `true`, `false`, `false`, `true`, `true`, `true`, `false`, `true` and `true`. If we took a very large number of samples from a $Bernoulli(0.7)$ distribution then the percentage of the samples equal to `true` would be very close to 70%.

Bernoulli distribution A probability distribution over a two-valued (binary) random variable. The Bernoulli distribution has one parameter p which is the probability of the value `true` and is written as $Bernoulli(p)$. As an example, $Bernoulli(0.5)$ represents the uncertainty in the outcome of a fair coin toss.

uniform distribution A probability distribution where every possible value is equally probable. For example, $Bernoulli(0.5)$ is a uniform distribution since `true` and `false` both have the same probability (of 0.5) and these are the only possible values.

point mass A distribution which gives probability 1 to one value and probability 0 to all other values, which means that the random variable is certain to have the specified value. For example, $Bernoulli(1)$ is a point mass indicating that the variable is certain to be `true`.

1.1 Incorporating evidence

Dr Bayes searches the mansion thoroughly. He finds that the only weapons available are an ornate ceremonial dagger and an old army revolver. "One of these must be the murder weapon", he concludes.

So far, we have considered just one random variable: `murderer`. But now that we have some new information about the possible murder weapons, we can introduce a new random variable, `weapon`, to represent the choice of murder weapon. This new variable can take two values: `revolver` or `dagger`. Given this new variable, the next step is to use probabilities to express its relationship to our existing `murderer` variable. This will allow us to reason about how these variables affect each other and to make progress in solving the murder.

Suppose Major Grey were the murderer. We might believe that the probability of his choosing a revolver rather than a dagger for the murder is, say, 90% on the basis that he is ex-military and would be familiar with the use of guns. But if instead Miss Auburn were the murderer, we might think the probability of her using a revolver would be much smaller, say 20%, on the basis that she is unlikely to be familiar with the operation of an old revolver and is therefore more likely to choose the dagger. This means that the probability distribution over the random variable `weapon` depends on whether the murderer is Major Grey or Miss Auburn. This is known as a **conditional probability distribution** because the probability values it gives vary depending on another random variable, in this case `murderer`. If Major Grey were the murderer, the conditional probability of choosing the revolver can be expressed like so:

$$P(\texttt{weapon} = \texttt{revolver}|\texttt{murderer} = \texttt{Grey}) = 0.9. \tag{1.6}$$

Here the quantity on the left side of this equation is read as "the probability that the weapon is the revolver *given* that the murderer is Grey". It describes a probability distribution over the quantity on the left side of the vertical 'conditioning' bar (in this case the value of `weapon`) which depends on the value of any quantities on the right hand side of the bar (in this case the value of `murderer`). We also say that the distribution over `weapon` is *conditioned* on the value of `murderer`.

Since the only other possibility for the weapon is a dagger, the probability that Major Grey would choose the dagger must be 10%, and hence

$$P(\texttt{weapon} = \texttt{dagger}|\texttt{murderer} = \texttt{Grey}) = 0.1. \tag{1.7}$$

Again, we can also express this information in pictorial form, as shown in Figure 1.2. Here we see a square with a total area of 1.0. The upper region, with area 0.9, corresponds to the conditional probability of the weapon being the revolver, while the lower region, with area 0.1, corresponds to the conditional probability of the weapon being the dagger. If we pick a point at random uniformly from within the square (in other words, sample from the distribution), there is a 90% probability that the weapon will be the revolver.

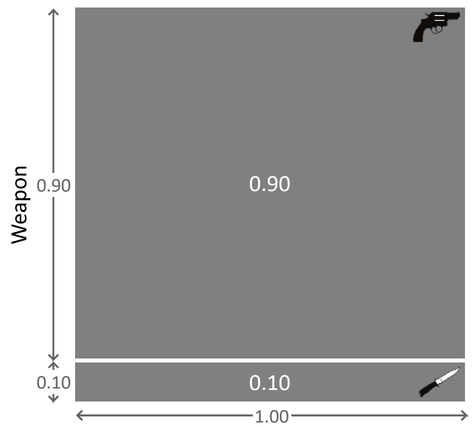


Figure 1.2: Representation of the probabilities for the two weapons, conditional on Major Grey being the murderer.

Now suppose instead that it was Miss Auburn who committed the murder. Recall that we considered the probability of her choosing the revolver was 20%. We can therefore write

$$P(\texttt{weapon} = \texttt{revolver}|\texttt{murderer} = \texttt{Auburn}) = 0.2. \tag{1.8}$$

Again, the only other choice of weapon is the dagger and so

$$P(\texttt{weapon} = \texttt{dagger}|\texttt{murderer} = \texttt{Auburn}) = 0.8. \tag{1.9}$$

This conditional probability distribution can be represented pictorially as shown in Figure 1.3.

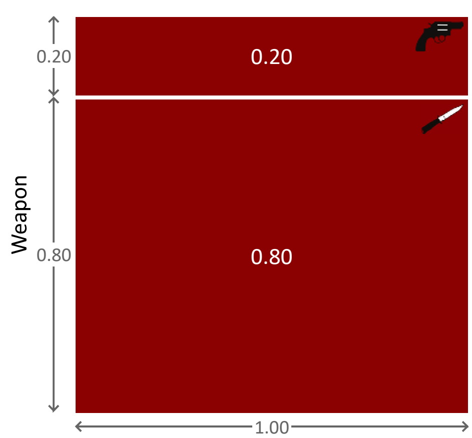


Figure 1.3: Representation of the probabilities for the two weapons, conditional on Miss Auburn being the murderer.

We can combine all of the above information into the more compact form

$$P(\texttt{weapon} = \texttt{revolver}|\texttt{murderer}) = \begin{cases} 0.9 & \text{if } \texttt{murderer} = \texttt{Grey} \\ 0.2 & \text{if } \texttt{murderer} = \texttt{Auburn}. \end{cases} \tag{1.10}$$

This can be expressed in an even more compact form as $P(\texttt{weapon}|\texttt{murderer})$. As before, we have a normalization constraint which is a consequence of the fact that, for each of the suspects, the weapon used must have been either the revolver or the dagger. This constraint can be written as

$$\sum_{\texttt{weapon}} P(\texttt{weapon}|\texttt{murderer}) = 1 \tag{1.11}$$

where the sum is over the two states of the random variable `weapon`, that is for `weapon=revolver` and for `weapon=dagger`, with `murderer` held at any fixed value (`Grey` or `Auburn`). Notice that we do not expect that the probabilities add up to 1 over the two states of the random variable `murderer`, which is why the two numbers in equation (1.10) do not add up to 1. These probabilities do not need to add up to 1, because they refer to the probability that the revolver was the murder weapon in two different circumstances: if Grey was the murderer and if Auburn was the murderer. For example, the probability of choosing the revolver could be high in both circumstances or low in both circumstances – so the normalization constraint does not apply.

Conditional probabilities can be written in the form of a **conditional probability table** (CPT) – which is the form we will often use in this book. For example, the conditional probability table for $P(\texttt{weapon}|\texttt{murderer})$ looks like this:

murderer	weapon=revolver	weapon=dagger
Auburn	0.200	0.800
Grey	0.900	0.100

Table 1.1: The conditional probability table for $P(\texttt{weapon}|\texttt{murderer})$. Table columns correspond to values of the conditioned variable `weapon`, rows correspond to values of the conditioning variable `murderer`, and table cells contain the conditional probability values. The normalization constraint means that the values in any row must add up to 1. We have also added blue bars to the table to provide a visual indication of the probability values.

As we just discussed, the normalization constraint means that the probabilities in the rows of Table 1.1 must add up to 1, but not the probabilities in the columns.

Independent variables

We have assumed that the probability of each choice of `weapon` changes depending on the value of `murderer`. We say that these two variables are *dependent*.

More commonly, we tend to focus on what variables do not affect each other, in which case we say they are **independent variables**. Consider for example, whether it is raining or not outside the Old Tudor Mansion at the time of the murder. It is reasonable to assume that this variable `raining` has no effect whatsoever on who the murderer is (nor is itself affected by who the murderer is). So we have assumed that the variables `murderer` and `raining` are independent. You can test this kind of assumption by asking the question "Does learning about the one variable, tell me anything about the other variable?". So in this case, the question is "Does learning whether it was raining or not, tell me anything about the identity of the murderer?", for which a reasonable answer is "No".

If we tried to write down a conditional probability for $P(\texttt{raining}|\texttt{murderer})$, then it would give the same probability for `raining` whether `murderer` was `Grey` or `Auburn`. If this were not true, learning about one variable would tell us something about the other variable, through a change in its probability distribution. We can express independence between these two variables mathematically.

$$P(\texttt{raining}|\texttt{murderer}) = P(\texttt{raining}) \tag{1.12}$$

What this equation says is that the probability of `raining` given knowledge of the `murderer` is exactly the same as the probability of `raining` without taking into account `murderer`. In other words, the two variables are independent. This also holds the other way around:

$$P(\texttt{murderer}|\texttt{raining}) = P(\texttt{murderer}) \tag{1.13}$$

Independence is an important concept in model-based machine learning, since any variable we do not explicitly include in our model is assumed to be independent of all variables in the model. We will see further examples of independence later in this chapter.

Let us take a moment to recap what we have achieved so far. In the first section, we specified the probability that the murderer was Major Grey (and therefore the complementary probability that the murderer was Miss Auburn). In this section, we also wrote down the probabilities for different choices of weapon for each of our suspects. In the next section, we will see how we can use all these probabilities to incorporate evidence from the crime scene and reason about the identity of the murderer.

Self assessment 1.1

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. To get familiar with thinking about conditional probabilities, estimate conditional probability tables for each of the following.
   (a) The probability of being late for work, conditioned on whether or not traffic is bad.

(b) The probability a user replies to an email, conditioned on whether or not he knows the sender.

(c) The probability that it will rain on a particular day, conditioned on whether or not it rained on the previous day.

Ensure that the rows of your conditional probability tables add up to one. If you can, compare your estimates for these probabilities with someone else's and discuss where and why you disagree.

2. Pick an example, like one of the ones above, from your life or work. You should choose an example where one binary (two-valued) variable affects another. Estimate the conditional probability table that represents how one of these variables affects the other.

3. For one of the events in question 1, write a program to print out 100 samples of the conditioned variable for each value of the conditioning variable. Print the samples side by side and compare the proportion of samples in which the event occurs for when the conditioning variable is true to when it is false. Does the frequency of events look consistent with your common sense in each case? If not, go back and refine your conditional probability table and try again.

Review of concepts introduced in this section

conditional probability distribution A probability distribution over some random variable `A` which changes its value depending on some other variable `B`, written as $P(\mathtt{A}|\mathtt{B})$. For example, if the probability of choosing each murder weapon (`weapon`) depends on who the murderer is (`murderer`), we can capture this in the conditional probability distribution $P(\mathtt{weapon}|\mathtt{murderer})$. Conditional probability distributions can also depend on more than one variable, for example $P(\mathtt{A}|\mathtt{B}, \mathtt{C}, \mathtt{D})$.

conditional probability table A table which defines a conditional probability, where the columns correspond to values of the conditioned variable and rows correspond to the values of the conditioning variable(s). For any setting of the conditioning variable(s), the probabilities over the conditioned variable must add up to 1 – so the values in any row must add up to 1. For example, here is a conditional probability table capturing the conditional probability of `weapon` given `murderer`:

murderer	weapon=revolver	weapon=dagger
Auburn	0.200	0.800
Grey	0.900	0.100

independent variables Two random variables are independent if learning about one does not provide any information about the other. Mathematically, two variables $\mathtt{A}$ and $\mathtt{B}$ are independent if

$$P(\mathtt{A}|\mathtt{B}) = P(\mathtt{A})$$
$$P(\mathtt{B}|\mathtt{A}) = P(\mathtt{B})$$

This is an important concept in model-based machine learning, since all variables in the model are assumed to be independent of any variable not in the model.

1.2 A model of a murder

Searching carefully around the library, Dr Bayes spots a bullet lodged in the book case. "Hmm, interesting", he says, "I think this could be an important clue".

So it seems that the murder weapon was the revolver, not the dagger. Our intuition is that this new evidence points more strongly towards Major Grey than it does to Miss Auburn, since the Major, with his military background, is more likely to have experience with a revolver than Miss Auburn. But how can we use this information?

A convenient way to think about the probabilities we have looked at so far is as a description of the process by which we believe the murder took place, taking account of the various sources of uncertainty. So, in this process, we first pick the murderer with the help of Figure 1.1. This shows that there is a 30% chance of choosing Major Grey and a 70% chance of choosing Miss Auburn. Let us suppose that Miss Auburn was the murderer. We can then refer to Figure 1.3 to pick which weapon she used. There is a 20% chance that she would have used the revolver and an 80% chance that she would have used the dagger. Let's consider the event of Miss Auburn picking the revolver. The probability of choosing Miss Auburn *and* the revolver is therefore 70% × 20% = 14%. This is the **joint probability** of choosing `Auburn` and `revolver`. If we repeat this exercise for the other three combinations of `murderer` and `weapon` we obtain the joint probability distribution over the two random variables, which we can illustrate pictorially as seen in Figure 1.4.

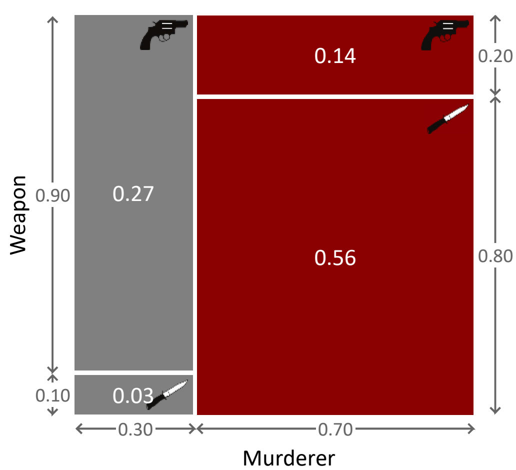


Figure 1.4: Representation of the joint probabilities for the two random variables `murderer` and `weapon`.

Figure 1.5 below shows how this joint distribution was constructed from the previous distributions we have defined. We have taken the left-hand slice of the P(`murderer`) square corresponding to Major Grey, and divided it vertically in proportion to the two regions of the conditional probability square for Grey. Likewise, we have taken the right-hand slice of the P(`murderer`) square corresponding Miss Auburn, and divided it vertically in proportion to the two regions of the conditional probability square for Auburn.

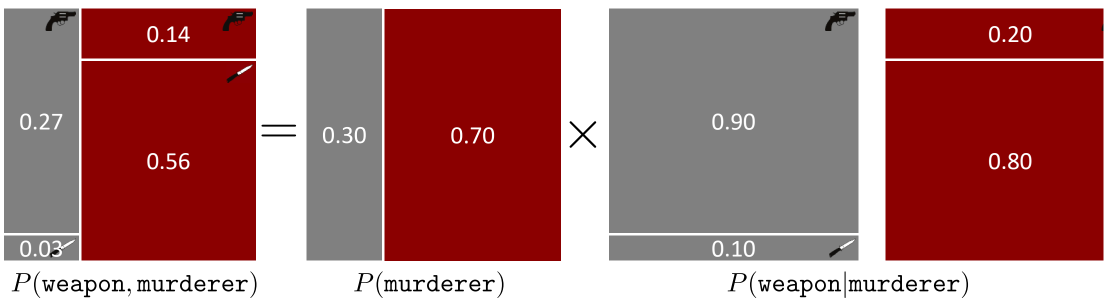


Figure 1.5: The joint distribution for our two-variable model, shown as a product of two factors.

We denote this joint probability distribution by $P(\texttt{weapon}, \texttt{murderer})$, which should be read as "the probability of `weapon` *and* `murderer`". In general, the joint distribution of two random variables `A` and `B` can be written $P(\texttt{A}, \texttt{B})$ and specifies the probability for each possible combination of settings of `A` and `B`. Because probabilities must sum to one, we have

$$\sum_{\texttt{A}} \sum_{\texttt{B}} P(\texttt{A}, \texttt{B}) = 1. \tag{1.14}$$

Here the notation $\sum_A$ denotes a sum over all possible states of the random variable `A`, and likewise for `B`. This corresponds to the total area of the square in Figure 1.4 being 1, and arises because we assume the world consists of one, and only one, combination of murderer and weapon. Picking a point randomly in this new square corresponds to sampling from the joint probability distribution.

1.2.1 Probabilistic models

We can now introduce the central concept of this book, the **probabilistic model**. A probabilistic model consists of:

- A set of random variables,
- A joint probability distribution over these variables (i.e. a distribution that assigns a probability to every configuration of these variables such that the probabilities add up to 1 over all possible configurations).

Once we have a probabilistic model, we can reason about the variables it contains, make predictions, learn about the values of some random variables given the values of others, and in general, answer any possible question that can be stated in terms of the random variables included in the model. This makes a probabilistic model an incredibly powerful tool for doing machine learning.

We can think of a probabilistic model as a set of assumptions we are making about the problem we are trying to solve, where any assumptions involving uncertainty are expressed using probabilities. The best way to understand how this is done, and how the model can be used to reason and make predictions, is by looking at example models. In this chapter, we give the example of a probabilistic model of a murder. In later chapters, we shall build a variety of more complex models for other applications. All the machine learning applications in this book will be solved solely through the use of probabilistic models.

1.2.2 Two rules for working with probabilistic models

So for our murder mystery, we have a probabilistic model with two variables `murderer` and `weapon` where the joint probability distribution over those variables is the one shown in Figure 1.4. To use this model, we now need to introduce two key rules which allow us to manipulate the probability distributions in a model.

From the discussion above, we see that the joint probability distribution for our model is obtained by taking the probability distribution over `murderer` and multiplying by the conditional distribution of `weapon`. This can be written in the form

$$P(\texttt{weapon}, \texttt{murderer}) = P(\texttt{murderer})P(\texttt{weapon}|\texttt{murderer}). \tag{1.15}$$

Equation (1.15) is an example of a very important result called the **product rule of probability**. The product rule says that the joint distribution of `A` and `B` can be written as the product of the distribution over `A` and the conditional distribution of `B` conditioned on the value of `A`, in the form

$$P(\texttt{A}, \texttt{B}) = P(\texttt{A})P(\texttt{B}|\texttt{A}). \tag{1.16}$$

Now suppose we sum up the values in the two left-hand regions of Figure 1.4 corresponding to Major Grey. Their total area is 0.3, as we expect because we know that the probability of Grey being the murderer is 0.3. The sum is over the different possibilities for the choice of weapon, so we can express this in the form

$$\sum_{\texttt{weapon}} P(\texttt{weapon}, \texttt{murderer} = \texttt{Grey}) = P(\texttt{murderer} = \texttt{Grey}). \tag{1.17}$$

Similarly, the entries in the second column, corresponding to the murderer being Miss Auburn, must add up to 0.7. Combining these together we can write

$$\sum_{\texttt{weapon}} P(\texttt{weapon}, \texttt{murderer}) = P(\texttt{murderer}). \tag{1.18}$$

This is an example of the **sum rule of probability**, which says that the probability distribution over a random variable $\mathtt{A}$ is obtained by summing the joint distribution $P(\mathtt{A},\mathtt{B})$ over all values of $\mathtt{B}$

$$P(\mathtt{A}) = \sum_{\mathtt{B}} P(\mathtt{A},\mathtt{B}). \tag{1.19}$$

In this context, the distribution $P(\mathtt{A})$ is known as the **marginal distribution** for $\mathtt{A}$ and the act of summing out $\mathtt{B}$ is called **marginalisation**. We can equally apply the sum rule to marginalise over the murderer to find the probability that each of the weapons was used, irrespective of who used them. If we sum the areas of the top two regions of Figure 1.4 we see that the probability of the weapon being the revolver was $0.27 + 0.14 = 0.41$, or 41%. Similarly, if we add up the areas of the bottom two regions we see that the probability that the weapon was the dagger is $0.03 + 0.56 = 0.59$ or 59%. The two marginal probabilities then add up to 1, which we expect since the weapon must have been either the revolver or the dagger.

The sum and product rules are very general. They apply not just when $\mathtt{A}$ and $\mathtt{B}$ are binary random variables, but also when they are multi-state random variables, and even when they are continuous (in which case the sums are replaced by integrations). Furthermore, $\mathtt{A}$ and $\mathtt{B}$ could each represent sets of several random variables. For example, if $\mathtt{B} \equiv \{\mathtt{C},\mathtt{D}\}$, then from the product rule (1.16) we have

$$P(\mathtt{A},\mathtt{C},\mathtt{D}) = P(\mathtt{A})P(\mathtt{C},\mathtt{D}|\mathtt{A}) \tag{1.20}$$

and similarly the sum rule (1.19) gives

$$P(\mathtt{A}) = \sum_{\mathtt{C}} \sum_{\mathtt{D}} P(\mathtt{A},\mathtt{C},\mathtt{D}). \tag{1.21}$$

The last result is particularly useful since it shows that we can find the marginal distribution for a particular random variable in a joint distribution by summing over all the other random variables, no matter how many there are.

Together, the product rule and sum rule provide the two key results that we will need throughout the book in order to manipulate and calculate probabilities. It is remarkable that the rich and powerful complexity of probabilistic modelling is all founded on these two simple rules.

1.2.3 Inference using the joint distribution

We now have the tools that we need to incorporate the fact that the weapon was the revolver. Intuitively, we expect that this should increase the probability that Grey was the murderer but to confirm this we need to calculate that updated probability. The process of computing revised probability distributions after we have observed the values of some the random variables, is called **inference**. Inference is the cornerstone of model-based machine learning – it can be used for reasoning about a model, learning from data, making predictions with a model – in fact any machine learning task can be achieved using inference.

We can do inference in our model using the joint probability distribution shown in Figure 1.4. Our model says that, before we observe which weapon was used to commit the crime, all points within this square are equally likely. However, we now know that the weapon was the revolver. We can therefore rule out the two lower regions which correspond to the weapon being the dagger, as illustrated in Figure 1.6.

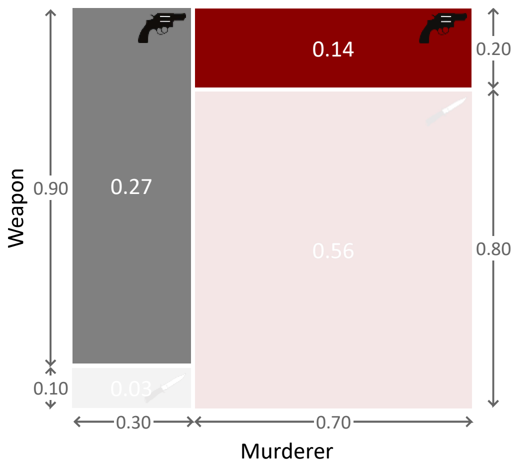


Figure 1.6: This shows the joint distribution from Figure 1.4 in which the regions corresponding to the dagger have been eliminated.

Because all points in the remaining two regions are equally likely, we see that the probability of the murderer being Major Grey is given by the fraction of the remaining area given by the grey box on the left.

$$P(\texttt{murderer} = \texttt{Grey}|\texttt{weapon} = \texttt{revolver}) = \frac{0.27}{0.27 + 0.14} \simeq 0.66$$

in other words a 66% probability. This is significantly higher than the 30% probability we had before observing that the weapon used was the revolver. We see that our intuition is therefore correct and it now looks more likely that Grey is the murderer rather than Auburn. The probability that we assigned to Grey being the murderer *before* seeing the evidence of the bullet is sometimes called the **prior probability** (or just the *prior*), while the revised probability *after* seeing the new evidence is called the **posterior probability** (or just the *posterior*).

The probability that Miss Auburn is the murderer is similarly given by

$$P(\texttt{murderer} = \texttt{Auburn}|\texttt{weapon} = \texttt{revolver}) = \frac{0.14}{0.27 + 0.14} \simeq 0.34.$$

Because the murderer is either Grey or Auburn these two probabilities again sum to 1. We can capture this pictorially by re-scaling the regions in Figure 1.6 to give the diagram shown in Figure 1.7.

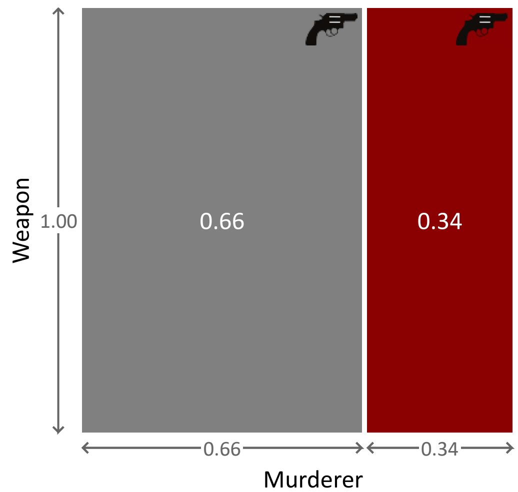


Figure 1.7: Representation of the posterior probabilities that Grey or Auburn was the murderer, given that the weapon is the revolver.

We have seen that, as new data, or evidence, is collected we can use the product and sum rules to revise the probabilities to reflect changing levels of uncertainty. The system can be viewed as having *learned* from that data.

So, after all this hard work, have we finally solved our murder mystery? Well, given the evidence so far it appears that Grey is more likely to be the murderer, but the probability of his guilt currently stands at 66% which feels too small for a conviction. But how high a probability would we need? To find an answer we turn to William Blackstone's principle of 1765:

> *"Better that ten guilty persons escape than one innocent suffer."*

We therefore need a probability of guilt for our murderer which exceeds $\frac{10}{10+1} \approx 91\%$. To achieve this level of proof we will need to gather more evidence from the crime scene, and to make a corresponding extension to our model in order to incorporate this new evidence. We'll look at how to do this in the next section.

Self assessment 1.2

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Check for yourself that the joint probabilities for the four areas in Figure 1.4 are correct and confirm that their total is 1. Use this figure to

compute the posterior probability over `murderer`, if the murder weapon had been the dagger rather than the revolver.

2. Choose one of the following scenarios (continued from the previous self assessment) or choose your own scenario

   (a) Whether you are late for work, depending on whether or not traffic is bad.

   (b) Whether a user replies to an email, depending on whether or not he knows the sender.

   (c) Whether it will rain on a particular day, depending on whether or not it rained on the previous day.

   For your selected scenario, pick a suitable prior probability for the conditioning variable (for example, whether the traffic is bad, whether the user knows the sender, whether it rained the previous day). Recall the conditional probability table that you estimated in the previous self assessment. Using the prior and this conditional distribution, use the product rule to calculate the joint distribution over the two variables in the scenario. Draw this joint distribution pictorially, like the example of Figure 1.4. Make sure you label each area with the probability value, and that these values all add up to 1.

3. Now assume that you know the value of the conditioned variable, for example, assume that you are late for work on a particular day. Now compute the posterior probability of the conditioning variable, for example, the probability that the traffic was bad on that day. You can achieve this using your diagram from the previous question, by crossing out the areas that don't apply and finding the fraction of the remaining area where the conditioning event happened.

4. For your joint probability distribution, write a program to print out 1,000 joint samples of both variables. Compute the fraction of samples that have each possible pair of values. Check that this is close to your joint probability table. Now change the program to only print out those samples which are consistent with your known value from the previous question (for example, samples where you are late for work). What fraction of these samples have each possible pair of values now? How does this compare to your answer to the previous question?

Review of concepts introduced in this section

joint probability A probability distribution over multiple variables which gives the probability of the variables jointly taking a particular configuration of values. For example, $P(\mathtt{A}, \mathtt{B}, \mathtt{C})$ is a joint distribution over the random variables `A`, `B`, and `C`.

probabilistic model A set of random variables combined with a joint distribution that assigns a probability to every configuration of these variables.

product rule of probability The rule that the joint distribution of $\texttt{A}$ and $\texttt{B}$ can be written as the product of the distribution over $\texttt{A}$ and the conditional distribution of $\texttt{B}$ conditioned on the value of $\texttt{A}$, in the form

$$P(\texttt{A},\texttt{B}) = P(\texttt{A})P(\texttt{B}|\texttt{A}).$$

sum rule of probability The rule that the probability distribution over a random variable $\texttt{A}$ is obtained by summing the joint distribution $P(\texttt{A},\texttt{B})$ over all values of $\texttt{B}$

$$P(\texttt{A}) = \sum_{\texttt{B}} P(\texttt{A},\texttt{B}).$$

marginal distribution The distribution over a random variable computed by using the sum rule to sum a joint distribution over all other variables in the distribution.

marginalisation The process of summing a joint distribution to compute a marginal distribution.

inference The process of computing probability distributions over certain specified random variables, usually after observing the value of some other variables in the model.

prior probability The probability distribution over a random variable prior to seeing any data. Careful choice of prior distributions is an important part of model design.

posterior probability The updated probability distribution over a random variable after some data has been taken into account. The aim of inference is to compute posterior probability distributions over variables of interest.

1.3 Working with larger models

We now wish to incorporate more evidence from the crime scene – for each new piece of evidence that we consider, we will need to introduce another random variable into our model. So far we've only had to cope with a model of just two random variables: `murderer` and `weapon`. For this two-variable model, we were able to write the joint distribution pictorially, like so:

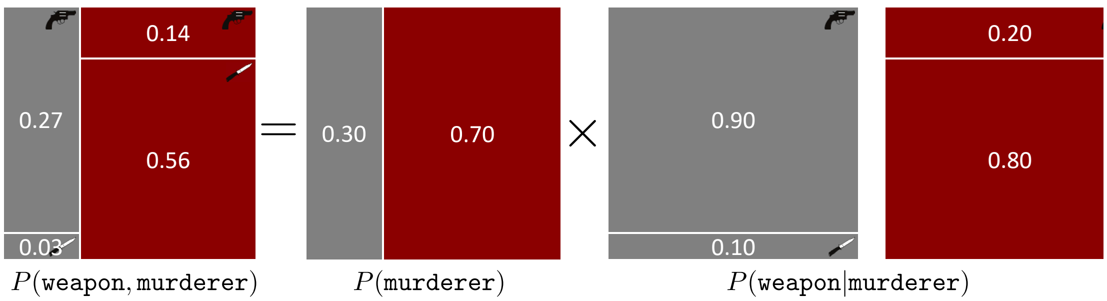


Figure 1.8: The joint distribution for our two-variable model, shown as a product of two factors.

Unfortunately, if we increase the number of random variables in our model beyond two (or maybe three), we cannot represent the joint distribution using this pictorial notation. But in real models there will typically be anywhere from hundreds to hundreds of millions of random variables. We need a different notation to represent and work with such large joint distributions.

The notation that we will use exploits the fact that most joint distributions can be written as a product of a number of terms or **factors** each of which refers to only a small number of variables. For example, our joint distribution above is the product of two factors: $P(\texttt{murderer})$ which refers to one variable and $P(\texttt{weapon}|\texttt{murderer})$ which refers to two variables. Even for joint distributions with millions of variables, the factors which make up the distribution usually refer to only a few of these variables. As a result, we can represent a complex joint distribution using a **factor graph** that shows which factors make up the distribution consists and what variables those factors refer to.

Figure 1.9 shows a factor graph for the two-variable joint distribution above. There are two types of node in the graph: a **variable node** for each variable in the model and a **factor node** for each factor in the joint distribution. Variable nodes are shown as white ellipses (or rounded boxes) containing the name of the variable. Factor nodes are small black squares, labelled with the factor that they represent. We connect each factor node to the variable nodes that it refers to. For example, the $P(\texttt{murderer})$ factor node is connected only to the `murderer` variable node since that is the only variable it refers to, whilst $P(\texttt{weapon}|\texttt{murderer})$ connects to both the `weapon` and `murderer` variable nodes, since it refers to both variables. Finally, if the factor defines a distribution over one of its variables, we draw an arrow on the edge pointing to that variable (the **child variable**). If the factor defines a conditional distribution, the other

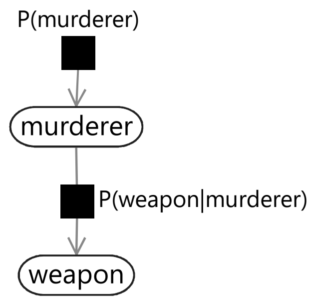


Figure 1.9: Factor graph for the murder mystery model. The model contains two random variables `murderer` and `weapon`, shown as white nodes, and two factors P(`murderer`) and P(`weapon`|`murderer`), shown as black squares.

edges from that factor connect to the variables being conditioned on (the **parent variables**) and do not have arrows.

The factor graph of Figure 1.9 provides a complete description of our joint probability, since it can be found by computing the product of the distributions represented by the factor nodes. As we look at more complex factor graphs throughout the book, it will always hold that the joint probability distribution over the random variables (represented by the variable nodes) can be written as the product of the factors (represented by the factor nodes). The joint distribution gives a complete specification of a model, because it defines the probability for every possible combination of values for all of the random variables in the model. Notice that in Figure 1.8 the joint distribution was represented explicitly, but in the factor graph it is represented only indirectly, via the factors.

Since we want our factor graphs to tell us as much as possible about the joint distribution, we should label the factors as precisely as possible. For example, since we know that P(`murderer`) defines a prior distribution of $Bernoulli(0.7)$ over `murderer`, we can label the factor "Bernoulli(0.7)". We do not need to mention the `murderer` variable in the factor label since the factor is only connected to the `murderer` variable node, and so the distribution must be over `murderer`. This allows more informative labelling of the factor graph, like so:

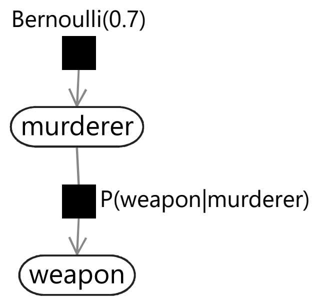


Figure 1.10: Factor graph representation of the murder mystery model with the *Bernoulli* prior over `murderer` labelled explicitly.

In this book, we will aim to label factors in our factor graphs so that the function represented by each factor is as clear as possible.

There is one final aspect of factor graph notation that we need to cover. When doing inference in our two-variable model, we observed the random variable `weapon` to have the value `revolver`. This step of observing random variables is such an important one in model-based machine learning that we introduce a special graphical notation to depict it. When a random variable is observed, the corresponding node in the factor graph is shaded (and sometimes also labelled with the observed value), as shown for our murder mystery in Figure 1.11.

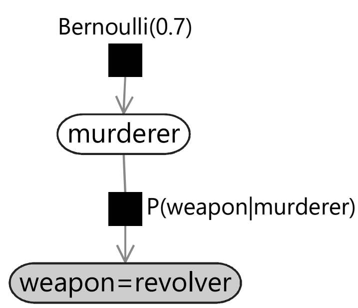


Figure 1.11: The factor graph for the murder mystery, with the `weapon` node shaded to indicate that this random variable has been observed, and is fixed to the value `revolver`.

Representing a probabilistic model using a factor graph gives many benefits:

- It provides a simple way to visualize the structure of a probabilistic model and see which variables influence each other.
- It can be used to motivate and design new models, by making appropriate modifications to the graph.
- The assumptions encoded in the model can be clearly seen and communicated to others.

- Insights into the properties of a model can be obtained by operations performed on the graph.
- Computations on the model (such as inference) can be performed by efficient algorithms that exploit the factor graph structure.

We shall illustrate these points in the context of specific examples throughout this book.

1.3.1 Inference without computing the joint distribution

Having observed the value of `weapon`, we previously computed the full joint distribution and used it to evaluate the posterior distribution of `murderer`. However, for most real-world models it is not possible to do this, since the joint distribution would be over too many variables to allow it to be computed directly. Instead, now that we have our joint distribution represented as a product of factors, we can arrive at the same result by using only the individual factors – in a way which is typically far more efficient to compute. The key lies in applying the product and sum rules of probability in an appropriate way. From the product rule (1.15) we have

$$P(\texttt{weapon}, \texttt{murderer}) = P(\texttt{weapon}|\texttt{murderer})P(\texttt{murderer}). \tag{1.22}$$

However, by symmetry we can equally well write

$$P(\texttt{weapon}, \texttt{murderer}) = P(\texttt{murderer}|\texttt{weapon})P(\texttt{weapon}). \tag{1.23}$$

Equating the right-hand sides of these two equations and re-arranging we obtain

$$P(\texttt{murderer}|\texttt{weapon}) = \frac{P(\texttt{weapon}|\texttt{murderer})P(\texttt{murderer})}{P(\texttt{weapon})}. \tag{1.24}$$

This is an example of **Bayes' theorem** or *Bayes' rule* Bayes [1763] which plays a fundamental role in many inference calculations (see Panel 1.1). Here $P(\texttt{murderer})$ is the prior probability distribution over the random variable `murderer` and is one of the things we specified when we defined our model for the murder mystery. Similarly, $P(\texttt{weapon}|\texttt{murderer})$ is also something we specified, and is called the **likelihood function** and should be viewed as a function of the random variable `murderer`. The quantity on the left-hand side $P(\texttt{murderer}|\texttt{weapon})$ is the posterior probability distribution over the `murderer` random variable, i.e. the distribution *after* we have observed the evidence of the revolver.

The denominator $P(\texttt{weapon})$ in equation (1.24) plays the role of a normalization constant and ensures that the left hand side of Bayes' theorem is correctly normalized (i.e. adds up to 1 when summed over all possible states of the random variable `murderer`). It can be computed from the prior and the likelihood using

$$P(\texttt{weapon}) = \sum_{\texttt{murderer}} P(\texttt{weapon}|\texttt{murderer})P(\texttt{murderer}) \tag{1.25}$$

which follows from the product and sum rules. When working with Bayes' rule, it is sometimes useful to drop this denominator $P(\texttt{weapon})$ and instead write

$$P(\texttt{murderer}|\texttt{weapon}) \propto P(\texttt{weapon}|\texttt{murderer})P(\texttt{murderer}) \tag{1.26}$$

where $\propto$ means that the left-hand side is proportional to the right-hand side (i.e. they are equal up to a constant that does not depend on the value of `murderer`). We do not need to compute the denominator because the normalization constraint tells us that the conditional probability distribution $P(\texttt{murderer}|\texttt{weapon})$ must add up to one across all values of `murderer`. Once we have evaluated the right hand side of (1.26) to give a number for each of the two values of `murderer`, we can scale these two numbers so that they sum up to one, to get the resulting posterior distribution.

Now let us apply Bayes' rule to the murder mystery problem. We know that `weapon=revolver`, so we can evaluate the right hand side of equation (1.26) for both `murderer=Grey` and `murderer=Auburn` giving:

$$\begin{aligned} P(\texttt{murderer} = \texttt{Grey}|\texttt{weapon} = \texttt{revolver}) &\propto 0.3 \times 0.9 = 0.27 \\ P(\texttt{murderer} = \texttt{Auburn}|\texttt{weapon} = \texttt{revolver}) &\propto 0.7 \times 0.2 = 0.14. \end{aligned}$$

These numbers sum to 0.41. To get probabilities, we need to scale both numbers to sum to 1 (by dividing by 0.41) which gives:

$$\begin{aligned} P(\texttt{murderer} = \texttt{Grey}|\texttt{weapon} = \texttt{revolver}) = \frac{0.27}{0.41} &\simeq 0.66 \\ P(\texttt{murderer} = \texttt{Auburn}|\texttt{weapon} = \texttt{revolver}) = \frac{0.14}{0.41} &\simeq 0.34. \end{aligned}$$

This is the same result as before. Although we have arrived at the same result by a different route, this latter approach using Bayes' theorem is preferable as we did not need to compute the joint distribution. With only two random variables so far in our murder mystery this might not look like a significant improvement, but as we go to more complex problems we will see that successive applications of the rules of probability allows us to work with small sub-sets of random variables – even in models with millions of variables!

Self assessment 1.3

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Use Bayes' theorem to compute the posterior probability over `murderer`, for the case that the murder weapon was the dagger rather than the revolver. Compare this to your answer from the previous self assessment.

2. For the scenario you chose in the previous self assessment, draw the factor graph corresponding to the joint distribution. Ensure that you label the factors as precisely as possible. Verify that the product of factors in the factor graph is equal to the joint distribution.

3. Repeat the inference task from the previous self assessment (computing the posterior probability of the conditioning variable) using Bayes' theorem rather than using the joint distribution. Check that you get the same answer as before.

Review of concepts introduced in this section

factors Functions (usually of a small number of variables) which are multiplied together to give a joint probability distribution (which may be over a large number of variables). Factors are represented as small black squares in a factor graph.

Panel 1.1 – Bayes' Theorem

Bayes' theorem allows us to express a conditional probability distribution such as $P(\mathtt{A}|\mathtt{B})$ in terms of the 'reversed' conditional distribution $P(\mathtt{B}|\mathtt{A})$:

$$P(\mathtt{A}|\mathtt{B}) = \frac{P(\mathtt{A})P(\mathtt{B}|\mathtt{A})}{P(\mathtt{B})}. \tag{1.27}$$

Bayes' theorem is particularly useful when we want to update the distribution of some uncertain quantity $\mathtt{A}$ when we are given some new information represented by the random variable $\mathtt{B}$. For instance, in the murder mystery we want to know the identity of the murderer $\mathtt{A}$ and we have just discovered the choice of weapon $\mathtt{B}$. If we didn't know $\mathtt{B}$ then our knowledge of $\mathtt{A}$ would be described by $P(\mathtt{A})$, which we call the *prior*. Once we know the value of $\mathtt{B}$ we can compute the revised distribution $P(\mathtt{A}|\mathtt{B})$ known as the *posterior*. They are related by the reversed conditional distribution $P(\mathtt{B}|\mathtt{A})$ which is known as the *likelihood*. Note that the likelihood should not be viewed as a probability distribution over $\mathtt{B}$, because the value of $\mathtt{B}$ is assumed to be known, but rather as a function of the random variable $\mathtt{A}$, and for this reason it is also known as the *likelihood function*. Note also that its sum over $\mathtt{A}$ does not necessarily equal 1.
We can also write Bayes' theorem in words:

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{normalizer}}. \tag{1.28}$$

Here the 'normalizer' is just the value of $P(\mathtt{B})$ and is the quantity which ensures that the posterior distribution is normalized. From the sum rule (1.19) it is given by

$$P(\mathtt{B}) = \sum_{\mathtt{A}} P(\mathtt{A})P(\mathtt{B}|\mathtt{A}) \tag{1.29}$$

and can therefore be computed from the prior and the likelihood function.

factor graph A representation of a probabilistic model which uses a graph with factor nodes (black squares) for each factor in the joint distribution and variable nodes (white, rounded) for each variable in the model. Edges connect each factor node to the variable nodes that it refers to.

variable node A node in a factor graph that represents a random variable in the model, shown as a white ellipse or rounded box containing the variable name.

factor node A node in a factor graph that represents a factor in the joint distribution of a model, shown as a small black square labelled with the factor name.

child variable For a factor node, the connected variable that the arrow points to. This indicates that the factor defines a probability distribution over this variable, possibly conditioned on the other variables connected to this factor. The child variable for a factor is usually drawn directly below the factor.

parent variables For a factor node, the connected variable(s) with edges that do not have arrows pointing to them. When a factor defines a conditional probability distribution, these are the variables that are conditioned on. The parent variables for a factor are usually drawn above the factor.

Bayes' theorem The fundamental theorem that lets us do efficient inference in probabilistic models. It defines how to update our belief about a random variable $\mathtt{A}$ after receiving new information $\mathtt{B}$, so that we move from our prior belief $P(\mathtt{A})$ to our posterior belief given $\mathtt{B}$, $P(\mathtt{A}|\mathtt{B})$.

$$P(\mathtt{A}|\mathtt{B}) = \frac{P(\mathtt{A})P(\mathtt{B}|\mathtt{A})}{P(\mathtt{B})}.$$

See Panel 1.1 for more details.

likelihood function A conditional probability viewed as a function of its conditioned variable. For example, $P(\mathtt{B}|\mathtt{A})$ can be viewed as a function of $\mathtt{A}$ when $\mathtt{B}$ is observed and we are interested in inferring $\mathtt{A}$. It is important to note that this not a distribution over $\mathtt{A}$, since $P(\mathtt{B}|\mathtt{A})$ does not have to sum to 1 over all values of $\mathtt{A}$. To get a distribution over $\mathtt{A}$ from a likelihood function, you need to apply Bayes' theorem (see Panel 1.1).

1.4 Extending the model

Dr Bayes pulls out his trusty magnifying glass and continues his investigation of the crime scene. As he examines the floor near Mr Black's body he discovers a hair lying on top of the pool of blood. "Aha" exclaims Dr Bayes "this hair must belong to someone who was in the room when the murder took place!" Looking more closely at the hair, Dr Bayes sees that it is not the lustrous red of Miss Auburn's vibrant locks, nor indeed the jet black of the victim's hair, but the distinguished silver of Major Grey!

Now that we are equipped with the concept of factor graphs, we can extend our model to incorporate this additional clue from the crime scene. The hair is powerful evidence indicating that Major Grey was present at the time of the murder, but there is also the possibility that the hair was stolen by Miss Auburn and planted at the crime scene to mislead our perceptive sleuth. As before, we can capture these thoughts quantitatively using a conditional probability distribution. Let us denote the new information by the random variable `hair`, which takes the value `true` if Major Grey's hair is discovered at the scene of the crime, and `false` otherwise. Clearly the discovery of the hair points much more strongly to Grey than to Auburn, but it does not rule out Auburn completely.

Suppose we think there is a 50% chance that Grey would accidentally leave one of his hairs at the crime scene if he were the murderer, but that there is only a 5% chance that Auburn would think to plant a grey hair if she were the murderer. The conditional probability distribution would then be

$$P(\texttt{hair} = \texttt{true}|\texttt{murderer}) = \begin{cases} 0.5 & \text{if } \texttt{murderer} = \texttt{Grey} \\ 0.05 & \text{if } \texttt{murderer} = \texttt{Auburn}. \end{cases} \tag{1.30}$$

As we have seen before, since this represents a conditional probability conditioned on the value of `murderer`, not a probability distribution over `murderer`, the numbers in (1.30) do not have to add up to one.

In writing the conditional probability this way, we have actually made an additional assumption: that the probability of one of Major Grey's hairs being found at the scene of the crime only depends on who committed the murder, and not anything else – including the choice of weapon that was used to commit the murder. This assumption has arisen because the conditional probability in (1.30) does not include `weapon` in the variables being conditioned on. Mathematically this assumption can be expressed as

$$P(\texttt{hair}|\texttt{weapon}, \texttt{murderer}) = P(\texttt{hair}|\texttt{murderer}). \tag{1.31}$$

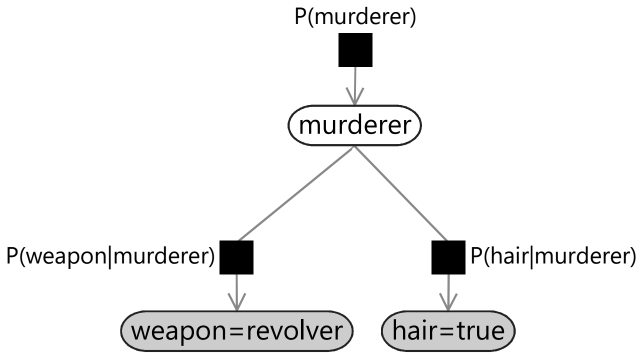


Figure 1.12: The factor graph for the murder mystery after the addition of the new evidence. Both the `weapon` node and the `hair` node are shaded to indicate that these random variables have been set to their observed values. Note the absence of an edge connecting the `weapon` random variable with the factor node representing $P(\texttt{hair}|\texttt{murderer})$.

which says that the distribution of `hair` is independent of the value of `weapon` once we have conditioned on the value of `murderer`. For this reason it is known as a **conditional independence** assumption. Notice that (1.31) has a similar form to the equations which hold when two variable are independent, e.g. (1.12), but has an additional conditioning variable on both sides.

The question to ask when considering a conditional independence assumption is "Does learning about one variable, tell me anything about the other variable, if I knew the value of the conditioning variable?". In this case that would be "Does learning about the hair, tell me anything about the choice of weapon, if I already knew who the murderer was?". Reasonably, the answer in this case might be that you could learn a little (for example, the dagger might mean the murderer had to get closer to the victim and so was more likely to drop a hair). However, for the sake of simplicity we assume that this conditional independence assumption holds.

Figure 1.12 shows the factor graph corresponding to our expanded model with the new `hair` variable and a new factor representing this conditional distribution. Our conditional independence assumption has a simple graphical interpretation, namely that there is no edge connecting the `weapon` node directly to the factor representing the conditional distribution $P(\texttt{hair}|\texttt{murderer})$. The only way to get from the `weapon` node to the `hair` node is via the `murderer` node. We see that the *missing* edges in the factor graph capture independence assumptions built into the model.

There is an alternative graphical representation of a model called a **Bayesian network** or *Bayes net* that emphasises such independence assumptions, at the cost of hiding information about the factors. It provides less detail about the model than a factor graph, but gives a good 'big picture' view of which variables directly and indirectly affect each other. See Panel 1.2 for more details.

Given the factor graph of Figure 1.12, we can write down the joint distribution as the product of three terms, one for each factor in the factor graph:

$$\begin{aligned} P(\texttt{murderer}, \texttt{weapon}, \texttt{hair}) &= P(\texttt{murderer})P(\texttt{weapon}|\texttt{murderer}) \\ &\quad P(\texttt{hair}|\texttt{murderer}). \end{aligned} \tag{1.32}$$

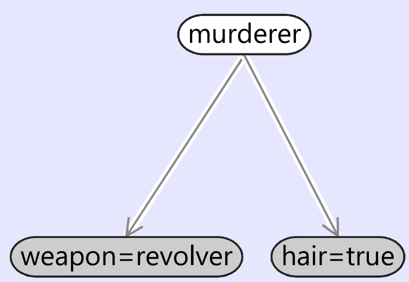
Check for yourself that each term on the right of equation (1.32) corresponds to one of the factor nodes in Figure 1.12.

1.4.1 Incremental inference

We want to compute the posterior distribution over `murderer` in this new model, given values of `weapon` and `hair`. Given that we have the result from the previous model, we'd like to make use of it – rather than start again from scratch. To get our posterior distribution in the previous model, we conditioned

Panel 1.2 – Bayesian Networks

A Bayesian network (or Bayes net) is a different way of using a graph to represent a probabilistic model. In a Bayes net, there are variable nodes corresponding to each variable in the model, but there are no factor nodes. Parent variables of a factor are connected directly to the child variable of the factor, using directed edges (arrows). For example, the Bayes net corresponding to the factor graph of our murder (Figure 1.12) looks like this:



As this figure shows, by hiding the factors, a Bayes net emphasises which variables there are and how they influence each other (directly or indirectly). Bayes nets can be very useful in the early stages of model design when you want to focus on what variables to include and which will affect each other, without yet getting into details of precisely *how* they affect each other.

The disadvantage of using a Bayes net is that it is an incomplete specification of a model – you also have to write down all the factor functions externally to the graph and consider the two together as making up the model. For this reason, we have chosen to use factor graphs in this book, since they provide a stand-alone description of the model.

on the value of `weapon`. To perform incremental inference in this new model, we can write down Bayes' rule but condition each term on the variable `weapon`:

$$P(\texttt{murderer}|\texttt{hair},\texttt{weapon}) = \frac{P(\texttt{murderer}|\texttt{weapon})P(\texttt{hair}|\texttt{murderer},\texttt{weapon})}{P(\texttt{hair}|\texttt{weapon})}. \tag{1.33}$$

We can use exactly the same trick as we did back in equation (1.26) to drop the denominator and replace the equals sign with a proportional sign $\propto$:

$$P(\texttt{murderer}|\texttt{weapon},\texttt{hair}) \propto P(\texttt{murderer}|\texttt{weapon})P(\texttt{hair}|\texttt{murderer},\texttt{weapon}). \tag{1.34}$$

Remembering that `hair` and `weapon` are conditionally indepedent given `murderer`, we can use equation (1.31) and drop `weapon` from the last term:

$$P(\texttt{murderer}|\texttt{weapon},\texttt{hair}) \propto P(\texttt{murderer}|\texttt{weapon})P(\texttt{hair}|\texttt{murderer}). \tag{1.35}$$

Since we know the values of `weapon` and `hair`, we can write in these observations:

$$\begin{aligned}&P(\texttt{murderer}|\texttt{weapon}=\texttt{revolver},\texttt{hair}=\texttt{true}) \propto \\ &\quad P(\texttt{murderer}|\texttt{weapon}=\texttt{revolver})P(\texttt{hair}=\texttt{true}|\texttt{murderer}).\end{aligned} \tag{1.36}$$

We can now compute the new posterior distribution for `murderer`. As before, each term depends only on the value of `murderer` and the overall normalization can be evaluated at the end. Substituting in the posterior we obtained in subsection 1.2.3 and our new conditional probability from equation (1.30) gives:

$$\begin{aligned}P(\texttt{murderer}=\texttt{Grey}|\texttt{weapon}=\texttt{rev.},\texttt{hair}=\texttt{true}) &\propto 0.66\times 0.50 = 0.33\\ P(\texttt{murderer}=\texttt{Auburn}|\texttt{weapon}=\texttt{rev.},\texttt{hair}=\texttt{true}) &\propto 0.34\times 0.05 = 0.017.\end{aligned}$$

The sum of these two numbers is 0.347, and dividing both numbers by their sum we obtain the normalized posterior probabilities in the form

$$\begin{aligned}P(\texttt{murderer}=\texttt{Grey}|\texttt{weapon}=\texttt{rev.},\texttt{hair}=\texttt{true}) &\simeq 0.95\\ P(\texttt{murderer}=\texttt{Auburn}|\texttt{weapon}=\texttt{rev.},\texttt{hair}=\texttt{true}) &\simeq 0.05.\end{aligned}$$

Taking account of all of the available evidence, the probability that Grey is the murderer is now 95%.

As a recap, we can plot how the probability distribution over `murderer` changed over the course of our murder investigation (Figure 1.13). Notice how the probability of `Grey` being the murderer started out low and increased as each new piece of evidence stacked against him. Similarly, notice how the probability of `Auburn` being the murderer evolved in exactly the opposite direction, due to the normalization constraint and the assumption that either one of the two suspects was the murderer. We could seek further evidence, in the hope that this would change the probability distribution to be even more confident (although, of course, evidence implicating Auburn would have the opposite effect). Instead, we will stop here – since 95% is greater than our threshold of 91% and so enough for a conviction!

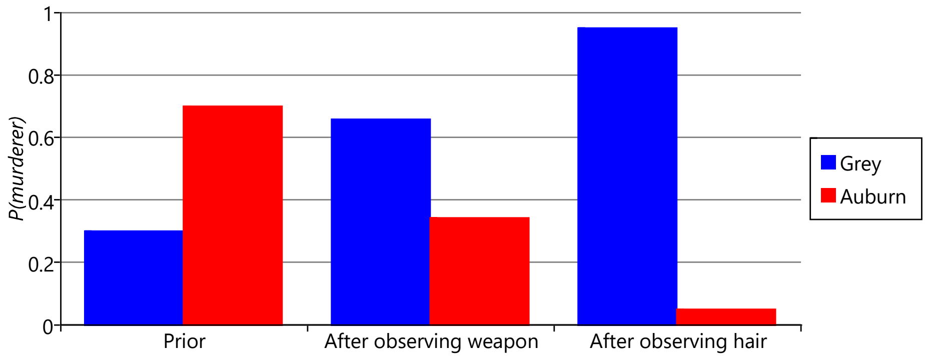


Figure 1.13: The evolution of $P(murderer)$ over the course of the murder investigation.

The model of the murder that we built up in this chapter contains various prior and conditional probabilities that we have set by hand. For real applications, however, we will usually have little idea of how to set such probability values and will instead need to *learn* them from data. In the next chapter we will see how such unknown probabilities can be expressed as random variables, whose values can be learned using the same probabilistic inference approach that we just used to solve a murder.

Self assessment 1.4

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Continuing your chosen scenario from previous self assessments, choose an additional variable that is affected by the conditioning variable. For example, if the conditioning variable is 'the traffic is bad', then an affected variable might be 'my boss is late for work'. Draw a factor graph for a larger model that includes this new variable, as well as the two previous variables. Define a conditional probability table for the new factor in the factor graph. Write down any conditional independence assumptions that you have made in choosing this model, along with a sentence justifying that choice of assumption.

2. Assume that the new variable in your factor graph is observed to have some particular value of your choice (for example, 'my boss is late for work' is observed to be true). Infer the posterior probability of the conditioning variable ('the traffic is bad') taking into account both this new observation and the observation of the other conditioned variable used in previous self assessments (for example, the observation that I am late for work).

3. Write a program to print out 1,000 joint samples of all three variables in your new model. Write down ahead of time how often you would

expect to see each triplet of values and then verify that this approximately matches the fraction of samples given by your program. Now change the program to only print out those samples which are consistent with your both observations from the previous question (for example, samples where you are late for work AND your boss is late for work). What fraction of these samples have each possible triplet of values now? How does this compare to your answer to the previous question?

4. Consider some other variables that might influence the three variables in your factor graph. For example, whether or not the traffic is bad might depend on whether it is raining, or whether there is an event happening nearby. Without writing down any conditional probabilities or specifying any factors, draw a Bayes net showing how the new variables influence your existing variables or each other. Each arrow in your Bayes net should mean that "the parent variable directly affects the child variable" or "the parent variable (partially) causes the child variable". If possible, present your Bayes network to someone else, and discuss it with them to see if they understand (and agree with) the assumptions you are making in terms of what variables to include in the model and what conditional independence assumptions you have made.

Review of concepts introduced in this section

conditional independence Two variables `A` and `B` are conditionally independent given a third variable `C`, if learning about `A` tells us nothing about `B` (and vice-versa) in the situation where we know the value of `C`. Put another way, it means that the value of `A` does not directly depend on the value of `B`, but only indirectly via the value of `C`. If `A` is conditionally independent of `B` given `C` then this can be exploited to simplify its conditional probability like so:

$$P(\mathtt{A}|\mathtt{B},\mathtt{C}) = P(\mathtt{A}|\mathtt{C}).$$

For example, the knowledge that a big sporting event is happening nearby (`B`) might lead you to expect congestion on your commute (`C`), which might increase your belief that you will be late for work (`A`). However, if you listen to the radio and find out that there is no congestion (so now you know `C`), then the knowledge of the sporting event (`B`) no longer influences your belief in how late you will be (`A`). This also applies the other way around, so someone observing whether you were late (`A`), who had also learned that there was no congestion (`C`) would be none the wiser as to whether a sporting event was happening (`B`).

Bayesian network A graphical model where nodes correspond to variables in the model and where edges show which variables directly influence each other. Factors are not shown, but the parent variables in a factor are connected directly to the child variable, using directed edges (arrows). See Panel 1.2.

Chapter 2

Assessing People's Skills

Throughout our lives, we are constantly assessing the skills and abilities of those around us. Who should I hire? Who should play on the team? Who can I ask for help? How can I best teach this person? Taking all that we know about someone and working out what they can and cannot do comes naturally to most of us. But how can we use model-based machine learning to do this automatically?

In this chapter, we will develop our first model of some real-world data. We will address the problem of assessing candidates for a job that requires certain skills. The idea is that candidates will take a multiple-choice test and we will use model-based machine learning to determine which skills each candidate has (and with what probability) given their answers in the test. We can then use this for tasks such as selecting a shortlist of candidates very likely to have a set of essential skills.

Each question in a test requires certain skills to answer. For a software development job, these skills might be knowledge of the programming language C# or the database query language SQL. Some of the questions might require multiple skills in order to be answered correctly. Figure 2.1 gives some example questions which have been marked with the skills required to answer them. Because our model could be used for many different types of job it must work with different tests and different skills, as long as these skill annotations are provided. It is important that the system should only use these annotations when presented with a new test – it must not require any additional information, for example, sample answers from people with known skills.

In order to assess which skills a candidate has, we will need to analyse their answers to the test. Since we know the skills needed for each question, this may

Software Development Skills Assessment

1. Which line of code creates a new Shape in C#? C#

```
a. Shape shape = new Shape();
b. Shape shape = Shape.new();
c. new Shape shape = Shape();
d. Shape shape = new Shape;
e. Shape shape = Shape();
```

2. Which SQL command is used to append a new row to a table in a database? SQL

```
a. ADD
b. INSERT
c. UPDATE
d. SET
e. INPUT
```

C#, SQL

3. After an SQL connection has been established using a SqlConnection object called "sql", which of the following will retrieve any rows in the "people" table with the name "bob"?

```
a. SqlCommand cmd = new SqlCommand("SELECT 'bob' FROM people", sql);
b. SqlCommand cmd = new SqlCommand("SELECT * FROM people WHERE name = 'bob'", sql);
c. SqlCommand cmd = new SqlCommand("SELECT * FROM people WHERE 'bob' IN name", sql);
d. SqlCommand cmd = sql.SqlCommand("SELECT * FROM people WHERE name = 'bob'");
e. SqlCommand cmd = sql.SqlCommand("SELECT 'bob' FROM people");
```

4. A developer wants to write a piece of software which

Figure 2.1: Part of a certification test used to assess software development skills. The questions have been annotated with the skills needed to answer them.

appear straightforward: we just need to check whether they are getting all the SQL questions right or all the C# questions wrong. But the real world is more complicated than this – even if someone knows C# they may make a mistake or misread a question; even if they do not know SQL they may guess the right answer by pure luck. In some cases, the test questions may be badly written or even outright wrong.

The situation is even more complicated for questions that need two (or more) skills. If someone gets a question that needs two skills right, it suggests that they are likely to have both skills. If they get it wrong, there are several possibilities: they could have one skill or the other (but probably not both) or they could have neither. Assessing which of these is the case requires looking at their answers to other questions and trying to find a consistent set of skills that is likely to give rise to all of the answers considered together. To do this kind of complex reasoning automatically, we need to design a model of how a person with particular skills answers a set of questions.

2.1 A model is a set of assumptions

When designing a model of some data, we must make assumptions about the process that gave rise to the data. In fact, we can say that the model *is* the set of assumptions and the set of assumptions *is* the model. The relationship between a model and the assumptions that it represents is so important that it is worth emphasising:

A model = A set of assumptions about the data

Selecting which assumptions to include in your model is a crucial part of model design. Incorrect assumptions will lead to models that give inaccurate predictions, due to these faulty assumptions. However, it is impossible to build a model without making at least *some* assumptions.

As you have seen in chapter 1, in this book we will use factor graphs to represent our models. As you progress through the book, you will learn how to construct the factor graph that encodes a chosen set of assumptions. Similarly, you will learn to look at a factor graph and work out which assumptions it represents. You can think of a factor graph as being a precise mathematical representation of a set of assumptions. For example, in chapter 1 we built up a factor graph that represented a precise set of assumptions about a murder mystery. For this application, we need to make assumptions about the process of a candidate answering some test questions if they have a particular skill set. This will define the relationship between a candidate's underlying skills and their test answers, which we can then invert to infer their skills from the test answers.

When designing a factor graph, we start by choosing which variables we want to have in the graph. At the very least, the graph must contain variables representing the data we actually have (whether the candidate got each question right) and any variables that we want to learn about (the skills). As we shall see, it is often useful to introduce other, intermediate, variables. Having chosen the variables, we can start adding factors to our graph to encode how these variables affect each other in the question-answering process. It is usually helpful to start with the variables we want to learn about (the skills) and work through the process to finish with the variables that we can actually measure (whether the candidate got the questions right).

So, starting with the skill variables, here is our first assumption:

1. A candidate has either mastered each skill or not.

Assumption 1 means that we can represent a candidate's skill as a binary (true/false) variable, which is `true` if the candidate has mastered the skill and `false` if they haven't. Variables which can take one of a fixed set of values (like all the variables we have seen so far) are called **discrete variables**. Later in the chapter, we will encounter **continuous variables** which can take any value in a continuous range of values, such as any real number between 0 and

1. As we shall see, continuous variables are useful for learning the probability of events, amongst many other uses.

We next need to make an assumption about the prior probability of a candidate having each of these skills.

(2) Before seeing any test results, it is equally likely that a candidate does or doesn't have any particular skill.

Assumption (2) means that the prior probability for each skill variable should be set neutrally to 50%, which is *Bernoulli*(0.5). To keep our factor graph small, we will start by considering a single candidate answering the three questions of Figure 2.1.

The above two assumptions, applied to the `csharp` and `sql` skills needed for these questions, give the following minimal factor graph:

Figure 2.2: Factor graph showing priors for the binary skill variables `csharp` and `sql`.

Remember that every factor graph represents a joint probability distribution over the variables in the graph. The joint distribution for this factor graph is:

$$P(\texttt{csharp}, \texttt{sql}) = \text{Bernoulli}(\texttt{csharp}; 0.5)\ \text{Bernoulli}(\texttt{sql}; 0.5). \tag{2.1}$$

Note that there is a term in the joint probability for every factor (black square) in the factor graph.

Continuing with the question-answering process, we must now make some assumptions about how a candidate's test answers relate to their skills. Suppose they have all the skills for a question, we should still allow that they may get it wrong some of the time. If we gave some SQL questions to a SQL expert, how many should we expect them to get right? Probably not all of them, but perhaps they would get 90% or so correct. We could check this assumption by asking some real experts to do such a quiz and seeing what scores they get, but for now we'll assume that getting one in ten wrong is reasonable:

(3) If a candidate has all of the skills needed for a question then they will usually get the question right, except one time in ten they will make a mistake.

For questions where the candidate lacks a necessary skill, we may assume that they guess at random:

(4) If a candidate doesn't have all the skills needed for a question, they will pick an answer at random. Because this is a multiple-choice exam with five answers, there's a one in five chance that they get the question right.

Assumption 3 and Assumption 4 tell us how to extend our factor graph to model the first two questions of Figure 2.1. We need to add in variables for each question that are `true` if the candidate got the question right and `false` if they got it wrong. Let's call these variables `isCorrect1` for the first question and `isCorrect2` for the second question. Based on our assumptions, if `csharp` is `true`, we expect `isCorrect1` to be `true` unless the candidate makes a mistake (since the first question only needs the `csharp` skill). Since we assume that mistakes happen only one time in ten, the probability that `isCorrect1` is `true` in this case is 90%. If `csharp` is `false`, then we assume that the candidate will only get the question right by one time in five, which is 20%. This gives us the following conditional probability table:

csharp	isCorrect1=true	isCorrect1=false
true	0.900	0.100
false	0.200	0.800

Table 2.1: Conditional probability table showing the probability of each value of `isCorrect1` conditioned on each of the two values of `csharp`.

We will call the factor representing this conditional probability table *AddNoise* since the output is a 'noisy' version of the input. Because our assumptions apply equally to all skills, we can use the same factor to relate `sql` to `isCorrect2`. This gives the following factor graph for the first two questions:

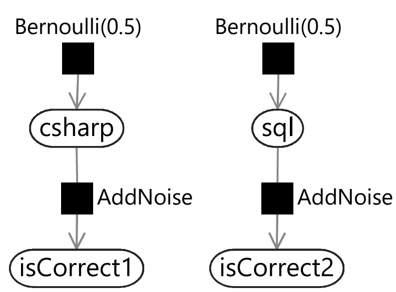


Figure 2.3: Factor graph for the first two questions in our test.

We can write down the joint probability distribution represented by this graph by including the two new terms for the *AddNoise* factors:

$$\begin{aligned} &P(\texttt{csharp}, \texttt{sql}, \texttt{isCorrect1}, \texttt{isCorrect2}) = \\ &\quad \text{Bernoulli}(\texttt{csharp}; 0.5)\ \text{Bernoulli}(\texttt{sql}; 0.5) \\ &\quad \text{AddNoise}(\texttt{isCorrect1}|\texttt{csharp})\ \text{AddNoise}(\texttt{isCorrect2}|\texttt{sql}). \end{aligned} \tag{2.2}$$

Modelling the third question is more complicated since this question requires both the `csharp` and `sql` skills. Assumption 3 and Assumption 4 refer to whether a candidate has "all the skills needed for a question". So for question 3, we need to include a new intermediate variable to represent whether the candidate has both the `csharp` and `sql` skills. We will call this binary variable `hasSkills`, which we want to be `true` if the candidate has both skills needed for the question and `false` otherwise. We achieve this by putting in an *And* factor connecting the two skill variables to the `hasSkills` variable. The *And* factor is defined so that $And(\mathtt{C}|\mathtt{A},\mathtt{B})$ is 1 if `C` is equal to `A` AND `B` and 0 otherwise. In other words, it forces the child variable `C` to be equal to (`A` AND `B`). A factor like *And*, where the child has a unique value given the parents, is called a **deterministic factor** (see Panel 2.1).

Here's a partial factor graph showing how the *And* factor can be used to make the `hasSkills` variable that we need:

Panel 2.1 – Deterministic factors

When building a model, we often want to include a variable which is a fixed function of some other variables in the model. For example, we may want a binary variable to be true if all of some other binary variables are true (AND) or if any of them are true (OR). For a continuous variable, we may want it to be the sum or product of some other continuous variables.
We can achieve this by putting a *deterministic* factor in our factor graph. The conditional probability distribution for a deterministic factor always has a value of either 1 or 0. It is 1 if the child variable is equal to the desired function of the parent variables and 0 otherwise. For example, if we want to add a variable `C` which is to be equal to `A` AND `B`, we can add a deterministic factor whose conditional probability distribution is:

A	B	C=false	C=true
false	false	1.000	0.000
false	true	1.000	0.000
true	false	1.000	0.000
true	true	0.000	1.000

Notice that whenever `C` is equal to `A` AND `B`, the conditional probability is 1 and it is 0 elsewhere. Since the overall joint probability includes this factor as one of its terms, the probability of any configuration of variables where `C` is not equal to `A` AND `B` must be zero. So the deterministic factor acts as a constraint that ensures `C`=(`A` AND `B`) is always true.
Throughout this book you will see that deterministic factors play a vital role in a wide variety of models.

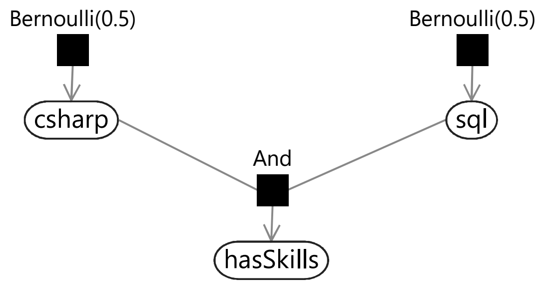


Figure 2.4: The *And* factor is a deterministic factor which constrains `hasSkills` to be true if `csharp` and `sql` are both true, and to be false in all other cases.

The joint probability distribution for this factor graph is:

$$P(\texttt{csharp}, \texttt{sql}, \texttt{hasSkills}) = \tag{2.3}$$
$$\text{Bernoulli}(\texttt{csharp}; 0.5)\ \text{Bernoulli}(\texttt{sql}; 0.5)\ \text{And}(\texttt{hasSkills}|\texttt{csharp}, \texttt{sql}).$$

The new *And* factor means that we now have a new *And* term in the joint probability distribution.

Now we can put everything together to build a factor graph for all three questions. We just need to connect `hasSkills` to our `isCorrect3` variable, once again using an *AddNoise* factor:

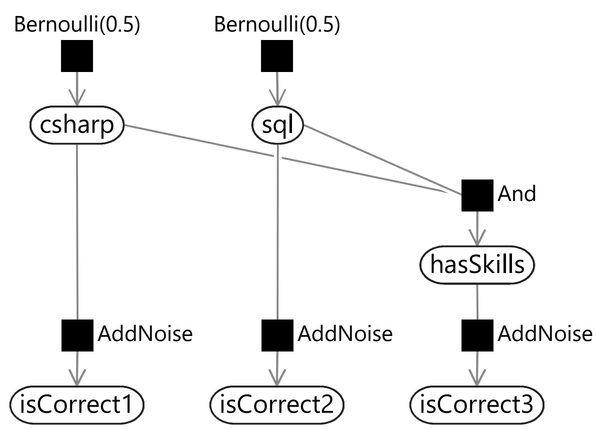


Figure 2.5: Factor graph for the three multiple choice questions of Figure 2.1.

The joint probability distribution for this factor graph is quite long because we now have a total of six factor nodes, meaning that it contains six terms:

$$P(\texttt{csharp}, \texttt{sql}, \texttt{hasSkills}, \texttt{isCorrect1}, \texttt{isCorrect2}, \texttt{isCorrect3}) = \tag{2.4}$$
$$\text{Bernoulli}(\texttt{csharp}; 0.5)\ \text{Bernoulli}(\texttt{sql}; 0.5)$$
$$\text{AddNoise}(\texttt{isCorrect1}|\texttt{csharp})\ \text{AddNoise}(\texttt{isCorrect2}|\texttt{sql})$$
$$\text{And}(\texttt{hasSkills}|\texttt{csharp}, \texttt{sql})\ \text{AddNoise}(\texttt{isCorrect3}|\texttt{hasSkills}).$$

Because joint probability distributions like this one are big and awkward to work with, it is usually easier to use factor graphs as a more readable and manageable way to express a model.

It is essential that any model contains variables corresponding to the observed data, and that these variables are of the same type. This allows the data to be attached to the model by fixing these variables to the corresponding observed data values. An inference calculation can then be used to find the marginal distributions for any other (unobserved) variable in the model. For our model, we need to ensure that we can attach our test results data to the model, which consists of a yes/no result for each question depending on whether the candidate got that question right. We can indeed attach this data to our model, because we have binary variables (`isCorrect1`, `isCorrect2`, `isCorrect3`) which we can set to be `true` if the candidate got the question right and `false` otherwise.

There is one more assumption being made in this model that has not yet been mentioned. In fact, it is normally one of the biggest assumptions made by any model! It is the assumed *scope* of the model: that is, the assumption that only the variables included in the model are relevant. For example, our model makes no mention of the mental state of the candidate (tired, stressed), or of the conditions in which they were performing the test, or whether it is possible that cheating was taking place, or whether the candidate even understands the language the questions are written in. By excluding these variables from our model, we have made the strong assumption that they are independent from (do not affect) the candidate's answers.

Poor assumptions about scope often lead to unsatisfactory results of the inference process, such as reduced accuracy in making predictions. The scope of a model is an assumption that should be critically assessed during the model design process, if only to identify aspects of the problem that are being ignored. So to be explicit, the last assumption for our learning skills model is:

5 Whether the candidate gets a question right depends only on what skills that candidate has and not on *anything* else.

We will not explicitly call out this assumption in future models, but it is good practice to consider carefully what variables are being ignored, whenever you are designing or using a model.

2.1.1 Questioning our assumptions

Having constructed the factor graph, let us pause for a moment and review the assumptions we have made so far. They are all shown together in Table 2.2.

1	Each candidate has either mastered each skill or not.
2	Before seeing any test results, it is equally likely that each candidate does or doesn't have any particular skill.
3	If a candidate has all of the skills needed for a question then they will get the question right, except one time in ten they will make a mistake.
4	If a candidate doesn't have all the skills needed for a question, they will pick an answer at random. Because this is a multiple-choice exam with five answers, there's a one in five chance that they get the question right.
5	Whether the candidate gets a question right depends only on what skills that candidate has and not on anything else.

Table 2.2: The five assumptions encoded in our model.

It is very important to review all modelling assumptions carefully to ensure that they are reasonable. For example, Assumption 1 is a simplifying assumption which reduces the degree of skill that a candidate has into a simple yes/no variable. It is usual to have to make such simplifying assumptions, which are not exactly incorrect but which make the model less precise. Simplifying assumptions can be made as long as you keep in mind that these may reduce the accuracy of the results. Assumption 2 seems apparently safe since it is just assuming ignorance. However, it is also assuming that each of the skill variables are independent, that is, knowing that someone has one particular skill doesn't tell you anything about whether they have any of the other skills. If some of the skills are related in some way, this may well not be the case. To keep the model simple, we will work with this assumption for now, but bear it in mind as a candidate for refinement later on. Assumption 3 and Assumption 4 are more subtle: is it really true that if the candidate has, say, two out of three skills needed for a question, then they are reduced to guesswork? We will continue to use these assumptions for now – later in the chapter we will show how to diagnose whether our model assumptions are causing problems and see how to revise them. Assumption 5, that no other variables are relevant, is reasonable assuming that there is a conscientious examiner administering the test. A good examiner will make sure that a candidate's answers genuinely reflect their skills and are not affected by external conditions or cheating.

Having reviewed our assumptions by eye, we can now try the model out to ensure that the assumptions continue to make sense when applied to realistic example data.

Self assessment 2.1

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Write down the conditional probability table for a deterministic factor which represents the OR function. The child variable `C` should be true if either of the parent variables `A` and `B` are true. Panel 2.1 should help.

2. Write down all the independence and conditional independence assumptions that you can find in Figure 2.5. For each assumption ask yourself whether it is reasonable – as discussed in chapter 1, for independence assumptions you need to ask yourself the question "does learning about A tell me anything about B?" and for conditional independence assumptions you need to ask "if I know X, does learning about A tell me anything about B?".

3. As mentioned above, there may be many other variables that affect the test outcomes (e.g. cheating, candidate's state of mind). Draw a Bayesian network that includes one or more of these additional variables, as well as all the variables in our current model. Your Bayes net should only include edges between variables that directly affect each other. It may be helpful to introduce intermediate variables as well. If possible, present your Bayes net to someone else and discuss whether they agree with the assumptions you have made.

Review of concepts introduced in this section

discrete variables Variables which can take one of a fixed set of values. For example, a binary variable can take only two values `true` or `false`.

continuous variables Variables which can take any value in a continuous range of values, for example, any real number between 0 and 1.

deterministic factor A factor defining a conditional probability which is always either 0 or 1. This means that the value of child variable can always be uniquely determined (i.e. computed) given the value of the parent variables. For example a factor representing the AND operation is a deterministic factor. See Panel 2.1 for more details.

2.2 Testing out the model

Having constructed a model, the first thing to do is to test it out with some simple example data to check that its behaviour is reasonable. Suppose a candidate knows C# but not SQL – we would expect them to get the first question right and the other two questions wrong. So let's test the model out for this case and see what skills it infers for that pattern of answers. For convenience, we'll use `isCorrect` to refer to the array [`isCorrect1`,`isCorrect2`,`isCorrect3`] and so we will consider the case where `isCorrect` is [`true`,`false`,`false`].

We want to infer the probability that the candidate has the `csharp` and `sql` skills, given this particular set of `isCorrect` values. This is an example of an **inference query** which is defined by the variables we want to infer (`csharp`, `sql`) and the variables we are conditioning on (`isCorrect`) along with their observed values. Because this example is quite small, we can work out the answer to this inference query by hand.

2.2.1 Doing inference by hand

Inference

Inference deep-dive
In this optional section, we perform inference in our model manually by marginalising the joint distribution. If you want to focus on modelling, feel free to skip this section.

As we saw in chapter 1, we can perform inference by marginalising the joint distribution (summing it over all the variables except the one we are interested in) while fixing the values of any observed variables. For the three-question factor graph, we wrote down the joint probability distribution in equation (2.4). Here it is again:

$$\begin{aligned} &P(\texttt{csharp}, \texttt{sql}, \texttt{hasSkills}, \texttt{isCorrect}) = \\ &\quad \text{Bernoulli}(\texttt{csharp}; 0.5)\ \text{Bernoulli}(\texttt{sql}; 0.5) \\ &\quad \text{AddNoise}(\texttt{isCorrect1}|\texttt{csharp})\ \text{AddNoise}(\texttt{isCorrect2}|\texttt{sql}) \\ &\quad \text{And}(\texttt{hasSkills}|\texttt{csharp}, \texttt{sql})\ \text{AddNoise}(\texttt{isCorrect3}|\texttt{hasSkills}). \end{aligned} \tag{2.5}$$

Before we start this inference calculation, we need to show how to compute a **product of distributions**. Suppose for some variable `x`, we know that:

$$P(\texttt{x}) \propto \text{Bernoulli}(\texttt{x}; 0.8)\ \text{Bernoulli}(\texttt{x}; 0.4). \tag{2.6}$$

This may look odd since we normally only associate one distribution with a variable but, as we'll see, products of distributions arise frequently when performing inference. Evaluating this expression for the two values of `x` gives:

$$P(\texttt{x}) \propto \begin{cases} 0.8 \times 0.4 = 0.32 & \text{if } \texttt{x} = \texttt{true} \\ 0.2 \times 0.6 = 0.12 & \text{if } \texttt{x} = \texttt{false}. \end{cases} \tag{2.7}$$

Since we know that $P(\mathtt{x} = \mathtt{true})$ and $P(\mathtt{x} = \mathtt{false})$ must add up to one, we can divide these values by $0.32 + 0.12 = 0.44$ to get:

$$P(\mathtt{x}) = \begin{cases} 0.727 & \text{if } \mathtt{x} = \mathtt{true} \\ 0.273 & \text{if } \mathtt{x} = \mathtt{false} \end{cases} = \text{Bernoulli}(\mathtt{x}; 0.727). \tag{2.8}$$

This calculation may feel familiar to you – it is very similar to the inference calculations that we performed in chapter 1.

In general, if want to multiply two Bernoulli distributions, we can use the rule that:

$$\text{Bernoulli}(\mathtt{x}; a)\ \text{Bernoulli}(\mathtt{x}; b) \propto \text{Bernoulli}\left(\mathtt{x}\ ;\ \frac{ab}{ab + (1-a)(1-b)}\right). \tag{2.9}$$

If, say, the second distribution is uniform (b=0.5), the result of the product is $\text{Bernoulli}(\mathtt{x}; a)$. In other words, the distribution $\text{Bernoulli}(\mathtt{x}; a)$ is unchanged by multiplying by a uniform distribution. In general, multiplying *any* distribution by the uniform distribution leaves it unchanged.

Armed with the ability to multiply distributions, we can now compute the probability that our example candidate has the `csharp` skill. The precise probability we want to compute is $P(\mathtt{csharp}|\mathtt{isCorrect} = [\mathtt{T}, \mathtt{F}, \mathtt{F}])$, where we have abbreviated `true` to `T` and `false` to `F`. As before, we can compute this by marginalising the joint distribution and fixing the observed values:

$$\begin{aligned} &P(\mathtt{csharp}|\mathtt{isCorrect} = [\mathtt{T}, \mathtt{F}, \mathtt{F}]) \propto \\ &\quad \sum_{\mathtt{sql}} \sum_{\mathtt{hasSkills}} P(\mathtt{csharp}, \mathtt{sql}, \mathtt{hasSkills}, \mathtt{isCorrect} = [\mathtt{T}, \mathtt{F}, \mathtt{F}]). \end{aligned} \tag{2.10}$$

As we saw in chapter 1, we use the proportional sign $\propto$ because we do not care about the scaling of the right hand side, only the ratio of its value when `csharp` is `true` to the value when `csharp` is `false`.

Now we put in the full expression for the joint probability from (2.5) and fix the values of all the observed variables. We can ignore the *Bernoulli*(0.5) terms since, as we just learned, multiplying a distribution by a uniform distribution leaves it unchanged. So the right hand side of (2.10) becomes

$$\begin{aligned} \propto \sum_{\mathtt{sql}} \sum_{\mathtt{hasSkills}} &\text{AddNoise}(\mathtt{isCorrect1} = \mathtt{T}|\mathtt{csharp}) \\ &\text{AddNoise}(\mathtt{isCorrect2} = \mathtt{F}|\mathtt{sql}) \\ &\text{And}(\mathtt{hasSkills}|\mathtt{csharp}, \mathtt{sql})\ \text{AddNoise}(\mathtt{isCorrect3} = \mathtt{F}|\mathtt{hasSkills}). \end{aligned} \tag{2.11}$$

Terms inside of each summation $\sum$ that do not mention the variable being summed over can be moved outside of the summation, because they have the same value for each term being summed. You can also think of this as moving the summation signs in towards the right:

$$\begin{aligned}\propto\ &\mathrm{AddNoise}(\mathtt{isCorrect1} = \mathtt{T}|\mathtt{csharp}) \\ &\sum_{\mathtt{sql}} \mathrm{AddNoise}(\mathtt{isCorrect2} = \mathtt{F}|\mathtt{sql}) \\ &\sum_{\mathtt{hasSkills}} \mathrm{And}(\mathtt{hasSkills}|\mathtt{csharp}, \mathtt{sql})\ \mathrm{AddNoise}(\mathtt{isCorrect3} = \mathtt{F}|\mathtt{hasSkills}).\end{aligned} \tag{2.12}$$

If you look at the first term here, you'll see that it is a function of `csharp` only, since `isCorrect1` is observed to be `true`. When `csharp` is `true`, this term has the value 0.9. When `csharp` is `false`, this term has the value 0.2. Since we only care about the relative sizes of these two numbers, we can replace this term by a *Bernoulli* term where the probability of `true` is $\frac{0.9}{0.9+0.2} = 0.818$ and the probability of `false` is therefore 1-0.818=0.182. Note that this has preserved the `true`/`false` ratio $0.818/0.182 = 0.9/0.2$.

Similarly the second *AddNoise* term has value 0.1 when `sql` is `true` and the value 0.8 when `sql` is `false`, so can be replaced by a *Bernoulli* term where the probability of `true` is $\frac{0.1}{0.1+0.8} = 0.111$. The final *AddNoise* term can also be replaced, giving:

$$\begin{aligned}\propto\ &\mathrm{Bernoulli}(\mathtt{csharp}; 0.818) \\ &\sum_{\mathtt{sql}} \mathrm{Bernoulli}(\mathtt{sql}; 0.111) \\ &\sum_{\mathtt{hasSkills}} \mathrm{And}(\mathtt{hasSkills}|\mathtt{csharp}, \mathtt{sql})\ \mathrm{Bernoulli}(\mathtt{hasSkills}; 0.111).\end{aligned} \tag{2.13}$$

For the deterministic *And* factor, we need to consider the four cases where the factor is not zero (which we saw in Panel 2.1) and plug in the *Bernoulli*(0.111) distributions for `sql` and `hasSkills` in each case:

csharp	sql	hasSkills	Bern(sql|0.111)	Bern(hasSkills|0.111)	Product
false	false	false	1-0.111	1-0.111	0.790
false	true	false	0.111	1-0.111	0.099
true	false	false	1-0.111	1-0.111	0.790
true	true	true	0.111	0.111	0.012

Table 2.3: Evaluation of the last three terms in (2.13). Each row of the table corresponds to one of the four cases where the *And* factor is 1 (rather than 0). The first three columns give the values of `csharp`, `sql` and `hasSkills`, which is just the truth table for AND. The next two columns give the corresponding values of the *Bernoulli* distributions for `sql` and `hasSkills` and the final column multiplies these together.

Looking at Table 2.3, we can see that when `csharp` is `true`, either both `sql` and `hasSkills` are `false` (with probability 0.790) or both `sql` and `hasSkills` are `true` (with probability 0.012). The sum of these is 0.802. When `csharp` is `false`, the corresponding sum is $0.790 + 0.099 = 0.889$. So we can replace the last three terms by a *Bernoulli* term with parameter $\frac{0.802}{0.802+0.889} = 0.474$.

$$\propto \text{Bernoulli}(\texttt{csharp}; 0.818)\ \text{Bernoulli}(\texttt{csharp}; 0.474) \tag{2.14}$$

Now we have a product of Bernoulli distributions, so we can use (2.9) to multiply them together. When `csharp` is `true`, this product has value $0.818 \times 0.474 = 0.388$. When `csharp` is `false`, the value is $(1 - 0.818) \times (1 - 0.474) = 0.096$. Therefore, the product of these two distributions is a *Bernoulli* whose parameter is $\frac{0.388}{0.388+0.096}$:

$$= \text{Bernoulli}(\texttt{csharp}; 0.802) \tag{2.15}$$

So we have calculated that the posterior probability that our candidate has the `csharp` skill to be 80.2%. If we work through a similar calculation for the `sql` skill, we find the posterior probability is 3.4%. Together these probabilities say that the candidate is likely to know C# but is unlikely to know SQL, which seems like a very reasonable inference given that the candidate only got the C# question right.

2.2.2 Doing inference by passing messages on the graph

INFERENCE

Inference deep-dive
Doing inference calculations manually takes a long time and it is easy to make mistakes. Instead, we can do the same calculation mechanically by using a **message passing algorithm**. This works by passing messages along the edges of the factor graph, where a message is a probability distribution over the variable that the edge is connected to. We will see that using a message passing algorithm lets us do the inference calculations automatically – a huge advantage of the model-based approach!

In this optional section, we show how inference can be performed using a message passing algorithm called belief propagation. If you want to focus on modelling, feel free to skip this section. Let us redo the inference calculation for the `csharp` skill using message passing – we'll describe the message passing process for this example first, and then look at the general form later on. The first step in the manual calculation was to fix the values of the observed variables. Using message passing, this corresponds to each observed variable sending out a message which is a point mass distribution at the observed value. In our case, each `isCorrect` variable sends the point mass *Bernoulli*(0) if it is observed to be `false` or the point mass *Bernoulli*(1) if it is observed to be `true`. This means that the three messages sent are as shown in Figure 2.6.

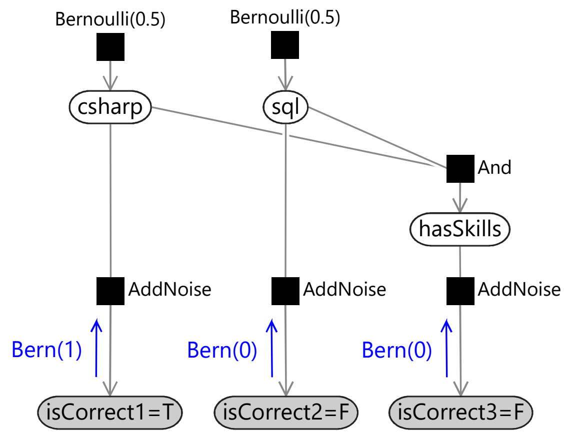


Figure 2.6: The messages sent from the observed variable nodes, which are shown shaded and labelled with their observed values. The message on any edge is a distribution over the variable that the edge is connected to. For example, the left hand $Bern(1)$ is short for $Bernoulli(\texttt{isCorrect1}; 1)$.

These point mass messages then arrive at the *AddNoise* factor nodes. The outgoing messages at each factor node can be computed separately as follows:

- The message up from the first *AddNoise* factor to `csharp` can be computed by writing $\text{AddNoise}(\texttt{isCorrect1} = \texttt{T}|\texttt{csharp})$ as a Bernoulli distribution over `csharp`. As we saw in the last section, the parameter of the Bernoulli is $p = \frac{0.9}{0.9+0.2} = 0.818$, so the upward message is $Bernoulli(0.818)$.

- The message up from the second *AddNoise* factor to `sql` can be computed by writing $\text{AddNoise}(\texttt{isCorrect2} = \texttt{F}|\texttt{sql})$ as a Bernoulli distribution over `sql`. The parameter of the Bernoulli is $p = \frac{0.1}{0.1+0.8} = 0.111$, so the upward message is $Bernoulli(0.111)$.

- The message up from the third *AddNoise* factor to `hasSkills` is the same as the second message, since it is computed for the same factor with the same incoming message. Hence, the third upward message is also $Bernoulli(0.111)$.

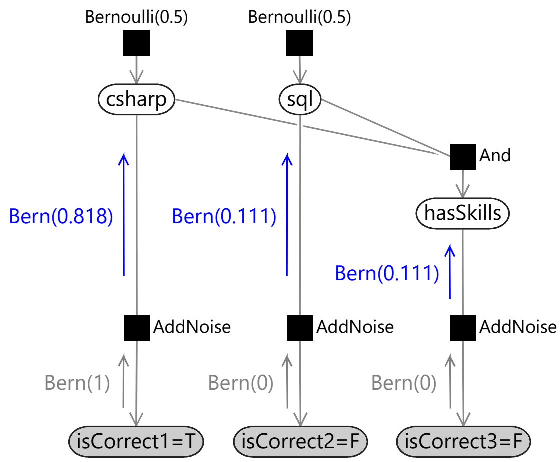


Figure 2.7: Outgoing messages from the *AddNoise* factor nodes.

Note that these three messages are exactly the three Bernoulli distributions we saw in in (2.13). Rather than working on the entire joint distribution, we have broken down the calculation into simple, repeatable message computations at the nodes in the factor graph.

The messages down from the *Bernoulli*(0.5) prior factors are just the prior distributions themselves:

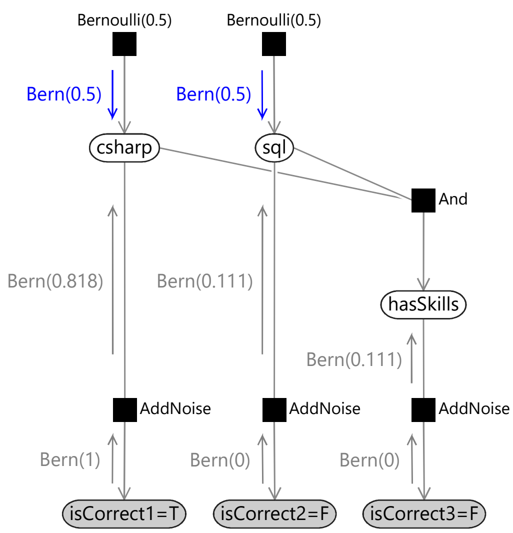


Figure 2.8: Messages from the *Bernoulli* prior factor nodes.

The outgoing message for any variable node is the product of the incoming messages on the other edges connected to that node. For the `sql` variable node we now have incoming messages on two edges, which means we can compute the outgoing message towards the *And* factor. This is *Bernoulli*(0.111) since the upward message is unchanged by multiplying by the uniform downward message *Bernoulli*(0.5). The `hasSkills` variable node is even simpler: since there is only one incoming message, the outgoing message is just a copy of it.

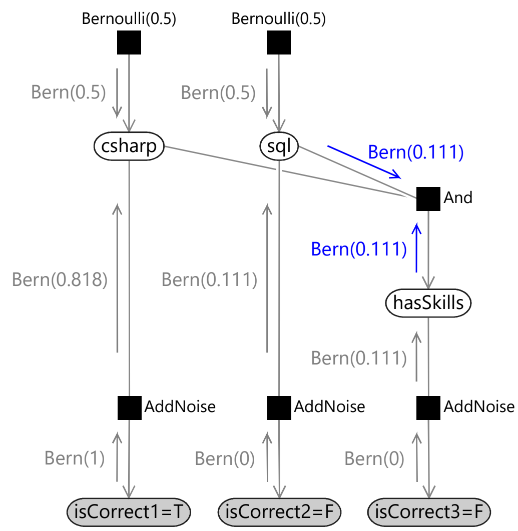


Figure 2.9: Messages out of the `sql` and `hasSkills` variable nodes.

Finally, we can compute the outgoing message from the *And* factor to the `csharp` variable. This is computed by multiplying the incoming messages by the factor function and summing over all variables other than the one being sent to (so we sum over `sql` and `hasSkills`):

$$\sum_{\texttt{sql}} \sum_{\texttt{hasSkills}} \text{And}(\texttt{hasSkills}|\texttt{csharp}, \texttt{sql}) \\ \text{Bernoulli}(\texttt{sql}; 0.111)\ \text{Bernoulli}(\texttt{hasSkills}; 0.111). \tag{2.16}$$

The summation gives the message *Bernoulli*(0.474), as we saw in equation (2.14).

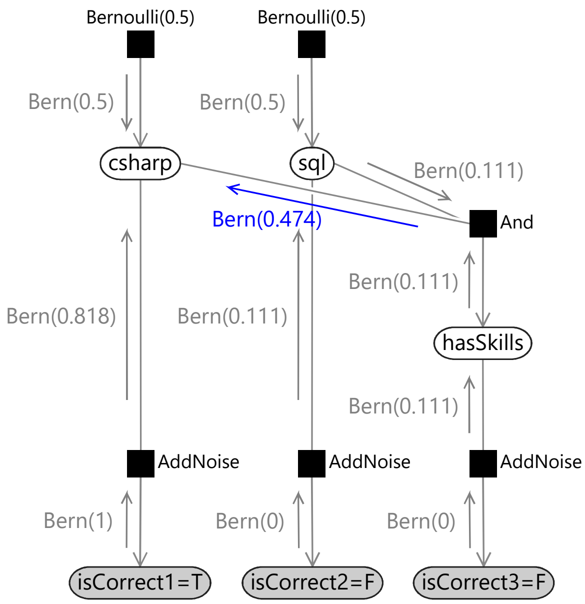


Figure 2.10: The final message toward the `csharp` variable node.

We now have all three incoming messages at the `csharp` variable node, which means we are ready to compute its posterior marginal. This is achieved by multiplying together the three messages – this is the calculation we performed in equation (2.14) and hence gives the same result *Bernoulli*(0.802) or 80.2%.

To compute the marginal for `sql`, we can re-use most of the messages we just calculated and so only need to compute two additional messages (shown in Figure 2.11). The first message, from `csharp` to the *And* factor, is the product of *Bernoulli*(0.818) and the uniform distribution *Bernoulli*(0.5), so the result is also *Bernoulli*(0.818).

The second message is from the *And* factor to `sql`. Again, we compute it by multiplying the incoming messages by the factor function and summing over all variables other than the one being sent to (so we sum over `csharp` and `hasSkills`):

$$\sum_{\texttt{csharp}} \sum_{\texttt{hasSkills}} \text{And}(\texttt{hasSkills}|\texttt{csharp}, \texttt{sql}) \\ \text{Bernoulli}(\texttt{csharp}; 0.818)\ \text{Bernoulli}(\texttt{hasSkills}; 0.111). \tag{2.17}$$

The summation gives the message *Bernoulli*(0.221), so the two new messages we have computed are those shown in Figure 2.11.

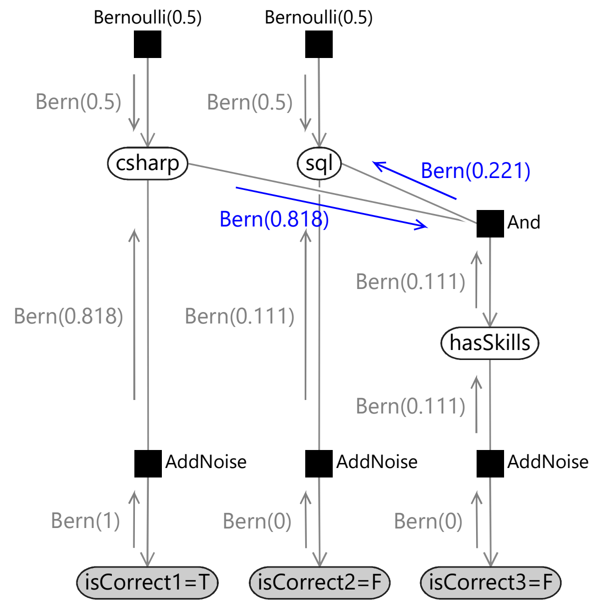


Figure 2.11: Additional messages needed to compute the marginal for the `sql` variable.

Multiplying this message into `sql` with the upward message from the *AddNoise* factor gives $Bernoulli(0.111) \times Bernoulli(0.221) \propto Bernoulli(0.034)$ or 3.4%, the same result as before. Note that again we have ignored the uniform $Bernoulli(0.5)$ message from the prior, since multiplying by a uniform distribution has no effect.

The message passing procedure we just saw arises from applying an algorithm called **belief propagation** [Pearl, 1988; Lauritzen and Spiegelhalter, 1988]. In belief propagation, messages are computed in one of three ways, depending on whether the message is coming from a factor node, an observed variable node or an unobserved variable node. The full algorithm is given in algorithm 2.1. The derivation of this algorithm can be found in Bishop [2006].

2.2.3 Using belief propagation to test out the model

The belief propagation algorithm allows us to do inference calculations entirely automatically for a given factor graph. This means that it is possible to completely automate the process of answering an inference query without writing any code or doing any hand calculation!

Using belief propagation, we can test out our model fully by automatically inferring the marginal distributions for the skills for every possible configuration of correct and incorrect answers. The results of doing this are shown in Table 2.4.

IsCorrect1	IsCorrect2	IsCorrect3	P(csharp)	P(sql)
☐	☐	☐	0.101	0.101
☑	☐	☐	0.802	0.034
☐	☑	☐	0.034	0.802
☑	☑	☐	0.561	0.561
☐	☐	☑	0.148	0.148
☑	☐	☑	0.862	0.326
☐	☑	☑	0.326	0.862
☑	☑	☑	0.946	0.946

Table 2.4: The posterior probabilities for the `csharp` and `sql` variables for all possible configurations of `isCorrect`. As before, the blue bars give a visual representation of the inferred probabilities.

Inspecting this table, we can see that the results appear to be sensible – the probability of having the `csharp` skill is generally higher when the candidate got the first question correct and similarly the probability of having the `sql` skill is generally higher when the candidate got the second question correct. Also, both

Algorithm 2.1: Belief Propagation

Input: factor graph, list of target variables to compute marginal distributions for.
Output: marginal distributions for target variables.

repeat
    foreach *node in the factor graph* **do**
        foreach *edge connected to the node* **do**
            If all needed incoming messages are available send the appropriate outgoing message below:
            - Variable node message: the product of all messages received on the other edges;
            - Factor node message: the product of all messages received on the other edges, multiplied by the factor function and summed over all variables except the one being sent to;
            - Observed node message: a point mass at the observed value;
        end
    end
until *target variables have received incoming messages on all edges*
Compute marginal distributions as the product of all incoming messages at each target variable node.

probabilities are higher when the third question is correct rather than incorrect.

Interestingly, the probability of having the `sql` skill is actually lower when only the first question is correct, than where the candidate got all the questions wrong (first and second rows of Table 2.4). This makes sense because getting the first question right means the candidate probably has the `csharp` skill, which makes it even more likely that the explanation for getting the third question wrong is that they *didn't* have the `sql` skill. This is an example of the kind of subtle reasoning which model-based machine learning can achieve, which can give it an advantage over simpler approaches. For example, if we just used the number of questions needing a particular skill that a person got right as an indicator of that skill, we would be ignoring potentially useful information coming from the other questions. In contrast, using a suitable model, we have exploited the fact that getting a `csharp` question right can actually *decrease* the probability of having the `sql` skill.

Self assessment 2.2

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Compute the product of the following pairs of Bernoulli distributions

   (a) $\text{Bernoulli}(\mathtt{x}; 0.3) \times \text{Bernoulli}(\mathtt{x}; 0.9)$

   (b) $\text{Bernoulli}(\mathtt{x}; 0.5) \times \text{Bernoulli}(\mathtt{x}; 0.2)$

   (c) $\text{Bernoulli}(\mathtt{x}; 0.5) \times \text{Bernoulli}(\mathtt{x}; 0.3)$

   (d) $\text{Bernoulli}(\mathtt{x}; 1.0) \times \text{Bernoulli}(\mathtt{x}; 0.2)$

   (e) $\text{Bernoulli}(\mathtt{x}; 1.0) \times \text{Bernoulli}(\mathtt{x}; 0.3)$

   Why can we not compute $\text{Bernoulli}(\mathtt{x}; 1.0) \times \text{Bernoulli}(\mathtt{x}; 0.0)$?

2. Write a program (or create a spreadsheet) to print out pairs of samples from two Bernoulli distributions with different parameters a and b. Now filter the output of the program to only show samples pairs which have the same value (i.e. where both samples are `true` or where both are `false`). Print out the fraction of these samples which are `true`. This process corresponds to multiplying the two Bernoulli distributions together and so the resulting fraction should be close to the value given by equation (2.9).

   Use your program to (approximately) verify your answers to the previous question. What does your program do when $a = 0.0$ and $b = 1.0$?

3. Manually compute the posterior probability for the `sql` skill, as we did for the `csharp` skill in subsection 2.2.1, and show that it comes to 3.4%.

4. Build this model in Infer.NET and reproduce the results in Table 2.4. For examples of how to construct a conditional probability table, it may be useful to refer to the wet grass/sprinkler/rain example in this thread.

You will also need to use the Infer.NET & operator for the *And* factor. This exercise demonstrates how inference calculations can be performed completely automatically given a model definition.

Review of concepts introduced in this section

inference query A query which defines an inference calculation to be done on a probabilistic model. It consists of the set of variables whose values that we know (along with those values) and another set of variables that we wish to infer posterior distributions for. An example of an inference query is if we may know that the variable `weapon` takes the value `revolver` and wish to infer the posterior distribution over the variable `murderer`.

product of distributions An operation which multiplies two (or more) probability distributions and then normalizes the result to sum to 1, giving a new probability distribution. This operation should not be confused with multiplying two different random variables together (which may happen using a deterministic factor in a model). Instead, a product of distributions involves two distributions over the *same* random variable. Products of distributions are used frequently during inference to combine multiple pieces of uncertain information about a particular variable which have come from different sources.

message passing algorithm An algorithm for doing inference calculations by passing messages over the edges of a graphical model, such as a factor graph. The messages are probability distributions over the variable that the edge is connected to. Belief propagation is a commonly used message passing algorithm.

belief propagation A message passing algorithm for computing posterior marginal distributions over variables in a factor graph. Belief propagation uses two different messages computations, one for messages from factors to variables and one for messages from variables to factors. Observed variables send point mass messages. See algorithm 2.1.

2.3 Loopiness

Let's now extend our model slightly by adding a fourth question which needs both skills. This new factor graph is shown in Figure 2.12, where we have added new `isCorrect4` and `hasSkills4` variables for the new question. Surely we can also do inference in this, very slightly larger, graph using belief propagation? In fact, we cannot.

The problem is that belief propagation can only send a message out of an (unobserved) node after we have received messages on all other edges of that node (algorithm 2.1). Given this constraint, we can only send all the messages in a graph if there are no **loops**, where a loop is a path through the graph which starts and finishes at the same node (without using the same edge twice). If the graph has a loop, then we cannot send any of the messages along the edges of the loop because that will always require one of the other messages in the loop to have been computed first.

Loops can be challenging.

If you look back at the old three-question factor graph (Figure 2.5) you'll see that it has no loops (a graph with no loops is called a **tree**) and so belief propagation worked without problems. However, our new graph does have a

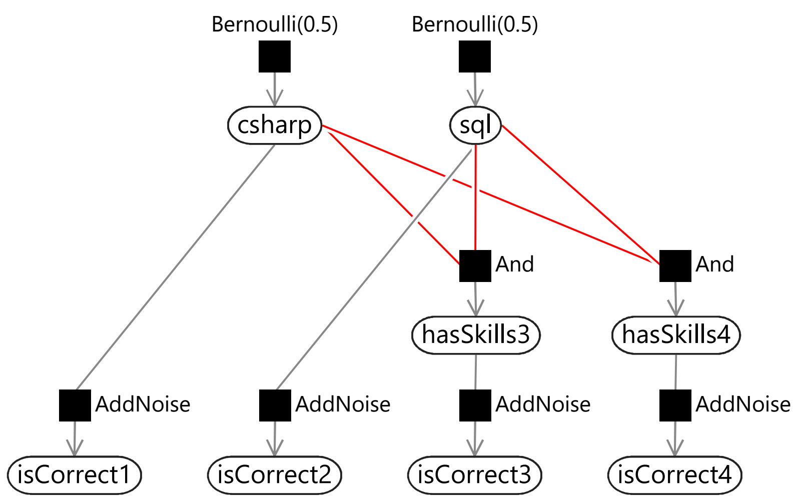


Figure 2.12: Factor graph for a four-question test. This graph contains a loop (shown in red) which means that we cannot apply belief propagation.

loop, which is marked in red in Figure 2.12. To do inference in such a **loopy graph**, we need to look beyond standard belief propagation.

To perform inference in loopy graphs, we need to get rid of the loops somehow. There are various methods to do this (see Panel 2.2) but they can all become too slow to use when dealing with large factor graphs. In most real applications the graphs are very large but, at the same time, inference needs to be performed quickly. The result is that such **exact inference** methods are often too slow to be useful.

The alternative is to look at methods that compute an approximation to the required marginal distributions, but which can do so in much less time. In this book, we will focus on such **approximate inference** approaches, since they have proven to be remarkably useful in a wide range of applications. For this particular loopy graph, we will introduce an approximate inference algorithm called **loopy belief propagation**.

2.3.1 Loopy belief propagation

INFERENCE

Inference deep-dive
In this optional section, we define the loopy belief propagation algorithm and use it to perform inference in our loopy model. If you want to focus on modelling, feel free to skip this section. Loopy belief propagation [Frey and MacKay, 1998] is identical to belief propagation until we come to a message that we cannot compute because it is in a loop. At that point, the loopy belief propagation algorithm computes the message anyway using a suitable initial value for any messages which are not yet available.

So, in loopy belief propagation, when we wish to compute a message m that depends on other messages which are not yet computed, we use a special initial message value for the unavailable messages. This initial value is usually the uniform distribution (such as $\mathit{Bernoulli}(0.5)$) but in some cases it may be preferable to use some other user-supplied distribution. These initial message values allows us to break the loop and compute m. Once we have computed m, we will be able to compute other messages around the loop and eventually we get back to the original node. At this point, all the incoming messages needed to compute m will have been computed, so we can recompute m using these values instead of the initial ones. But because m has changed in value, we can then go around the loop computing all the messages again. Which will bring us back to recomputing m, and so on. After a number of iterations around the loop, this procedure often leads to the value of message m not changing – we say that it has **converged**. At this point, we can stop sending any further messages, since there will be no further changes to the computed marginal distributions.

The complete loopy belief propagation algorithm is given as algorithm 2.2 – it requires as input a message-passing schedule, which we will discuss shortly. Loopy belief propagation is not guaranteed to give the exactly correct result but it often gives results that are very close. Unlike exact inference methods, however, loopy belief propagation is still fast when applied to large models, which is a very desirable property in real applications.

Panel 2.2 – Exact Inference in Loopy Graphs

To perform inference calculations exactly in loopy graphs, we need to find a way to remove the loops and so convert the graph into a tree. Once we have a tree, we can run belief propagation as normal. There are two common approaches for removing loops from a loopy graph:

1. **Remove loops by merging variables together**

   In our example, we could replace the variables `csharp` and `sql` by a single variable with four states FF, TF, FT, TT. We would also need to modify and in some cases combine all the factors connected to either variable. The resulting factor graph would no longer contain a loop. This approach is the basis of the *junction tree algorithm* Lauritzen and Spiegelhalter [1988] which merges variables to create a *junction tree*, on which belief propagation is applied. The junction tree algorithm was used successfully in many early machine learning applications, but it does become unusably slow to run when a large number of variables need to be merged together, as is often the case with today's applications. This is because the number of states in the merged node is the product of the number of states of the individual variables. This product quickly becomes unmanageably large as more variables are merged together.

2. **Remove loops by observing a variable in the loop**

   If we observe `csharp` to be `true`, then the outward messages from the `csharp` variable can be sent, because they are just point masses. This has the effect of cutting the loop. The downside is that to get any marginal you now have to run inference twice, once with `csharp` set to `true` and once with it set to `false` and then combine the two answers. For graphs with many loops, we would need to observe multiple variables to ensure all loops were cut. This is the basis of a method called *cutset conditioning* Pearl [1988]; Suermondt and Cooper [1990], where the *cutset* is the set of variables that are observed (conditioned on) in order to cut all loops. Like the junction tree algorithm, cutset conditioning can be unusably slow when the cutset is large since we need to re-run inference for every configuration of the variables in the cutset. The number of configurations of the cutset is again the product of the number of states of the individual variables, which quickly becomes unmanageably large as the number of variables in the cutset increases.

Choosing a message-passing schedule

An important consequence of using loopy belief propagation is that we now need to provide a **message-passing schedule**, that is, we need to say the order in which messages will be calculated. This is in contrast to belief propagation

Algorithm 2.2: Loopy Belief Propagation

Input: factor graph, list of target variables to compute marginals for, **message-passing schedule**, initial message values (optional).
Output: marginal distributions for target variables.

Initialise all messages to uniform (or initial values, if provided).
repeat
  foreach *edge in the message-passing schedule* **do**
    Send the appropriate message below:
    - Variable node message: the product of all messages received on the other edges;
    - Factor node message: the product of all messages received on the other edges, multiplied by the factor function and summed over all variables except the one being sent to;
    - Observed node message: a point mass at the observed value;
  end
until *all messages have converged*
Compute marginal distributions as the product of all incoming messages at each target variable node.

where the schedule is fixed, since a message can be sent only at the point when all the incoming messages it depends on are received. A schedule for loopy belief propagation needs to be iterative, in that parts of it will have to be repeated until message passing has converged.

The choice of schedule can have a significant impact on the accuracy of inference and on the rate of convergence. Some guidelines for choosing a good schedule are:

- Message computations should use as few initial message values as possible. In other words, the schedule should be as close to the belief propagation schedule as possible and initial message values should only be used where absolutely necessary to break loops. Following this guideline will tend to make the converged marginal distributions more accurate.

- Messages should be sent sequentially around loops within each iteration. Following this guideline will make inference converge faster – if instead it takes two iterations to send a message round any loop, then the inference algorithm will tend to take twice as long to converge.

There are other factors that may influence the choice of schedule: for example, when running inference on a distributed cluster you may want to minimize the number of messages that pass between cluster nodes. Manually designing a message-passing schedule in a complex graph can be challenging – thankfully, there are automatic scheduling algorithms available that can produce good schedules for a large range of factor graphs, such as those used in Infer.NET [Minka et al., 2014].

2.3.2 Applying loopy belief propagation to our model

Let's now apply loopy belief propagation to solve our model of Figure 2.12, assuming that the candidate also gets the fourth question wrong (so that `isCorrect4` is `false`). We'll start by laying out the model a bit differently to make the loop really clear – see Figure 2.13a. Now we need to pick a message-passing schedule for this model. A schedule which follows the guidelines above is:

1. Send messages towards the loop from the `isCorrect` observed nodes and the Bernoulli priors (Figure 2.13b);

2. Send messages clockwise around the loop until convergence (Figure 2.13c). We need to use one initial message to break the loop (shown in green);

3. Send messages anticlockwise around the loop until convergence (Figure 2.13d). We must also use one initial message (again in green).

In fact, the messages in the clockwise and anti-clockwise loops do not affect each other since the messages in a particular direction only depend on incoming messages running in the same direction. So we can execute steps 2 and 3 of this schedule in either order (or even in parallel!).

For the first step of the schedule, the actual messages passed are shown in (Figure 2.13b). The messages sent around the loop clockwise A, B, C, D are shown in Table 2.5 for first five iterations around the loop. By the fourth iteration the messages are no longer changing, which means that they have converged (and so we could have stopped after four iterations).

Iteration	A	B	C	D
1	0.360	0.066	0.485	0.809
2	0.226	0.035	0.492	0.813
3	0.224	0.035	0.492	0.814
4	0.224	0.035	0.492	0.814
5	0.224	0.035	0.492	0.814

Table 2.5: The messages sent around the loop in the first five iterations of message passing – the numbers shown are the parameters of the Bernoulli distribution of each message. By the fourth iteration, the messages have stopped changing, showing that the algorithm has converged rapidly.

The messages for the anti-clockwise loop A', B', C', D' turn out to be identical to the corresponding A, B, C, D messages, because the messages from `hasSkills3` and `hasSkills4` are the same. Given these messages, the only remaining step is to multiply together the incoming messages at `csharp` and `sql` to get the marginal distributions.

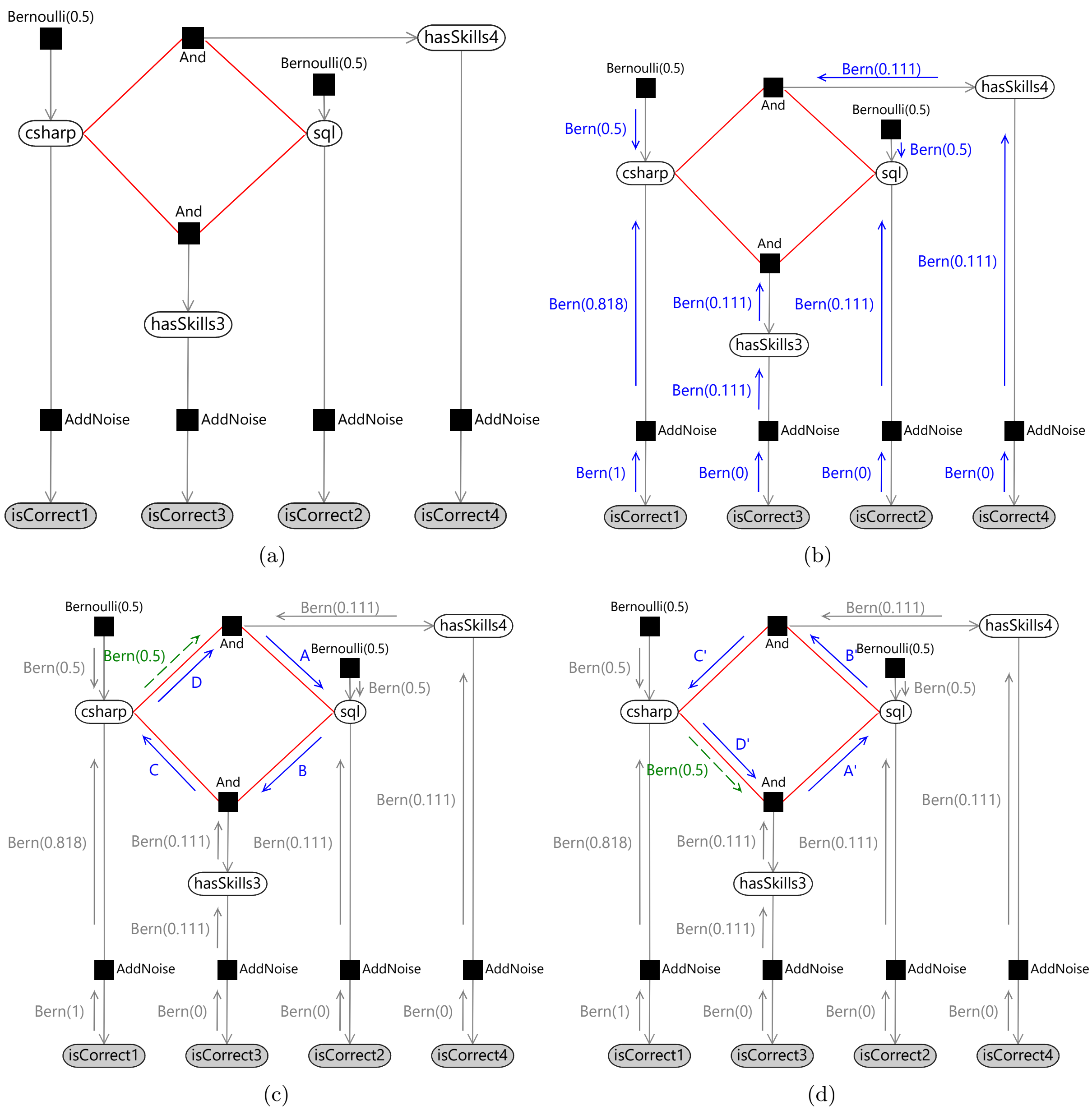


Figure 2.13: **Loopy belief propagation in the four-question factor graph** (a) The factor graph of Figure 2.12 rearranged to show the loop more clearly. (b) The first stage of loopy belief propagation, showing messages being passed inwards toward the loop. (c,d) The second and third stages of loopy belief propagation where messages are passed clockwise or anti-clockwise around the loop. In each case, the first message (A or A') is computed using a uniform initial message (green dashed arrow).

Loopy belief propagation gives the marginal distributions for `csharp` and `sql` as *Bernoulli*(0.809) and *Bernoulli*(0.010) respectively. If we use an exact inference method to compute the true posterior marginals, we get *Bernoulli*(0.800) and *Bernoulli*(0.024), showing that our approximate answers are reasonably close to the exact solution. For the purposes of this application, we are interested in whether a candidate has a skill or not but can tolerate the predicted probability being off by a percentage point or two, if it can make the system run quickly. This illustrates why approximate inference methods can be so useful when tackling large-scale inference problems. However, it is always worth investigating what inaccuracies are being introduced by using an approximate inference method. Later on, in subsection 2.5.1, we'll look at one possible way of doing this.

Another reason for using approximate inference methods is that they let us do inference in much more complex models than is possible using exact inference. The accuracy gain achieved by using a better model, that more precisely represents the data, usually far exceeds the accuracy loss caused by doing approximate inference. Or as the mathematician John Tukey put it,

> *"Far better an approximate answer to the right question... than an exact answer to the wrong one."*

Self assessment 2.3

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Draw a factor graph for a six-question test which assesses three skills. Identify all the loops in your network. If there are no loops, add more questions until there are.

2. For your six-question test, design a message-passing schedule which uses as few initial messages as possible (one per loop). Remember that a message cannot be sent from a node unless messages have been received on all edges connected to that node (except for observed variable nodes).

3. Extend your three question Infer.NET model from the previous self assessment, to include the fourth question of Figure 2.12. Use the TraceMessages attribute to see what messages Infer.NET is sending and confirm that they match the schedule and values shown in Table 2.5.

Review of concepts introduced in this section

loops A loop is a path through a graph starting and ending at the same node which does not go over any edge more than once. For example, see the loop highlighted in red in Figure 2.13a.

tree A graph which does not contain any loops, such as the factor graphs of Figure 2.4 and Figure 2.5. When a graph is a tree, belief propagation can be used to give exact marginal distributions.

loopy graph A graph which contains at least one loop. For example, the graph of Figure 2.12 contains a loop, which may be seen more clearly when it is laid out as shown in Figure 2.13a. Loopy graphs present greater difficulties when performing inference calculations – for example, belief propagation no longer gives exact marginal distributions.

exact inference an inference calculation which exactly computes the desired posterior marginal distribution or distributions. Exact inference is usually only possible for relatively small models or for models which have a particular structure, such as a tree. See also Panel 2.2.

approximate inference an inference calculation which aims to closely approximate the desired posterior marginal distribution, used when exact inference will take too long or is not possible. For most useful models, exact inference is not possible or would be very slow, so some kind of approximate inference method will be needed.

loopy belief propagation an approximate inference algorithm which applies the belief propagation algorithm to a loopy graph by initialising messages in loops and then iterating repeatedly. The loopy belief propagation algorithm is defined in algorithm 2.2.

converged The state of an iterative algorithm when further iterations do not lead to any change. When an iterative algorithm has converged, there is no point in performing further iterations and so the algorithm can be stopped. Some convergence criteria must be used to determine whether the algorithm has converged – these usually allow for small changes (for example, in messages) to account for numerical inaccuracies or to stop the algorithm when it has approximately converged, to save on computation.

message-passing schedule The order in which messages are calculated and passed in a message passing algorithm. The result of the message passing algorithm can change dramatically depending on the order in which messages are passed and so it is important to use an appropriate schedule. Often, a schedule will be iterative – in other words, it will consist of an ordering of messages to be computed repeatedly until the algorithm converges.

2.4 Moving to real data

Now that we have fully tested out our model on example data, we are ready to work with some real data. We asked 22 volunteers to complete an assessment test consisting of 48 questions, intended to assess seven different development skills. Many of the questions required two skills, because they needed both the knowledge of a software development concept (such as object-oriented programming) and a knowledge of the programming language that the question used (such as C#).

As well as completing the test, we also asked each volunteer to say which development skills they consider that they have. These self-assessed skills will be used as **ground truth** for the skill variables – that is, we will consider them to be the true values of the variables. Such ground truth data will be used to assess the accuracy of our system in inferring the skills automatically from the volunteers' answers. The ground truth data should be reasonably reliable since the volunteers have no incentive to exaggerate their skills: the results were kept anonymous so that the reported skills and answers could not be linked to any particular volunteer. However, it is plausible that some volunteers may over- or under-estimate their own skills and we will need to bear this in mind when using these data to assess our accuracy.

Part of the raw data that we collected is shown in Table 2.6.

#	S1	S2	S3	S4	S5	S6	S7	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12	Q13	Q14	Q15	Q16	Q17	Q18	Q19	Q20	Q21	Q22	Q23	Q24	Q25	Q26	Q2
ANS								2	4	3	3	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	4	2	2	2	4	
P1	☑	☑	☑	☑	☐	☑	☑	2	4	3	3	4	3	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	5	2	2	2	4	
P2	☑	☑	☑	☑	☐	☐	☑	1	4	3	3	4	1	4	5	1	5	1	5	1	4	3	3	5	3	2	3	4	5	5	2	2	4	
P3	☐	☐	☐	☑	☐	☑	☐	3	4	5	2	4	5	4	5	1	5	5	3	2	5	5	1	2	1	2	3	1	5	1	1	4	4	
P4	☑	☑	☐	☑	☐	☐	☐	2	4	3	3	4	3	4	5	1	5	1	1	2	4	3	1	2	3	2	3	2	2	2	2	2	4	
P5	☑	☑	☐	☐	☐	☐	☑	2	4	3	3	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	5	2	2	2	4	
P6	☐	☐	☐	☐	☐	☐	☐	1	3	3	5	3	4	5	2	5	2	1	4	2	2	4	4	5	1	3	2	1	3	1	2	3	5	
P7	☑	☑	☐	☐	☐	☐	☐	2	4	3	3	4	1	4	5	1	5	1	1	1	2	3	1	2	3	2	3	4	5	2	2	2	4	
P8	☑	☑	☐	☐	☐	☐	☑	2	4	5	2	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	4	2	2	2	4	
P9	☑	☑	☐	☐	☑	☑	☑	2	4	1	3	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	2	2	1	2	5	
P10	☑	☑	☐	☐	☐	☑	☑	2	4	3	3	4	1	4	5	1	5	1	1	2	4	3	1	2	3	2	2	1	5	2	2	2	4	
P11	☑	☑	☐	☐	☐	☐	☑	1	4	3	3	4	3	4	5	1	5	3	1	1	4	3	1	2	3	2	3	4	5	4	2	2	4	
P12	☐	☐	☐	☐	☑	☐	☐	1	1	1	3	4	1	4	5	1	5	1	5	5	2	2	1	5	3	2	3	4	5	2	2	2	4	...
P13	☑	☑	☐	☐	☐	☐	☐	2	4	3	3	4	3	4	5	1	5	1	1	1	2	3	1	2	3	2	3	4	2	2	2	2	4	
P14	☑	☑	☐	☐	☐	☑	☐	2	5	3	3	5	5	4	5	1	5	1	1	5	2	3	1	2	3	2	3	2	4	2	3	2	4	
P15	☑	☐	☐	☐	☐	☐	☐	2	4	3	3	4	3	4	5	1	5	4	5	1	2	3	5	2	3	2	4	4	1	2	3	2	4	
P16	☑	☑	☐	☐	☑	☑	☑	2	4	3	5	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	5	5	2	2	4	
P17	☑	☑	☐	☐	☐	☐	☑	2	4	3	3	4	1	4	5	1	5	1	1	1	4	3	1	2	3	3	3	4	5	2	2	2	4	
P18	☑	☑	☐	☐	☐	☐	☑	2	4	3	3	4	3	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	2	2	2	2	4	
P19	☑	☑	☐	☐	☑	☐	☑	2	4	5	3	4	3	4	2	1	5	1	5	1	4	3	1	2	3	2	3	4	3	2	2	2	4	
P20	☑	☑	☑	☑	☐	☑	☑	2	4	3	3	4	1	4	5	1	5	1	1	1	4	3	1	2	3	2	3	4	4	2	2	2	4	
P21	☑	☑	☐	☑	☑	☑	☑	2	4	3	3	4	1	3	5	1	5	1	1	1	4	3	1	2	3	2	3	4	5	2	2	2	4	
P22	☑	☑	☑	☑	☐	☑	☐	2	4	4	3	4	1	4	5	1	5	1	1	1	3	3	1	2	4	2	3	4	5	5	2	2	4	

Table 2.6: Part of the raw data collected from volunteers completing a real assessment test. This data consists of the self-assessed skills (S1-S7) and the answers to each question (Q1-Q48). The first row of data gives the correct answers to each question. Each subsequent row gives the data for one of the participants.

In this machine learning application, we need the system to be able to work with any test supplied to it, without having to gather new ground truth data for each new test. This means that we cannot use the ground truth data when doing inference in our model, since we will not have this kind of data in practice. Learning without using ground truth data is called **unsupervised learning**. We still need ground truth data when developing our system, however, since we need to evaluate how well the system works. We will evaluate it on this particular test, with the assumption that it will then work with similar accuracy on new, unseen tests.

2.4.1 Visualising the data

When working on a new data set it is *essential* to spend time looking at the data by visualising it in various ways (see Panel 2.3 for why this is so important). So let's now look at making a **visualisation** of our test answers.

The crucial elements of a good visualisation are (i) it is a faithful representation of the underlying data, (ii) it makes at least one aspect of the data very clear, (iii) it stands alone (does not require any explanatory text) and (iv) it is otherwise as simple as possible. There are entire books on the topic (such

Panel 2.3 – The importance of visualisation

Machine learning algorithms often don't fail when there is an error in the code, but instead continue silently on to give inaccurate results. Visualisations of data, of the inference process, and of results provide a very effective way of detecting and understanding such errors.
Visualisations are also important because:

- They let you discover issues with the data, such as mistakes in the data entry, missing data, mislabelled data, data that was saved in the wrong format or data which is being loaded incorrectly.
- They let you see patterns in the data, even before any model is created or any inference calculations are done. Carefully designed visualisations can expose a useful pattern in much the same way that a carefully designed model can expose one.
- They let you communicate the results of your work to others, to help convince them that your system is working well or to demonstrate that it is extracting useful information from the data.

Rather than asking "do I need to visualise this data?", a better question is "can I afford NOT to visualise this data?". Any time you choose not to visualise some data, some part of the inference process or some results, there is a (high) chance that you are missing something important. **A good rule of thumb is that it is worth spending at least 20% of your time on making visualisations.**

as Tufte [1986]), as well as useful websites (these are constantly changing – use your search engine!) and commercial visualisation software (such as Tableau). In addition, most programming languages have visualisation and charting libraries available, particularly those languages focused on data science such as R, Python and Matlab. In this book we aim to illustrate what makes a good visualisation by example, through the various figures illustrating each case study. For example, in Table 2.4 the use of bars to represent probabilities, as well as numbers, makes it easier to see the relationship between which questions were correct and the inferred skill probabilities.

We want to visualise whether each person got each question right or wrong, along with the skills needed for that question (as provided by the person who wrote the test). For the skills needed, we can use a grid where a white square means the skill is needed and a black square means it is not needed (Figure 2.14a). Similarly for the answers, we can use another grid where white means the answer was right and black means it was wrong (Figure 2.14b). To make it easier to spot the relationship between the skills and the answers, we can align the two grids, giving the visualisation of Figure 2.14.

Already this visualisation is telling us a lot about the data: it lets us see which questions are easy (columns that are nearly all white) and which are hard (columns that are nearly all black). Similarly, it lets us identify individuals who are doing well or badly and gives us a sense of the variation between people. Most usefully, it shows us that people often get questions wrong in runs. In our test consecutive questions usually need similar skills, so a run of wrong questions can be explained by the lack of a corresponding skill. These runs are reassuring since this is the kind of pattern we would expect if the data followed the assumptions of our model.

A difficulty with this visualisation is that we have to look back and forth between the two grids to discover the relationship between the answers to a question and the skills needed for a question. It is not particularly easy, for example, to identify the set of skills needed for the questions that a particular person got wrong. To address this, we could try to create a visualisation that contains the information in both of the grids. One way to do this is to associate a colour with each skill and colour the wrong answers appropriately, as shown in Figure 2.15:

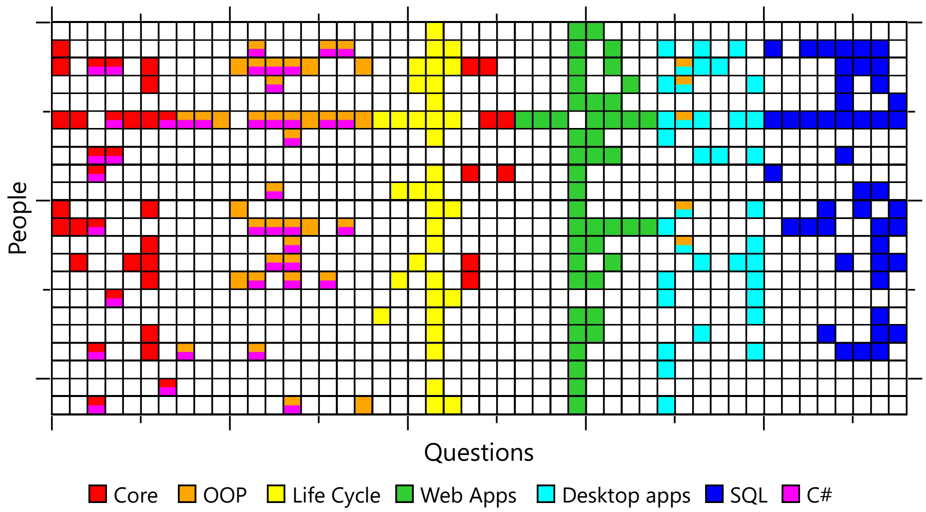
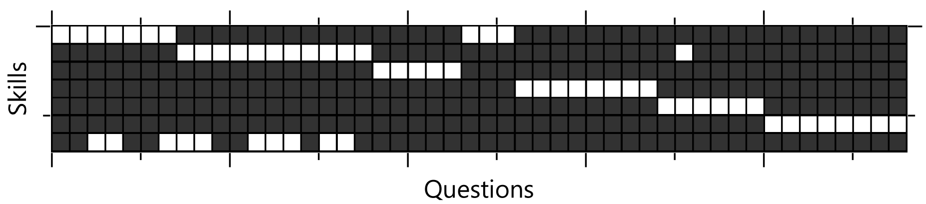
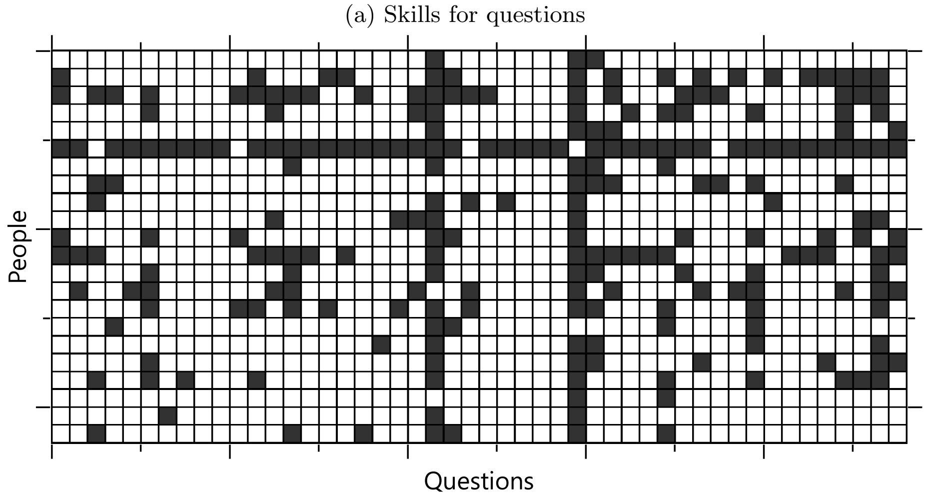


Figure 2.15: A visualisation of the same data as Figure 2.14 but using only a single, coloured grid, to make it easier to see associations between wrong questions and skills.



(a) Skills for questions



(b) Responses

Figure 2.14: Visualisation of the answer data and skills needed for each question. (a) Each row corresponds to a skill and each column to a question. White squares show which skills are needed for each question (b) Each row corresponds to a person and again each column corresponds to a question. Here, white squares show which questions each person got correct.

This visualisation makes it easier to spot patterns of wrong answers associated with the same skill, without constantly switching focus between two grids. We could instead have chosen to highlight the correct answers but in this case it is more useful to focus on the wrong answers since these are rarer, and so more interesting. For example, we can see that those people who got some orange (Object Oriented Programming) questions wrong often got many other orange questions wrong, since orange grid cells often appear in blocks. This is very suggestive of the absence of an underlying skill influencing the answers to all these questions. Conversely for the cyan (Desktop apps) questions there seems to be less block structure, suggesting that our assumption of one skill influencing all these questions is weaker in this case.

2.4.2 A factor graph for the whole test

Reassured that our data looks plausible, we would now like to run inference on a factor graph for this assessment test. We've already seen factor graphs for three questions (Figure 2.5) and for four questions (Figure 2.12) where there were just two skills being modelled. But if we tried to draw a factor graph for all 48 questions and all seven skills in the same way, it would be huge and not particularly useful. To avoid such overly large factor graphs, we can represent repeated structure in the graph using a **plate**. Here is an example of using a plate used to represent the prior over five skill variables:

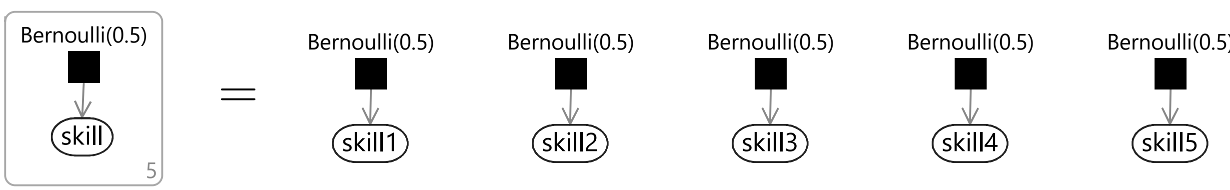


Figure 2.16: Using a plate to represent repeated structure in a factor graph

The factor graph on the left with a plate is equivalent to the factor graph on the right without a plate. The plate is shown as a rectangle with the number of repetitions in the bottom right corner – which in this case is 5. Variable and factor nodes contained in the plate are considered to be replicated 5 times. Where a variable has been replicated inside a plate it becomes a **variable array** of length 5 – so in this example `skill` is an array with elements `skill`[0], `skill`[1], `skill`[2], `skill`[3] and `skill`[4]. Note that we use index 0 to refer to the first element of an array.

Figure 2.17 shows how we can use plates to draw a compact factor graph for the entire test. There are two plates in the graph, one across the skills and one across the questions. Instead of putting in actual numbers for the number of repetitions, we have used variables called `skills` and `questions`. This gives us a factor graph which is configurable for any number of skills and any number of questions and so could be used for any test. For our particular test, we will set `skills` to 7 and `questions` to 48.

Figure 2.17 has also introduced the *Subarray* factor connecting two new variables `skillsNeeded` and `relevantSkills`, both of which are arrays inside the questions plate. The `skillsNeeded` array must be provided (indicated by the grey shading) and contains the information of which skills are needed for each question. Each element of `skillsNeeded` is itself a small array of integers specifying the indices of the skills needed for that question - so for a question that needs the first and third skills this will be $[0, 2]$. The *Subarray* factor uses this information to pull out the relevant subarray of the `skill` array and put it into the corresponding element of the `relevantSkills` array. Continuing our example, this would mean that the element of `relevantSkills` would contain the subarray [`skill`[0], `skill`[2]]. From this point on, the factor graph is as before: `hasSkills` is an AND of the elements of `relevantSkills` and `isCorrect` is then a noisy version of `hasSkills`.

2.4.3 Our first results

We are now ready to get our first results on a real data set. It's taken a while to get here, because of the time we have spent testing out the model on small examples and visualising the data. But, by doing these tasks, we can be

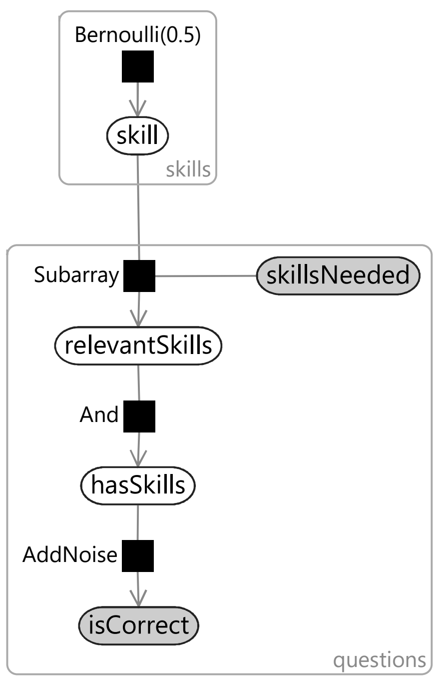
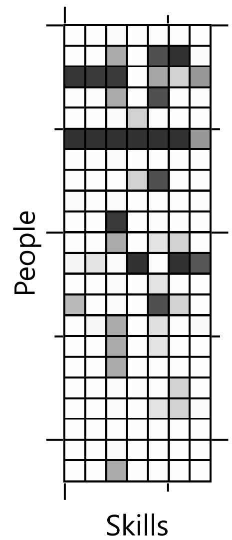
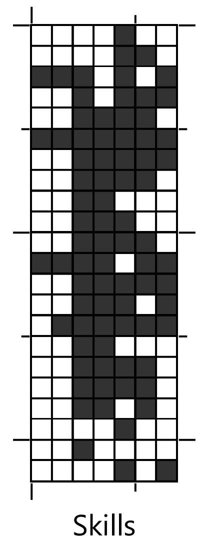


Figure 2.17: A factor graph for the entire test, constructed using plates and the *Subarray* factor.



(a) Inferred skills



(b) Self-assessed skills

Figure 2.18: Initial results of applying our model to real assessment data. (a) Computed probability of each person having each skill, where white corresponds to probability 1.0, black to probability 0.0 and shades of grey indicate intermediate probability values. (b) Ground truth self-assessed skills where white indicates that the person assessed that they have the skill and black indicates that they do not. Unfortunately, the inferred skills have little similarity to the self-assessed skills.

confident that our inference results will be meaningful from the start.

We can apply loopy belief propagation to the factor graph of Figure 2.17 separately for each person, with `isCorrect` set to that person's answers. For each skill, this will give the probability that the person has that skill. Repeating this for each person leads to a matrix of results which is shown in the visualisation on the left of Figure 2.18, where the rows correspond to different people and the columns correspond to different skills. For comparison, we include the self-assessed skills for the same people on the right of the figure.

There is clearly something very wrong with these inference results! The inferred skills show little similarity to the self-assessed skills. There are a couple of people where the inferred skills seem reasonable – such as the people on the 3rd and 6th rows. However, for most people, the system has inferred that they have almost all the skills, whether they do or not. How can this happen after all our careful testing and preparation?

In fact, the first time a machine learning system is applied to real data, it is very common that the results are not as intended. The challenge is to find out what is wrong and to fix it.

Self assessment 2.4

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Create an alternative visualisation of the data set of Table 2.6 which shows which people get the most questions right and which questions the most people get right. For example, you could sort the rows and columns of Figure 2.14 or Figure 2.15. What does your new visualization show that was not apparent in the visualisations used in this section? Note: the data set can be downloaded in Excel or CSV form using the buttons by the online version of the table.

2. Implement the factor graph with plates from Figure 2.17 using Infer.NET. You will need to use Variable arrays, ForEach loops and the Subarray factor. Apply your factor graph to the data set and verify that you get the results shown in Figure 2.18a.

Review of concepts introduced in this section

ground truth A data set which includes values for variables which we want to predict or infer, used for evaluating the prediction accuracy of a model and/or for training a model. Ground truth data is usually expensive or difficult to collect and so is a valuable and scarce commodity in most machine learning projects.

unsupervised learning Learning which doesn't use labelled (ground truth) data but instead aims to discover patterns in unlabelled data automatically, without manual guidance.

visualisation A pictorial representation of some data or inference result which allows patterns or problems to be detected, understood, communicated and acted upon. Visualisation is a very important part of machine learning, as discussed in Panel 2.3.

plate A container in a factor graph which compactly represents a number of repetitions of the contained nodes and edges. The plate is drawn as a rectangle and labelled in the bottom right hand corner with the number of repetitions. For example, see Figure 2.16.

variable array an ordered collection of variables where individual variables are identified by their position in the ordering (starting at zero). For example, a variable array called `skill` of length 5 would contain five variables: `skill`[0], `skill`[1], `skill`[2], `skill`[3], and `skill`[4].

2.5 Diagnosing the problem

When a machine learning system is not working there are generally three possible reasons: bad data, bad model, or bad inference. Here are some common causes of problems under each of these three headings:

Bad data: data items have been entered, stored or loaded incorrectly; the data items are incomplete or mislabelled; data values are too noisy to be useful; the data is biased or unrepresentative of how the system will be used; it is the wrong data for the task; there is insufficient data to make accurate predictions.

Bad model: one or more of the modelling assumptions are wrong – that is, not consistent with the actual process that generated the data; the model makes too many simplifying assumptions; the model contains insufficient assumptions to make accurate predictions given the amount of available data.

Bad inference: the inference code contains a bug; the message-passing schedule is bad; the inference has not converged; there are numerical problems (e.g. rounding, overflow); the approximate inference algorithm is not accurate enough.

In our case, we can be fairly confident that the data is good because we have inspected and visualised it carefully. So it seems likely that either the model or the inference is causing the problem. We'll start by checking that the inference algorithm, loopy belief propagation, is working correctly.

2.5.1 Checking the inference algorithm

To see if inference is working correctly, we need to be able to separate out any problems caused by inference issues from any problems caused by our model not matching the data. To achieve this separation, we can generate a new *synthetic* data set which is guaranteed to match the model exactly. If we get poor results using this data set it suggests that there is an inference problem. We will create this synthetic data set by sampling from the joint distribution specified by the model, which guarantees that the data is consistent with the model (refer to chapter 1 for a reminder of what sampling is). We can generate samples by running the data generation process specified by the model – a process called **ancestral sampling**, as defined by algorithm 2.3 (see also Bishop [2006]).

Looking at the factor graph of Figure 2.17, we run ancestral sampling following the arrows from top to bottom (from ancestor to descendent), by sampling a value for each variable given its parents in the graph. If a variable is the child variable of a deterministic factor, then we just compute its value from the values of its parent variables using the function encoded by the deterministic factor (such as the AND function).

So, starting at the top, we sample a value for each element of the `skill` array from a $Bernoulli(0.5)$ distribution – in other words we pick `true` with

Algorithm 2.3: Ancestral sampling

Input: factor graph
Output: sampled values for each variable in the graph

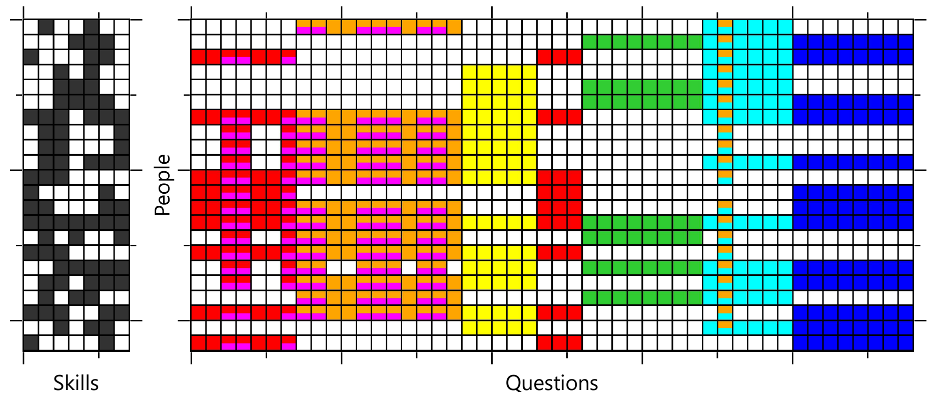
Order variables from top to bottom so that parent variables come before child variables.
foreach *variable v in this ordering* **do**
    If `v` has parent variables, retrieve their sampled values (which must already exist due to the ordering).
    Sample a value for `v` from the parent factor function, conditioned on the retrieved parent values, if any. If the parent factor is deterministic (such as an *And* factor) this simplifies to just computing the child value from the parent values.
    Store the sampled value.
end

50% probability and `false` otherwise. For the `relevantSkills` array element for a question we just pull out the already-sampled values of the `skill` array that are relevant to that question. These values are then ANDed together to give `hasSkills`. Figure 2.19 gives an example set of 22 samples for the `skill` and `hasSkills` arrays. To get a data set with multiple rows we just repeat the entire sampling process for each row. Notice how, for each row, `hasSkills` is always the same for questions that require the same skills (are the same colour).

The final stage of ancestral sampling in our model requires sampling each element of `isCorrect` given its parent element of `hasSkills`. Where `hasSkills` is `true` we sample from *Bernoulli*(0.9) and where `hasSkills` is `false` we sample from *Bernoulli*(0.2) (following Table 2.1). The result of performing this step gives the `isCorrect` samples of Figure 2.19c. Notice that these samples end up looking like a noisy version of the `hasSkills` samples – about one in ten white squares has been flipped to colour and about one in five coloured squares has been flipped to white.

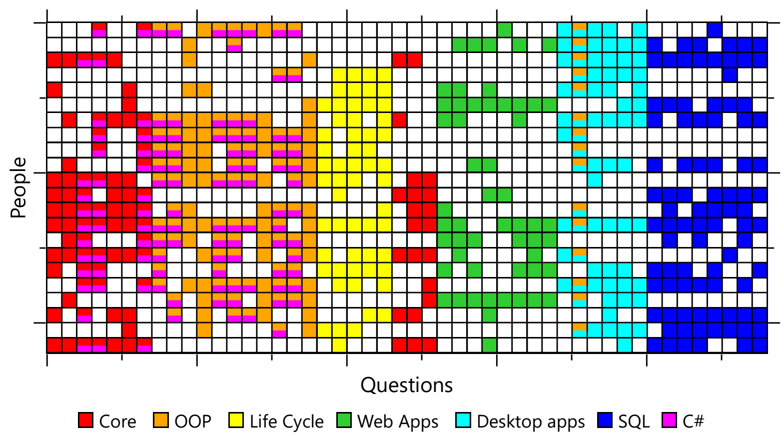
We now have an entire sampled data set, which we can run our inference algorithm on to test if it is working correctly. The inferred skill probabilities are shown in Figure 2.20 next to the actual skills that we sampled. Unlike with the real data, the results are pretty convincing: the inferred skills look very similar to the actual sampled skills. So, when we run inference on a data set that conforms perfectly to our model, the results are good. This suggests that the inference algorithm is working well and the problem must instead be that our model does not match the real data.

An important and subtle point is that the inferred skills are close *but not identical* to the sampled skills, even though the data is perfectly matched to the model. This is because there is still some remaining uncertainty in the skills even given all the answers in the test. For example, the posterior probability of skill 7 (C#) is uncertain in the cases where the individual does not have skill 1 (Core) or skill 2 (OOP). This makes sense because the C# skill is only tested



(a) Sampled `skill` array

(b) `hasSkills` array computed from sampled `skill` array



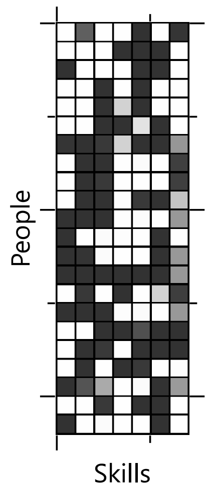
(c) Sampled `isCorrect` array

Figure 2.19: Synthetic data set created using ancestral sampling. First the `skill` array was sampled and then the `hasSkill` array was computed from it. The `isCorrect` array was then sampled given the `hasSkill` array, which has the effect of making it a noisy version of `hasSkill`.

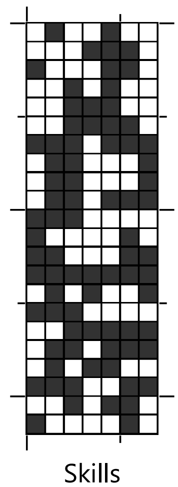
in combination with these first two skills – if a person does not have them then they will get the associated questions wrong, whether or not they know C#. So in this case, the inference algorithm is correct to be uncertain about whether or not the person has the C# skill. We could use this information to improve the test, such as by adding questions that directly test the C# skill by itself.

2.5.2 Working out what is wrong with the model

We have determined that our model assumptions are not matching the data – now we need to identify which assumption(s) are at fault. We can again use



(a) Inferred skills



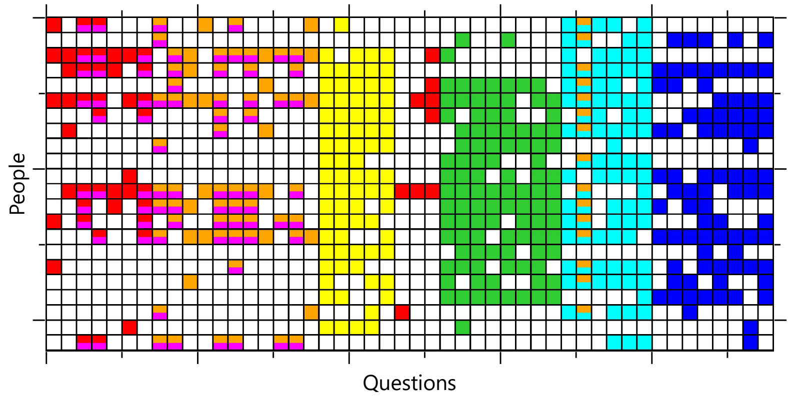
(b) Sampled skills

Figure 2.20: Skills inferred from a sample data set shown next to the actual sampled skills for that data set. The inferred skills are close to the actual skills, suggesting that the inference algorithm is working well.

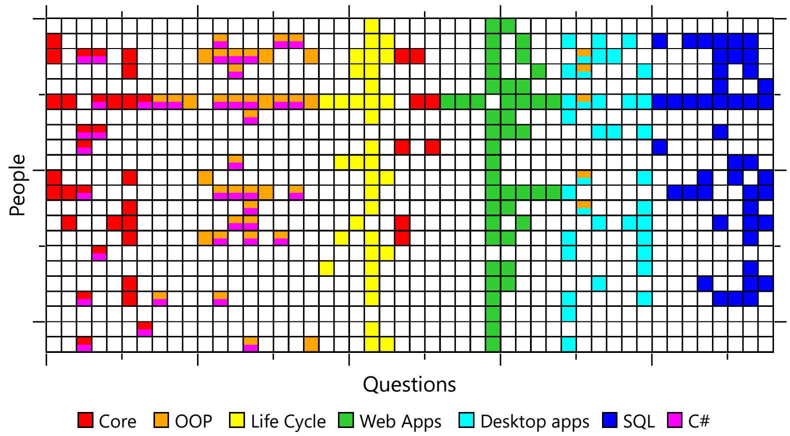
sampling to achieve this but rather than sampling the `skill` array, we can set it to the true (self-assessed) values. If we then sample the `isCorrect` array, it will show us which answers the model is expecting people to get wrong if they had these skills. By comparing this to the actual `isCorrect` array from our data set, we can see where the model's assumptions differ from reality. Figure 2.21 shows that the actual `isCorrect` data looks quite different to the sampled data. The biggest difference appears to be that our volunteers got many more questions right than our model is predicting, given their stated skills. This suggests that they are able to guess the answer to a question much more often than the 1-in-5 times that our model assumes. On reflection, this makes sense – even if someone doesn't have the skill to answer a question they may be able to eliminate some answers on the basis of general knowledge or intelligent guesswork.

We can investigate this further by computing the fraction of times that our model predicts our volunteers should get each question right, given their self-assessed skills, and then compare it to the fraction of times they actually got it right (Figure 2.22).

For a few questions, the fraction of people who got them correct matches that predicted by the model – but for most questions the actual fraction is higher than the predicted fraction. This suggests that some questions are easier to guess than others and that they can be guessed correctly more often than 1-in-5 times. So we need to change our assumptions (and our model) to allow different guess probabilities for different questions. We can modify our fourth assumption as follows:



(a) Sampled `isCorrect` array given true (self-assessed) skills



(b) Observed `isCorrect` array from our data set

Figure 2.21: The modelling problem can be diagnosed by comparing (a) the `isCorrect` data sampled from the model given the self-assessed skills and (b) the observed `isCorrect` data showing which questions the volunteers actually got wrong.

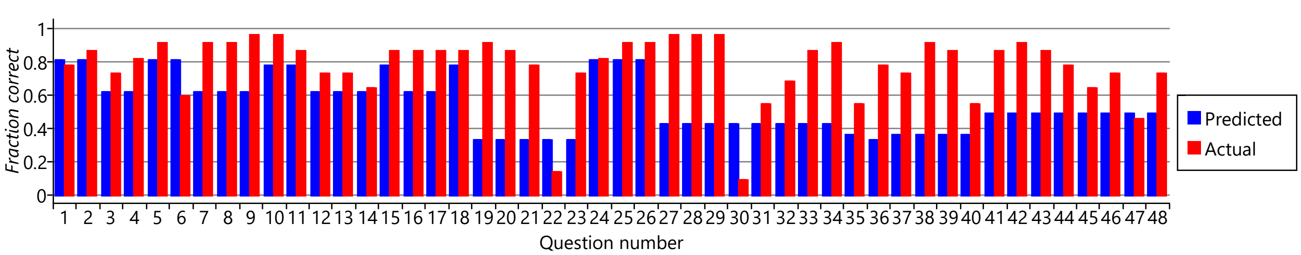


Figure 2.22: The fraction of people the model predicts will get each question right given their self-assessed skills (blue) compared to the fraction that actually got it right (red), for each of the 48 questions in the test.

4 If a candidate doesn't have all the skills needed for a question, they will ~~pick an answer at random~~ guess an answer, where the probability that they guess correctly is about 20% for most questions but could vary up to about 60% for very guessable questions.

This assumption means that, rather than having a fixed guess probability for all questions, we need to extend our model to *learn* a different guess probability for each question.

Self assessment 2.5

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Make a check list of the causes of problems with machine learning systems (either data problems, model problems or inference problems). Rank the causes in the order which you think are most likely to occur. Now if you are working on a machine learning problem in the future, this check list could be useful when diagnosing the root cause of the problem.

2. Write a program to implement ancestral sampling in the skills model, as was described in this section, and use it to make a synthetic data set. Visualise this data set, for example, using the visualisation you developed in the previous self assessment. Check that your samples look similar to the samples from Figure 2.19.

3. Try changing a couple of the probability values that we have chosen in the model, such as the prior probability of having a skill or the probability of guessing the answer. Run your sampling program again and see how the synthetic data set changes. You could imagine repeating this procedure until the synthetic data looks as much like the real data as possible given the model assumptions. This would be quite inefficient, so we instead learn these probability values as part of the inference algorithm, as we shall see in the next section.

Review of concepts introduced in this section

ancestral sampling A process of producing samples from a probabilistic model by first sampling variables which have no parents using their prior distributions, then sampling their child variables conditioned on these sampled values, then sampling the children's child variables similarly and so on. Ancestral sampling is defined in algorithm 2.3. For an example of ancestral sampling, see subsection 2.5.1.

2.6 Learning the guess probabilities

You might expect that inferring the guess probabilities would require very different techniques than we have used so far. In fact, our approach will be exactly the same: we add the probability values we want to learn as new continuous random variables in our model and use probabilistic inference to compute their posterior distributions. This demonstrates the power of the model-based approach – whenever we want to know something, we introduce it as a random variable in our model and compute it using a standard inference algorithm.

Let's see how to modify our model to include the guess probabilities as random variables. To keep things consistent, we'll also add in a variable for the mistake probability (actually the no-mistake probability) but we'll keep this fixed at a 10% chance of making a mistake. To start with, we'll change how we write the *AddNoise* factor. Figure 2.23 shows how the existing *AddNoise* factor (which has the guess and no-mistake probabilities hard-coded at 0.2 and 0.9 respectively) can be replaced by a general *Table* factor which takes these probabilities as additional arguments. We can then set these arguments using two new random variables, which we name as `probGuess` and `probNoMistake`. Inferring the posterior distribution over the variable `probGuess` will allow us to learn the guess probability for a question. But before we can do this, we must first see what kind of distribution we can use to represent the uncertainty in such a variable.

2.6.1 Representing uncertainty in continuous values

The two new variables `probGuess` and `probNoMistake` have a different type to the ones we have encountered so far: previously all of our variables have been binary (two-valued) whereas these new variables are continuous (real-valued) in the interval 0.0 to 1.0 inclusive. This means we cannot use a Bernoulli distribution to represent their uncertainty. In fact, because our variables are continuous, we need to use a distribution based on a **probability density function** – if you are not familiar with this term, read Panel 2.4.

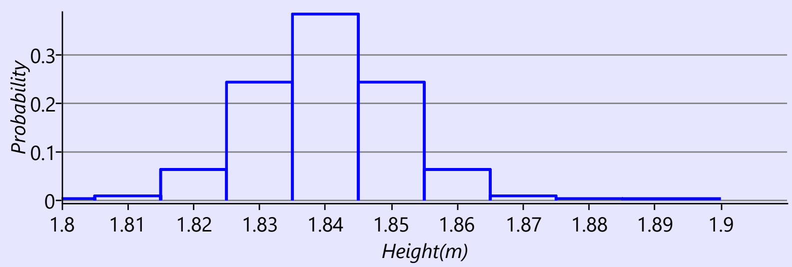
We need a distribution whose density function can represent both our prior assumption "the probability that they guess correctly is about 20% for most questions but could vary up to about 60% for very guessable questions" and also the posterior over the guess probabilities, once we have learned from the data. The distribution should also be restricted to the range 0.0 to 1.0 inclusive. A suitable function would be one that could model a single 'bump' that lies in this range, since the bump could be broad from 20%-60% for the prior and then could become narrow around a particular value for the learned posterior. A distribution called the **beta distribution** meets these requirements. It has the following density function:

$$Beta(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha, \beta)} \tag{2.18}$$

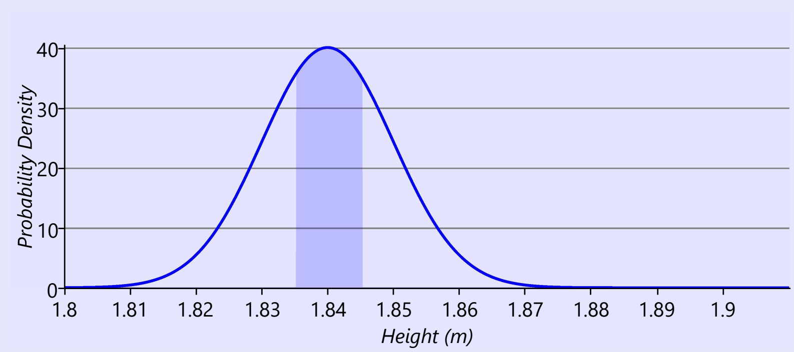
Panel 2.4 – Probability Density Functions

When we want to represent the uncertainty in a continuous variable, such as a person's height, apparently reasonable statements like "There is an 80% chance that his height is 1.84m" don't actually make sense. To see why, consider the mathematically equivalent statement "There is an 80% chance that his height is 1.840000000. . . m". This statement seems very unreasonable, because it suggests that, no matter how many additional decimal places we measure the height to, we will always get zeroes. In fact, the more decimal places we measure, the more likely it is that we will find a non-zero. If we could keep measuring to infinite precision, the probability of getting exactly 1.84000. . . (or any particular value) would effectively vanish to nothing.

So rather than refer to the probability of a continuous variable taking on a particular value, we instead refer to the probability that its value lies in a particular range, such as the range from 1.835m to 1.845m. In everyday language, we convey this by the accuracy with which we express a number, so when we say "1.84m", we often mean "1.84m to the nearest centimetre", that is, anywhere between 1.835m and 1.845m. We could represent a distribution over a continuous value, by giving a set of such ranges along with the probability that the value lies in each range, such that the probabilities add up to one. For example:



This approach can be useful but often also causes problems: it introduces a lot of parameters to learn (one per range); it can be difficult to choose a sensible set of ranges; there are discontinuities as we move from one range to another; and it is hard to impose smoothness, that is, that probabilities associated with neighbouring ranges should be similar. A better solution is to define a function, such that the area under the function between any two values gives the probability of being in that range of values. Such a function is called a **probability density function** (pdf). For example, this plot shows a Gaussian pdf (we'll learn much more about Gaussians in chapter 3):



Notice that the y-axis now goes up well above 1, since a probability density is not limited to be between 0 and 1. Instead, the total area under the function is required to be 1.0. The area of the shaded region between 1.835m and 1.845m is 0.383, which gives the probability that the height lies between these two values. Similarly, computing the area under the pdf between *any* two points gives the probability that the height lies between those points.

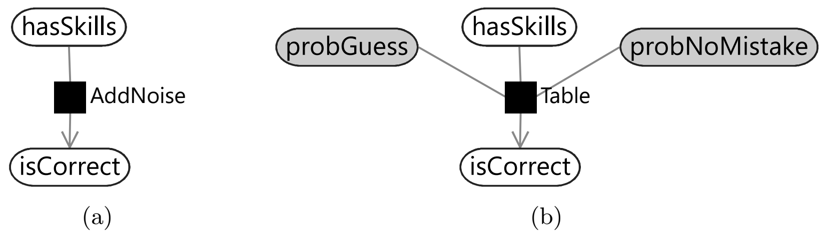


Figure 2.23: Two ways of writing the *AddNoise* factor: (a) As a custom factor with the guess and mistake probabilities 'built-in'. (b) Using a general purpose *Table* factor which has arguments for the probability that the child is `true` given that the parent is `false` (left argument) or given the parent is `true` (right argument). This way of writing the factor allows the arguments to be included as variables in the graph.

where B() is the beta function that the distribution is named after, which is used to ensure the area under the function is 1.0. The beta density function has two parameters, α and β that between them control the position and width of the bump – Figure 2.24a shows a set of beta pdfs for different values of these parameters. The parameters α and β must be positive, that is, greater than zero. The mean value $\frac{\alpha}{\alpha+\beta}$ dictates where the centre of mass of the bump is located and the sum $\alpha+\beta$ controls how broad the bump is – larger $\alpha+\beta$ means a narrower bump. We can configure a beta distribution to encode our prior assumption by choosing $\alpha = 2.5$ and $\beta = 7.5$, which gives the density function shown in Figure 2.24b.

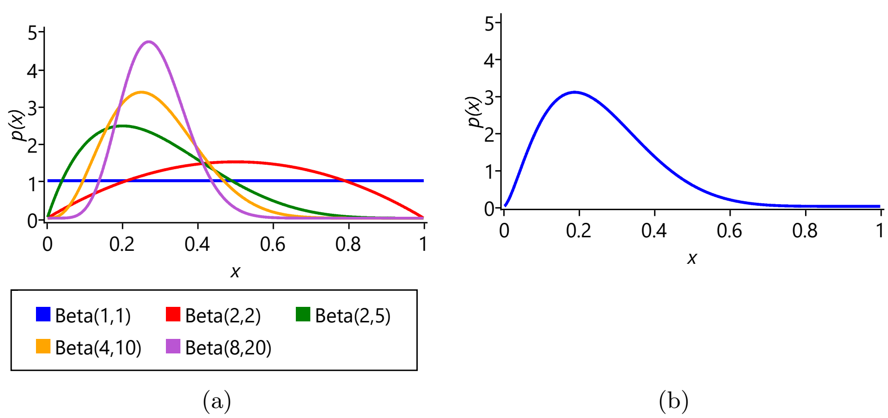


Figure 2.24: (a) Example beta distributions for different values of the parameters α and β. (b) The *Beta*(2.5,7.5) distribution which we can use as a prior for the probability of guessing a question correctly. The peak of the distribution is at around 0.2 but it extends to the right up to around 0.6 to allow for questions that are easier to guess.

We want to extend our factor graph so that the prior probability of each `probGuess` variable is:

$$p(\texttt{probGuess}) = \mathrm{Beta}(\texttt{probGuess}; 2.5, 7.5) \tag{2.19}$$

Notice the notation here: we use a lower-case p to denote a probability density for a continuous variable, where previously we have used an upper-case P to denote the probability distribution for a discrete variable. This notation acts as a reminder of whether we are dealing with continuous densities or discrete distributions.

Taking the factor graph of Figure 2.17, we can extend it to have the guess probabilities included as variables in the graph with this distribution as the prior. One other change is needed: to infer the guess probabilities, we need to look at the data across as many people as possible (it would be very inaccurate to try to estimate a guess probability from just one person's answer!). So we must now extend the factor graph to model everyone's results at once, that is, the entire dataset. To do this, we add a new plate to our factor graph which replicates all variables that are specific to each person (which are: `skill`, `relevantSkills`, `hasSkills` and `isCorrect`). Since we are assuming that the guess probabilities for a question are the same for everyone, `probGuess` is placed outside the new plate, but inside the questions plate. Since the no-mistake probability is assumed to be the same for everyone and for all questions, `probNoMistake` is placed outside of all plates. The final factor graph, of the entire data set, is shown in Figure 2.25.

We can run inference on this graph to learn the guess probabilities. Even now that we have continuous variables, we can essentially run loopy belief propagation on the graph. The only modification we need is a change to ensure that the uncertainty in our guess probabilities is always represented as a beta distribution (this modified form is called expectation propagation and will be described fully in the next chapter). After running inference, we get a beta distribution for each question representing the uncertain value of the guess probability for that question. The beta distributions for some of the questions are shown in Figure 2.26 (we show only every fifth question, so that the figure is not overwhelmed by too many curves). The first thing to note is that the distributions are all still quite wide, indicating that there is still substantial uncertainty in the guess probabilities. This is not too surprising since the data set contains relatively few people and we only learn about question's guess probability from the subset of those people who are inferred not to have the skills needed for a question. For question 1, where we assume pretty much everyone has the (Core) skill needed, the posterior distribution is very close to the prior (compare the curve to Figure 2.24b) since there is hardly any data to learn the guess probability from, as almost no one is guessing this question. Several of the questions (such as 11, 16 and 26) have posteriors that are shifted slightly to the right from the prior, suggesting that these are a bit easier to guess than 1-in-5. Most interestingly, the guess probabilities for some questions have been inferred to be either quite low (questions 6, 31) or quite high (question 21, 36, 41). We

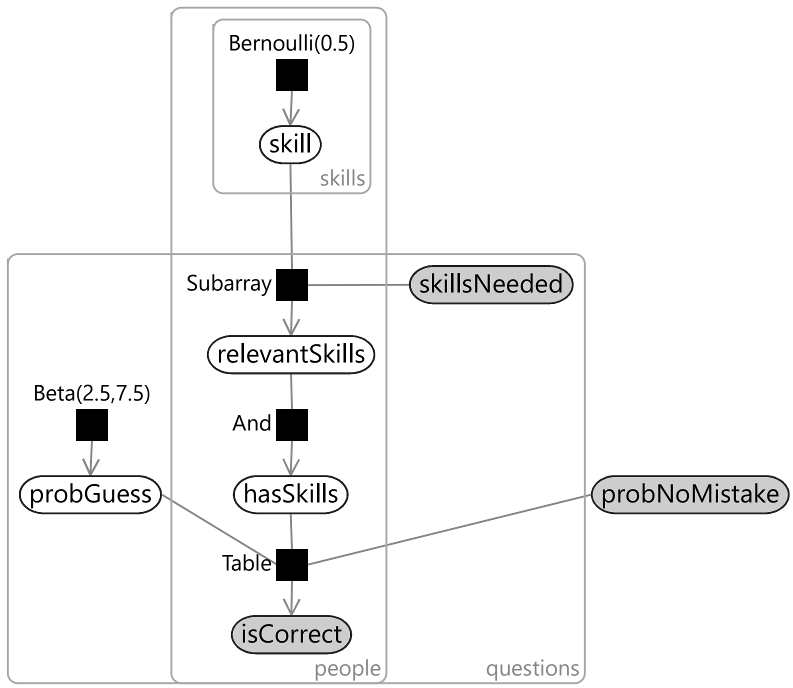


Figure 2.25: A factor graph for the entire data set, for all people who took the test. The guess probabilities for each question appear as a variable array with an appropriate beta prior.

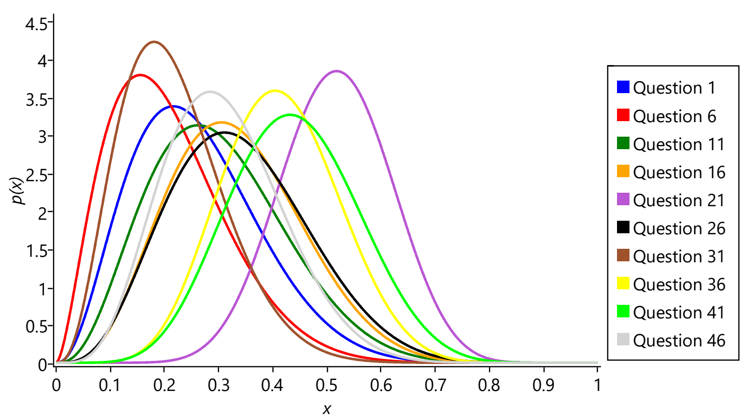


Figure 2.26: Posterior beta distributions over `probGuess` for every fifth question.

can plot the posteriors over the guess probabilities for all of the questions by plotting the mean (the centre of mass) of each along with error bars showing the uncertainty (Figure 2.27). This shows that a substantial number have a guess probability which is higher than 0.2.

Just as a reminder – we have learned these guess probabilities without knowing which people had which skills, that is, without using any ground truth data. Since it doesn't have ground truth, the model has had to use all the assumptions that we built into it, in order to infer the guess probabilities.

We can now investigate whether learning the guess probabilities has improved the accuracy of the skills we infer for each person. Figure 2.28 shows the inferred skill posteriors for the old model and for the new model with learned guess probabilities. Visually, it is clear that the new probabilities are closer to the ground truth skills, which is great news!

2.6.2 Measuring progress

As well as visually inspecting the improvements, it is also important to measure the improvements numerically. To do this, we must choose an **evaluation metric** which we will use to measure how well we are doing. For the task of inferring an applicant's skills, our evaluation metric should measure how close the inferred skill probabilities are to the ground truth skills. A common metric to use is the probability of the ground truth values under the inferred distributions. Sometimes it is convenient to take the logarithm of the probability, since this gives a more manageable number when the probability is very small. When we

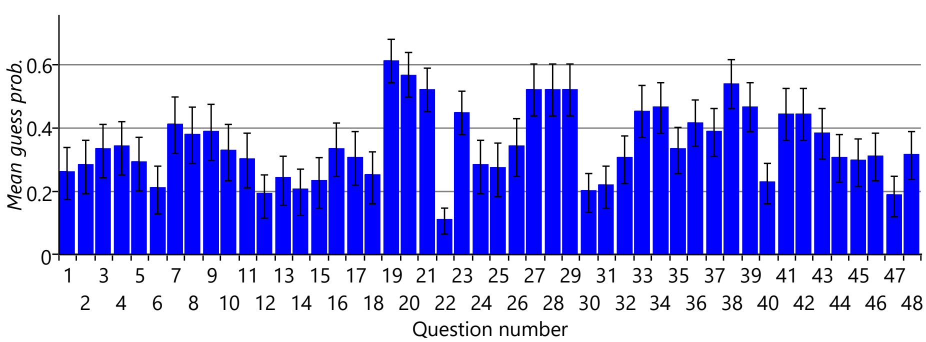
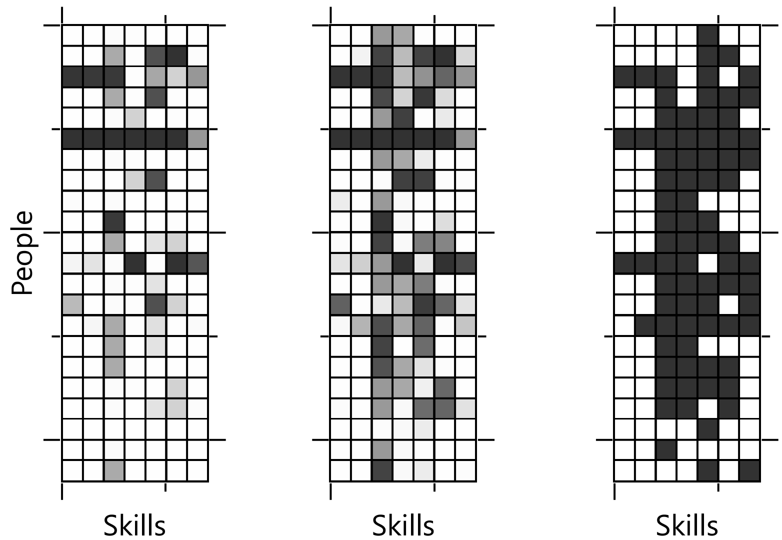


Figure 2.27: The inferred guess probabilities. The blue bar shows the mean of the posterior distribution over the guess probability for each question. The black lines are called error bars and indicate the uncertainty in the inferred guess probabilities. The top and bottom of the error bars show the upper and lower quartiles of the posterior distribution, that is, the values where there is 25% chance of the guess probability being above or below the value respectively. As we suspected, the variation in the mean shows that some questions are much easier to guess than others.



(a) Old inferred skills (b) New inferred skills (c) Self-assessed skills

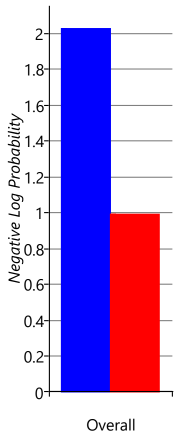
Figure 2.28: Skill posteriors for (a) the original model and (b) the new model with learned guess probabilities, as compared to (c) the ground truth skills. Qualitatively, the skills inferred by the new model are closer to the self-assessed skills.

use the logarithm of the probability, the metric is referred to as the **log probability**. So, if the inferred probability of a person having a particular skill is p, then the log probability is $\log p$ if the person has the skill and $\log(1-p)$ if they don't. If the person does have the skill then the best possible prediction is $p = 1.0$, which gives log probability of $\log 1.0 = 0$ (the logarithm of one is zero). A less confident prediction, such as $p = 0.8$ will give a log probability with a negative value, in this case $\log 0.8 = -0.097$. The worst possible prediction of $p = 0.0$ gives a log probability of negative infinity. This tells us two things about this metric:

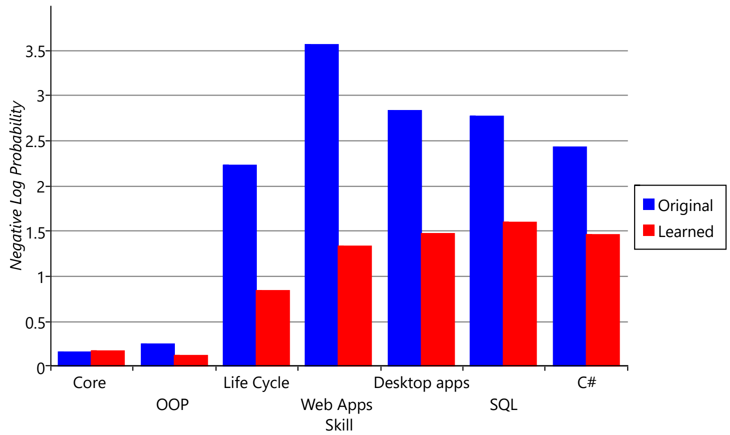
1. Since the perfect log probability is zero, and real systems are less than perfect, the log probability will in practice have a negative value. For this reason, it is common to use the negative log probability and consider lower values (values closer to 0) to be better.

2. This metric penalises confidently wrong predictions very heavily, because the logarithm gives very large negative values when the probability of the ground truth is very close to zero. This should be taken into account particularly where there are likely to be errors in the ground truth.

It is useful to combine the individual log probability values into a single overall metric. To do this, the log probabilities for each skill and each person can be either averaged or added together to get an overall log probability – we will use



(a)



(b)

Figure 2.29: (a) Overall negative log probability for the original model and the model with learned guess probabilities. The lower red bar indicates that the learning the guess probabilities gives a substantially better model, according to this metric. (b) Negative log probability for each skill, showing that the improvement varies from skill to skill.

averaging since it makes the numbers more manageable. Notice that the best possible overall score (zero) is achieved by having $p = 1$ where the person has the skill and $p = 0$ where they don't – in other words, by having the inferred skill probability matrix exactly match the ground truth skill matrix.

Figure 2.29a shows the negative log probability averaged across skills and people, for the original and improved models. The score for the improved model is substantially lower, indicating that it is making quantitatively much better predictions of the skill probabilities. We can investigate this further by breaking down the overall negative log probability into the contributions for the different skills (Figure 2.29b). This shows that learning the guess probabilities improves the log probrability metric for all skills except the Core skill where it is about the same. This is because almost everyone has the Core skill and so the original model (which predicted that everyone has every skill) actually did well for this skill. But in general, in terms of log probability our new results are a substantial improvement over the original inferred skills.

2.6.3 A different way of measuring progress

It is good practice to use more than one evaluation metric when assessing the accuracy of a machine learning system. This is because each metric will provide different information about how the system is performing and there will be less emphasis on increasing any particular metric. No metric is perfect – focusing too much on increasing any one metric is a bad idea since it can end up exposing flaws in the metric rather than actually improving the system. This is succinctly

		Prediction		
		Positive	Negative	
Ground truth	Positive	**True positive (TP)**	**False negative (FN)**	**True positive rate** $\frac{\#TP}{\#TP + \#FN}$
	Negative	**False positive (FP)**	**True negative (TN)**	**False positive rate** $\frac{\#FP}{\#FP + \#TN}$

Table 2.7: The terms *positive* and *negative* are used for the predicted and ground truth values to avoid confusion with *true* and *false* which are used to say if the prediction was correct or not. True and false positive rates are calculated for a particular set of predictions (the # means 'number of').

expressed by **Goodhart's law** which can be stated as

> *"When a measure becomes a target, it ceases to be a good measure."*

Using multiple evaluation metrics will help us avoid becoming victims of Goodhart's law.

When deciding on a second evaluation metric to use, we need to think about how our system is to be used. One scenario is to use the system to select a short list of candidates very likely to have a particular skill. Another is to filter out candidates who are very unlikely to have the skill, to make a 'long list'. For both of these scenarios, we might only care about the ordering of people by their skill probabilities, not on the actual value of these probabilities. In each case, we would select the top N people, but for the shortlist N would be small, whereas for the long list N would be large. For any number of selected candidates, we can compute:

- the fraction of candidates who have the skill that are correctly selected – this is the **true positive rate** or TPR,
- the fraction of candidates who don't have the skill that are incorrectly selected – this is the **false positive rate** or FPR.

The terminology of true and false positive predictions and their corresponding rates is summarised in Table 2.7.

In general, there is a trade-off between having a high TPR and a low FPR. For a shortlist, if we want everyone on the list to have the skill (FPR=0) we would have to tolerate missing a few people with the skill (TPR less than 1). For a long list, if we want to include all people with the skill (TPR=1) we would have to tolerate including some people without the skill (FPR above 0). A **receiver operating characteristic curve**, or ROC curve, lets us visualise this trade-off by plotting TPR against FPR for all possible lengths of list N. The ROC curves for the original and improved models are shown in Figure 2.30, where the TPR and FPR have been computed across all skills merged together. We could also have plotted ROC curves for individual skills but, since our data set is relatively small, the curves would be quite bumpy, making it hard to interpret and compare them.

Figure 2.30 immediately reveals something surprising that the log probability metric did not: the original model does very well and our new model only has a slightly higher ROC curve. It appears that whilst the skill probabilities computed by the first model were generally too high, they were still giving a good *ordering* on the candidates. That is, the people who had a particular skill had higher inferred skill probabilities than the people who did not, even though the probabilities themselves were not very accurate. A system which gives inaccurate probabilities is said to have poor **calibration**. The log probability metric is sensitive to bad calibration while the ROC curve is not. Using both metrics together lets us see that learning the guess probabilities improved the calibration of the model substantially but improved the predicted ordering only slightly. We will discuss calibration in more detail in chapter 4, particularly in Panel 4.3.

The ROC curve can be used as an evaluation metric by computing the area under the curve (AUC), since in general a higher area implies a better ranking. A perfect ranking would have an AUC of 1.0 (see the 'Perfect' line of Figure 2.30). It is usually a good idea to look at the ROC curve as well as computing the

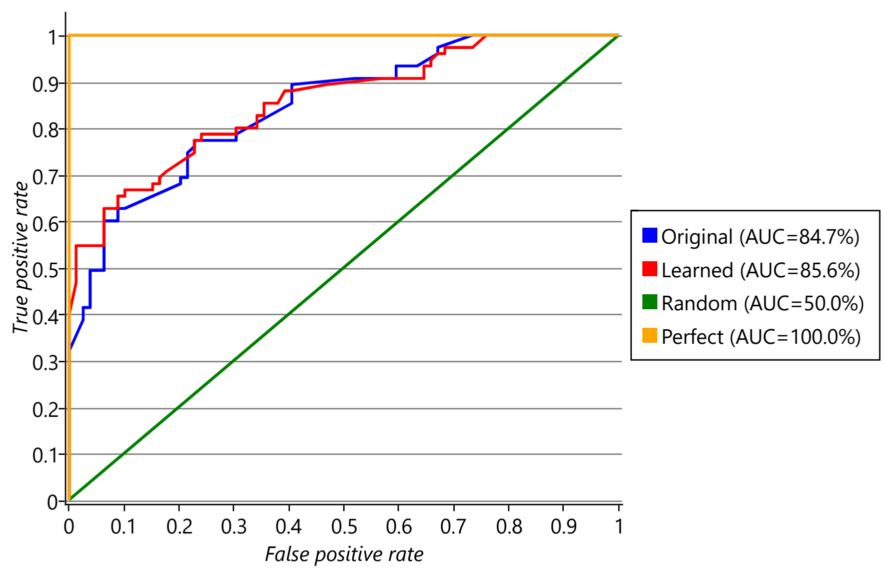


Figure 2.30: Receiver Operating Characteristic curves for all skills combined for the original model and the model with learned guess probabilities. Surprisingly, the original model has only a slightly worse ROC curve than the improved one. For comparison, curves for the best possible results (Perfect) and for a random prediction (Random) are also shown.

AUC since it gives more detail about how well a system would work in different scenarios, such as for making a short or long list.

Our improved system has a very respectable AUC of 0.86, substantially improved log probability scores across all skills and has been visually checked to give reasonable results. It would now be ready to be tried out for real.

2.6.4 Finishing up

In this chapter, we've gone through the process of building a model-based machine learning system from scratch. We've seen how to build a model from a set of assumptions, how to run inference, how to diagnose and fix a problem and how to evaluate results. As it happens, the model we have developed in this chapter has been used previously in the field of psychometrics (the science of measuring mental capacities and processes). For example, Junker and Sijtsma [2001] consider two models DINA (Deterministic Inputs, Noisy And) which is essentially the same as our model and NIDA (Noisy Inputs, Deterministic And) which is a similar model but the *AddNoise* factors are applied to the inputs of the *And* factor rather than the output. Using this second model has the effect of increasing a person's chance of getting a question right if they have some, but not all, of the skills needed for the question.

Of course, there is always room for improving our model. For example, we could learn the probability of making a mistake for each question, as well as the probability of guessing the answer. We could investigate different assumptions about what happens when a person has some but not all of the skills needed for a question (like the NIDA model mentioned above). We could consider modelling whether having certain skills makes it more likely to have other skills. Or we could reconsider the simplifying assumption that the skills are binary and instead model them as a continuous variable representing the degree of skill that a person has. In the next case study, we will do exactly that and represent skills using continuous variables, to solve a very different problem – but first, we will have a short interlude while we look at the *process* of solving machine learning problems.

Self assessment 2.6

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. *[This exercise shows where the beta distribution shape comes from and is well worth doing!]* Suppose we have a question which has an actual guess probability of 30%, but we do not know this. To try and find it out, we take $N = 10$ people who do not have the skills needed for that question and see how many of them get it right through guesswork.

   (a) Write a program to sample the number of people that get the question right (T). You should sample 10 times from a *Bernoulli*(0.3) and count the number of `true` samples. Before you run your sampler, what sort of samples would you expect to get from it?

(b) In reality, if we had the answers from only 10 people, we would have only one sample count to use to work on the guess probability. For example, we might know that three people got the question right, so that $T = 3$. How much would this tell us about the actual guess probability? We can write another sampling program to work it out. First, sample a possible guess probability between 0.0 and 1.0. Then, given this sampled guess probability, compute a sample of the number of people that would get the question right, had this been the true guess probability. If your sampled count matches the true count T (in other words, is equal to 3), then you 'accept it' and store the sampled guess probability. Otherwise you 'reject it' and throw it away. Repeat the process until you have 10,000 accepted samples.

(c) Plot a histogram of the accepted samples using 50 bins between 0.0 and 1.0. You should see that the histogram has the shape of a beta distribution!! In fact, your program is sampling from a $Beta(T + 1, (N - T) + 1)$ distribution.

(d) Using this information, change N and T in your program to recreate the beta distributions of Figure 2.24a. Explore what happens when you increase N whilst keeping T/N fixed (your beta distribution should get narrower). This should match the intuition that the more people you have data for, the more accurately you can assess the guess probability.

2. Plot a receiver operating characteristic curve for the results you got for the original model in the previous self assessment. You will need to sort the predicted skill probabilities whilst keeping track of the ground truth for each prediction. Then scan down the sorted list computing the true positive rate and false positive rate at each point. Verify that it looks like the Original ROC curve of Figure 2.30. Now make a perfect predictor (by cheating and using the ground truth). Plot the ROC curve for this perfect predictor and check that it looks like the Perfect line of Figure 2.30. If you want, you can repeat this for a random predictor (the results should approximate the diagonal line of Figure 2.30).

Review of concepts introduced in this section

probability density function A function used to define the probability distribution over a continuous random variable. The probability that the variable will take a value within a given range is given by the area under the probability density function in that range. See Panel 2.4 for more details.

beta distribution A probability distribution over a continuous random variable between 0 and 1 (inclusive) whose probability density function is

$$Beta(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}.$$

The beta distribution has two parameters α and β which control the position and width of the peak of the distribution. The mean value $\frac{\alpha}{\alpha+\beta}$ gives the position of the centre of mass of the distribution and the sum $\alpha + \beta$ controls how spread out the distribution is (larger $\alpha + \beta$ means a narrower distribution).

evaluation metric A measurement of the accuracy of a machine learning system used to assess how well the machine learning system is performing. An evaluation metric can be used to compare two different systems, to compare different versions of the same system or to assess if a system meets some desired target accuracy.

log probability (or *log-prob*) The logarithm of the probability of the ground truth value of a random variable, under the inferred distribution for that variable. Used as an evaluation metric for evaluating uncertain predictions made by a machine learning system. Larger log-prob values mean that the prediction is better, since it gives higher probability to the correct value. Since the log-prob is a negative number (or zero), it is common to use the negative log-prob, in which case smaller values indicate better accuracy. For example, see Figure 2.29.

Goodhart's law A law which warns about focusing too much on any particular evaluation metric and which can be stated as *"When a measure becomes a target, it ceases to be a good measure"*.

true positive rate The fraction of positive items that are correctly predicted as positive. Higher true positive rates indicate better prediction accuracy. See also Table 2.7.

false positive rate The fraction of negative items that are incorrectly predicted as positive. Higher false positive rates indicate worse prediction accuracy. See also Table 2.7.

receiver operating characteristic curve A receiver operating characteristic (ROC) curve is a plot of true positive rate against false positive rate which indicates the accuracy of predicting a binary variable. A perfect predictor has an ROC curve that goes vertically up the left hand side of the plot and then horizontally across the top (see plot below), whilst a random predictor has an ROC curve which is a diagonal line (again, see plot). In general, the higher the area under the ROC curve, the better the predictor.

calibration The accuracy of probabilities predicted by a machine learning system. For example, in a well-calibrated system, a prediction made with 90% probability should be correct roughly 90% of the time. Calibration can be assessed by looking at repeated predictions by the same system. In a poorly-calibrated system the predicted probabilities will not correspond closely to the actual fractions of predictions that are correct. Being poorly calibrated is usually a sign of an incorrect assumption in the model and so is always worth investigating – even if a system is being used in a way that is not sensitive to calibration (for example, if we are ranking by predicted probability rather than using the actual value of the probability). See Panel 4.3 for more details.

Interlude: the machine learning life cycle

In tackling our murder mystery back in chapter 1, we first gathered evidence from the crime scene and then used our own knowledge to construct a probabilistic model of the murder. We incorporated the crime scene evidence into the model, in the form of observed variables, and performed inference to answer the query of interest: what is the probability of each suspect being the murderer? We then assessed whether the results of inference were good enough – that is, was the probability high enough to consider the murder solved? When it was not, we then gathered additional data, extended the model, re-ran inference and finally reached our target probability.

In assessing skills of job candidates in chapter 2, we gathered data from people taking a real test and visualised this data. We then built a model based on our knowledge of how people take tests. We ran inference and assessed that the results were not good enough. We diagnosed the problem, extended the model and then evaluated both the original and the extended models to quantify the improvement and check that the improved model met our success criteria.

We can generalise from these two examples to define the steps needed for any model-based machine learning application:

1. **Gather data** for training and evaluating the model.
2. **Gather knowledge** to help make appropriate modelling assumptions.
3. **Visualise** the data to understand it better, check for data issues and gain insight into useful modelling assumptions.
4. **Construct a model** which captures knowledge about the problem domain, consistent with your understanding of the data.
5. **Perform inference** to make predictions over the variables of interest using the data to fix the values of other variables.
6. **Evaluate results** using some evaluation metric, to see if they meet the success criteria for the target application.

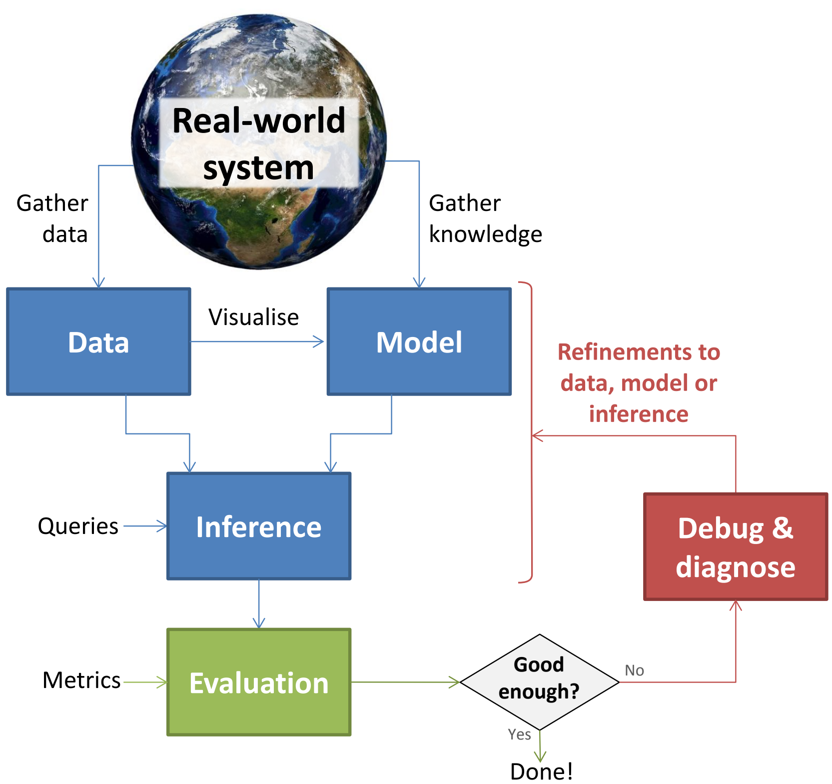
In the (usual) case that the system does not meet the success criteria the first time around, there are then two additional steps needed:

7. **Diagnose issues** which are reducing prediction accuracy. Visualisation is a powerful tool for bringing to light problems with data, models or inference algorithms. Inference issues can also be diagnosed using synthetic data sampled from the model (as we saw in chapter 2). At this stage, is may also be necessary to diagnose performance issues if the inference algorithm is taking too long to complete.

8. **Refine the system** – this could mean refining the data, model, visualisations, inference or evaluation.

These two stages need to be repeated until the system is performing at a level necessary for the intended application. Model-based machine learning can make this repeated refinement process much quicker when using automatic inference software, since it is easy to extend or modify a model and inference can then be immediately applied to the modified model. This allows for rapid exploration of a number of models each of which would be very slow to code up by hand.

The stages of this *machine learning life cycle* can be illustrated in a flow chart:



As we move on to our next case study, keep this life cycle flowchart in mind – it will continue to be useful as a template for solving machine learning problems.

Chapter 3

Meeting Your Match

The Xbox Live® online gaming service is used by tens of millions of players around the world to play against each other in a wide variety of games. Such a system must be able to match players with other players of comparable skill level in order that they have an enjoyable gaming experience. So how can we create an automated system to match players of similar ability at a particular type of game?

One of the great advantages of the online world for gaming is the ready availability of opponents at any time of day or night. An important requirement for Xbox Live is the capability to find opponents with comparable skill levels, in order that players have an enjoyable gaming experience, and so the system must have a way of estimating the skills of players. However, this presents some significant challenges – in particular, a game is not always won by the stronger player. Many games involve an element of chance, and in a particular game luck may favour the weaker player. More generally, a player's performance can vary from one game to the next, due to factors such as tiredness or fluctuating enthusiasm. We therefore cannot assume that the winner of a particular game has a higher skill level than the loser. On the other hand we do expect a stronger player to win against a weaker player more often than they lose, so the game outcome clearly gives us some information about the players' relative skills.

Figure 3.1: Xbox Live®provides a real-time matchmaking service for online gaming.

Another challenge concerns new players to the game. We have little idea of their ability until we see the outcomes of some games. New players are not always poor players – they may have played under different identities or have experience of other similar games. Either way, it is essential to have reasonably reliable assessments of their skills after only a few games so that they can be matched against players of comparable skill. This ensures that new players have a good gaming experience and so are more likely to continue to subscribe to Xbox Live. Rapid assessment of skills is therefore important to the commercial success of the service.

A final challenge arises when we have games played by teams of players. We observe that one team wins and the other loses, and we must use this information to learn about the skills of the individual players. At first it might seem impossible to solve this 'credit assignment' problem. But we can make use of the fact that, particularly in online games, the composition of teams changes frequently and so over the course of multiple games we can disambiguate the contributions of individual players to the successes and failures of the teams in which they play.

We will need to work with the data available in Xbox Live, when doing match-making amongst the players. Table 3.1 shows a sample of the kind of data that we need to work with, in this case from the Xbox game Halo 2.

Player1	Player2	Player1Score	Player2Score	Outcome	Id	Variant
Gamer00123	Gamer00103	0	2	Player2Win	282203	Slayer
Gamer00044	Gamer00094	2	4	Player2Win	282201	Slayer
Gamer00139	Gamer00074	2	5	Player2Win	282205	Slayer
Gamer00095	Gamer00140	2	2	Draw	282211	Slayer
Gamer00120	Gamer00141	5	1	Player1Win	282209	Slayer
Gamer00142	Gamer00143	5	2	Player1Win	282208	Slayer
Gamer00144	Gamer00122	1	1	Draw	282212	Slayer
Gamer00116	Gamer00145	5	0	Player1Win	282207	Slayer

Table 3.1: Sample of the available data, showing ten games in the 'Head to Head' variant of Halo2. The columns give the anonymized player ids, their scores, the game outcome, the game id and the variant of the game that was played.

So in summary, our goal is to use data of the above form to infer the skills of individual players, in order to match players against others of a similar skill level in future games. A secondary goal is to use the inferred skill levels in order to create 'leader boards' showing the ranking of players within a tournament or league. The system must also allow for the fact that players may play one-on-one or may work together in teams. Furthermore, we must solve this problem in a way that makes efficient use of the game outcome results so that we can arrive at an accurate assessment of a player's skill after observing a relatively small number of games involving that player.

3.1 Modelling the outcome of games

Our goal is to build a system which can assess the skills of players in online gaming. As a first step towards this, we need to look at the simpler problem of predicting the outcome of a game where we already know the skills of the players involved. This will allow us to develop many of the concepts required to solve the more complex problem of determining skills.

Suppose that Jill is going to play a game of Halo against Fred on Xbox Live. In chapter 2 we represented a person's software development skills by using a binary variable for each skill, indicating whether the person possessed that particular skill or not. Clearly this approach is insufficient when we consider a person's skill at a typical Xbox game such as Halo. There is a wide spectrum of possible skill levels, and it is more appropriate to represent a person's skill using a continuous value. The first of our modelling assumptions is therefore:

(1) Each player has a skill value, represented by a continuous variable.

The stronger player is not always the winner.

We denote the skill of Jill by `Jskill` and the skill of Fred by `Fskill`. Let us suppose that Fred has a skill level of `Fskill` = 12.5 while Jill has a skill of `Jskill` = 15. These numbers appear to be completely arbitrary, and the scale on which we measure skill is indeed arbitrary. What matters, however, is how the skill values compare between players, and we shall see in a moment how to give meaning to such numbers. We have given Jill a higher skill value to indicate that she is the stronger player. But now we run into the first of our challenges, which is that the stronger player in a game such as Halo is not always the winner. If Jill and Fred were to play lots of games against each other we would expect Jill to win more than half of them, but not necessarily to win them all. We can capture the variability in the outcome of a game by introducing the notion of a *performance* for each player, which expresses how well they played on a particular game. The player with the higher performance for a specific game will be the winner of that game. A player with a high skill level will tend to have a high performance, but their actual performance will vary from one game to another. As with skill, the performance is most naturally expressed using a continuous quantity. We denote Jill's performance by `Jperf` and Fred's performance by `Fperf`. Figure 3.2 shows `Jperf` plotted against `Fperf`. For points lying in the region above the diagonal line Jill is the winner, while below the diagonal line Fred is the winner.

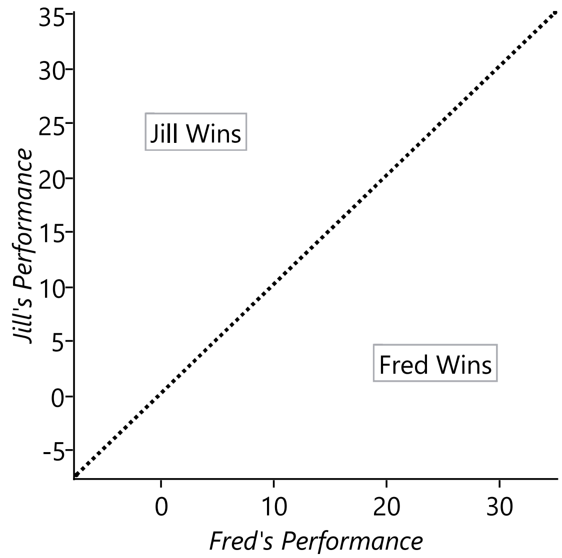


Figure 3.2: Schematic illustration of the values of Jill's performance and Fred's performance showing the areas in which Jill would be the winner and in which Fred would be the winner.

We can think of a person's skill as their average performance across many games. For example, Jill has a skill level of 15 so her performance will have an average value of 15 but on a particular game it might be higher or lower. Once again we have to deal with uncertainty, and we shall do this using a suitable probability distribution. We anticipate that larger departures of performance from the average will be less common, and therefore have lower probability, than values which are closer to the average. Intuitively the performance should therefore take the form of a 'bell curve' as illustrated in Figure 3.3 in which the probability of a given performance value falls off on either side of the skill value.

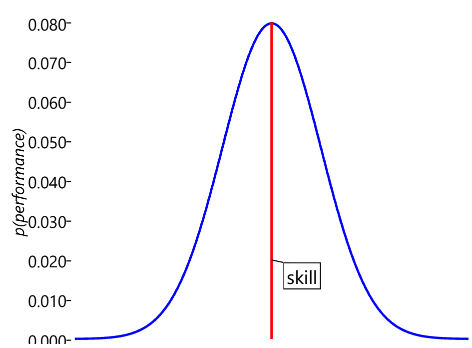


Figure 3.3: Schematic illustration of a 'bell curve' showing how the performance of a player can vary randomly around their skill value.

Because performance is a continuous quantity, this bell curve is an example of a probability density, which we encountered previously in Panel 2.4. Although we have sketched the general shape of the bell curve, to make further progress we need to define a specific form for this curve. There are many possible choices, but there is one which stands out as special in having some very useful mathematical properties. It is called the *Gaussian probability density* and is the density function for the **Gaussian distribution**. In fact, the Gaussian distribution has so many nice properties that it is one of the most widely used distributions in the fields of machine learning and statistics. A particular Gaussian distribution is completely characterized by just two numbers: the centre value of the distribution, known as the **mean**, and the **standard deviation**, which determines how wide the curve is. These concepts are discussed in more detail in Panel 3.1. Figure 3.4 shows a plot of the Gaussian distribution, illustrating the interpretation of the mean and the standard deviation.

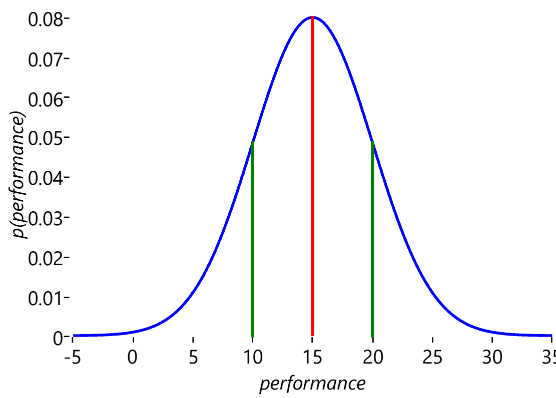


Figure 3.4: Plot of the Gaussian distribution having mean of 15 and standard deviation of 5, showing the mean (red line) and the values which differ from the mean by plus-or-minus one standard deviation (green lines). There is roughly a 68.2% probability of a random variable with this distribution having a value lying within one standard deviation of the mean (i.e. between the two green lines), a 95.4% probability of the value lying within two standard deviations of the mean (i.e. between 5 and 25), and a 99.7% probability of the value lying within 3 standard deviations of the mean (i.e. between 0 and 30).

To understand the scale of the values on the vertical axis of Figure 3.4, remember that the total area under a probability distribution curve must be one. Note that the distribution is symmetrical about its maximum point – because there is equal probability of being on either side of this point, the performance at this central point is also the mean performance.

In standard notation, we write the mean as μ and the standard deviation as σ. Using this notation the Gaussian density function can be written as

$$Gaussian(x; \mu, \sigma^2) = \frac{1}{(2\pi)^{1/2}\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}. \tag{3.1}$$

The left hand side says that $Gaussian(x; \mu, \sigma^2)$ is a probability distribution over x whose value is dependent on the values of μ and σ. It is often convenient to work with the square of the standard deviation, which we call the **variance** and which we denote by σ^2 (see Panel 3.1). We shall also sometimes use the reciprocal of the variance $\tau = 1/\sigma^2$ which is known as the **precision**. For the most part we shall use standard deviation since this lives on the same scale (i.e. has the same units) as x.

Sometimes when we are using a Gaussian distribution it will be clear which variable the distribution applies to. In such cases, we can simplify the notation and instead of writing $Gaussian(x; \mu, \sigma^2)$ we simply write $Gaussian(\mu, \sigma^2)$. It is important to appreciate that is simply a shorthand notation and does not represent a distribution over μ and σ^2.

Now let's see how we can apply the Gaussian distribution to model a single game of Halo between Jill and Fred. Figure 3.5 shows the Gaussian distributions which describe the probabilities of various performances being achieved by Jill and Fred in their Halo game. Here we have chosen the standard deviations of

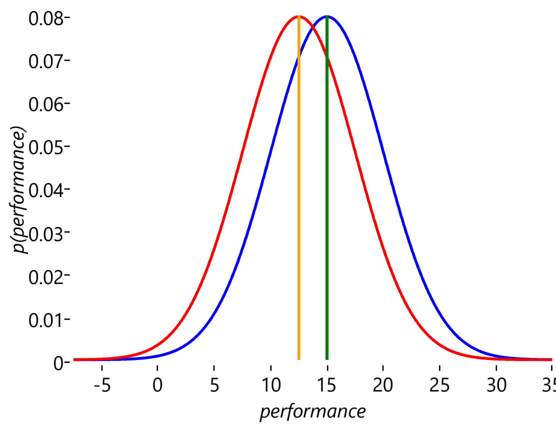


Figure 3.5: Plot of the Gaussian distributions of performance for Jill and Fred.

the two Gaussians to be the same, with $\texttt{perfSD} = 5$ (where '`perfSD`' denotes the standard deviation of the performance distribution). We shall discuss the significance of this choice shortly. The first question we can ask is: "what is the probability that Jill will be the winner?". Note that there is considerable overlap between the two distributions, which implies that there is a significant chance that the performance value for Fred would be higher than that for Jill and hence that he will win the game, even though Jill has a higher skill value. You can also see that if the curves were more separated (for example, if Jill had a much higher skill), then the chance of Fred winning would be reduced.

We have introduced two further assumptions into our model, and it is worth making these explicit:

② Each player has a performance value for each game, which varies from game to game such that the average value is equal to the skill of that

Panel 3.1 – Mean, Variance, and Standard Deviation

Suppose we make multiple measurements of some quantity x, resulting in a set of values $x_1, x_2, \ldots, x_N$. For example, we might measure the heights of adults in the population. It can be very useful to summarise the properties of this set of values by computing some simple **statistics**. One well-known statistic is called the *mean*, and is defined by

$$\begin{aligned} \texttt{mean} &= \frac{x_1 + x_2 + \ldots + x_N}{N} \\ &= \frac{1}{N}\sum_{n=1}^{N} x_n. \end{aligned} \tag{3.2}$$

The mean is therefore simply the average of the values. Another useful statistic is the variance which measures how much the values vary around the mean value, and is defined by

$$\begin{aligned} \texttt{variance} &= \frac{(x_1 - \texttt{mean})^2 + \ldots + (x_N - \texttt{mean})^2}{N} \\ &= \frac{1}{N}\sum_{n=1}^{N} (x_n - \texttt{mean})^2. \end{aligned} \tag{3.3}$$

If the heights of our adults are measured in metres, then the units of the mean height would again be metres, whereas the variance would have the units of metres-squared. It is usually more useful to measure variation from the mean in the same units that we measure the mean in, and so we can instead use the standard deviation, which is given by the square root of the variance

$$\texttt{standard deviation} = \sqrt{\texttt{variance}}. \tag{3.4}$$

The standard deviation would then have the units of metres, and would be a more easily interpretable quantity because it would tell us directly about the variability of heights within the population. For example, in a particular population of people the mean height might be 1.64 metres and the standard deviation might be 0.35 metres.

There is an important connection between the statistics of a data set and the parameters of the probability distribution that gave rise to that data set. Consider the Gaussian distribution in equation (3.1). If we take a very large number of samples from this distribution, then the mean and variance statistics of the samples will be almost exactly equal to the mean and variance parameters of the distribution (see Bishop [2006]). In fact, this is why the parameters of the Gaussian distribution are called the 'mean' and 'variance' parameters. In general, the statistics of a very large set of samples from any distribution can be computed directly from the distribution's parameters, without actually having to do any sampling.

player. The variation in performance, which is the same for all players, is symmetrically distributed around the mean value and is more likely to be close to the mean than to be far from the mean.

3. The player with the highest performance value wins the game.

As written, assumption Assumption 2 expresses the qualitative knowledge that a domain expert in online games might possess, and corresponds to a bell-shaped performance distribution. This needs to be refined into a specific mathematical form and for this we choose the Gaussian, although we might anticipate that other bell-shaped distributions would give qualitatively similar results.

This is a good moment to introduce our first factor graph for this chapter. To construct this graph we start with the variable nodes for each random variable in our problem. So far we have two variables: the performance of Fred, which we denote by the continuous variable `Fperf`, and the performance for Jill, denoted by `Jperf`. Each of these is described by a Gaussian distribution whose mean is the skill of the corresponding player, and with a common standard deviation of 5, and therefore a variance of 5^2:

$$\begin{aligned} p(\texttt{Jperf}) &= \text{Gaussian}(\texttt{Jperf}; 15, 5^2) \\ p(\texttt{Fperf}) &= \text{Gaussian}(\texttt{Fperf}; 12.5, 5^2). \end{aligned} \tag{3.5}$$

Note that, as in section 2.6, we are using a lower-case p to denote a probability density for a continuous variable, and will use an upper-case P to denote the probability distribution for a discrete variable.

The other uncertain quantity is the winner of the game. For this we can use a binary variable `JillWins` which takes the value `true` if Jill is the winner and the value `false` if Fred is the winner. The value of this variable is determined by which of the two variables `Jperf` and `Fperf` is larger – it will be `true` is `Jperf` is larger or otherwise `false`. Using `T` for `true` and `F` for `false` as before, we can express this distribution by

$$P(\texttt{JillWins} = \texttt{T}|\texttt{Jperf}, \texttt{Fperf}) = \begin{cases} 1 & \text{if } \texttt{Jperf} > \texttt{Fperf}, \\ 0 & \text{otherwise.} \end{cases} \tag{3.6}$$

Since probabilities sum to one, we then have

$$P(\texttt{JillWins} = \texttt{F}|\texttt{Jperf}, \texttt{Fperf}) = 1 - P(\texttt{JillWins} = \texttt{T}|\texttt{Jperf}, \texttt{Fperf}). \tag{3.7}$$

We shall refer to the conditional probability in equation (3.6) as the *GreaterThan* factor, which we shall denote the by '¿' when drawing factor graphs. Note that this is a deterministic factor since the value of the child variable is fixed if the values of both parent variables are known. Using this factor, we are now ready to draw the factor graph. This has three variable nodes, each with a corresponding factor node, and is shown in Figure 3.6.

We asked for the probability that Jill would win this game of Halo. We can find an approximate answer to this question by using ancestral sampling (which

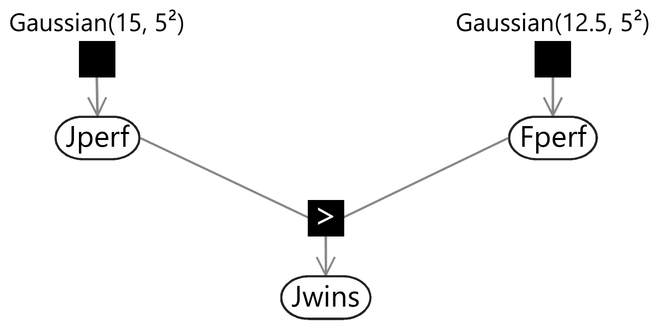


Figure 3.6: Basic model of performance difference between two players Fred and Jill, having known skills, in a specific game.

was introduced back in subsection 2.5.1). To apply ancestral sampling in our factor graph we must first sample from the parent variables `Jperf` and `Fperf` and then compute the value of the child variable `Jwins`.

Consider first the sampling of the performance `Jperf` for Jill. There are standard numerical techniques for generating random numbers having a Gaussian distribution of specified mean and variance. If we generate five samples from $Gaussian(x; 15, 5^2)$ and plot them as a histogram we obtain the result shown in Figure 3.7a. Note that we have divided the height of each bar in the histogram by the total number of samples (in this case 5) and also by the width of the histogram bins (in this case 10). This ensures that the total area under the histogram is one. If we increase the number of samples to 50, as seen in Figure 3.7b, we see that the histogram roughly approximates the bell curve of a Gaussian. By increasing the number of samples we obtain a more accurate approximation, as shown in Figure 3.7c for the case of 500 samples, and in Figure 3.7d for 5,000 such samples. We see that we need to draw a relatively large number of samples in order to obtain a good approximation to the Gaussian. When using ancestral sampling we therefore need to use a lot of samples in order to obtain reasonably accurate results. This makes ancestral sampling computationally very inefficient, although it is a straightforward technique which provides a useful way to help understand the model or generate synthetic datasets from the model.

Having seen how to sample from a single Gaussian distribution we can now consider ancestral sampling from the complete graph in Figure 3.6 representing a single game of Halo between Jill and Fred. We first select a performance `Jperf` for Jill on this specific game, corresponding to the top-level variable node on the factor graph, by drawing a value from the Gaussian distribution

$$p(\texttt{Jperf}) = \text{Gaussian}(\texttt{Jperf}; 15, 5^2). \tag{3.8}$$

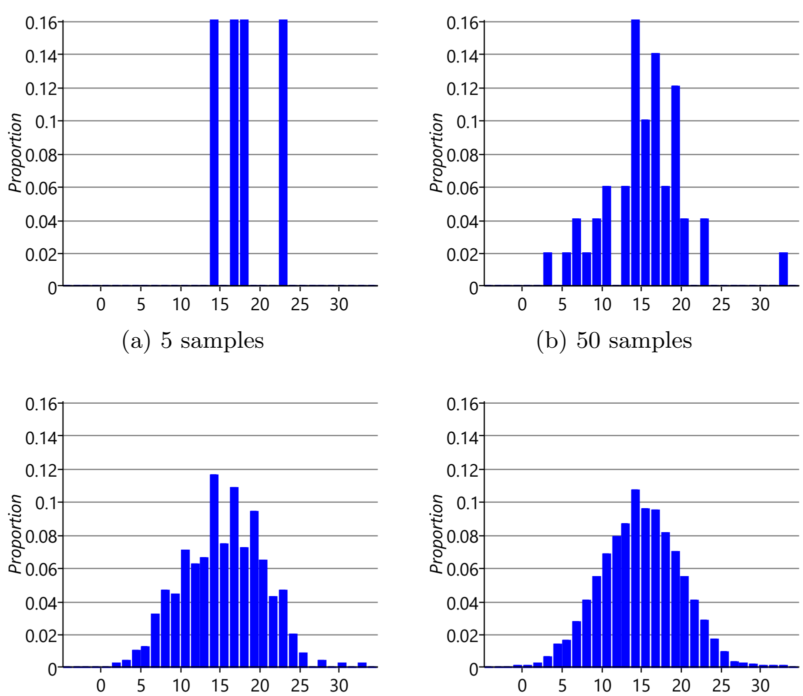
Independently, we choose a performance value `Fperf` for Fred, which is also a top-level variable node, by drawing a sample from the Gaussian distribution

$$p(\texttt{Fperf}) = \text{Gaussian}(\texttt{Fperf}; 12.5, 5^2). \tag{3.9}$$

We then compute the value of the remaining variable `JillWins` using these sampled values. This involves comparing the two performance values, and if `Jperf` is greater than `Fperf` then `JillWins` is `true`, otherwise `JillWins` is `false`. If we repeat this sampling process many times, then the fraction of times that `JillWins` is `true` gives (approximately) the probability of Jill winning a game. The larger the number of samples over which we average, the more accurate this approximation will be. Figure 3.8 shows a scatter plot of the performances of our two players across 1,000 samples.

For each game we independently select the performance of each of our two players by generating random values according to their respective Gaussian distributions. Each of these games is shown as a point on the scatter plot. Also shown is the 45-degree line along which the two performances are equal. Points lying below this line represent games in which Fred is the winner, while points lying above the line are those for which Jill is the winner. We see that the majority of points lie above the line, as we expect because Jill has a higher skill value. By simply counting the number of points we find that Jill wins 63.1% of the time.

Of course this is only an approximate estimate of the probability of Jill



(a) 5 samples

(b) 50 samples

(c) 500 samples

(d) 5,000 samples

Figure 3.7: Histograms of samples drawn from the Gaussian distribution with mean of 15 and standard deviation of 5 shown in Figure 3.4.

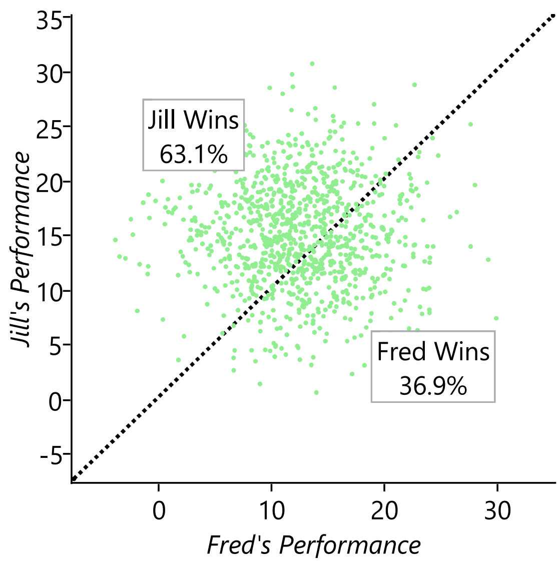


Figure 3.8: Samples of Jill and Fred's performances overlaid on the schematic illustration from Figure 3.2

winning. We can find the exact result mathematically [Moser, 2010] by making use of the equation for the Gaussian distribution (3.1), which tells us that the probability of Jill being the winner is given by

$$P(\texttt{Jperf} > \texttt{Fperf}|\texttt{Jskill}, \texttt{Fskill}) = \mathit{CumGauss}\left(\frac{\texttt{Jskill} - \texttt{Fskill}}{\sqrt{2}\texttt{perfSD}}\right). \tag{3.10}$$

Here *CumGauss* denotes the **cumulative Gaussian function** which is illustrated in Figure 3.9

Using a numerical evaluation of this function we find that the probability of Jill winning the game is 63.8%, which is close to the value (63.1%) we obtained by ancestral sampling.

We noted earlier that the scale on which skill is measured is essentially arbitrary. If we add a fixed constant onto the skills of all the players this would leave the probabilities of winning unchanged since, from equation (3.10), they depend only on the difference in skill values. Likewise, if we multiplied all the skill values by the same constant, and at the same time we multiplied the parameter `perfSD` by the same constant, then again the probabilities of winning would be unchanged. All that matters is the difference in skill values measured in relation to the value of `perfSD`.

We have now built a model which can predict the outcome of a game for two players of known skills. In the next section we will look at how to extend this model to go in the opposite direction: to predict the player skills given the outcome of one or more games.

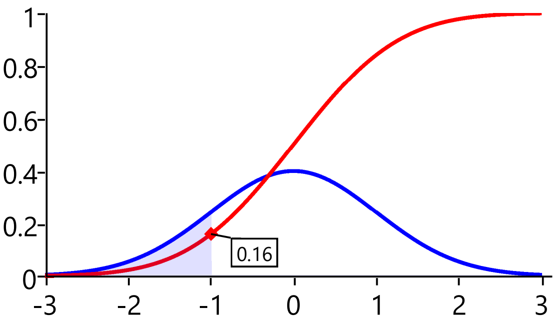


Figure 3.9: The blue curve shows a Gaussian distribution with mean of zero and a standard deviation of one. The area under this Gaussian from $-\infty$ up to the point x is known as the cumulative Gaussian distribution and is shown, as a function of x, by the red curve. For example, at $x = -1$ the area of the shaded region has the value 0.16, as indicated.

Self assessment 3.1

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Write a program or create a spreadsheet which produces 10,000 samples from a Gaussian with zero mean and a standard deviation of 1 (most languages/spreadsheets have built in functions or available libraries for sampling from a Gaussian). Compute the percentage of these samples which lie between -1 and 1, between -2 and 2 and between -3 and 3. You should find that these percentages are close to those given in the caption of Figure 3.4.

2. Construct a histogram of the samples created in the previous exercise (like the ones in Figure 3.7) and verify that it resembles a bell-shaped curve.

3. Compute the mean, standard deviation and variance of your samples, referring to Panel 3.1. The mean should be close to zero and the standard deviation and variance should both be close to 1 (since $1^2 = 1$).

4. Produce a second set of 10,000 samples from a Gaussian with mean 1 and standard deviation 1. Plot a scatter plot like Figure 3.8 where the X co-ordinate of each point is a sample from the first set and the Y co-ordinate is the corresponding sample from the second set (pairing the first sample from each set, the second sample from each set and so on). Compute the fraction of samples which lie above the diagonal line where X=Y.

5. Using Infer.NET, create double variables `X` and `Y` with priors of *Gaussian*(0,1) and *Gaussian*(*1*, *1*) respectively. Define a third random variable `Ywins` equal to `Y` $>$ `X`. Compute the posterior distribution over `Ywins` and verify that it is close to the fraction of samples above the diagonal in the previous exercise.

Review of concepts introduced in this section

Gaussian distribution A specific form of probability density over a continuous variable that has many useful mathematical properties. It is governed by two parameters – the mean and the standard deviation. The mathematical definition of a Gaussian is given by equation (3.1)

mean The average of a set of values. See Panel 3.1 for a more detailed discussion of the mean and related concepts.

standard deviation The square root of the variance.

variance A measure of how much a set of numbers vary around their average value. The variance, and related quantities, are discussed in Panel 3.1.

precision The reciprocal of the variance.

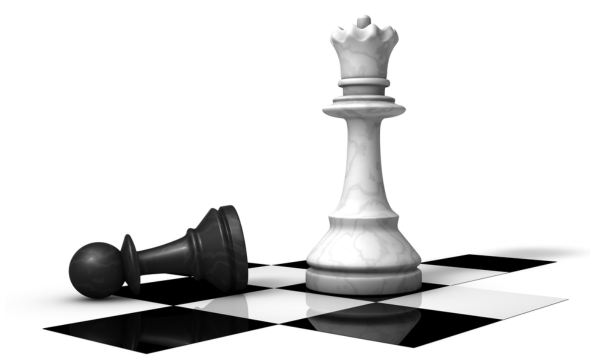
statistics A statistic is a function of a set of data values. For instance the mean is a statistic whose value is the average of a set of values. Statistics can be useful for summarising a large data set compactly.

cumulative Gaussian function The value of the cumulative Gaussian function at a point x is equal to the area under a zero-mean unit-variance Gaussian from minus infinity up to the point x. It follows from this definition that the gradient of the cumulative Gaussian function is given by the Gaussian distribution.

3.2 Inferring the players' skills

The discussion so far has assumed that we know the skills of Jill and Fred. These skills were then used to compute the probability that each of the players would be the winner. In practice, we have to reason backwards: we observe the outcome of the game and we wish to use this information to learn something about the skill values of the players. We therefore turn to the problem of assessing player skill.

The original Xbox was launched in 2001, and was followed a year later by an online gaming service Xbox Live. This required a matchmaking feature which in turn needed a way of determining the relative skills of players. To address this requirement, the Xbox online service adopted a widely used algorithm called Elo [Elo, 1978], which is used (with various modifications) by most of the major international chess organizations as well as by representative bodies of many other sports. The Elo algorithm is summarized in Panel 3.2.



The Elo algorithm is widely used in chess.

One merit of the Elo system is that it is relatively easy for players to compute the skill updates for themselves. In Xbox Live, however, the skill calculations are automated – and so more complex but more accurate methods become possible. Furthermore, the Elo algorithm does not handle more than two players, nor does it apply to games played by teams of players, and so it was not directly applicable to many of the games on Xbox Live. There was a significant motivation, therefore, to find improved methods to assess player skills which are able to give accurate skill values after relatively few games have been played. When the successor games console the Xbox 360 was launched in 2005 it was decided to replace the Elo algorithm with an approach built on a probabilistic model of the skill assessment problem, known as the TrueSkill®system [Herbrich et al., 2007]. TrueSkill has been used as the skill rating and matchmaking system on Xbox Live continuously since 2005, processing the outcomes of millions of games per day. As well as overcoming the above limitations of the Elo system, the modelling of uncertainty in the players' skills in TrueSkill leads to a significant improvement in the efficiency with which skill is assessed [Herbrich et al., 2007]. In the remainder of this chapter we explain how the TrueSkill model was constructed. For more details of the mathematics behind TrueSkill see Moser [2010].

Panel 3.2 – The Elo Algorithm

The skill of a player is an uncertain quantity and so we should model this using a probability distribution. However, it is instructive to see first what happens if we simply treat the skill as a number whose value gets updated when we learn the outcome of a game. We will see how far we can get, and what sort of problems we encounter, and this will help us understand some of the benefits of using a model-based approach.

Given the outcome of a game it would seem reasonable to increase the skill value for the winner and decrease the skill value for the loser. What is less clear, however, is how big an adjustment we should make. Intuitively we can reason as follows. Suppose that Jill is the winner of the game. If Jill's skill is significantly higher than Fred's, then it is unsurprising that Jill should be the winner, and so the change in skill values should be relatively small. If the skills are similar then a larger change would be justified. However, if Jill's skill is significantly less than Fred's then the game outcome is very surprising. The outcome suggests that our current assessments of the skill values are not very accurate, and therefore that we should make a much larger adjustment in skill values. Put concisely, the degree of surprise gives an indication of how big a change in skill values should be made.

Let us define the winner of a game to have a score of 1 and the loser to have a score of 0. If we now imagine Jill and Fred playing lots of games against each other then the average score for Jill after playing lots of games against Fred is the same as the probability that she will win. This can be obtained from equation (3.10), and is given by [Elo, 1978]:

$$\texttt{Jscore} = \mathit{CumGauss}\left(\frac{\texttt{Jskill} - \texttt{Fskill}}{\sqrt{2}\texttt{perfSD}}\right) \tag{3.11}$$

where, as before, `perfSD` is an arbitrary constant which sets the scale of the skill variables. We refer to this average score as the *expected score* for Jill. Similarly, the expected score for Fred is $(1 - \texttt{Jscore})$. We can then define the degree of surprise as the difference between the actual score of a player against a particular opponent and the expected score for that game. Thus, if it turns out that Jill is the winner, then the surprise for Jill is $(1 - \texttt{Jscore})$ while for Fred it is $0 - (1 - \texttt{Jscore})$. The change in skill value can then be made proportional to this degree of surprise, so that

$$\texttt{Jskill}^{(\text{new})} = \texttt{Jskill} + K(1 - \texttt{Jscore}) \tag{3.12}$$

$$\begin{aligned} \texttt{Fskill}^{(\text{new})} &= \texttt{Fskill} + K(0 - (1 - \texttt{Jscore})) \\ &= \texttt{Fskill} - K(1 - \texttt{Jscore}) \end{aligned} \tag{3.13}$$

Here K is an arbitrary coefficient which determines how much the players skills change as a result of each game. Elo has some limitations which are relevant to our matchmaking problem. For instance, it does not apply to team games, or to games involving more than two players. Furthermore, because Elo is an algorithm, rather than a model, it is not immediately obvious how it should be modified in order to overcome such limitations. By contrast, in our probabilistic modelling approach, when the assumptions of the model are not satisfied, we change the assumptions and then construct the corresponding modified model. We shall see how to do this in practice in section 3.4.

3.2.1 A probabilistic model: TrueSkill

We have already noted that skill is an uncertain quantity, and should therefore be included in the model as a random variable. We need to define a suitable prior distribution for this variable. This distribution captures our prior knowledge about a player's skill before they have played any games. Since we know very little about a player before they play any games, this distribution needs to be broad and cover the full range of skills that a new player might have. Because skill is a continuous variable we can once again use a Gaussian distribution to define this prior. This represents a modification to our first modelling assumption, which becomes:

① Each player has a skill value, represented by a continuous variable with a broad prior distribution.

For a new player, this distribution will represent our (significant) uncertainty in their skill value. Again, we make this modelling assumption precise through the choice of a Gaussian distribution. Once a new player has played a game, we aim to use the outcome of the game to infer the updated skill distribution for the player (and also for any other players in the game). This involves solving a probabilistic inference problem to calculate the posterior distribution of each player's skill, taking account of the new information provided by the result of the game. Although the prior distribution is Gaussian, the corresponding posterior distribution may not be Gaussian. However, we shall see that there is considerable benefit in approximating the exact posterior distribution by a Gaussian. This Gaussian posterior will act as the effective prior distribution for the next game played by that player. We will discuss this idea in greater detail later in the chapter.

For the moment, let us return to our game of Halo between Jill and Fred. We will suppose that some games have already been played, and that the uncertainty in the skills of our two players are represented by Gaussian distributions. Earlier in this chapter we used skill values for Jill and Fred of 12.5 and 15 respectively, which are quite small in relation to the standard deviation in performance of 5, and therefore help to illustrate the influence of these quantities on the probability of a win for Jill. For the remainder of the chapter we shall use values which are more realistic for a pair of real players and so we assume the mean for Jill is 120 while that for Fred 100. We will also suppose that standard deviation of the skill distribution for Jill is 40, while for Fred it is 5. This would typically arise if Jill is a relatively new player and so there is a lot of uncertainty in her skill whereas Fred is a more established player whose skill is more precisely known. We must therefore extend our model for a specific game of Halo by introducing two more uncertain variables `Jskill` and `Fskill`: the skills of Jill and Fred. Each of these variables has its own Gaussian distribution and therefore its own factor in the factor graph. The factor graph for our extended model is shown in Figure 3.10.

At this point it is convenient to summarise the assumptions that are encoded in the model represented in Figure 3.10. They are all shown together in

Figure 3.11.

> ① Each player has a skill value, represented by a continuous variable with a broad Gaussian distribution.
>
> ② Each player has a performance value for each game, which varies from game to game such that the average value is equal to the skill of that player. The variation in performance, which is the same for all players, is symmetrically distributed around the mean value and is more likely to be close to the mean than to be far from the mean.
>
> ③ The player with the higher performance value wins the game.

Figure 3.11: The three assumptions encoded in our model.

Having stated our modelling assumptions explicitly, it is worth taking a moment to review them. Assumption ① says that a player's ability at a particular type of game can be expressed as a single continuous variable. This seems reasonable for most situations, but we could imagine a more complex description of a player's abilities which, for example, distinguishes between their skill in attack and their skill at defence. This might be important in team games (discussed later) where a strong team may require a balance of players with strong attack skills and those with good defensive skills. We also assumed a Gaussian prior for the skill variable. This is the simplest probabilistic model we could have for a continuous skill variable, and it brings some nice analytical and engineering properties. However, if we looked at the skills of a large population of players

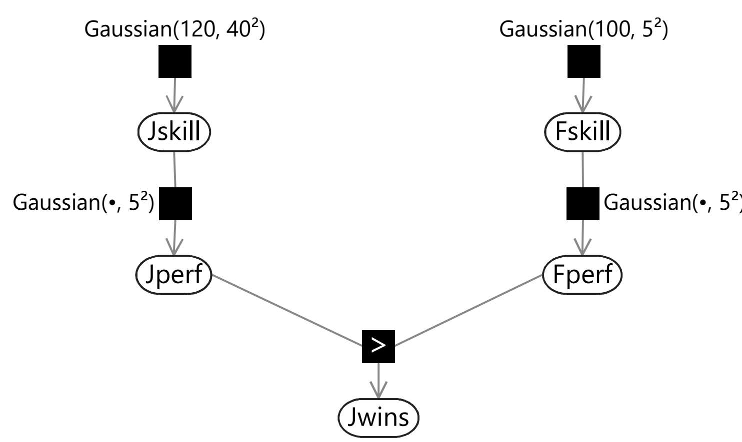


Figure 3.10: TrueSkill model for two players in a game, with unknown skills. Here we have used the notation $Gaussian(\cdot, 5^2)$ to describe a factor whose distribution is Gaussian with a mean given by the parent variable, in this case the corresponding skill variable, and a standard deviation of 5.

we might find a rather non-Gaussian distribution of skills, for example, new players may often have low skill but, if they have played a similar game before, may occasionally have a high skill.

Similarly, Assumption (2) considers a single performance variable and again assumes it has a Gaussian distribution. It might well be the case that players can sometimes have a seriously 'off' day when their performance is way below their skill value, while it would be very unlikely for a player to perform dramatically higher than their skill value. This suggests that the performance distribution might be non-symmetrical. Another aspect that could be improved is the assumption that the variance is the same for all players – it is likely that some players are more consistent than others and so would have correspondingly lower variance.

Finally, Assumption (3) says that the game outcome is determined purely by the performance values. If we had introduced multiple variables to characterize the skill of a player, there would presumably each have a corresponding performance variable (such as how the player performed in attack or defence), and we would need to define how these would be combined in order to determine the outcome of a game.

3.2.2 Inference in the TrueSkill model

Inference

Inference deep-dive

In this optional section, we see how to do exact inference in the model as defined so far, and then we see why exact inference is not useable in practice. If you want to focus on modelling, feel free to skip this section.

Now that we have the factor graph describing our model, we can set the variable `Jwins` according to the observed game outcome and run inference in order to compute the marginal posterior distributions of the skill variables `Jskill` and `Fskill`. The graph has a tree structure (there are no loops) and so we have already seen in chapter 2 that we can solve this problem using belief propagation.

Consider the evaluation of the posterior distribution for `Jskill` in the case where Jill won the game (`Jwins` is `true`). Using the belief propagation algorithm we have to evaluate the messages shown in Figure 3.12. Message (1) is just given by the Gaussian factor itself. Similarly, message (2) is just the product of all incoming messages on other edges of the `Fskill` node, and since there is only one incoming message this is just copied to the output message. These first two messages are summarized in Figure 3.13.

Next we have to compute message (3) in Figure 3.12. The belief propagation algorithm tells us to multiply the incoming message (2) by the Gaussian factor and then sum over the variable `Fskill`. In this case the summation becomes an integration because `Fskill` is a continuous variable. We can gain some insight into this step by once again considering a generative viewpoint based on sampling. Imagine that we draw samples from the Gaussian distribution over `Fskill`. Each sample is a specific value of `Fskill` and forms the mean of a Gaussian distribution over `Fperf`. In Figure 3.14a we consider three samples

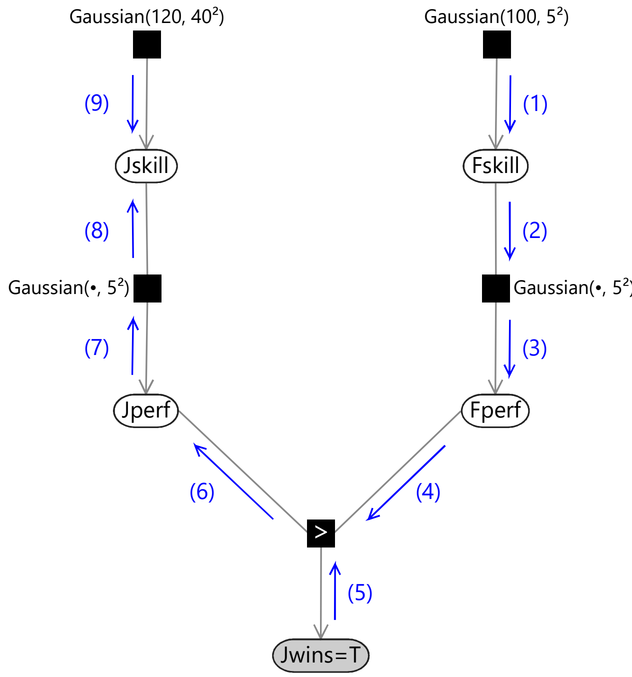


Figure 3.12: The messages which arise in the application of belief propagation to the evaluation of the updated distribution for `Jskill`.

of `Fskill` and plot the corresponding distributions over `Fperf`. To compute the desired outgoing message we then average these samples, giving the result shown in Figure 3.14b. This represents an approximation to the marginalization over `Fskill`, and would become exact if we considered an infinite number of samples instead of just three.

The sampling approximation becomes more accurate as we increase the number of samples, as shown in Figure 3.14c and Figure 3.14d. In this final figure the resulting distribution looks almost Gaussian. This is not a coincidence, and in fact the calculation of the outgoing message can be worked out exactly (see Equation (2.115) in Bishop [2006]) with the result that the outgoing message is also a Gaussian whose mean is the mean of the distribution of `Fskill` and whose variance is the sum of the variances of `Fskill` and `Fperf`: $5^2 + 5^2$. This process of 'smearing' out one Gaussian using the other Gaussian is an example of a mathematical operation called **convolution**. Message (4) is just a copy of message (3) as there is only one incoming message to the `Fperf` node. These messages are illustrated in Figure 3.15.

Message (5) in Figure 3.12 is just the Bernoulli distribution with its probability mass concentrated on the value `true`. To compute message (6) we take the *GreaterThan* factor, multiply by the two incoming messages, and then sum over `Jwins` and integrate over `Fperf`. Since we are considering the case where

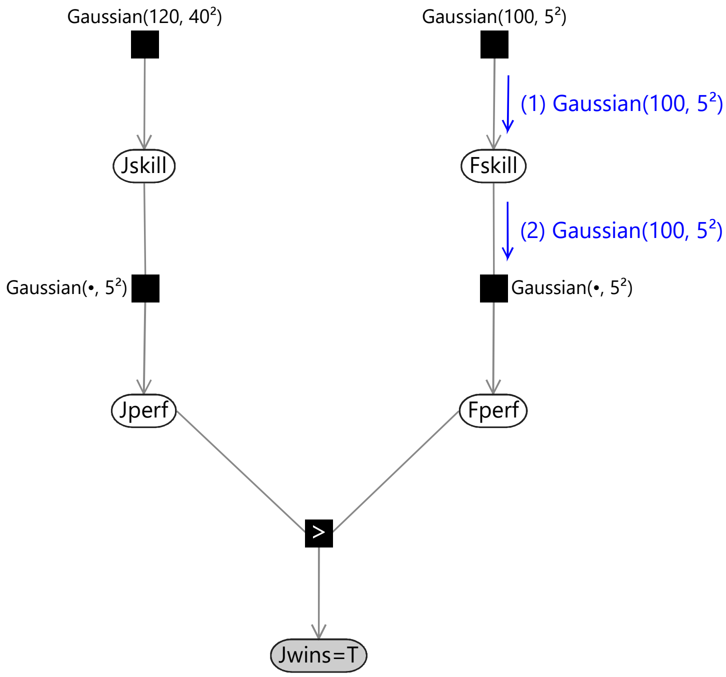
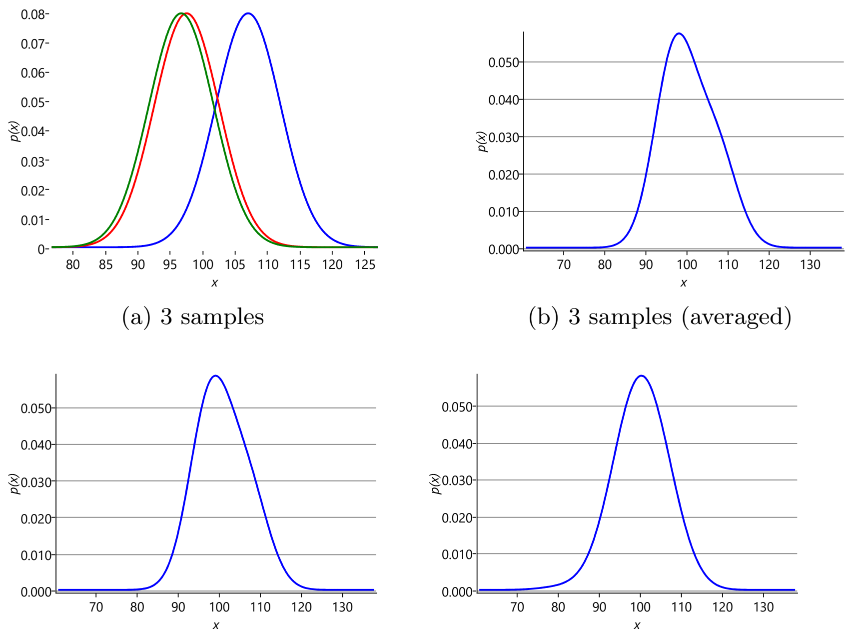


Figure 3.13: Messages (1) and (2) in the application of belief propagation to the evaluation of the updated distribution for `Jskill`.

Jill is the winner, message (5) evaluates to zero for `Jwins` = `false` and one for `Jwins` = `true`. The sum over `Jwins` then multiplies by zero those regions of the performance space which correspond to Fred being the winner. This is illustrated in Figure 3.16 which shows the result of multiplying the *GreaterThan* factor by the two incoming messages and then summing over `Jwins`.

Finally we have to integrate over `Fperf` in order to generate the outgoing message (6) which itself is a function of `Jperf`. This message is shown in Figure 3.17. The reader should take a moment to confirm that shape of this function is what would be expected from integrating Figure 3.16 over the variable `Fperf`. Mathematically, for each value of `Jperf` a truncated Gaussian distribution is being integrated, this is equivalent to the evaluation of the cumulative Gaussian that we introduced back in equation (3.10), and so this message can be evaluated analytically (indeed, this is how Figure 3.17 was plotted).

We can also understand this message intuitively. Suppose we knew that `Fperf` was exactly 100, given that Jill won, this tells us that Jill's performance `Jperf` must be some number greater than 100. This would mean a message in the form of a step, with the value zero below 100 and some positive constant above it. Since, we don't know that `Fperf` is exactly 100, but only know that it is likely to be near 100, this smears out the step into the smooth function of Figure 3.17.



(a) 3 samples

(b) 3 samples (averaged)

(c) 6 samples (averaged)

(d) 100 samples (averaged)

Figure 3.14: Illustration of the sampling approximation to the computation of message (3) in Figure 3.12. Panel (a) shows three Gaussians whose means have themselves been sampled from $Gaussian(100, 5^2)$, while panel (b) shows the average of these three samples. As we increase the number of samples, so the average gets progressively closer to being Gaussian, as seen in panels (c) and (d).

Message (7) is just a copy of message (6) since there is only one incoming message to the `Jperf` node. These messages are illustrated in Figure 3.18 Message (8) is found by multiplying the Gaussian factor describing the performance variability by the incoming message (7) and then integrating over `Jperf`. This again is a convolution, and has an exact solution again in the form of a cumulative Gaussian. Effectively it is a blurred version of the incoming cumulative Gaussian message which has been smeared out by the variance of the Gaussian performance factor. Finally, message (9) is the prior Gaussian distribution given by the skill factor itself. These messages are summarized in Figure 3.19.

To obtain the marginal distribution of `Jskill` we then multiply messages (8) and (9). Because this is the product of a Gaussian and a cumulative Gaussian the result is a bump-like distribution but it is not symmetrical and therefore is not a Gaussian. These messages, and the resulting marginal distribution for `Jskill`, are shown in Figure 3.20.

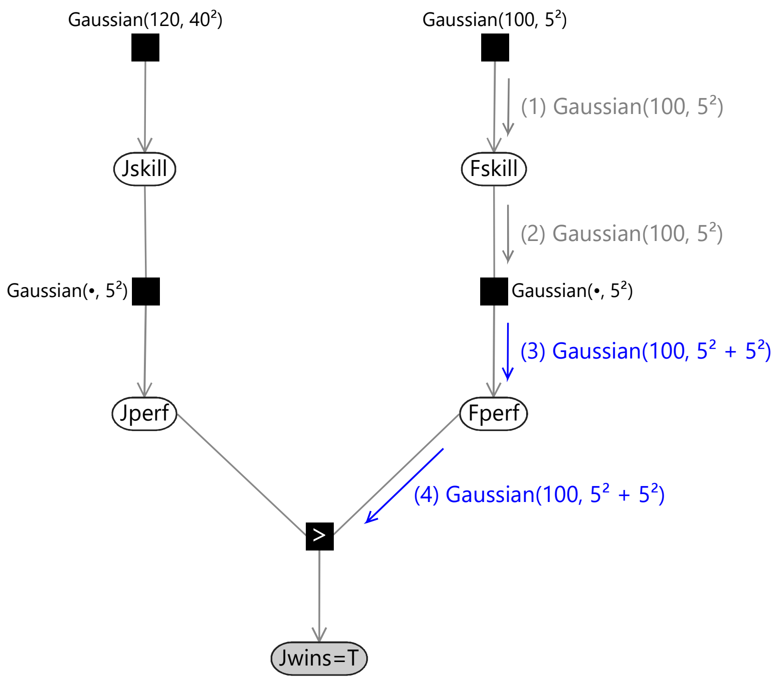


Figure 3.15: Messages (3) and (4) in the application of belief propagation to the evaluation of the updated distribution for `Jskill`.

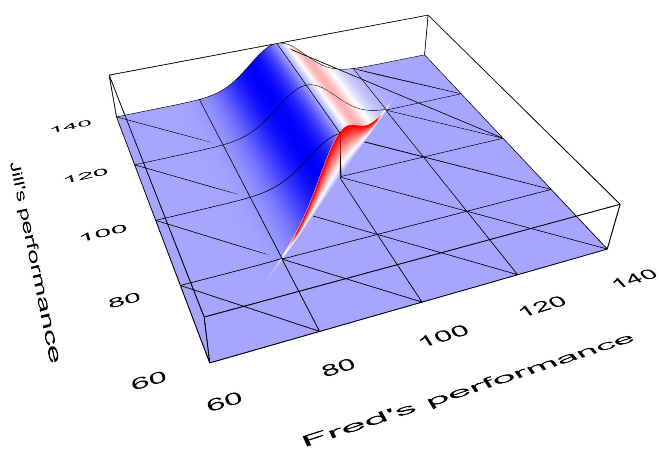


Figure 3.16: Plot of the result of multiplying the *GreaterThan* factor by messages (4) and (5) and then summing over message (5). Note that this plot represents an un-normalized distribution, and so no vertical scale has been shown.

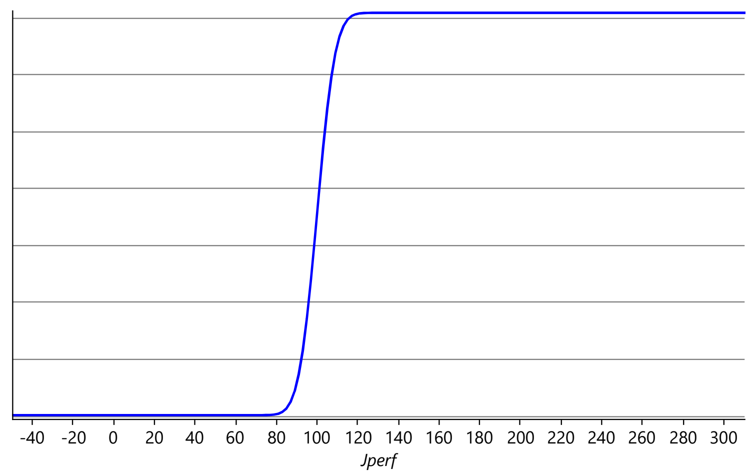


Figure 3.17: The exact Belief Propagation message (6) from the *GreaterThan* factor to the `Jperf` variable, which is given by a cumulative Gaussian.

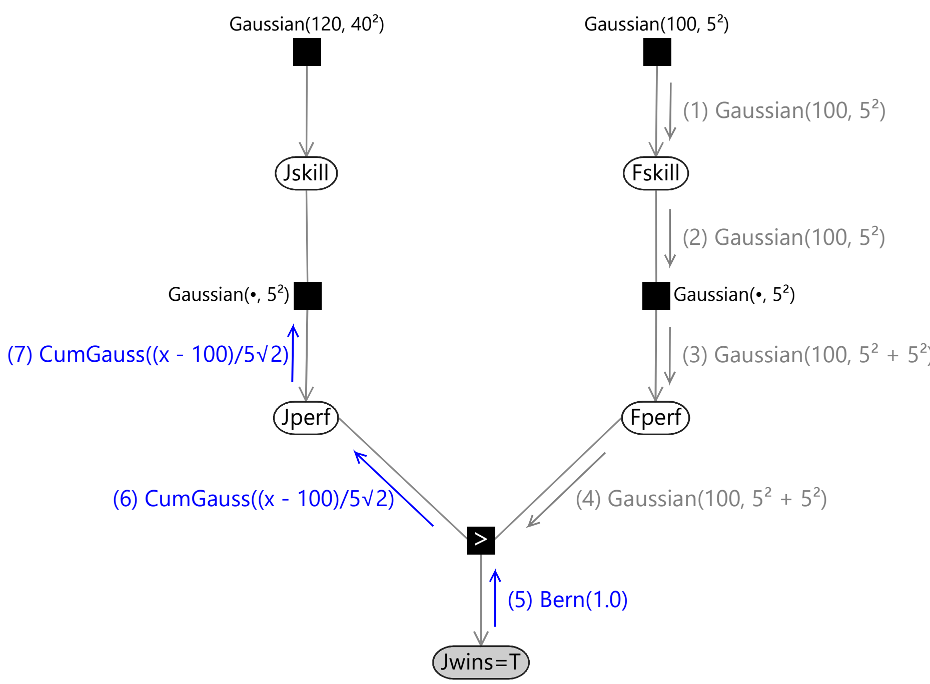


Figure 3.18: Messages (5), (6), and (7) in the application of belief propagation to the evaluation of the updated distribution for `Jskill`.

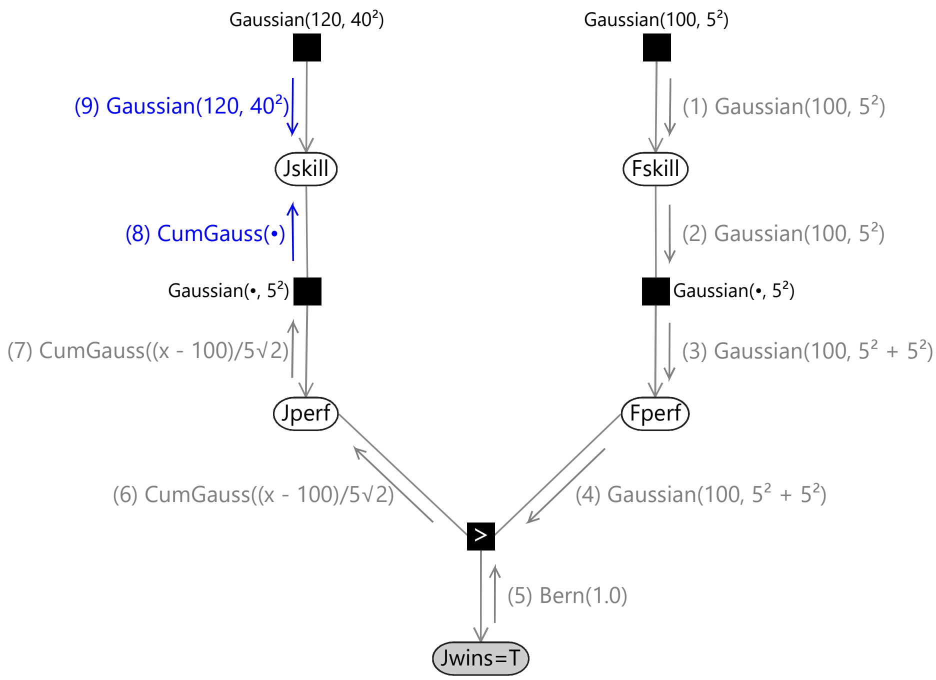


Figure 3.19: Messages (8) and (9) in the application of belief propagation to the evaluation of the updated distribution for `Jskill`.

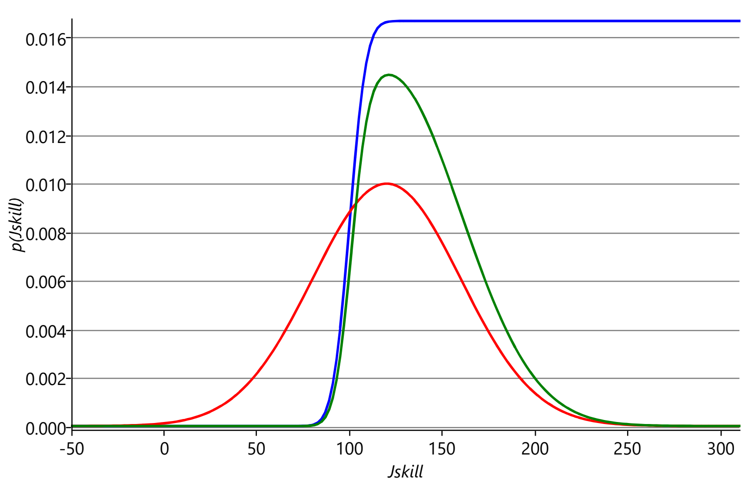


Figure 3.20: Plot of the exact message (8) in blue, the exact message (9) in red. Also shown in green is the product of these two messages, which gives the exact marginal over `Jskill`. Note that this exact marginal is non-Gaussian.

3.2.3 A problem with using exact inference

We seem to have solved the problem of finding the posterior distribution for `Jskill`. Clearly, we can also pass messages in the opposite direction around the graph to obtain the corresponding posterior distribution for `Fskill`. These posterior distributions can be expressed exactly as the product of a Gaussian and a cumulative Gaussian. However, there is a major problem which becomes apparent if we imagine, say, Jill going on to play another game with a new player. Before the game with Fred, our uncertainty in the value of `Jskill` was expressed as a Gaussian distribution, which has two parameters (the mean and the variance). After she has played against Fred the corresponding posterior distribution is expressed as the product of a Gaussian and a cumulative Gaussian and therefore has four parameters, where the two additional parameters come from the cumulative Gaussian. Now suppose that Jill plays another game of Halo against Alice. We can again represent this by a factor graph similar to Figure 3.10, except that the factor describing our current uncertainty in `Jskill` is now the posterior distribution resulting from the game against Fred. When we run inference in this new graph, to take account of the outcome of the game against Alice, the new posterior marginal will be given by the product of messages into the node `Jskill` and will therefore consist of the original product of a Gaussian and a cumulative Gaussian times another cumulative Gaussian resulting from the game with Alice. This gives a posterior distribution for `Jskill` which now has six parameters. Each time Jill plays a game of Halo the distribution over her skill value requires two additional parameters to represent it, and the number of parameters continues to grow as she plays more and more games. Clearly this is not a practical framework to use in an engineering application.

Notice that this problem would not arise if the posterior distribution for the variable of interest had the same form as the prior distribution. In some probabilistic models we are able to choose a form of prior distribution, known as a **conjugate** prior, such that the posterior ends up having the same form as the prior. For example, suppose we have a model containing a random variable `x` for the probability-of-true parameter of a Bernoulli distribution. The conjugate prior for `x` is then the beta distribution, as explained in more detail in Panel 3.3. In our TrueSkill model, the presence of the *GreaterThan* factor, means that the Gaussian is not a conjugate distribution for `Jskill`. We must therefore introduce some form of approximation. In the next section, we will describe a powerful algorithm that extends belief propagation by allowing messages to be approximated even when they are not conjugate. This algorithm will not only solve the inference problem with this model, but turns out to be applicable to a wide variety of other probabilistic models as well.

Self assessment 3.2

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

Panel 3.3 – Conjugate Distribution Example

We can illustrate the idea of a conjugate distribution by considering the following example. Suppose we are selling items through a web page and we want to know the probability that a user will click on the 'buy' button. Let us denote this probability by x. The probability that they won't click is then $1-x$. Note that this is just the Bernoulli distribution that we saw in chapter 1. Suppose we collect data from multiple visitors to our web page, and we find that N of them click on the button and M of them do not. If we assume that the visits to the web page are independent, then the conditional probability of seeing this data, given the value of x, is obtained by multiplying the probabilities of each click/non-click event, so that

$$P(\texttt{data}|x) = x^N(1-x)^M. \tag{3.14}$$

If we wish to learn the value of x from this data, we need to define a prior probability density $p(x)$. There is a particular form for this prior which makes the calculation especially easy, namely if we choose $p(x)$ to have the form

$$p(x) \propto x^A(1-x)^B \tag{3.15}$$

where A and B are parameters. In this case the corresponding posterior distribution is then, from Bayes' rule,

$$\begin{aligned} p(x|\texttt{data}) &\propto P(\texttt{data}|x)p(x) \\ &\propto x^{A+N}(1-x)^{B+M} \end{aligned} \tag{3.16}$$

and so the posterior distribution has the same functional form as the prior distribution, but with A replaced by $A+N$ and B replaced by $B+M$. The prior distribution (3.15) is said to be *conjugate* to the Bernoulli distribution. In fact, you can see that this is exactly the beta distribution that we introduced in section 2.6.

There are many other examples of conjugate distributions [Bishop, 2006]. For instance, the conjugate prior for the mean of a Gaussian is just another Gaussian, while the conjugate prior for the precision of a Gaussian is called a Gamma distribution, which we will meet in chapter 4. For the simple murder mystery of chapter 1 the prior distribution was a Bernoulli, which is conjugate to the conditional distribution representing the probability of the murder weapon given the identity of the murderer.

When running inference on a factor graph, we can think of conjugacy as a local property between pairs of nodes. To prevent message complexity from growing, we will need to find an approximation to an outgoing message whenever we have a non-conjugate relationship between a parent distribution and the corresponding child distribution.

1. Reproduce Figure 3.14 by plotting the average of K Gaussian distributions each with standard deviation is 5 and with mean is given by a sample from a $Gaussian(100, 5^2)$. Do this for $K = 3$,$K = 6$ and $K = 100$.

2. Referring to Panel 3.3, use Bayes' theorem to compute the posterior distribution over x (the probability of clicking on the buy button) given that $N = 20$ people do click on the button but $M = 100$ people do not click on it. Assume a $Beta(1, 1)$ prior distribution. Notice that this is a conjugate prior and so the posterior distribution is also a beta distribution.

3. *[Advanced]* Show that the convolution of two Gaussian distributions is also a Gaussian distribution whose variance is the sum of the variances of the two original distributions. Section 2.3.3 in Bishop [2006] should help.

Review of concepts introduced in this section

convolution The convolution of a function f with a function g measures the overlap between f and a version of g which is translated by an amount a. It is expressed as a function of a.

conjugate For a given likelihood function, a prior distribution is said to be conjugate if the corresponding posterior distribution has the same functional form as the prior.

3.3 A solution: expectation propagation

INFERENCE

Inference deep-dive
In this optional section, we introduce the approximate inference technique of expectation propagation, which we will use extensively in this book. If you want to focus on modelling, feel free to skip this section.

We have seen that belief propagation allows us to calculate the exact marginal posterior distribution for the variable `Jskill` in the model described by Figure 3.10. Whereas the prior distribution for `Jskill` is a Gaussian described by two parameters, the posterior distribution requires four parameters and is non-Gaussian. To solve the problem of the proliferation of parameters we now need a way to approximate this true posterior by a distribution having a fixed number of parameters, and for this we choose the Gaussian. The posterior distribution will then have the same functional form as the prior, mimicking the behaviour of a conjugate prior. If we can achieve this, we will be able to treat the resulting approximate posterior distribution as the prior distribution for the next game. Then the skill for each player will at all times be represented by a Gaussian distribution governed by just two parameters.

The first question is how to approximate a non-Gaussian distribution by a Gaussian. A simple solution is to find the mean and the variance of the non-Gaussian distribution and then to choose as our approximation a Gaussian having the same mean and variance. This turns out to be a sensible approximation, which can be derived formally by optimizing a measure of the dissimilarity of two probability distributions [Bishop, 2006; Minka, 2005].

We might be tempted then just to approximate the exact posterior distribution for `Jskill` by a Gaussian. Although this will work satisfactorily for the factor graph of Figure 3.10 it will break down again as we go to more complex factor graphs (such as those we will encounter later in this chapter). Messages with simple functional forms tend to become more complex as a result of passing through factors. As we extend our model to larger and more sophisticated graphs we quickly arrive at situations where messages cannot be evaluated exactly. Such problems can be avoided by making our approximations *locally* at each factor node, so that all messages have the desired distribution type. This ensures that factors can be composed together into arbitrary graphs, as long as each factor is capable of sending approximate messages to all neighbouring variable nodes using the appropriate types of distribution. Returning to Figure 3.12 (which is reproduced in Figure 3.21 for convenience), we see that message (6) was the first message that we encountered which was non-Gaussian. Our goal is therefore to approximate message (6) by a Gaussian, thereby ensuring that all subsequent messages will also be Gaussian distributions.

While this seems like a desirable goal, there also seems to be a significant obstacle – the exact form of message (6) as seen in Figure 3.17 does not look at all Gaussian! In fact, its mean and variance are not even well defined (they are both infinite). The key to finding a sensible Gaussian approximation is to notice that the approximate version of message (6) will subsequently be passed through the graph as modified forms of messages (7) and (8) and will

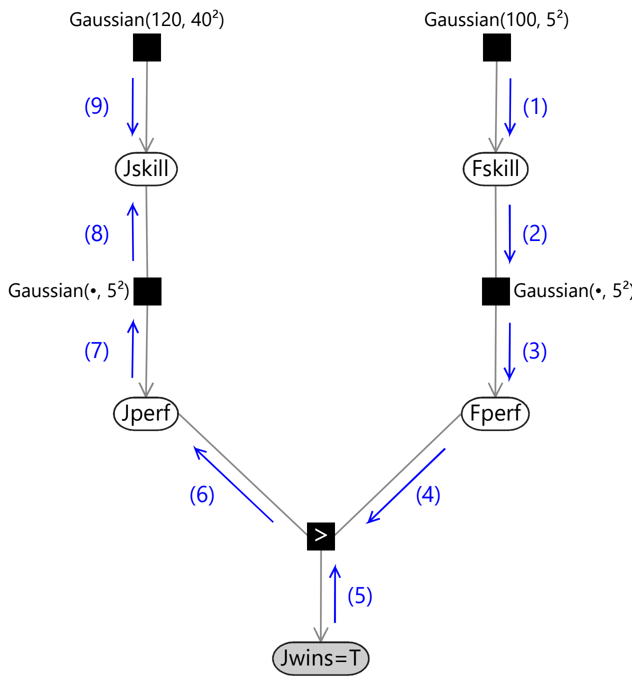


Figure 3.21: The messages which arise in the application of belief propagation to the evaluation of the updated distribution for `Jskill`. (Reproduced from Figure 3.12.)

then be multiplied by the downward message (9) in order to determine the (approximate) posterior distribution of `Jskill`. Our goal will therefore be to make the Gaussian approximation to message (6) over `Jperf` be most accurate in those regions which are considered more probable by the information coming from other parts of the graph. As we have just discussed, however, we need to keep our approximation local to the region of the graph where the message is generated. Message (6) is sent to the node `Jperf` and so we can choose our approximation so as to maximize the accuracy of the marginal distribution of `Jperf`. This is obtained by multiplying message (6) by the downward message on the same edge in the graph, which can be evaluated as shown in Figure 3.22. Note that these same messages are needed to find the posterior marginal for `Fskill`, so there is no additional overhead introduced by evaluating them.

Let's consider the piece of the factor graph close to the `Jperf` node in more detail, as seen in Figure 3.23. Here e denotes the exact message (6) as seen previous in Figure 3.20, c denotes the downward 'context' message, and g denotes our desired Gaussian approximation to message e. These messages are all just functions of the variable `Jperf`. We have already seen that we cannot simply approximate message e by a Gaussian since message e has infinite mean and variance. Instead we make a Gaussian approximation for the marginal distribu-

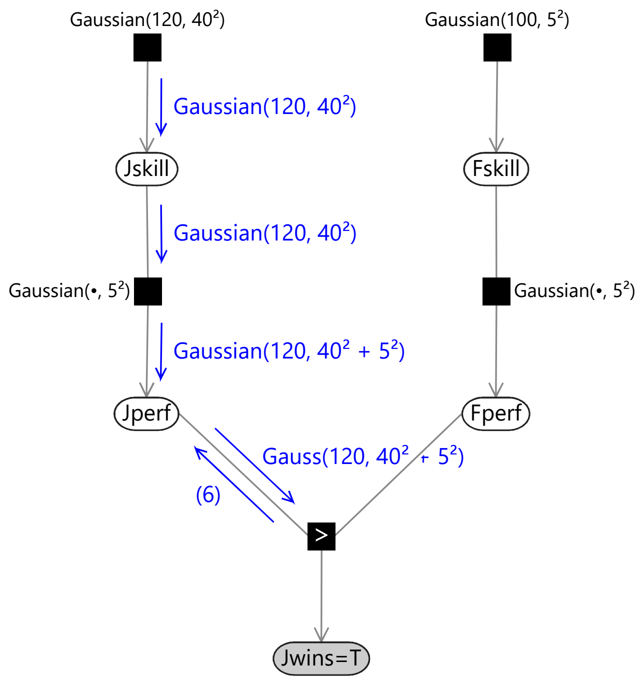


Figure 3.22: Evaluation of the context message that will be used to find a Gaussian approximation for message (6).

tion of `Jperf`. The exact marginal is given by the product of incoming messages ce. We therefore define our approximate message g to be such that the product of the messages c and g gives a marginal distribution for `Jperf` which is a best Gaussian approximation to the true marginal, so that

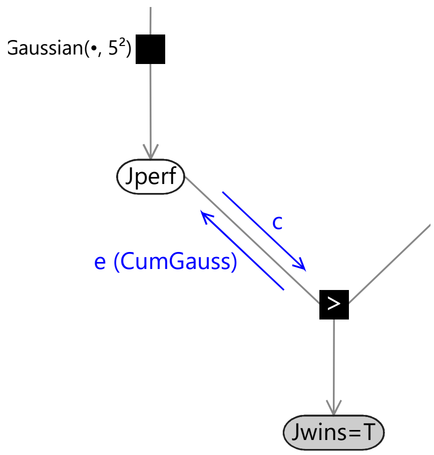
$$cg = \mathrm{Proj}\,(ce)\,. \tag{3.17}$$

Here Proj() denotes 'projection' and represents the process of replacing a non-Gaussian distribution with a Gaussian having the same mean and variance. This can be viewed as projecting the exact message onto the 'nearest' message within the family of Gaussian distributions. Dividing both sides by c we then obtain

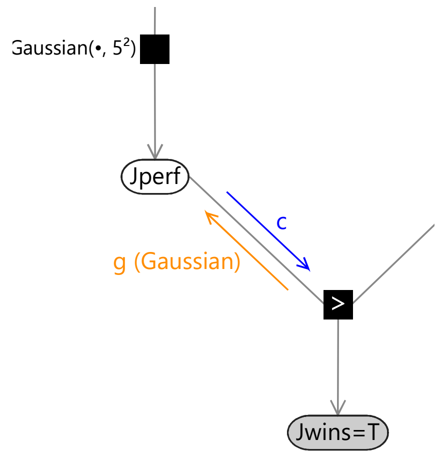
$$g = \frac{\mathrm{Proj}\,(ce)}{c}. \tag{3.18}$$

Details of the mathematics of how to do this are discussed in Herbrich et al. [2007] and Moser [2010].

We therefore find a Gaussian approximation g to the exact e message (6) as follows. First we compute the exact outgoing message (6) as before. This is shown in blue in Figure 3.24. Then we multiply this by the incoming message context message c which is shown in red in Figure 3.24. This gives a distribution, shown in green in Figure 3.24 which is non-Gaussian but which is localised



(a)



(b)

Figure 3.23: Detail of the factor graph around the `Jperf` node, showing the messages involved (a) when running belief propagation (b) when making a local Gaussian approximation to the upward message from the *GreaterThan* factor.

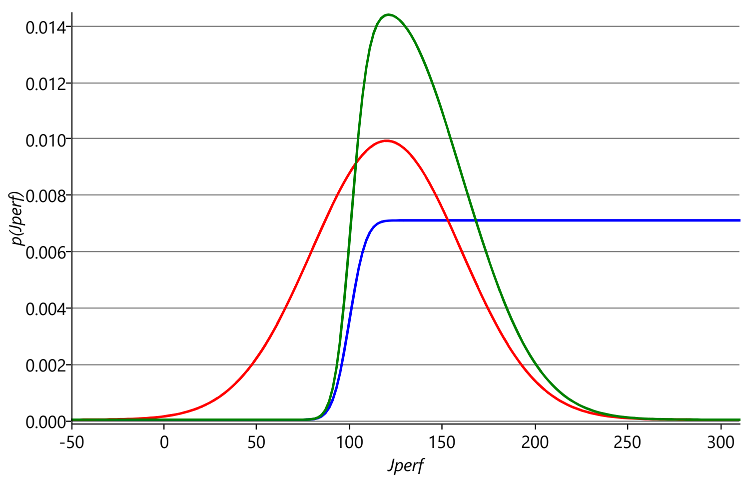


Figure 3.24: Plot of the exact outgoing message (6) in blue, the incoming Gaussian context message in red, and the product of these two messages in green.

and therefore has finite mean and variance and so can be approximated by a Gaussian. This curve is repeated in Figure 3.25 which also shows the Gaussian distribution which has the same mean and variance. Finally, we divide this Gaussian distribution by the incoming context message c to generate our approximate outgoing g message. Because both of these functions are Gaussian, and because the ratio of two Gaussians is itself a Gaussian [Bishop, 2006], the

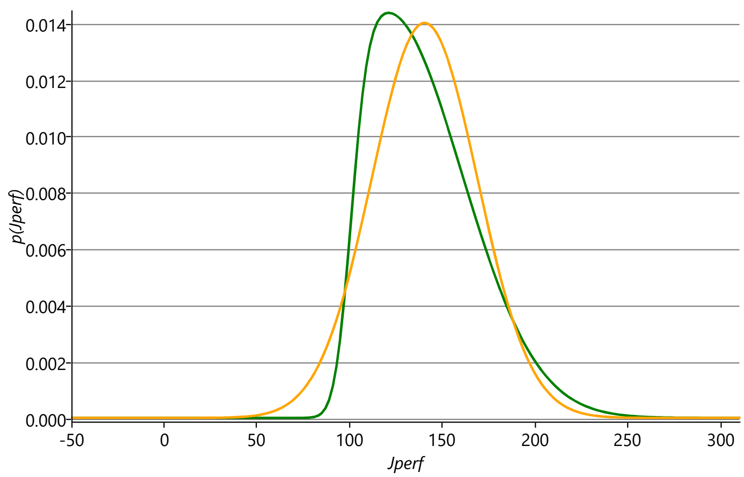


Figure 3.25: The product, shown in green, of the true belief propagation and incoming context messages as in Figure 3.24, together with the Gaussian approximation, shown in orange.

resulting outgoing message will be Gaussian, which was our original goal. For our specific example, this message is a Gaussian with mean 160.4 and standard deviation 40.2. The computation of the approximate message is summarised in Figure 3.26.

We see that overall we multiplied by the incoming context message, then made the Gaussian approximation, then finally divided out the context message again. The evidence provided by the incoming message is therefore used only to determine the region over which the Gaussian approximation should be accurate, but is not directly incorporated into the approximated message. If we happened to have a conjugate distribution, then the projection operation would be unnecessary and the context message would have no effect.

This approach of using an incoming message to provide the context in which to approximate the corresponding outgoing message is known as **expectation propagation** (or EP). We see that the approximation is being made locally at the factor node, and in a way that is independent of the structure of the remainder of the graph. This technique can therefore be applied, without modification, to arbitrarily structured graphs as long as each factor is consistently sending and receiving messages with the required distribution types, in this case Gaussians. The expectation propagation algorithm is summarised in algorithm 3.1.

Now that we have found a suitable Gaussian approximation to the outgoing message (6) we can continue to pass messages along the graph to give the corresponding approximate message (7) as shown in Figure 3.27.

Evaluation of the new (approximate) version of message (8) again involves the convolution of a Gaussian with a Gaussian, with the result shown in Figure 3.28. The downward message (9) is unchanged, and so we can finally compute the Gaussian approximation to the posterior distribution of `Jskill` as the

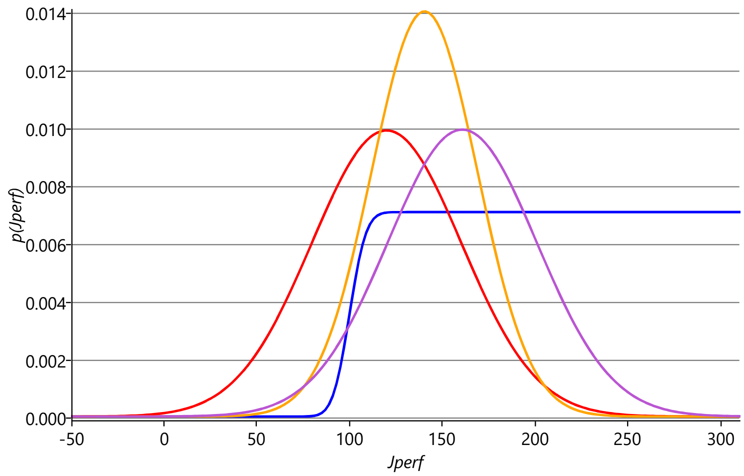


Figure 3.26: The steps involved in computing the Gaussian approximation to message (6). The blue curve shows the exact message (6), the red curve shows the incoming Gaussian context message, the orange curve shows the Gaussian approximation to the product of true message and context message, and the purple curve shows the result of dividing the orange curve by the red context message. This purple curve represents the outgoing Gaussian approximation for message (6).

product of two Gaussians, which gives the final result of a Gaussian with mean 140.1 and standard deviation 28.5.

3.3.1 Applying expectation propagation

Let's see what happens to the skill distributions when we apply expectation propagation to our game of Halo between Jill and Fred. First we suppose that Jill is the winner of the game. In Figure 3.29 we see the prior and posterior distributions of skill for Jill and Fred. Because Jill is the winner, the mean of the skill distribution for Jill increases, while the mean of the skill distribution for Fred decreases. The increase in mean is quite large for Jill, whereas the mean for Fred hardly decreases at all. This difference is due to the greater certainty in `Fskill` compared to that for `Jskill`. Intuitatively we are using the known skill of Fred to estimate the skill of Jill. This is a crucial difference compared to Elo, where the changes in skill estimates are equal and opposite for the two players. This difference arises because we are modelling the uncertainty in each player's skill rather than using a point estimate as in Elo. We also see from Figure 3.29 that the standard deviation for Jill's skill distributions decreases as a result of this game. This is because we have learned something about her skill and therefore the degree of uncertainty is reduced.

Alternatively, if Fred were to have won the game, we have the results shown

Algorithm 3.1: Expectation Propagation

Input: factor graph, list of target variables to compute marginals for, message-passing schedule, initial message values (optional), **choice of approximating distributions for each edge**.
Output: marginal distributions for target variables.

Initialise all messages to uniform (or initial values, if provided).
repeat
  foreach *edge in the message-passing schedule* **do**
    Send the appropriate message below:
    - Variable node message: the product of all messages received on the other edges;
    - Factor node message: Compute the belief propagation message (see algorithm 2.1). Multiply by the context message (the message coming towards the factor on this edge). Project into the desired distribution type for this edge using moment matching. Divide out the context message.
    - Observed node message: a point mass at the observed value;
  end
until *all messages have converged*
Compute marginal distributions as the product of all incoming messages at each target variable node.

in Figure 3.30, This result is more surprising, since we believed Jill to be the stronger player. Intuitively we would expect the adjustments of the skill distributions therefore to be greater, which is indeed the case. We see that the shift in the means of the distributions is larger than in Figure 3.29. In fact the change in the mean of the distribution of `Jskill` is so large that it is now less than the mean of `Fskill`. Again, the standard deviations of Jill's skill has decreased, reflecting a reduction in uncertainty due to the incorporation of new evidence.

Because the skill updates in TrueSkill model depend on the variance of the skill distribution, TrueSkill is able to make relatively large changes to the distributions of new players. Furthermore, this happens automatically as a consequence of running inference in our model. By contrast, the updates in Elo are governed by the update parameter K. In practice, this problem is addressed in Elo by altering the value of the update parameter K according to the number of games played. For instance, FIDE (the World Chess Federation) uses $K = 30$ for new players (this was increased from the previous value of 25 in July 2011 to accelerate the rating changes for early players). Once a player has played 30 games, this switches to $K = 15$ as long as their rating remains below 2,400, and becomes $K = 10$ once players have achieved a rating of 2,400. By tracking uncertainty in a model-based approach, we can avoid the need for such ad-hoc parameter changes.

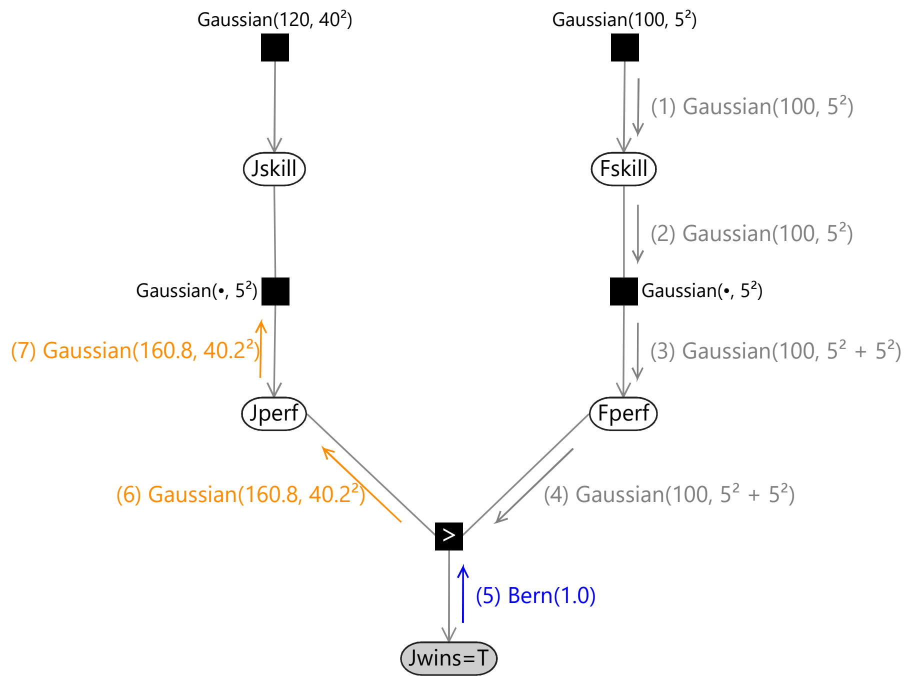


Figure 3.27: Messages (5), (6), and (7) in the application of expectation propagation to the evaluation of the updated distribution for `Jskill`. Note that messages (6) and (7), which are highlighted in orange, differ from the exact messages in Figure 3.18.

3.3.2 Multiple games

So far in this section we have developed a probabilistic model for a single game of Halo between Jill and Fred. In practice we will have a large pool of players, and individual games will take place between pairs of players from within that pool. When we try to assess the skill of a player we potentially have available the results of all the games ever played by that player against a range of different opponents. We might also have available the results of all the games played by those opponents, many of which might involve yet other players, and so on. In principle, all of this information is relevant and could help us to assess the original player's skill. Furthermore, every time there is a new game outcome we could include this additional information and update the skill of the player even if they themselves haven't played any new games. This new information could be relevant even if it involves a game between other players since it could influence the assessment of their skills, and hence the relative skill of our player.

We could in principle handle this by constructing a very large factor graph expressing all of the games played so far. Each player would have a single variable representing their skill value, but multiple variables (one for each game they have played) representing their performances on each of the games. This

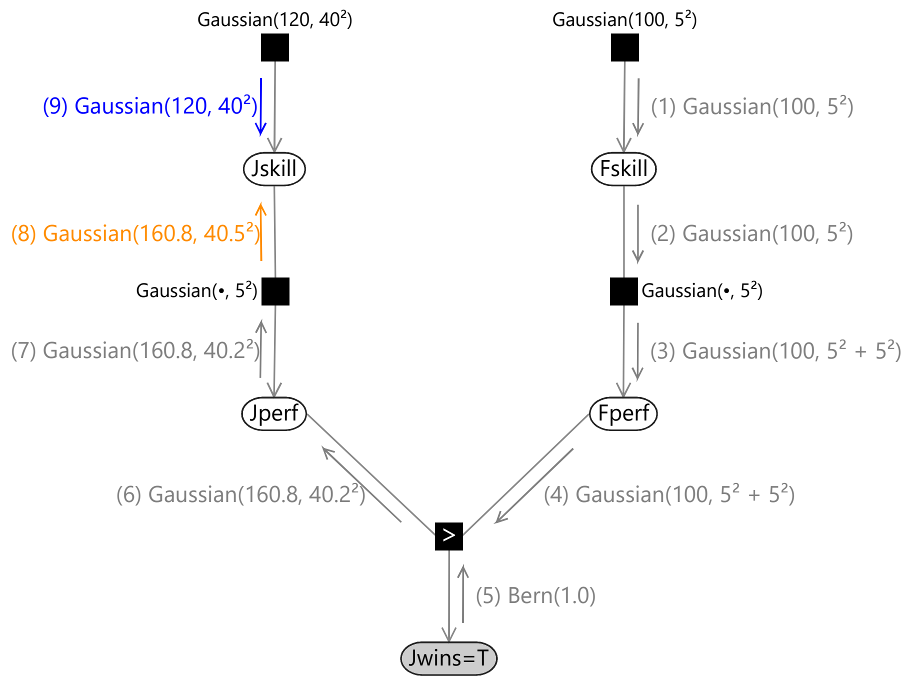


Figure 3.28: Messages (8) and (9) in the application of expectation propagation to the evaluation of the updated distribution for `Jskill`. Note that in addition to messages (6) and (7), message (8) (in orange) also differs from the exact message from Figure 3.19.

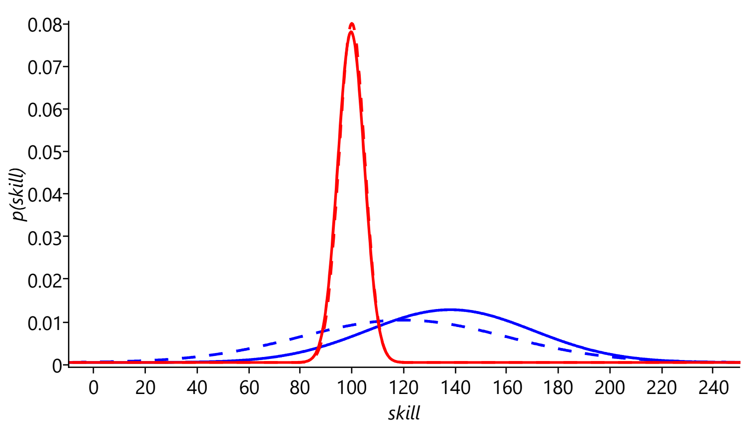


Figure 3.29: The result of applying the TrueSkill model for a game between Jill (blue) and Fred (red) for the case where Jill is the winner. The prior distributions are shown as dashed curves, and the corresponding posterior distributions are shown as solid curves.

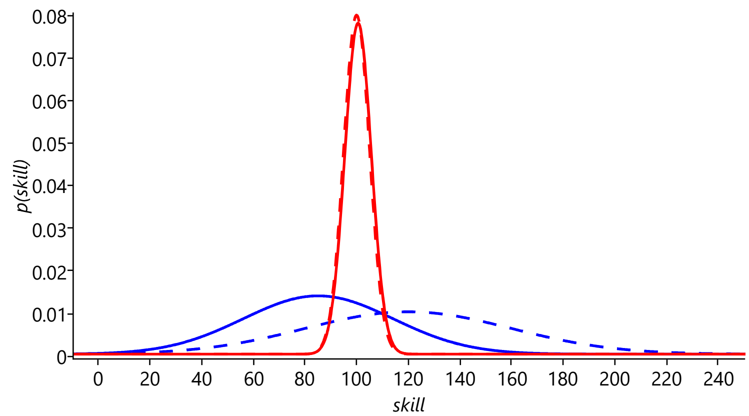


Figure 3.30: As in Figure 3.29 but for the case where Fred is the winner. The prior distributions (dashed lines) are the same as before.

would be a complex graph with multiple loops, and we could run loopy belief propagation, using the expectation propagation approximation, to keep the messages within the Gaussian family of distributions, until a suitable convergence criterion is satisfied. This would give a posterior skill distribution for each of the players, which takes account of all of the games played. If a new game is then played we would start again with a new, larger factor graph and re-run inference in order to obtain the new posterior distributions of every player.

In practice, an approach which takes account of all previous game outcomes in order to update the skills of all the players would be completely infeasible. Instead we can use an approximate inference approach known as **online learning** (sometimes called *filtering*) in which each player's skill distribution gets updated only when a game outcome is obtained which involves that player. We therefore need only store the mean and variance of the Gaussian skill distribution for each player. When a player plays a new game, we run inference using this current Gaussian skill distribution as the prior, and the resulting posterior distribution is then stored and forms the prior for the next game. Each single game is therefore described by a graph of the form shown in Figure 3.10.

This particular form of online inference algorithm, based on local projection onto the Gaussian distribution in which each data point (i.e. game outcome) is used only once, is also known as *Gaussian Density Filtering* Maybeck [1982]; Opper [1998]. It can be viewed as a special case of expectation propagation in which a specific choice is made for the message-passing schedule: namely that messages are only passed forwards in time from older games to newer games, but never in the reverse direction.

It is worth noting that, if we consider the full factor graph describing all games played so far, then the order in which those games had been played would have been irrelevant. When doing online learning, however, the ordering becomes significant and can influence the assessed skills. We have to live with this, however, as only online learning would be feasible in a practical system.

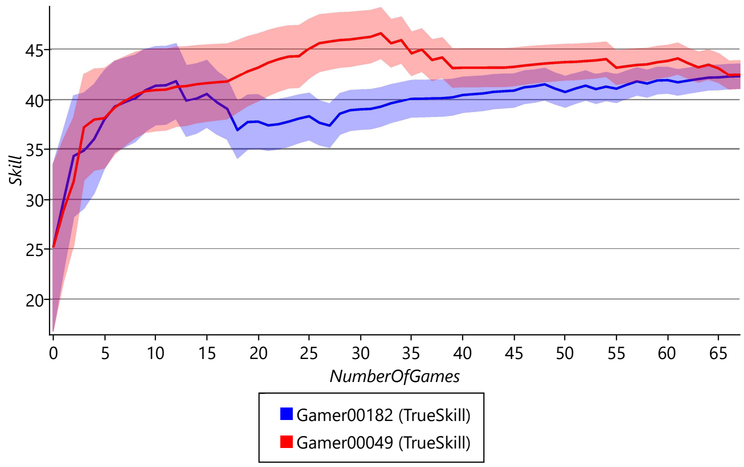


Figure 3.31: Trajectories of skill distributions of two of the top players in the Halo2 head-to-head dataset, showing the mean and the one-standard-deviation envelopes. The horizontal axis shows the number of games played by the corresponding player.

We can illustrate the behaviour of online learning in our model using data taken from the game *Halo 2* on Xbox Live. We use a data set involving 1,650 players which contains the outcomes of 5,915 games. Each game is a head-to-head contest in which a pair of players play against each other. Figure 3.31 shows how the skill distributions for two of the top players varies as a function of the number of game outcomes played by each of the two players. We see that the initial skill distributions are the same, because all player skills have the same prior distribution before any games are played. As an increasing number of games are played, we see that the standard deviation of the skill distributions decreases. This reduction in uncertainty as a result of observing the outcome of games is the effect we saw earlier in Figure 3.29 and Figure 3.30.

The model we have constructed in this section represents a single game between two players. However, many games on Xbox Live have a more elaborate structure, and so we turn next to a number of model extensions which allow for these additional complexities.

Self assessment 3.3

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Reproduce Figure 3.24 by evaluating the (red) Gaussian context message and the (blue) exact CumGauss message at `Jperf` values of -50, -49 . . . 0,1,2 . . . 299,300. Plot the two lines you get with `Jperf` on the x axis and the evaluated messages on the y axis. You will need to rescale the CumGauss message to get it to fit (remember that the scale of this message

does not matter since it is an improper distribution). To get the (green) product message corresponding to the exact marginal for `Jperf`, first multiply your two messages together at each `Jperf` value. Then rescale the result so that the area under the line is 1 (you can achieve this roughly by rescaling to make the sum of the value at each point equal to 1). Plot this result as a third line on your axes.

2. Compute the mean and standard deviation of the exact marginal product message that you just computed. The mean can be well approximated by summing the product of the message at each point times the `Jperf` value at each point. The variance (which is the square of the standard deviation) can be approximated similarly using the mnemonic "the mean of the square minus the square of the mean" (see Wikipedia). First, you need to compute the "mean of the square" which can be approximated by sum of the product of the message at each point times the *square of* the `Jperf` value at each point. Then subtract off "the square of the mean" which refers to the mean you just computed. This gives the variance, which you can take the square root of to get the standard deviation. You have now computed the mean and standard deviation of the Gaussian approximation to the marginal for `Jperf`. You can check your result against the Gaussian in Figure 3.25.

3. Finally, we need to divide this Gaussian distribution (whose mean and standard deviation you just found in the previous exercise) by the Gaussian context message. You can refer to [Bishop, 2006] for how to do this. You can check your result against message (6) in Figure 3.27. Congratulations! You have now successfully calculated an expectation propagation message!

4. Now we can use Infer.NET to do the expectation propagation calculations for us. Implement the Trueskill model in Infer.NET, setting the skill distributions for Jill and Fred to the ones used in this section (this How to guide might help). Compute the posterior marginal distributions for Jill and Fred for the two outcomes where Jill wins the game and where Fred wins the game. Plot your results and check them against Figure 3.29 and Figure 3.30.

Review of concepts introduced in this section

expectation propagation An approximate message-passing algorithm that extends belief propagation by allowing messages to be approximated by the closest distribution in a particular family, such as a Gaussian distribution. This approximation is done either to ensure that the inference algorithm remains tractable or to speed up the inference process. See algorithm 3.1.

online learning An approach to machine learning in which data points are considered one at a time, with model parameter distributions updated after each data point.

3.4 Extensions to the core model

So far, we have constructed a probabilistic model of a game played between two players which results in a win for one of the players. To handle the variety of games needed by Xbox Live, we need to extend our model to deal with a number of additional complexities. In particular, real games can end in draws, can involve more than two players, and can be played between teams of people. We will now show how our initial model can be extended to take account of these complexities. This flexibility nicely illustrates the power of a model-based approach to machine learning.

The original Xbox online gaming service used the Elo algorithm to estimate the skills of players. However, in spite of its popularity, the Elo system suffers from some significant limitations. In particular:

- Elo does not handle draws
- Elo does not handle team games
- Elo does not handle games with more than two players

Various modifications to the basic Elo system, mostly heuristic in nature, have been proposed to deal with the issues of draws, team games, and multiple players. A draw, for example, can be represented as a score of 1/2 in computing the skill updates. The fundamental problem is that, since Elo is an algorithm rather than a model, it is difficult to see what assumptions are being made by making changes to the algorithm. Without understanding the assumptions underlying the each change it is hard to predict how well the resulting algorithm will work – and, more importantly, extremely hard to diagnose problems with the algorithm when they arise. A model-based approach allows such extensions to be incorporated in a transparent way, giving rise to a solution which can handle all of the above complexities – whilst remaining both understandable and maintainable.

3.4.1 What if a game can end in a draw?

In our current model, the player with the higher performance value on a particular game is the winner of that game. For games which can also end in a draw, we can modify this assumption by introducing the concept of a *draw margin*, such that a player is the winner only if their performance exceeds that of the other player by at least the value of the draw margin. Mathematically this can be expressed as

$$\begin{array}{rll} \text{if} & \texttt{Jperf} > \texttt{Fperf} + \texttt{drawMargin} & \text{Jill wins} \\ \text{else if} & \texttt{Fperf} > \texttt{Jperf} + \texttt{drawMargin} & \text{Fred wins} \\ \text{else} & & \text{game drawn.} \end{array} \tag{3.19}$$

This is illustrated in Figure 3.32.

We have therefore modified Assumption 3 to read:

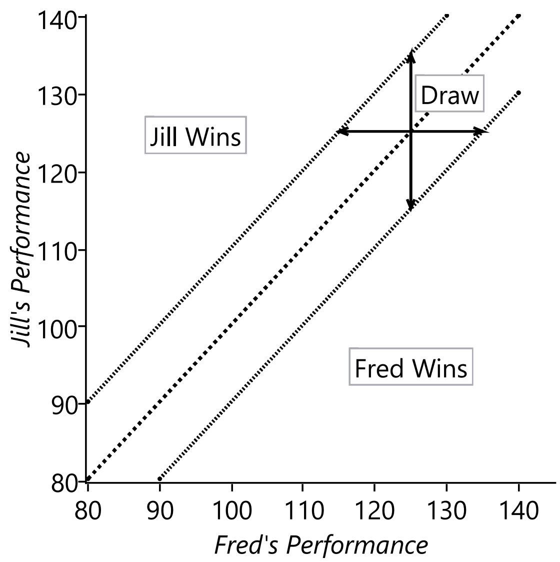


Figure 3.32: Schematic illustration of the regions in performance space where Jill is the winner, where Fred is the winner, and where the game ends in a draw.

③ The player with the higher performance value wins the game, unless the difference between their performance and that of their opponent is less than the draw margin, in which case the game is drawn.

The value of the draw margin represents a new parameter in our model, and we may not know the appropriate value. This is particularly true if we introduce a new type of game, or if we modify the rules for an existing game, where we have yet to see any game results. To solve this problem we simply treat the draw margin as a new random variable `drawMargin` whose value is to be learned from data. Because `drawMargin` is a continuous variable, it is chosen to be a Gaussian. This can be expressed as a factor graph, as shown in Figure 3.33. The variable `Jwins` is replaced by `outcome` which is a discrete variable that takes one of the values `JillWins`, `Draw`, or `FredWins`. The *WinLoseDraw* factor is simply a function whose value is 1 if the three values of `Jperf`, `drawMargin`, and `Fperf` are consistent with the value of `outcome` and is 0 otherwise. We need to make some modifications to the evaluation of messages sent out from this factor. These will not be discussed in detail here, and instead the interested reader can refer to this excellent blog post and Herbrich et al. [2007].

In order to simplify the subsequent discussion of other extensions to the core model, we will ignore the draw modification in the remaining factor graphs in this chapter, although all subsequent models can be similarly modified to include draws if required.

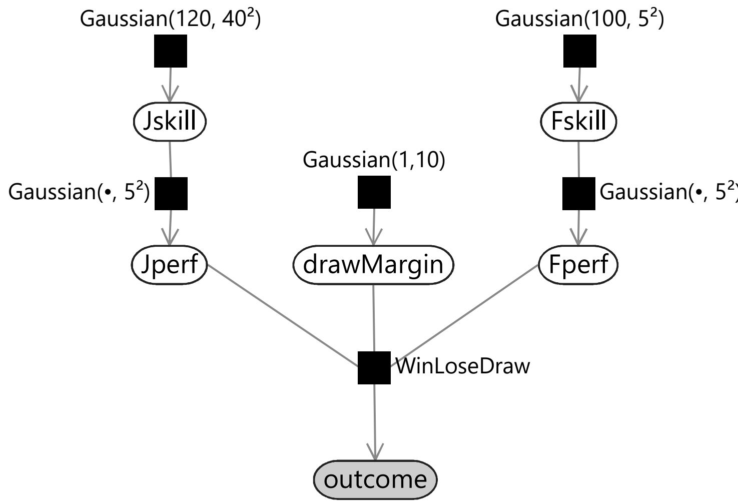


Figure 3.33: TrueSkill model for a game between two players which includes the possibility of a draw.

3.4.2 What if we have more than two players in a game?

Suppose we now have more than two players in a game, such as in the Halo game 'Free for All' in which eight players simultaneously play against each other. The outcome of such a game is now an ordering amongst the players involved in the game. With our model-based approach, incorporating a change such as this involves just making a suitable assumption, constructing the corresponding factor graph and then running our inference algorithm. Our new Assumption 3 can be stated as

3. The order of players in the game outcome is the same as the ordering of their performance values in that game.

Games with more than two players require a more complex model

If there are N players in the game then this assumption can be captured in a factor graph using $N-1$ *GreaterThan* factors to describe the player ordering. This is illustrated for the case of three players in Figure 3.34. Note that we could have introduced a separate 'greater-than' factor for each possible pair of players. For N players there are $N(N-1)/2$ such factors. However, these additional

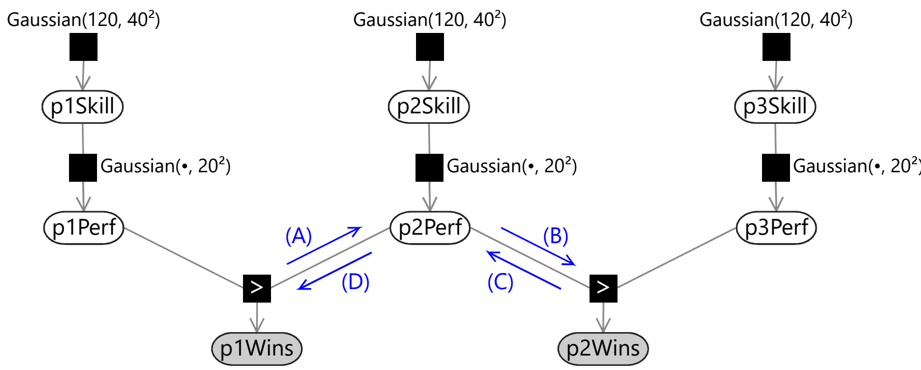


Figure 3.34: Factor graph for a game involving three players. Also shown are some of the messages which arise in the use of expectation propagation applied to this graph.

factors contain only redundant information and lead to an unnecessarily complex graph. The ordering of N players can be expressed using $N-1$ greater than factors, provided these are chosen to connect the pairs of adjacent players in the ordering sequence. In effect, because we know the outcome of the game, we can choose a relatively simple graph which captures this.

INFERENCE

Inference deep-dive
In this optional section, we show why the use of expectation propagation, even for a tree-structured graph, can require iterative solution. If you want to focus on modelling, feel free to skip this section. The extension to more than two players introduces an interesting effect related to our expectation propagation algorithm. We saw in subsection 2.2.2 that if our factor graph has a tree structure then belief propagation gives exact marginal distributions after a single sweep through the graph (with one message passed in each direction across every link). Similarly, if we now apply expectation propagation to the two-player graph of Figure 3.10 this again requires only a single pass in each direction. This is because the 'context' messages for the expectation propagation approximation are fixed. However, the situation becomes more complex when we have more than two players. The graph of Figure 3.34 has a tree structure, with no loops, and so exact belief propagation would require only a single pass. However, consider the evaluation of outgoing message (A) using expectation propagation. This requires the incoming message (D) to provide the 'context' for the approximation. However, message (D) depends on message (C) which itself is evaluated using expectation propagation using message (B) as context, and message (B) in turn depends on message (A). Expectation propagation therefore requires that we iterate these messages until we reach some suitable convergence criterion (in which the changes to the messages fall below some threshold). We therefore modify our message-passing schedule so that we first pass messages downwards from the skill nodes to the performance nodes (as before), then we perform multiple passes back and forth amongst the

performance nodes until we achieve convergence, and then finally pass messages upwards to the skill nodes in order to evaluate posterior skill marginals.

Remember that in Figure 3.29 and Figure 3.30 we saw how the shift of the distributions between prior and posterior were larger in the case where the weaker player (Fred) won the game. Now we repeat the experiment, except with a third player (Steve), whose prior skill distribution is $Gaussian(140, 40^2)$ (keeping Jill as $Gaussian(120, 20^2)$ and Fred as $Gaussian(100, 40^2)$ as before), and run the multi-player TrueSkill model on a single game with the outcome Jill 1st, Fred 2nd, Steve 3rd. The results of this are shown in Figure 3.35. Firstly, note that since Steve was expected to be the strongest player, but in fact came last, his posterior mean has moved markedly downwards (to below the other two players). Secondly, note that the changes in the means of Jill and Fred are in the same direction as in Figure 3.29, but are more pronounced than before. This again is because the overall game result is more surprising. In Figure 3.36 we begin with the same priors, but now observe a single game

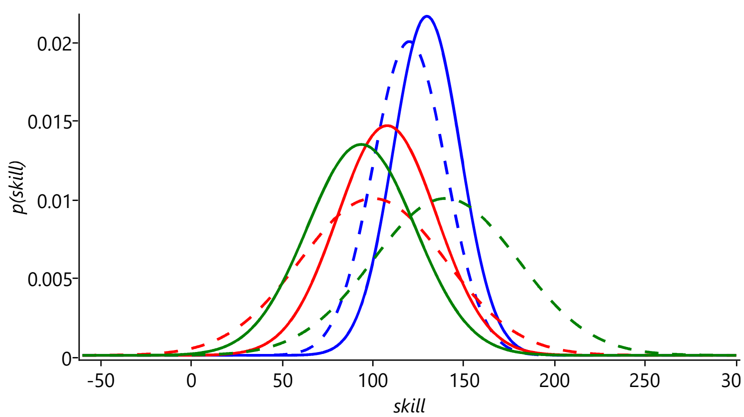


Figure 3.35: The result of applying the TrueSkill model for a three player game between Jill (blue), Fred (red), and Steve (green) for the case where Jill is the winner, Fred comes second and Steve comes last. The prior distributions are shown as dashed curves, and the corresponding posterior distributions are shown as solid curves.

with outcome Jill 2nd, Fred 1st, Steve 3rd. Note that since Fred and Steve's prior skills were equidistant from Jill's, and their prior variances were equal, their posterior means have shifted by the same amount, and so they appear to have "swapped" places. A further consequence of this symmetry is that since Jill neither won nor lost, her skill mean has not moved, although the variance of her skill is reduced due to the new information provided by the game outcome.

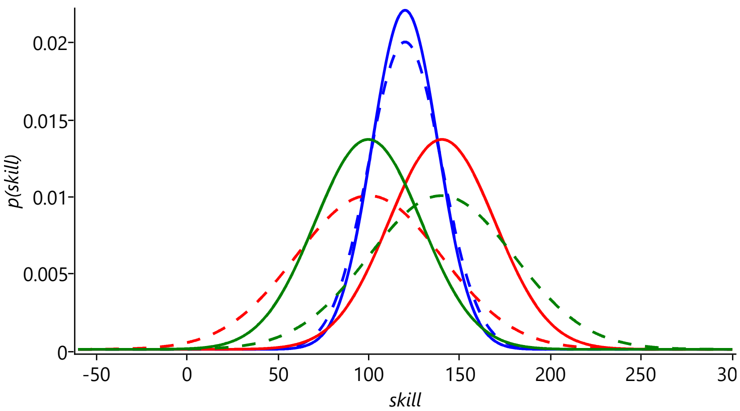


Figure 3.36: As in Figure 3.35 but for the case where Fred is the winner, followed by Jill and then Steve came last.

3.4.3 What if the games are played by teams?

Many of the games available on Xbox Live can be played by teams of players. For example, in Halo, another type of game is played between two teams each consisting of eight players. The outcome of the game simply says which team is the winner and which team is the loser, and the challenge is to use this outcome information to revise the skill distributions for each of the individual players. This is an example of a **credit assignment problem** in which we have to work out how the credit for a victory (or blame for a defeat) should be attributed to individual players when only the outcome for the overall team is given. The solution is similar to the last two situations: we make an assumption about how the individual player skills combine to affect the game outcome, we construct a probabilistic model which encodes this assumption and then run inference to update the skill distributions. There is no need to invent new algorithms or design new heuristics.

Here is one suitable assumption which we could use when modelling team games, which would replace Assumption 3:

3 The performance of a team is the sum of the performances of its members, and the team with the highest performance value wins the game.

We can now build a factor graph corresponding to this assumption. For example, consider a game between two teams, each of which involves two

The performance of a team depends on the skills of the individual players.

players. The factor graph for this is shown in Figure 3.37.

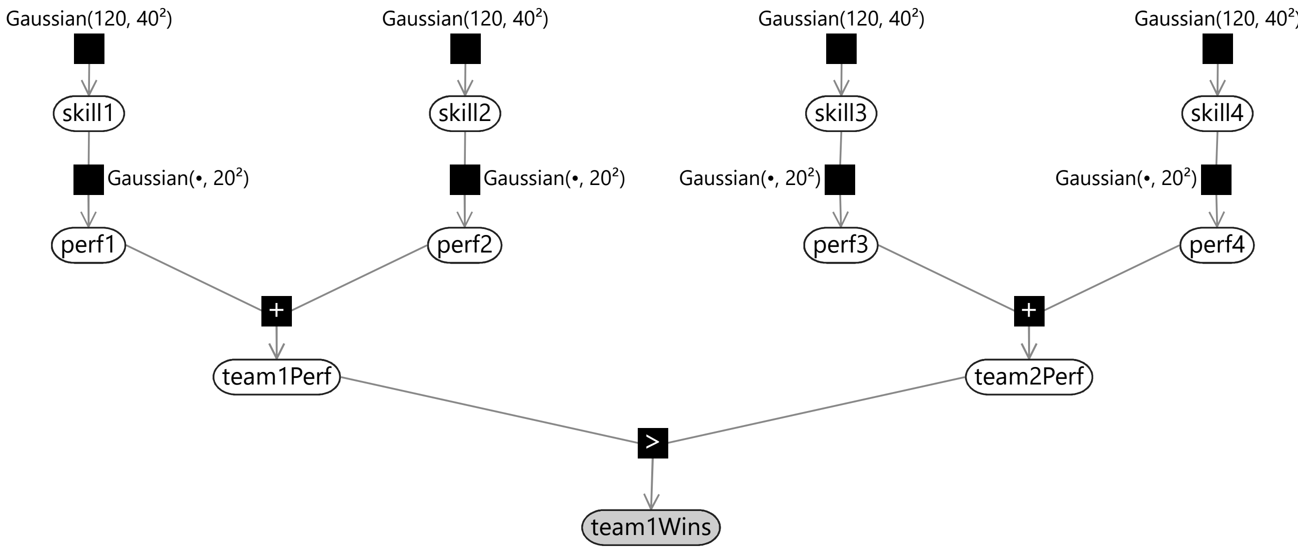


Figure 3.37: A factor graph of the TrueSkill model for two teams. The first team consists of players 1 and 2, and the second team consists of players 3 and 4.

The performance of a team is determined by the performance of the players who comprise that team. Our assumption above was that the team performance is given by the sum of the performances of the individual players. This might be appropriate for collaborative team games such as Halo. However, other assumptions might be appropriate in other kinds of game. For example, in a race where only the fastest player determines the team outcome, we might make the alternative assumption

③ The performance of a team is equal to the highest performance of any of its members, and the team with the highest performance value wins the game.

In this section we have discussed various modifications to the core TrueSkill model, namely the inclusion of draws, the extension to multiple players, and the extension to team games. These modifications can be combined as required, for example to allow a game between multiple teams that includes draws, by constructing the appropriate factor graph and then running expectation propagation. This highlights not only the flexibility of the model-based approach to machine learning, but also the ease with which modifications can be incorporated. As long as the model builder is able to describe the process by which the data is generated, it is usually straightforward to formulate the corresponding model. By contrast, when a solution is expressed only as an algorithm, it may be far from clear how the algorithm should be modified to account for changes in the problem specification. In the next section, we conclude our discussion of the online game matchmaking problem by a further modification to the model in which we relax the assumption that the skills of the players are fixed.

Self assessment 3.4

The following exercises will help embed the concepts you have learned in this section. It may help to refer back to the text or to the concept summary below.

1. Sketch out a factor graph for a model which allows draws, two-player teams and multiple teams. You will need to combine the factor graphs of Figure 3.33, Figure 3.34 and Figure 3.37. Your sketch can be quite rough – for example, you should name factors (e.g. "Gaussian") but there is no need to provide any numbers for factor parameters.

2. Extend your Infer.NET model from the previous self assessment to have three players and reproduce the results from Figure 3.35 and Figure 3.36.

3. *[Project idea]* There is a wide variety of sports results data available on the web. Find a suitable set of data and build an appropriate model to infer the skills of the teams or players involved. Rank the teams or players by the inferred skill and decide if you think the model has inferred a good ranking. If not, diagnose why not and explore modifications to your model to address the issue.

Review of concepts introduced in this section

credit assignment problem The problem of allocating a reward amongst a set of entities, such as people, all of which have contributed to the outcome.

3.5 Allowing the skills to vary

At this point we seem to have found a comprehensive solution to the problem posed at the start of the chapter. We have a probabilistic model of games between multiple teams of players including draws, in which simpler situations (two players, individuals instead of teams, games without draws) arise as special cases. However, when this system was deployed for real beta testers, it was found that its matchmaking was not always satisfactory. In particular, the skill values for some players seemed to 'get stuck' at low values, even as the players played and improved a lot, leading to poor matchmaking.

To understand the reason for this we note that the assumptions encoded in our model do not allow for the possibility that the skill of a player could change over time. In particular, Assumption 1 says that "each player has a skill value" – in other words, each player has a single skill value with no mention of this skill value being allowed to change. Since players' skills do change over time, this assumption will not apply to real data. For example, as a player gains experience in playing a particular type of game, we might anticipate that their skill will improve. Conversely, an experienced player's skill might deteriorate if they play infrequently and get out of practice.

You may think that our online learning process updates our skill distribution for a player over time and so would allow the skill to change. This is a common misconception about online learning, but it is not true. Our current model assumes that the skill of a player is a *fixed*, but unknown, quantity. Online learning does not represent the modelling of an evolving skill value, but rather an updating of the uncertainty in this unknown fixed-across-time skill.

Skill increases with practice.

3.5.1 Reproducing the problem

To deal with players having changing skills, we will need to change the model. But first, we need to reproduce the problem, so that we can check later that we have fixed it. To do this we can create a synthetic data set. In this data set, we synthesise results of games involving a pool of one hundred players. The first player, Elliot, has an initial skill fixed at 110, and this skill value is increased in steps as shown by the red line in Figure 3.38. The remaining 99 players have fixed skill values which are drawn from a Gaussian with mean 125 and standard deviation 10. For each game, two players are selected at random and their performances on this game are evaluated by adding Gaussian noise to their skill values with standard deviation 5. This just corresponds to running ancestral sampling on the model in Figure 3.6 (just like we did to create a synthetic data set in subsection 2.5.1).

Given this synthetic data set, we can then run online learning using the model in Figure 3.10 in which the game outcomes are known and the skills are

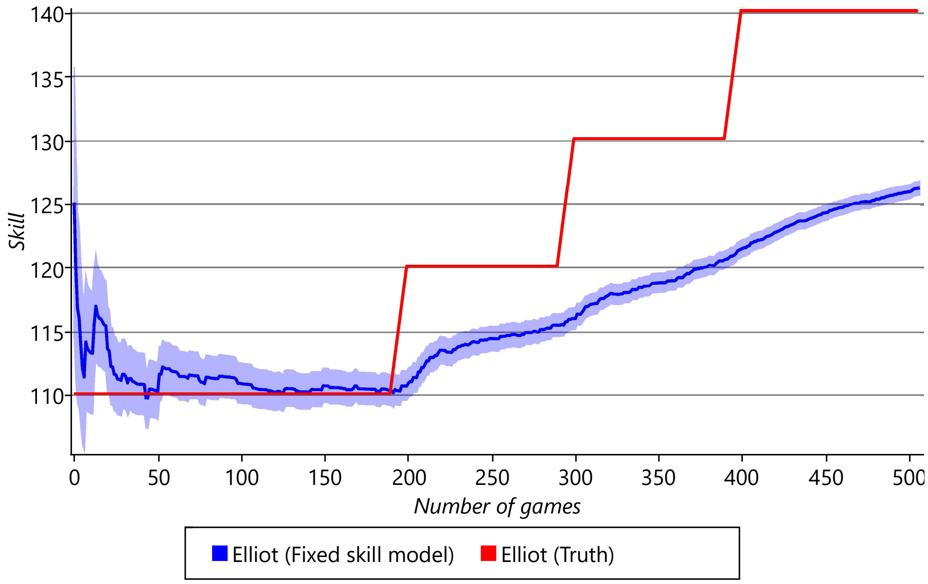


Figure 3.38: The red curve shows the skill value for player Elliot in a synthetic data set drawn from a pool of 100 players. All other players have fixed skills (not shown). The blue line shows the mean of the inferred Gaussian skill distribution for Elliot under our model, which assumes that Elliot's skill is fixed. The blue shaded region shows the plus/minus one-standard-deviation region around the mean of this distribution.

unknown. Figure 3.38 shows the inferred skill distribution for Elliot under this model. We see that our model cannot account for the changes in Elliot's skill: the estimated skill mean does not match the trajectory of the true skill, and the variances of the estimates are wildly overconfident. Due to the small variance, the update to the skill mean is small, and so the evolution of the skill mean is too slow. This is unsurprising as a key assumption of the model, namely that the skill of each player is constant, is incorrect.

To address this problem, we need to change the incorrect assumption in our model. Rather than assuming a fixed skill, we need to allow for the skill to change by a typically small amount from game to game. We can therefore replace Assumption 1 with:

1. Each player has a skill value, represented by a continuous variable, given by their skill value in their previous game plus some change in skill which has a zero-mean bell-shaped distribution.

Whereas previously a player had a single skill variable, there is now a separate skill variable for each game. We assume that the skill value for a particular player in a specific game is given by the skill value from the previous game involving that player with the addition of some change in value having, on

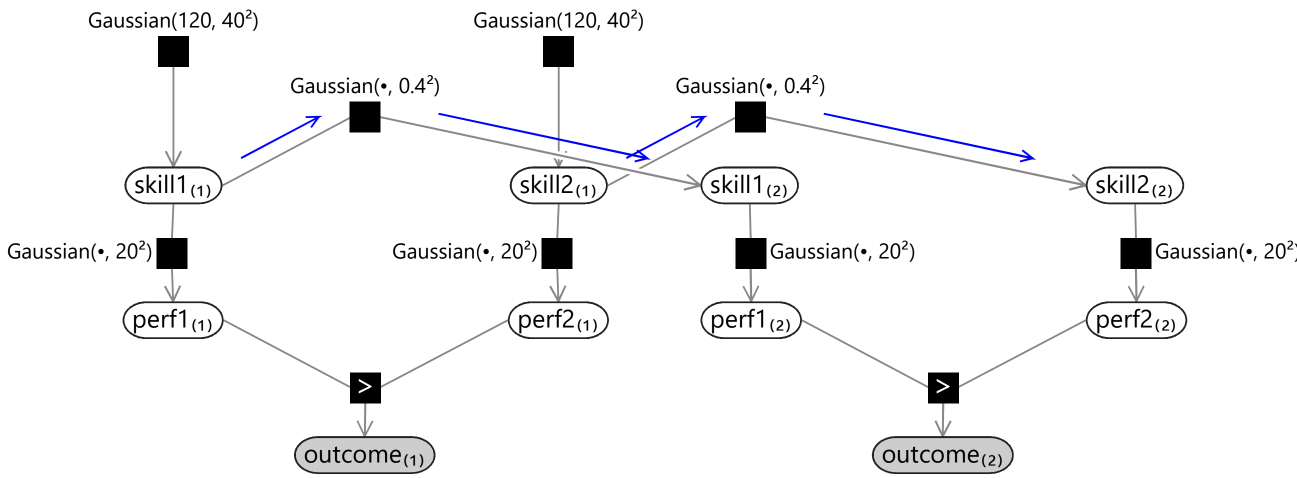


Figure 3.39: A factor graph for two players and two successive games in which the skill values are allowed to change from one game to the next.

average, the value of zero. Again, we make this assumption mathematically precise by choosing this distribution to be a zero-mean Gaussian. If we denote the skill of player in their previous game by $\texttt{skill}^{(\text{old})}$ and their skill in the current game by $\texttt{skill}^{(\text{new})}$, then we are assuming that

$$\texttt{skill}^{(\text{new})} = \texttt{skill}^{(\text{old})} + \texttt{skillChange} \tag{3.20}$$

where

$$p(\texttt{skillChange}) = \mathit{Gaussian}(0, \texttt{SkillChangeVariance}). \tag{3.21}$$

From these two equations it follows that [Bishop, 2006]

$$p\left(\texttt{skill}^{(\text{new})}\right) = \mathit{Gaussian}\left(\texttt{skill}^{(\text{old})}, \texttt{SkillChangeVariance}\right). \tag{3.22}$$

This allows us to express our new assumption in the form of a factor graph. For example, in the case of two players who play two successive games against each other, the factor graph would be given by Figure 3.39. The prior distribution for skill of player 1 in the second game, denoted $\texttt{skill1}_{(2)}$, is given by a Gaussian distribution whose mean, instead of being fixed, is now given by the skill of that player in the previous game, denoted by $\texttt{skill1}_{(1)}$.

Inference in this model, using the online learning approximation, can be done as follows. We run our inference algorithm, based on expectation propagation, for the first game using a graph of the form shown in Figure 3.10, to give posterior Gaussian skill distributions for each of the players. Then we send messages through the Gaussian factors connecting the two games, as indicated in blue in Figure 3.39. The incoming messages to these factors are the skill distributions coming from the first game. The subsequent outgoing messages to the new skill variables are, because of the convolution computed for the Gaussian factor, broadened versions of these skill distributions. These are then used as the prior skill distribution for this new game. Because we are broadening the prior in the new game, we are essentially saying that we know less about the skill of the player. This in turn means the new game outcome will lead to a greater change in skill and so we will be better at tracking changes in skill. It may seem strange that we can improve the behaviour of our system by *increasing* the uncertainty in our skill variable, but this arises because we have modified the model to correspond more closely to reality. In the time since the last game, the player's skill may indeed have changed and we are now correctly modelling this possibility.

We can now test out this modified model on our synthetic data set. We use a `SkillChangeVariance` of 0.16 which encodes our belief that the change in skill from one game to the next should be small. The results are shown by the green curve in Figure 3.40.

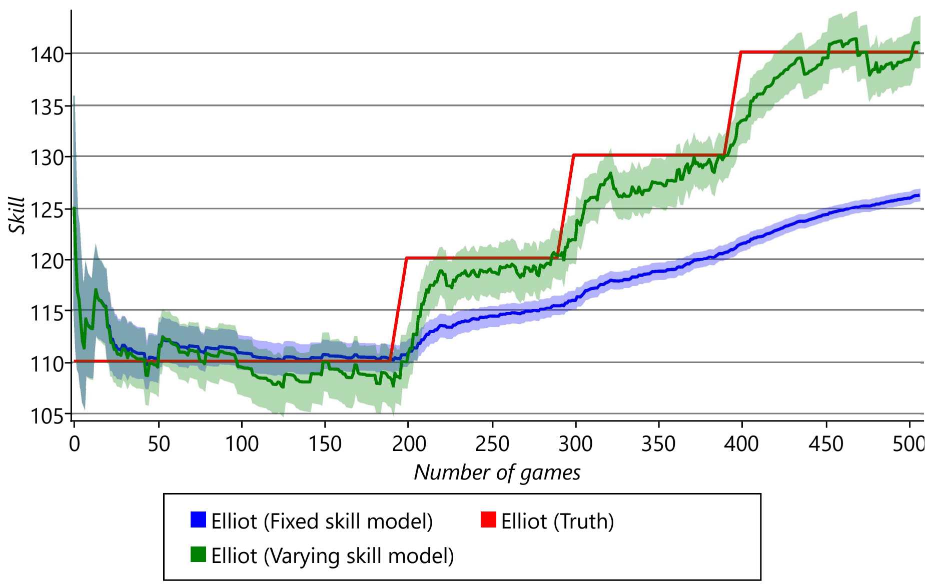


Figure 3.40: This shows the same information as in Figure 3.38 with the addition in green of the distribution of inferred skill for Elliot using a model in which skill values are allowed to evolve over time.

We see that the changing skill of Elliot is tracked much better when we allow for varying skills in our model – we have solved the problem of tracking time-varying skills!

This particular model, in which we assume a Gaussian-distributed change is added at each stage is known as the *Kalman filter* [Kalman, 1960; Zarchan and Musoff, 2005] and is widely used in signal processing. Note that we do not need to know anything about Kalman filters, or to be familiar with the literature or with the associated algorithms or terminology, in order to use them in our application. We just write down the model corresponding to our assumptions and run online message passing, and this will implement the standard Kalman filtering equations automatically.

Rather than doing online learning in this model, we could instead perform full inference on a large factor graph with multiple games. In this case, we would have messages which pass forward through time and those which pass backwards through time. The first are the (Kalman) filtering equations as before and the second are called the *Kalman smoothing* equations. Again, these arise automatically without requiring any specific knowledge of Kalman filters. This technique has been used to apply the TrueSkill model to the history of chess to work out the relative strengths of different historical chess players, even though they lived decades apart! You can read all about this in Dangauthier et al. [2007].

3.5.2 The final model

Now that we have adapted the model to cope with varying skills, it meets all the requirements of the Xbox Live team. With all extensions combined, here is the full set of assumptions built into our model:

1. Each player has a skill value, represented by a continuous variable, given by their skill value in their previous game plus some change in skill which has a zero-mean bell-shaped distribution.

2. Each player has a performance value for each game, which varies from game to game such that the average value is equal to the skill of that player. The variation in performance, which is the same for all players, is symmetrically distributed around the mean value and is more likely to be close to the mean than to be far from the mean.

3. The performance of a team is given by the sum of the performances of the players within that team.

4. The order of teams in the game outcome is the same as the ordering of their performance values in that game, unless the magnitude of the difference in performance between two teams is below a threshold in which case those teams draw.

Figure 3.41: The four assumptions encoded in our final model.

This model encompasses the variety of different game types which arise including teams and multiple players, it allows for draws and it tracks the evolution of player skills

over time. When this full model was deployed it gave good user feedback during extensive beta testing and so when Xbox 360 launched in November 2005, the online skill rating system was switched from Elo to TrueSkill. Since then, the skill distributions inferred by TrueSkill have been used to perform real-time matchmaking. The role of the model is to infer the skills, while the decision on how to use those skills to perform matchmaking is a separate question. Typically this is done by selecting players for which the game outcome is most uncertain. Note that this also tends to produce matches whose outcomes are the most informative in terms of learning the skills of the players. The matchmaking process must also take account of the need to provide players with opponents within a reasonably short time, and so there is a natural trade-off between how long a player waits for a game to be set up, and the closeness in match to their opponents. One of the powerful aspects of decomposing the matchmaking problem into the two stages of skill inference and matchmaking decision is that changes to the matchmaking criteria are easy to implement and do not require any changes to the more complex modelling and inference code. As discussed in the introduction the ability to match players against others of similar ability, and to do so quickly and accurately, is a key feature of this very successful service.

The inferred skills produced by TrueSkill are also used for a second, distinct purpose which is to construct 'leader boards' showing the ranking of players within a particular type of game. For this purpose, we need to define a single skill value for each player, based on the inferred Gaussian skill distribution. One possibility would be to use the mean of the distribution, but this fails to take account of the uncertainty, and could lead to a player having an artificially high (or low) position on the leader board. Instead, the displayed skill value for a player is taken to be the mean of their distribution minus three times the standard deviation of their distribution. This is a conservative choice and implies that their actual skill is, with high probability, no lower than their displayed skill. Thus a player can make progress up the leader board both by increasing the mean of their distribution (by winning games against other players) and by reducing the uncertainty in their skill (by playing lots of games).

We have seen how TrueSkill continually adapts to track the skill level of individual players. In the next chapter we shall see another example of a model which adapts to individual users, but in the context of a very different kind of application: a model that helps to de-clutter your email inbox.

Chapter 4

Uncluttering Your Inbox

More and more people are becoming overwhelmed by their email. It is not unusual for a busy person to receive many hundreds of new emails every day. As a result, people are having to spend longer processing their emails – and are more likely to miss an important email because it gets lost in a constant stream of new emails. Can model-based machine learning help to reduce this information overload?

The average office worker spends almost three hours a day processing their email. About 90% of this time is spent either reading incoming email or managing existing email – only the remaining 10% is spent writing or replying to emails [Outlook team, 2008]. An automatic tool to speed up reading and managing email would free up a lot of people's time, allowing them to focus on important tasks and avoid the stress of information overload.

Microsoft Exchange is an email server used to power more than 300 million mailboxes worldwide [Radicati and Hoang, 2010]. The Exchange team are keen to use machine learning to help people to manage their mail and improve their productivity. In this chapter, we will look at how model-based machine learning was used by the Exchange team to separate out the clutter from a user's inbox, allowing users to focus on their important emails and reducing the time taken to process incoming email.

The idea was to decide if a user thinks an email was clutter or not, based on the actions the user takes on the email. For example, emails that are never read or quickly deleted are likely to be considered as clutter by the user. Now suppose we had a machine learning system that could predict what actions a user would take on a new email – for example, the system would predict whether a user would reply to an email, delete it or leave it unread. Given such a machine learning system we could then remove from the inbox emails that are unlikely to be read or acted upon. Such clutter emails could then be placed in a separate location where they could be easily reviewed and processed in one go, at a convenient time for the user.

To achieve this goal, the team needed a system that could take a number of older emails that a user had already taken action on and learn which actions the user would be likely to take on emails with different characteristics. The system was to consider many aspects of the email: who sent the email, who was on the To and Cc lines, what the subject was, what was written in the email, whether there were any attachments and so on. The trained system was then to be applied to incoming mails to predict the probability of the user performing various actions on each email. The Exchange team considered it essential that the system make personalised predictions. Unlike junk mail, which emails are clutter is a personal thing: what is clutter for one user might not be clutter for another. For example, a project update email might be clutter for someone not on the project but might be important to read for someone who is working on the project.

In this chapter, we'll use model-based machine learning to develop a personalised system that meets the needs of the Exchange team. We will focus on building a system to predict whether a user will reply to an incoming email. However, the resulting system will be general enough to predict many other kinds of actions and so can be used to predict whether or not a user will consider an email to be clutter. In particular, we will see how to:

- Manage email data and privacy issues,
- Develop a model for predicting actions personalized to each user,
- Use information about an email to drive the model,
- Evaluate the model both in numerical terms and in terms of user experience,
- Extend the model to address various problems as they arise.

4.1 Collecting and managing email data

For the purposes of writing this chapter, we developed a tool for collecting all of a person's email received in a given time period. We then used the tool to collect emails from 10 volunteers who kindly agreed to share their email data (in an anonymised form, as we shall discuss shortly). This was quite a time consuming process and so we need to plan carefully about how we are going to use this precious email data. For example, we need to decide which data we will use to train on and which data we will use to evaluate the system's accuracy. It is *very* important that the data used for training is not used for evaluation. If training data is used for evaluation it can give misleadingly high accuracy results – because it is much easier to make a prediction for an email when you've already been told the correct answer! To avoid this, we need to divide our data into different data sets:

- A **training set** which we will use to train the model.
- A separate **test set** which we will use to assess the prediction accuracy for each user and so indicate what we might expect to achieve for real users.

If you were to evaluate a trained model on its training set, it will tend to give higher accuracy results than on a test set. The amount that the accuracy is higher on the training set indicates how much the model has learned that is specific to the particular data in the training set, rather than to that type of data in general. We say that a model is **overfitting** to the training data, if its accuracy is significantly higher on the training set than on a test set.

If we were only planning to evaluate our system once, these two data sets would be sufficient. However, we expect to make repeated changes to our system, and to evaluate each change to see if it improves prediction accuracy. If we were to evaluate on the test set many times, making only the changes that improve the test set accuracy, we would run the risk of overfitting to the test set. This is because the process of repeatedly making changes that increase the test set accuracy could be picking up on patterns that are specific to the test and training set combined but not to general data of the same type. This overfitting would mean that the accuracy reported on the test set would no longer be representative of what we might expect for real users. To avoid overfitting, we will instead divide our data into three, giving a third data set:

- A **validation set** which we will use to evaluate prediction accuracy during the process of developing the system.

We can evaluate on the validation set as many times as we like to make decisions about which changes to make to our system. Once we have a final system, we will then evaluate once on the test set. If it turns out that the model has been overfitting to the validation set, then the accuracy results on the test set will be lower, indicating that the real user accuracy will be lower than we might have expected from the validation set accuracy numbers.

If the test set accuracy is not yet sufficient, it would then be necessary to make further changes to the system. These can again be assessed on the validation set. At some point, a new candidate system would be ready for test set evaluation. Strictly speaking, a fresh test set should be used at this point. In practice, it is usually okay to evaluate on a test set a small number of times, bearing in mind that the numbers may be slightly optimistic. However, if used too much, a test set can become useless due to the possibility of overfitting, at which point it would then be necessary to gather a fresh test set.

For the email data that we collected, we can divide each user's emails into training, validation and test sets. Since the goal is to make predictions on email arriving in the user's inbox, we exclude emails in the user's Sent Mail and Junk folders from these data sets, since such emails did not arrive in the inbox. We also exclude emails which were automatically moved by a rule, since such emails also did not appear in the inbox. Table 4.1 gives the sizes of the training, validation and test sets for each user, after removing such non-inbox emails.

4.1.1 Learning from confidential data

Table 4.1 highlights another challenge when working with email data – it is highly personal and private data! Email data is an example of **personally identifiable information** (PII), which is information that could be used to identify or learn about a particular person. For an email, personally identifiable information includes the names and email addresses on the email along with the actual words of the subjects and email bodies. Knowing which senders a particular user ignores or replies to, for example, would be very sensitive data.

	Train	Validation	Test	User Total
User35CB8E5	1,995	2,005	657	4,657
UserCE3FDB4	1,067	1,067	356	2,490
User6AACED	1,827	1,822	600	4,249
User7E601F9	531	528	173	1,232
User68251CD	600	602	198	1,400
User223AECA	532	532	179	1,243
UserFF0F29E	2,202	2,199	729	5,130
User25C0488	1,181	1,182	393	2,756
User811E39F	1,574	1,565	513	3,652
User10628A6	485	485	163	1,133
Total	11,994	11,987	3,961	27,942
Average	1278.77778	1278	422	2978.77778

Table 4.1: Number of emails in the training, validation and test sets for each user and overall.

In any system that uses PII, it is essential to ensure that such data is kept confidential.

In a machine learning system, this need for confidentiality appears to conflict with the need to understand the data deeply, monitor the performance of the system, find bugs and make improvements. The main technique used to resolve this conflict is some kind of **anonymisation**, where the data is transformed to remove any PII whilst retaining the underlying patterns that the machine learning system can learn from. For example, names and email addresses can be anonymised by replacing them with arbitrary codes. For this project, we anonymise all user identities using an alphanumeric hash code like 'User35CB8E5', as shown in Table 4.1. This type of anonymisation removes PII (or at least makes it extremely difficult to identify the user involved) but preserves information relevant to making predictions, such as how often the user replies to each person.

In some cases, anonymisation is hard to achieve. For example, if we anonymised the subject and body on a word-by-word basis, this anonymisation could potentially be reversed using a word frequency dictionary. For this reason, we have removed the email bodies and subject lines from the data used for this chapter, so that we can make it available for download while protecting the confidentiality of our volunteers. We will retain the lengths of the subject lines and body text, since they are useful for making predictions but do not break confidentiality. If you wish to experiment with a more complete email data set, there are a few such available, an example of which is the Enron email dataset. Notice that, even in this case, some emails were deleted "as part of a redaction effort due to requests from affected employees", demonstrating again the sensitive nature of email data! For cases like these where anonymisation cannot easily be achieved, there is an exciting new method under development called *homomorphic encryption* which makes it possible to do machine learning on encrypted data without decrypting the data first. This approach is at the research stage only, so is not yet ready for use in a real application (but read more in Panel 4.1 if you are curious).

Using our anonymised and pruned data set means that we can inspect, refine, or debug any part of the system without seeing any confidential information. In some cases, this anonymisation can make it hard to understand the system's behaviour or to debug problems. It is therefore useful to have a small non-anonymised data set to work with in such cases. For this chapter we used a selection of our own emails for this purpose. For a deployed system, you can also ask real users to voluntarily supply a very limited amount of what would normally be confidential information (for example, a single email), in order to debug an issue they are reporting with that email (such as an incorrect prediction).

Now that we have training and validation data sets in a suitably anonymised form, we are ready to start developing our model.

Review of concepts introduced in this section

training set The part of the collected data which will be used for model training.

test set The part of the collected data which will be used to assess a trained model's accuracy. This evaluation should be performed infrequently, ideally only once, to avoid overfitting to the test set.

overfitting The situation where a trained model has learned too much about patterns in the data that are specific to the training set, rather than patterns relating to general data of the same form. If a model is overfitting, its prediction accuracy on data sets other than the training set is reduced.

validation set The part of the collected data which will be used to assess a trained model's accuracy as the model is being developed. Typically the validation set is used repeatedly to decide whether or not to make changes to the model. This runs the risk of overfitting to the validation set, which is why it is important also to have a separate test set.

personally identifiable information Any information about a person which could be used to identify who they are or to learn confidential information about them.

anonymisation A process where data is transformed to remove any personally identifiable information, whilst retaining enough information to be useful. For example, email addresses can be anonymised by replacing them by a randomly generated string, such that the same address is always replaced by the same string. This allows patterns of email use to be identified without associating those patterns with any given sender or recipient.

Panel 4.1 – Homomorphic encryption

Homomorphic encryption is a type of data encryption that allows certain algorithms to run directly on the encrypted data, giving encrypted results, without ever being decrypted! At the moment there are practical restrictions on the kinds of algorithms that can be run on the data – for example, they may be required to consist only of additions or multiplications (and a limited number of these). There is currently also a significant computational cost to running algorithms this way. Despite these limitations, it is possible to run inference algorithms using homomorphic encryption – for example, Graepel et al. [2013] describe a classification algorithm which runs entirely on encrypted data.
Although still at the research stage, homomorphic encryption has great potential for allowing machine learning algorithms to be run on confidential data.

4.2 A model for classification

The problem of predicting a label, such as ‘reply’ or ‘not reply’, for a data item is called **classification**. Systems that perform classification are known as **classifiers**, and are probably the most widely used machine learning algorithms today. There are many different classification algorithms available and, for a particular prediction task, some will work better than others. A common approach to solving a classification problem is to try several different classification algorithms and see which one works the best. This approach ignores the underlying reason that the classification algorithms are making different predictions on the same data: that each algorithm is implicitly making different assumptions about the data. Unfortunately, these assumptions are hidden away inside each algorithm.

You may be surprised to learn that many classification algorithms can be interpreted as doing approximate inference in some probabilistic model. So rather than running a classification algorithm, we can instead build the corresponding model and use an inference algorithm to do classification. Why would we do this instead of using the classification algorithm? Because a model-based approach to classification gives us several benefits:

- The assumptions in the classifier are made explicit. This helps us to understand what the classifier is doing, which can allow us to improve how we use it to achieve better prediction accuracy.

- We can modify the model to improve its accuracy or give it new capabilities, beyond those of the original classifier.

- We can use standard inference algorithms both to train the model and to make predictions with it. This is particularly useful when modifying the model, since the training and prediction algorithms remain in sync with the modified model.

These are not small benefits – in this chapter you will see how all three will be crucial in delivering a successful system. We will show how to construct the model for a widely used classifier from scratch, by making a series of assumptions about how the label arises given a data item. We will then show how to extend this initial classification model, to achieve various capabilities needed by the email classification system. Throughout the evolution of the model we will rely on standard inference algorithms for training and prediction.

Before we start constructing the model, we first need to understand how a classifier with a fixed set of assumptions could possibly be applied to many different problems. This is possible because classifiers require the input data to be transformed into a form which matches the fixed assumptions encoded in the classifier. This transformation is achieved using a set of features (a **feature set**), where a **feature** is a function that acts on a data item to return one or more values, which are usually binary or continuous values. In our case we will use continuous feature values – for example, a feature that returns 1.0 if the user is mentioned on the To line of the email or 0.0 otherwise (we'll call this the *ToLine* feature). It is these feature values, rather than the data item itself, that are fed into the classifier. So, rather than changing the assumptions in the classifier, we can use features to transform the data so that it matches the assumptions already built in to the classifier.

Another important simplification that a classifier makes is that it only ever makes predictions about the label variable assuming that the corresponding values for the features are known. Because it always conditions on these known feature values, the model only needs to represent the conditional probability $P(\text{label}|\text{features})$ rather than the joint distribution $P(\text{label}, \text{features})$. Because it represents a conditional probability, this kind of model is called a **conditional model**. It is convenient to build a conditional model because we do not need to model the data being conditioned on (the feature values) but only the probability of the label given these values. This brings us to our first modelling assumption.

1 The feature values can always be calculated, for any email.

By always, we mean *always*: during training, when doing prediction, for every single email ever encountered by the system. Although convenient, the assumption that the feature values can always be calculated makes it difficult to handle missing data. For example, if the sender of an email is not known, any features requiring the sender cannot be calculated. Strictly, this would mean we would be unable to make a prediction. In practice, people commonly provide a default feature value if the true value is not available, even though this is not the correct thing to do. For example in the sender case it is equivalent to treating all emails with missing senders as if they came from a particular 'unknown' sender. The correct thing to do would be to make a joint model of the feature values and marginalise over any missing values – but, if data is rarely missing, the simpler approach is often sufficiently good – indeed it is what we shall use here.

4.2.1 A one-feature classification model

We will start by building a model that uses only one feature to predict whether a user will reply to an email: whether the user is on the To line or not (the *ToLine* feature). Since we are building a conditional model, we only need to consider the process of generating the label (whether the user replied to the email or not) from the feature value. The variable we are trying to generate is therefore a binary label that is `true` if the user replied to the mail or `false` otherwise – we will call this variable `repliedTo`. This `repliedTo` variable is the variable that we will observe when training the model and which we will infer when making predictions.

It would be difficult to define the process of generating this binary `repliedTo` variable directly from the continuous feature values, since it is not itself a continuous variable. Instead, we introduce an intermediate variable that is continuous, which we shall call the *score*. We will assume that the score will be higher for emails which having a higher probability of reply and lower for emails which have a lower probability of reply. Here is the assumption:

② Each email has an associated continuous score which is higher when there is a higher probability of the user replying to the email.

Notice that, unlike a probability, the continuous score value is not required to lie between zero and one but can take on any continuous value. This makes it an easier quantity to model since we do not have to worry about keeping its value constrained to be between zero and one.

We are now ready to make an assumption about how the feature value for an email affects its score.

③ If an email's feature value changes by x, then its score will change by $weight \times x$ for some fixed, continuous weight.

This assumption says that the score for an email is either always higher if the feature value increases (if the weight is positive) or always lower if the feature value increases (if the weight is negative) or is not affected by the feature value (if the weight is zero). The size of any change in score is controlled by the size of the weight: a larger weight means a particular change in feature value produces a larger change in the score. Remember that, according to our previous assumption, a higher score means a higher reply probability and lower score means a lower reply probability.

To build a factor graph to represent Assumption ③ we first need a continuous `featureValue` variable to hold the value of the feature for each email (so it will be inside a plate across the emails). Since this variable will always be observed, we always show it shaded in the factor graph (Figure 4.1). We also introduce a continuous `weight` variable for the feature weight mentioned in the assumption. Because this weight is fixed, it is the same for all emails and so lies outside the emails plate. We can then model Assumption ③ by multiplying the `featureValue` by the `weight`, using a deterministic multiplication factor and storing the result in continuous `score` variable. The factor graph for a single feature modelled in this way is shown in Figure 4.1.

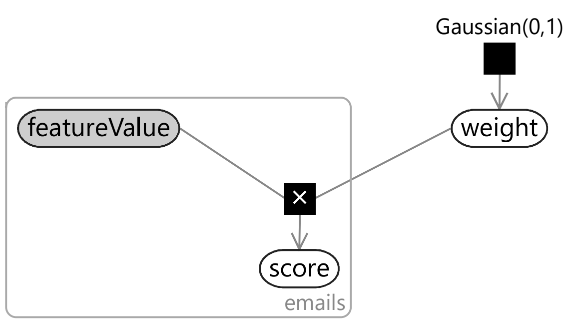


Figure 4.1: Factor graph for a single feature. Each email has a `featureValue` which is multiplied by a single common `weight` to give a `score` for that email. A positive `weight` means that the score increases if the feature value increases. A negative `weight` means that the score decreases if the feature value increases. A higher score corresponds to a higher probability that the email is replied to.

In drawing the factor graph, we've had to assume some prior distribution for `weight`. In this case, we have assumed that the weight is drawn from a Gaussian distribution with zero mean, so that it is equally likely to be positive or negative.

④ The weight for a feature is equally likely to be positive or negative.

We have also the prior distribution to be Gaussian with variance 1.0 (so the standard deviation is also 1.0). This choice means that the weight will most often be in the range from -1.0 to 1.0, occasionally be outside this in the range -2.0 to 2.0 and very occasionally be outside even that range (as we saw in Figure 3.4). We could equally have chosen any value for the variance, which would have led to different ranges of weight values so there is no implied assumption here. The effect of this choice will depend on the feature values which multiply the weight to give the score and also on how we use the score, which we will look at next.

We now have a continuous `score` variable which is higher for emails that are more likely to be replied to and lower for emails that are less likely to be replied to. Next we need to convert the `score` into a binary `repliedTo` variable. A simple way to do this is to threshold the `score` – if it is above some threshold then `repliedTo` is `true`, otherwise `false`. We can do this by adding a continuous `threshold` variable and use the deterministic *GreaterThan* factor that we met in the previous chapter:

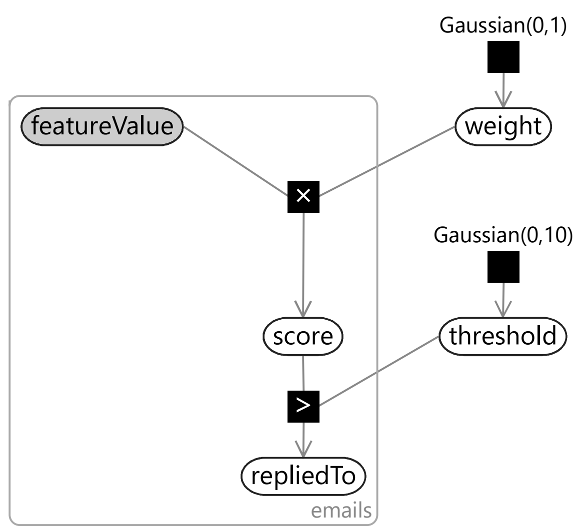


Figure 4.2: Factor graph of Figure 4.1 extended so that if the `score` is greater than a `threshold` the binary `repliedTo` variable is true, otherwise it is false.

Here we've chosen a $Gaussian(0, 10)$ prior for the `threshold` – we'll discuss this choice of prior shortly. Now suppose we try to train this one-feature model on the training set for one of our users. We can train the model using probabilistic inference as usual. First we fix the value of `repliedTo` for each email (by seeing if the user actually did reply to the email)and also the *ToLine* `featureValue` – which is always available since we can calculate it from the email To line. Given these two observed values for each email, we can train by inferring the posterior distributions for `weight` and `threshold`.

Unfortunately, if we attempt to run inference on this model then any inference algorithm we try will fail. This is because some of the observed values have zero probability under the model. In other words, there is no way that the data-generating process encoded by our model could have generated the observed data values. When your data has zero probability under your model, it is a sure sign that the model is wrong!

The issue is that the model is wildly overconfident. For any `weight` and `threshold` values, it will always predict `repliedTo` to be true with 100% certainty if the `score` is greater than the `threshold` and predict `repliedTo` to be false with 100% certainty otherwise. If we plot the reply probability against the `score`, it abruptly moves from 0% to 100% as the `score` passes the `threshold` (see the blue line in Figure 4.3). We will only be successful in training such a model if we are able to find some `weight` and `threshold` that *perfectly* classifies the training set – in other words gives a `score` above the `threshold` for all replied-to training emails and a score below the `threshold` for all emails that were not replied to. As an example, this would be possible if the user replied to every single email where they were on the To line and did not reply to every single other email. If there is even a single email where this is not the case, then its observed label will have zero probability under the model. For example, suppose a not-replied-to email has a `score` above the `threshold` – the prediction will be that `repliedTo` is `true` with probability 1.0 and so has zero probability of being `false`. But in this case `repliedTo` is observed to be `false`, which has zero probability and is therefore impossible under the model.

Looking back, Assumption 2 said that the reply probability would always be higher for emails with a higher score. But in fact, in our current model, this assumption does not hold – if we have two positive scores one higher than the other, they will both have the same 100% probability of reply. So our model is instead encoding the assumption that the reply probability abruptly changes from 0 to 100% as the score increases – it is this overly strong assumption that is causing training to fail.

To better represent Assumption 2, we need the reply probability to increase smoothly as the score increases. The red curve in Figure 4.3 shows a much smoother relationship between the score and the reply probability. This curve may look familiar to you, it is the cumulative density function for a Gaussian distribution, like the ones that we saw in Figure 3.9 in the previous chapter. We'd like to change our model to use this smooth curve. We can achieve this by adding a Gaussian-distributed random value

Adding noise to a model can be helpful when it does not perfectly represent the data.

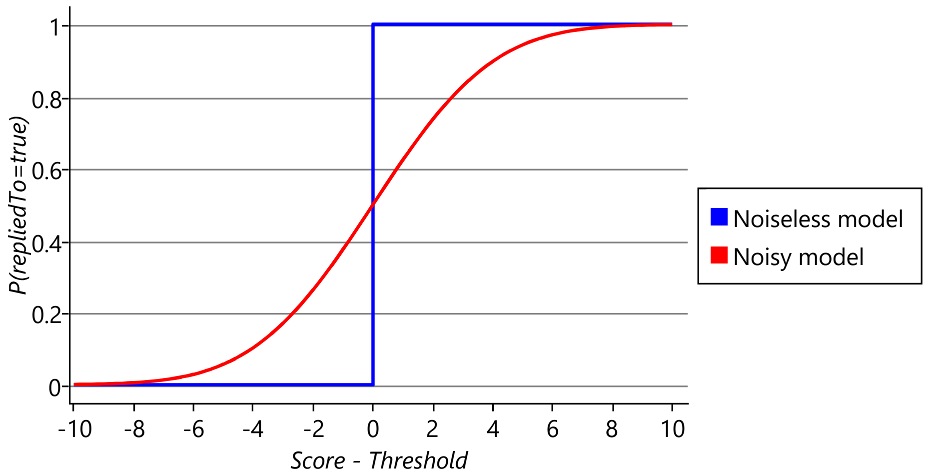


Figure 4.3: Plot of the predicted probability of reply as the score varies relative to the threshold for the noiseless model of Figure 4.2 and a noisy score model which adds Gaussian noise to the score before thresholding it. For the noiseless model, the reply probability abruptly changes from 0.0 to 1.0 as the score passes the threshold. In contrast, for the noisy model, the reply probability varies smoothly from near 0.0 to near 1.0 over a range of score values (from about -8 to +8).

to the `score` before we threshold it. These are called 'noise' values, because they take the clean 0% or 100% prediction and make it 'noisy'. Now, even if the `score` is below the threshold, there is a small probability that the noisy version will be above the threshold (and vice versa) so that the model can tolerate misclassified training examples. The exact probability that this will happen will depend on how far the score is below the threshold and the probability that the added Gaussian noise will push it above the threshold. This probability is given by the cumulative density function for the Gaussian noise, and so you end up with the curve shown in Figure 4.3.

Since the predicted probability varies smoothly from 0.0 to 1.0 over a range of score values, the model can now vary the confidence of its predictions, rather than always predicting 0% or 100%. The range of values that this happens over (the steepness of the curve) is determined by the variance of the Gaussian noise. The plot in Figure 4.3 is for a noise variance of 10, which is the value that we will use in our model, for reasons we will discuss in a moment. So let's add a new continuous variable called `noisyScore` and give it a Gaussian distribution whose mean is at `score` and whose variance is 10. This gives the factor graph of Figure 4.4.

In choosing a variance of 10, we have set how much the score needs to change in order to change the predicted probability. Remember that our weights are normally in the range -1.0 to 1.0, sometimes in the range -2.0 to 2.0 and

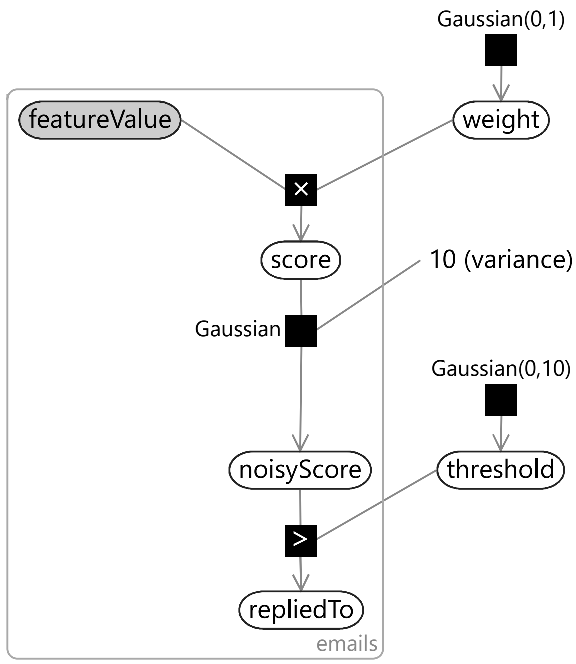


Figure 4.4: Factor graph of a classification model with one feature. The model uses a *Gaussian* factor to introduce uncertainty in the prediction of `repliedTo` for a particular `score`.

occasionally outside this range. Looking at Figure 4.3 you can see that to change the predicted probability from a 'don't know' prediction of 50% to a confident prediction of, say, 85% means that the score needs to change by about 3.0. If we choose feature values in the range -1.0 to 1.0 (which we will), this means that we are making the following assumption:

5. A single feature normally has a small effect on the reply probability, sometimes has an intermediate effect and occasionally has a large effect.

This assumption prevents our classification model from becoming too confident in its predictions too quickly. For example, suppose the system sees a few emails with a particular feature value, say *ToLine*=1.0, which are then all replied to. How confident should the system be at predicting reply for the next email with *ToLine*=1.0? The choice of noise variance encodes our assumption of this confidence. Setting the noise variance to a high value means that the system would need to see a lot of emails to learn a large weight for a feature and so would make underconfident predictions. Setting the noise variance too low would have the opposite effect and the system would make confident predictions after only a few training emails. A variance of 10 is a suitable intermediate value that avoids making either under- or over-confident predictions.

We can now try training this new model on the emails of one of our users, say,

ToLine	P(repliedTo=true)
0	0.008
1	0.112

(a)

ToLine	Replied to	Not replied to	Fraction replied to
0	19	3,046	0.006
1	111	824	0.119

(b)

Table 4.2: (a) Predicted probability of reply for our one-feature model, for each feature value. (b) For each feature value: the number of emails that were replied to, the number of emails that were not replied to and the fraction of emails that were replied to for the emails of User35CB8E5. Reassuringly, these fractions are close to the predicted probabilities of the learned model.

User35CB8E5. As in chapter 3, we can use expectation propagation to perform inference. This gives Gaussian distributions over `weight` and `threshold` of $Gaussian(3.77{,}0.028)$ and $Gaussian(7.63{,}0.019)$ respectively.

We can now use these Gaussian distributions to make predictions on a new email (or several emails), using online learning, as we saw in chapter 3. To do this, we replace the priors over `weight` and `threshold` with the learned posterior distributions. Then we fix the feature values for each email and run inference to compute the marginal distribution over `repliedTo`. Since we've only got one feature in our model and it only has two possible values, the model can only make two possible predictions for the reply probability, one for each feature value. Given the above Gaussian distributions for the `weight` and `threshold`, the predicted probability of reply for the two values of the *ToLine* feature are shown in Table 4.2a. As we might have expected, the predicted probability of reply is higher when the user is on the To line (*ToLine*=1.0) than when the user is not on the To line (*ToLine*=0.0).

To check whether these predicted probabilities are reasonable, we can compute the actual fraction of emails with each feature value that were replied to in the training set. The predicted probabilities should be close to these fractions. The counts of replied-to and not-replied-to emails with each feature value are shown in Table 4.2b, along with the fraction replied to computed from these counts.

These computed fractions are very close to the predicted probabilities, which gives us some reassurance that we have learned correctly from our data set. Effectively, we have provided a long-winded way of learning the conditional probability table given in Table 4.2a! However, if we want to use multiple features in our model, then we cannot use a conditional probability table, since it would become unmanageably large as the number of features increased. Instead, we will use the `score` variables to provide a different, scalable approach for combining features, as we will see in the next section.

Review of concepts introduced in this section

classification The task of predicting one of a fixed number of labels for a given data item. For example, predicting whether or not a user will reply to a particular email or whether a web site visitor will click on a particular link. So, in classification, the aim is to make predictions about a discrete variable in the model.

classifiers Systems that perform classification, in other words, which predict a label for a data item (or a distribution over labels if the classifier is probabilistic). Classifiers are probably the best known and most widely used machine learning systems today.

feature set A set of features that together are used to transform a data item into a form more suitable to use with a particular model or algorithm. Feature sets are usually used with classifiers but can also be used with many other types of models and algorithms.

feature A function which computes a value when given a data item. Features can return a single binary or real value or can return multiple values. A feature is usually used as part of a feature set to transform a data item into a form more suitable to use with a particular model or algorithm.

conditional model A model which represents a conditional probability rather than a joint probability. Conditional models require that the values of the variables being conditioned on are always known. The advantage of a conditional model is that the model can be simpler since it does not need to model the variables being conditioned on.

4.3 Modelling multiple features

With just one feature, our classification model is not very accurate at predicting reply, so we will now extend it to handle multiple features. We can do this by changing the model so that multiple features contribute to the `score` for an email. We just need to decide how to do this, which involves making an additional assumption:

(6) A particular change in one feature's value will cause the same change in score, no matter what the values of the other features are.

Let's consider this assumption applied to the *ToLine* feature and consider changing it from 0.0 to 1.0. This assumption says that the change in score due to this change in feature value is always the same, no matter what the other feature values are. This assumption can be encoded in the model by ensuring that the contribution of the ToLine feature to the score is always added on to the contributions from all the other features. Since the same argument holds for each of the other features as well, this assumption means that the score for an email must be the sum of the score contributions from each of the individual features.

So, in our multi-feature model (Figure 4.5), we have a `featureScore` array to hold the score contribution for each feature for each email. We can then use a deterministic summation factor to add the contributions together to give the total `score`. Since we still want Assumption (3) to hold for each feature, the `featureScore` for a feature can be defined, as before, as the product of the `featureValue` and the feature `weight`. Notice that we have added a new plate across the features, which contains the weight for the feature, the feature value and the feature score. The value and the score are also in the emails plate, since they vary from email to email, whilst the weight is outside since it is shared among all emails.

We now have a model which can combine together an entire set of features. This means we are free to put in as many features as we like, to try to predict as accurately as possible whether a user will reply to an email. More than that, we are assuming that anything we do not put in as a feature is not relevant to the prediction. This is our final assumption:

(7) Whether the user will reply to an email depends only on the values of the features and not on anything else.

As before, now that we have a complete model, it is a good exercise to go back and review all the assumptions that we have made whilst building the model. The full set of assumptions is shown in Table 4.3.

Assumption (1) arises because we chose to build a conditional model, and so we need to always condition on the feature values.

In our model, we have used the red curve of Figure 4.3 to satisfy Assumption (2). Viewed as a function that computes the score given the reply probability, this curve is called the *probit function*. It is named this way because the units of the score have historically been called 'probability units' or 'probits'.

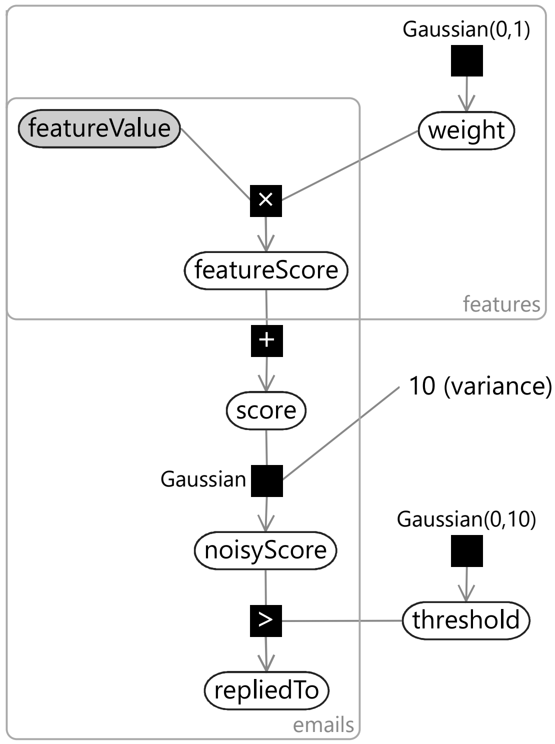


Figure 4.5: Factor graph of a classification model with multiple features. Variables within the features plate are duplicated for each feature, so there is a separate `weight` for each feature and, for each email, a separate `featureValue` and `featureScore`. The `featureScore` values for each feature are summed to give an overall `score` for each email.

Since **regression** is the term for predicting a continuous value (in this case, the score) from some feature values, the model as a whole is known as a *probit regression* model (or in its fully probabilistic form as the *Bayes Point Machine* [Herbrich et al., 2001]). There are other functions that we could have used to satisfy Assumption 2 – the most well-known is the **logistic function**, which equals $1/(1+e^{-x})$ and has a very similar S-shape (see Figure 4.6 to see just how similar!). If we had used the logistic function instead of the probit function, we would have made a *logistic regression* model – a very widely used classifier. In practice, both models are extremely similar – we used a probit model because it allowed us to build on the factors and ideas that you learned about in the previous chapter.

Assumption 3, taken together with Assumption 6, means that the score must be a **linear function** of the feature values. For example, if we had two features, the score would be $\texttt{weight}_1 \times \texttt{featureValue}_1 + \texttt{weight}_2 \times \texttt{featureValue}_2$. For any particular score, the feature values that give rise to that score lie on a

1	The feature values can always be calculated, for any email.
2	Each email has an associated continuous score which is higher when there is a higher probability of the user replying to the email.
3	If an email's feature value changes by x, then its score will change by $weight \times x$ for some fixed, continuous weight.
4	The weight for a feature is equally likely to be positive or negative.
5	A single feature normally has a small effect on the reply probability, sometimes has an intermediate effect and occasionally has a large effect.
6	A particular change in one feature's value will cause the same change in score, no matter what the values of the other features are.
7	Whether the user will reply to an email depends only on the values of the features and not on *anything* else.

Table 4.3: The seven assumptions encoded in our classification model.

line in a plot of the first feature value against the second, which is why we use the term linear. Any classifier based around a linear function is called a *linear classifier*.

Assumption 4 and Assumption 5 are reasonable statements about how features affect the predicted probability. However, Assumption 6 places some

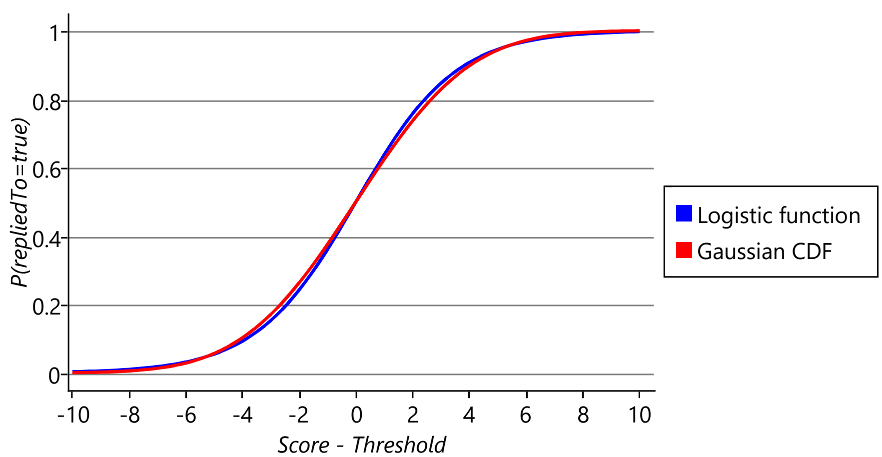


Figure 4.6: The logistic function scaled horizontally to match the Gaussian CDF from Figure 4.3. The similarity of the two functions means that our probit regression model behaves very similarly to a logistic regression model.

subtle but important limitations on what the classifier can learn, which are worth understanding. These are explored and explained in Panel 4.2.

Finally, Assumption 7 states that our feature set contains all of the information that is relevant to predicting whether a user will reply to an email. We'll see how to develop a feature set to satisfy this assumption as closely as possible in the next section, but first we need to understand better the role that the feature set plays.

4.3.1 Features are part of the model

To use our classification model, we will need to choose a set of features to transform the data, so that it better conforms to the model assumptions of Table 4.3. Another way of looking at this is that the assumptions of the *combined* feature set and classification model must hold in the data. From a model-based machine learning perspective, this means that the feature set combined with the classification model form a larger overall model. In this way of looking at things, the feature set is the part of this overall model that is usually easy to change (by changing the feature calculation code) whereas the classification part is the part that is usually hard to change (for example, if you are using off-the-shelf classifier software there is no easy way to change it).

We can represent this overall combined model in a factor graph by including the feature calculations in the graph, as shown in Figure 4.7. The `email` variable holds all the data about the email itself (you can think of it as an email object). The feature calculations appear as deterministic *ComputeFeature* factors inside of the features plate, each of which computes the feature value for the feature, given the `email`. Notice that, although only `email` is shown as observed (shaded), `featureValue` is effectively observed as well since it is deterministically computed from `email`.

Panel 4.2 – How features combine together

n 6 is quite a strong assumption about how features combine together. To investigate the effect umption, consider a two-feature model with the existing *ToLine* feature and a new feature called *ger*. This new *FromManager* feature has a value of 1.0 if the sender is the user's manager and 0.0 Suppose a particular user replies to 80% of emails from their manager, but only if they are on the To y are not on the To line, then they treat it like any other email where they are on the Cc line. To h a user, we will create a synthetic data set to represent our hypothetical user's email data. For email *nManager* is zero, we will take User35CB8E5's data set from Table 4.2b. We will then add 500 new mails where *FromManager* is 1, such that the user is on the To line exactly half of the time, giving the the table below. The final column of this table gives the predicted probabilities for each combination for a model trained on this data.

ToLine	FromManager	Replied to	Not replied to	Fraction replied to	P(repliedTo=true)
0	0	19	3,046	0.006	0.004
1	0	111	824	0.119	0.144
0	1	2	248	0.008	0.108
1	1	200	50	0.800	0.646

uite a big difference between the predicted probability of reply and the actual fraction replied to. le, the predicted probability for emails from the user's manager where the user is on the To line is ow: 64.6% not 80%. Similarly, the prediction is too high (10.8% not 0.8%) for emails from the user's here the user is not on the To line. These inaccurate predictions occur because there is no setting of and `threshold` variables that can make the predicted probability match the actual reply fraction. n 6 says the change in score for *FromManager* must be the same when *ToLine* is 1.0 as for when).0. But, to match the data, we need the change in score to be higher when *ToLine* is 1.0 than when

n changing the model to remove Assumption 6, we can work around this limitation by adding a new t is 1.0 only if *ToLine* and *FromManager* are both 1.0 (an AND of the two features). This new feature s own `weight` associated with it, which means there can now be a different score for manager emails ser is on the To line to when they are not on the To line. If we train such a three-feature model, we predictions shown here:

oLine	FromManager	And	Replied to	Not replied to	Fraction replied to	P(repliedTo=true)
0	0	0	19	3,046	0.006	0.007
1	0	0	111	824	0.119	0.119
0	1	0	2	248	0.008	0.024
1	1	1	200	50	0.800	0.766

ted probabilities are now much closer to the actual reply fractions in each case, meaning that the is making more accurate predictions than the old one. Any remaining discrepancies are due to n 5, which controls the size of effect of any single feature.

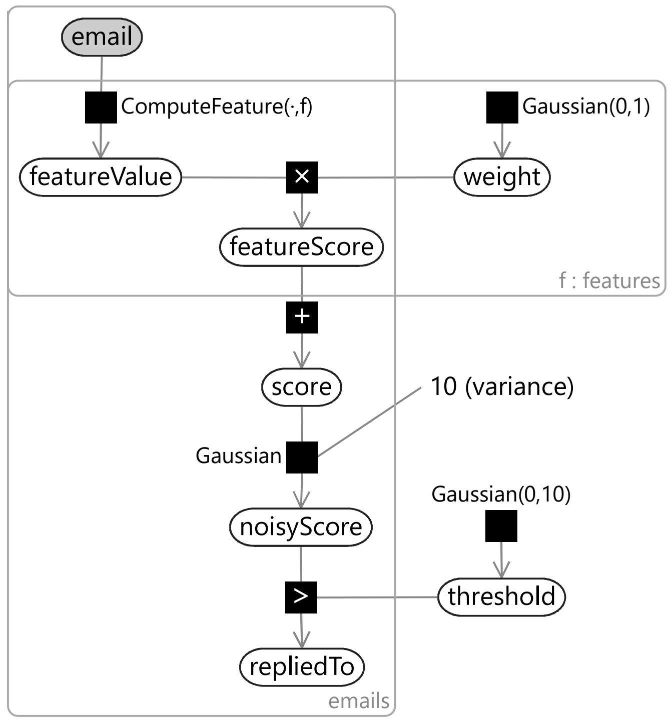


Figure 4.7: Factor graph of a model which includes both feature calculation and classification. The *ComputeFeature* factor takes as arguments the current feature f and the email being considered and computes the value of feature f for that email.

If the feature set really is part of the model, we must use the same approach for designing a feature set, as for designing a model. This means that we need to visualise and understand the data, be conscious of assumptions being represented, specify evaluation metrics and success criteria, and repeatedly refine and improve the feature set until the success criteria are met (in other words, we need to follow the machine learning life cycle). This is exactly the process we will follow next.

Review of concepts introduced in this section

regression The task of predicting a real-valued quantity (for example, a house price or a temperature) given the attributes of a particular data item (such as a house or a city). In regression, the aim is to make predictions about a continuous variable in the model.

logistic function The function $f(x) = 1/(1 + e^{-x})$ which is often used to transform unbounded continuous values into continuous values between 0 and 1. It has an S-shape similar to that of the cumulative Gaussian (see Figure 4.6).

linear function Any function of one or more variables $f(x_1, \ldots, x_k)$ which can be written in the form $f(x_1, \ldots, x_k) = a + b_1x_1 + \ldots + b_kx_k$. A linear function of just one variable can therefore be written as $f(x) = a + bx$. Plotting $f(x)$ against x for this equation gives a straight line which is why the term *linear* is used to describe this family of functions.

4.4 Designing a feature set

To use our classification model, we need to choose a set of features to transform the data, so that it conforms as closely as possible to the assumptions built into the model (Table 4.3). For example, to satisfy Assumption 7 (that features contain all relevant information about the user's actions) we need to make sure that our feature set includes all features relevant to predicting reply. Since pretty much any part of an email may help with making such a prediction, this means that we will have to encode almost all aspects of the email in our features. This will include who sent the email, the recipients of the email on the To and Cc lines, the subject of the email and the main body of the email, along with information about the conversation the email belongs to.

When designing a new feature, we need to ensure that:

- the feature picks up on some informative aspect of the data,
- the feature output is of the right form to feed into the model,
- the feature provides new information about the label over and above that provided by existing features.

In this section, we will show how to design several features for our feature set, while ensuring that they meet the first two of these criteria. In the next section we will show how to check the third criterion by evaluating the system with and without certain features.

4.4.1 Features with many states

So far, we have represented where the user appears on the email using a *ToLine* feature. This feature has only two states: the user is either on the To line or not. So the feature ignores whether the user is on the Cc line, even though we might expect a user to be more likely to reply to an email if they appear on the Cc line than if they do not appear at all. The feature also ignores the position of the user on the To/Cc line. If the user is first on the To line we might expect them to be more likely to reply than if they are at the end of a long list of recipients. We can check these intuitions using our data set by finding the actual fraction of all training/validation emails that were replied to in a number of cases: when the user is first, second or later than second on the To line, when the user is first or elsewhere on the Cc line and when the user is not on either the To or Cc lines (for example, if they received the email via a distribution list). Figure 4.8 shows a plot of these fractions, showing that the probability of reply does vary substantially depending on which of these cases applies. This plot demonstrates that a feature that was able to distinguish these cases would indeed pick up on an informative aspect of the data (our first criterion above). When assessing reply fractions, such as those in Figure 4.8, it is important to take into account how many emails the fraction is computed from, since a fraction computed from a small number of emails would not be very accurate. To check this, in Figure 4.8 we show the number of emails in brackets below each bar label, demonstrating that each has sufficient emails to compute the fraction accurately and so we can rely on the computed values.

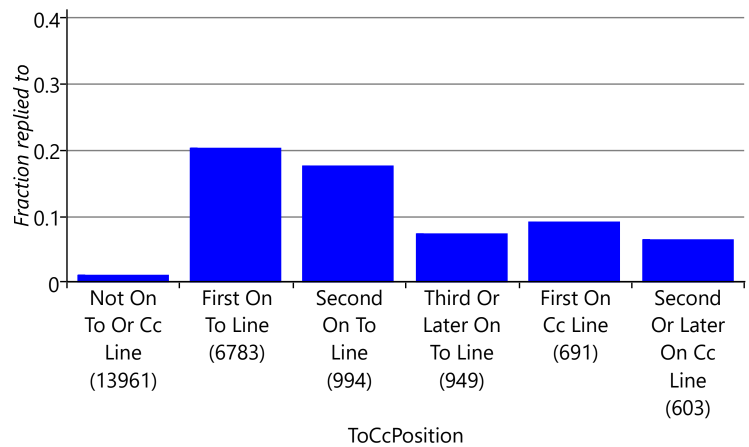


Figure 4.8: Fraction of emails that were replied to, for each of six possible positions of the user on the To or Cc line. The number of emails with the user in each position is shown in brackets (the fraction replied to is a fraction of these emails that were replied to). The plot shows that, for our data set, being first on the To line indicates the highest probability of reply, but that this reduces if the user is second or later. It also shows that if the user is not mentioned on the To or Cc line, the reply probability is very low.

We can improve our feature to capture cues like this by giving it multiple states, one for each of the bars of Figure 4.8. So the states will be: {`NotOnToOrCcLine`, `FirstOnToLine`, `SecondOnToLine`, `ThirdOrLaterOnToLine`, `FirstOnCcLine`, `SecondOrLaterOnCcLine`}. Now we just need to work out what the output of the feature should be, to be suitable for our model (the second criterion). We could try returning a value of 0.0 for `NotOnToOrCcLine`, 1.0 for `FirstOnToLine` and so on up to a value of 5.0 for `SecondOrLaterOnCcLine`. But, according to Assumption 3 (that the score changes by the weight times the feature value) this would mean that the probability of reply would either steadily increase or steadily decrease as the value changes from 0.0 through to 5.0. However, Figure 4.8 shows that this is not the case since the reply fraction goes up and down as we go from left to right, and so such an assumption would be incorrect. In general, we would want to avoid making assumptions which depend on the ordering of some states that do not have an inherent ordering, such as in this case. Instead we would like to be able to learn how the reply probability is affected separately for each state.

To achieve this we can modify the feature to output *multiple* feature values, one for each state, where the value is 1.0 for the state that applies to a particular email and 0.0 for all other states. So an email where the user is first on the

To line would be represented by the feature values $\{0.0, 1.0, 0.0, 0.0, 0.0, 0.0\}$. Similarly an email where the user is first on the Cc line would be represented by the feature values $\{0.0, 0.0, 0.0, 0.0, 1.0, 0.0\}$. By doing this, we have effectively created a group of related binary features – however it is much more convenient to think of them as a single *ToCcPosition* feature which outputs multiple values. To avoid confusion in terminology, we will refer to the different elements of such a feature as **feature buckets** – so the *ToCcPosition* feature contains 6 feature buckets. Using this terminology, the plate across the features in our factor graph should now be interpreted as being across all buckets of all features, so that each bucket has its own `featureValue` and its own associated `weight`. This means that the `weight` can be different for each bucket of our *ToCcPosition* feature and so we are no longer assuming that the reply probability steadily increases or decreases across the buckets.

4.4.2 Numeric features

We also need to create features that encode numeric quantities, such as the number of characters in the email body. If we used the number of characters directly as the feature value, we would be assuming that longer emails mean either always higher or always lower reply probability than shorter emails. But in fact we might expect the user to be unlikely to respond to a very short email ("Thanks") or a very long email (such as a newsletter), but may be likely to respond to emails whose length is somewhere in between. Again, we can investigate these beliefs by plotting the fraction of emails replied to for various body lengths. To get a useful plot, it is necessary to divide body lengths for longer emails into bins, in order to get enough emails to estimate the reply fraction reliably. In Figure 4.9, we have used bins such that each bin is roughly double the size of the previous one, along with a catch-all bin for all very long emails (more than 1023 characters).

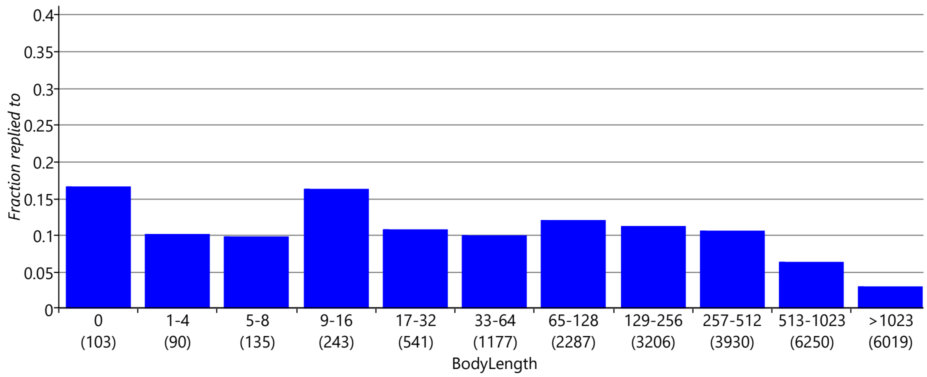


Figure 4.9: Fraction of emails that were replied to, for various ranges of body lengths, given by the number of characters in the email body. The number of emails falling into each bin is shown in brackets. Zero-length emails are likely to have their message in the subject line and so have quite a high reply fraction. For other emails, the reply fraction peaks at around 9-16 characters and then generally decreases, until it is very low for very long emails.

There are several aspects of this plot that are worthy of comment. Zero-length emails have a quite high reply probability, probably because these are emails where the message was in the subject. As we anticipated, very short emails have relatively low reply probability and this increases to a peak in the 9-16 characters and is then roughly constant until we get to very long emails of 513 characters or more where the reply probability starts to tail off. To pick up on these changes in the probability of reply, we can use the same approach as we just used for *ToCcPosition* and treat each bin of our plot as a different feature bucket. This gives us a *BodyLength* feature with 11 buckets. Emails whose length fall into a particular bin, such as 33-64 characters, all map to a single bucket. This mapping encodes the assumption that the reply probability does not depend on the exact body length but only on which bin that length falls into.

4.4.3 Features with many, many states

We might expect that the sender of an email would be one of the most useful properties for predicting whether a user will reply or not. But why rely on belief, when we can use data? Figure 4.10 shows the fraction of emails replied to for the twenty most frequent senders for User35CB8E5. As you can see there is substantial variation in reply fraction from one sender to another: some senders have no replies at all, whilst others have a high fraction of replies. A similar pattern holds for the other users in our data set. So indeed, the sender is a very useful cue for predicting reply.

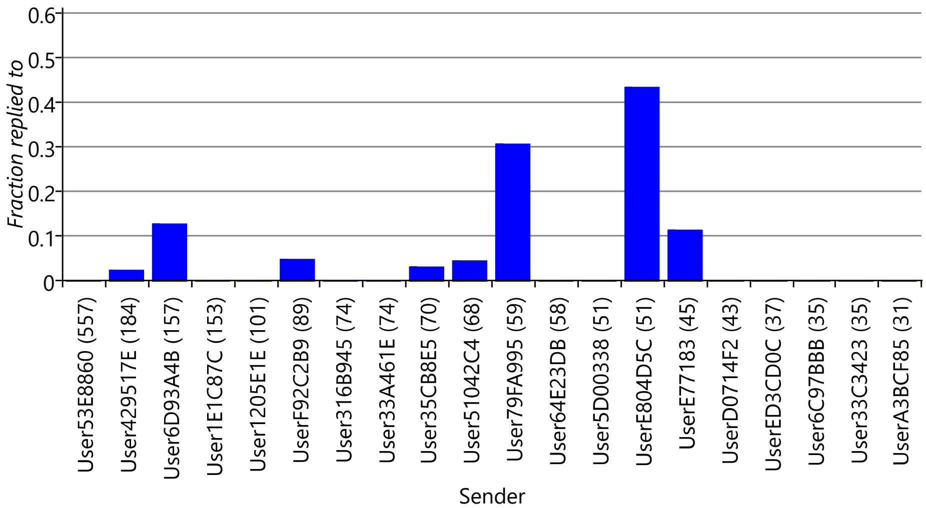


Figure 4.10: Fraction of emails replied to for the 20 most common senders for User35CB8E5 (the number of emails from each sender is shown in brackets). Reply fraction varies significantly from sender to sender, indicating that this is a very useful cue for predicting reply. As discussed in section 4.1, the sender identities have been anonymised to preserve the privacy of the user.

To incorporate the sender information into the feature set, we can use a multi-state *Sender* feature, with one state for each sender in the data set. For example, User35CB8E5 has 658 unique senders in the training and validation sets combined. This would lead to a feature with 658 buckets of which 657 would have value 0.0 and the bucket corresponding to the actual sender would have value 1.0. Since so many of the feature bucket values would be zero, it is much more efficient to change our factor graph to only include the feature buckets that are actually 'active' (non-zero). A suitably modified factor graph is shown in Figure 4.11.

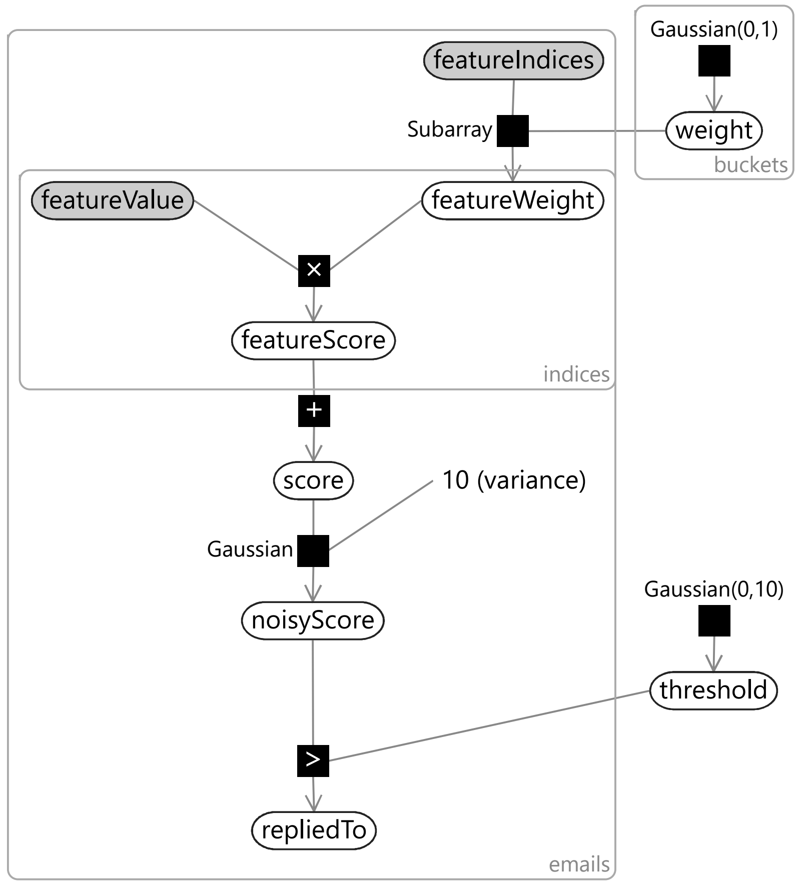
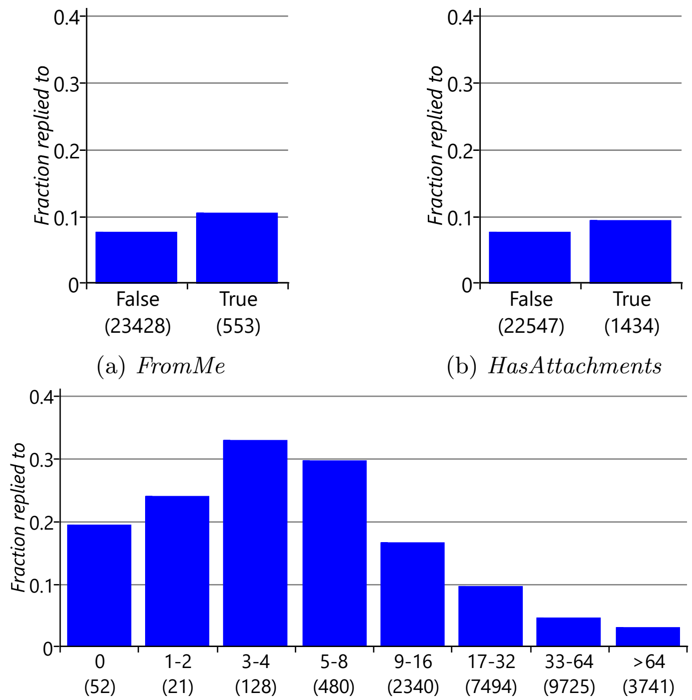


Figure 4.11: Modified factor graph which represents only non-zero feature buckets. The `featureIndices` variable contains the indices of feature buckets that have non-zero values. The `featureValues` variable contains the corresponding values for those buckets. The *Subarray* factor is used to pull out the relevant elements of the `weight` array, which are placed into the `featureWeight` array.

In this modified graph, the feature values for an email are represented by the indices of non-zero values (`featureIndices`) along with the corresponding values at these indices (`featureValues`). We use the *Subarray* factor that we introduced back in section 2.4 to pull out the weights for the active buckets (`featureWeight`) from the full weights array (`weight`). This new factor graph allows features like the *Sender* feature to be added without causing a substantial slow-down in training and classification times. For example, training on User35CB8E5's training set takes 9.2 seconds using the old factor graph but just 0.43 seconds using this new factor graph. This speed up would be even greater if we had trained on more emails, since there would be more unique senders.

4.4.4 An initial feature set

Now that we know how to encode all the different types of data properties, we can complete our initial feature set, ready to start experimenting with. To encode remaining data properties, we add three further features: *FromMe*, *HasAttachments* and *SubjectLength* whose feature buckets and reply fractions are shown in Figure 4.12.



(a) *FromMe* (b) *HasAttachments* (c) *SubjectLength*

Figure 4.12: Fraction of emails that were replied to for each feature bucket, for the three new features. The number of emails falling into each feature bucket is shown in brackets.

As we discussed back in section 4.1, we removed the content of the subject lines and email bodies from the data set and so cannot add any features to encode the actual words of the subject or of the email body. To build the classifier for the Exchange project, anonymised subject and body words were used from voluntarily provided data. As you might expect, including such subject and body word features did indeed help substantially with predictive accuracy.

Our initial feature set, with six features, is shown in Table 4.4.

	Description	#Buckets
FromMe	Whether the message is from you	1
ToCcPosition	Your position on the To or Cc lines	6
HasAttachments	Whether the message has attachments	1
BodyLength	The number of new characters in the body text	11
SubjectLength	The number of characters in the subject	8
Sender	Who the message is from	(varies)

Table 4.4: An initial set of features for predicting reply on an email. For each feature, we show the feature type, a brief description and the number of feature buckets for that feature (where this number is fixed).

Now that we have a classification model and a feature set, we are ready to see how well they work together to predict whether a user will reply to a new email.

Review of concepts introduced in this section

feature buckets Labels which identify the values for a feature that returns multiple values. For example, the *ToCcPosition* feature in Figure 4.8 has six feature buckets: `NotOnToOrCcLine`, `FirstOnToLine`, `SecondOnToLine`, `ThirdOrLaterOnToLine`, `FirstOnCcLine` and `SecondOrLaterOnCcLine`. For this feature the value associated with one of the buckets will be 1.0 and the other values will be 0.0, but for other features multiple buckets may have non-zero values.

4.5 Evaluating and improving the feature set

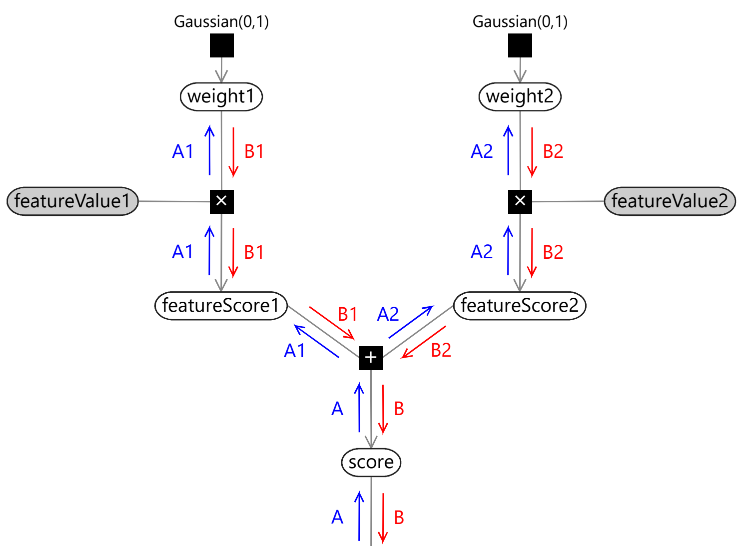
Using our newly-completed model and feature set, we can train a personalised classifier for each user in our data set. To be precise, for each user's training set, we compute the active feature buckets `featureIndices` for each email, along with their feature values `featureValue`. Given these observed variables, we can then apply expectation propagation to learn a posterior `weight` distribution for each bucket, along with a single posterior distribution over the value of the `threshold`. But first we need to look at how to schedule message passing for our model.

4.5.1 Parallel and sequential schedules

INFERENCE

Inference deep-dive
In this optional section, we look at how to schedule the expectation propagation messages for our model. If you want to go straight to look at the results of running expectation propagation, feel free to skip this section.

When running expectation propagation in this model, it is important to choose a good message-passing schedule. In this kind of model, a poor schedule can easily cause the message-passing algorithm to fail to converge or to converge very slowly. When you have a model with repeated structures (such as our classification model), there are two main kinds of message-passing schedule that can be used: sequential or parallel. To understand these two kinds of schedule, let's look at message passing on a simplified form of our model with two features and two weights:



In this figure, rather than using a plate across the buckets, we have instead duplicated the part of the model for each weight. When doing message passing in this model, two choices of schedule are:

- A *sequential schedule* which processes the two weights in turn. For the first weight, this schedule passes messages in the order A, A1, B1, B. After processing this weight, message-passing happens in the bottom piece of the graph (not shown). The schedule then moves on to the second weight, passing messages in the order A, A2, B2, B.

- A *parallel schedule* which processes the two weights at once. In this schedule, first the messages marked A are passed. Then both sets of messages (A1 and B1) and (A2 and B2) are passed, where the messages from the plus factor are computed using the previous B1 and B2 messages. Finally, the message marked B are passed.

To see the difference between the two schedules, look at how the first A2 message coming out of the plus factor is calculated. In the sequential schedule, it is calculated using the B1 message that has just been updated in this iteration of the schedule. In the parallel schedule, it uses the B1 message calculated in the previous iteration, in other words, an older version of the message. As a result, the parallel schedule converges more slowly than the sequential schedule and is also more likely to fail to converge at all. So why would we ever want to use a parallel schedule? The main reason is if you want to distribute your inference computation in parallel across a number of machines in order to speed it up. In this case, the best option is to use a combined schedule which is sequential on the section of model processed within each machine but which is parallel across machines.

4.5.2 Visualising the learned weights

To ensure this sequential schedule is working well, we can visualise the learned weight distributions to check that they match up to our expectations. Figure 4.13 shows the learned Gaussian distributions over the weights for each feature bucket for User35CB8E5 (to save space, only the fifteen most frequent Sender weights are shown).

Looking at each weight in turn, we can see that more positive weights generally correspond to those feature buckets that we would expect to have a higher probability of reply, given the histograms in the previous section. For example, looking at the *SubjectLength* histogram of Figure 4.12c, you can see that the positive and negative learned weights correspond to the peaks and troughs of the histogram. You can also see that the error bars are narrower for common feature buckets like *SubjectLength*[33-64] than for rare feature buckets like *SubjectLength*[1-2]. This is to be expected since, if there are fewer emails with a particular feature bucket active, there is less information about the weight for that bucket and so the learned weight posterior is more uncertain. For very rare buckets, there are so few relevant emails in the training set that we should expect the `weight` posterior to be very close to the *Gaussian*(0,1) prior. You can see this is true for *SubjectLength*[1-2], for example, whose weight mean is close

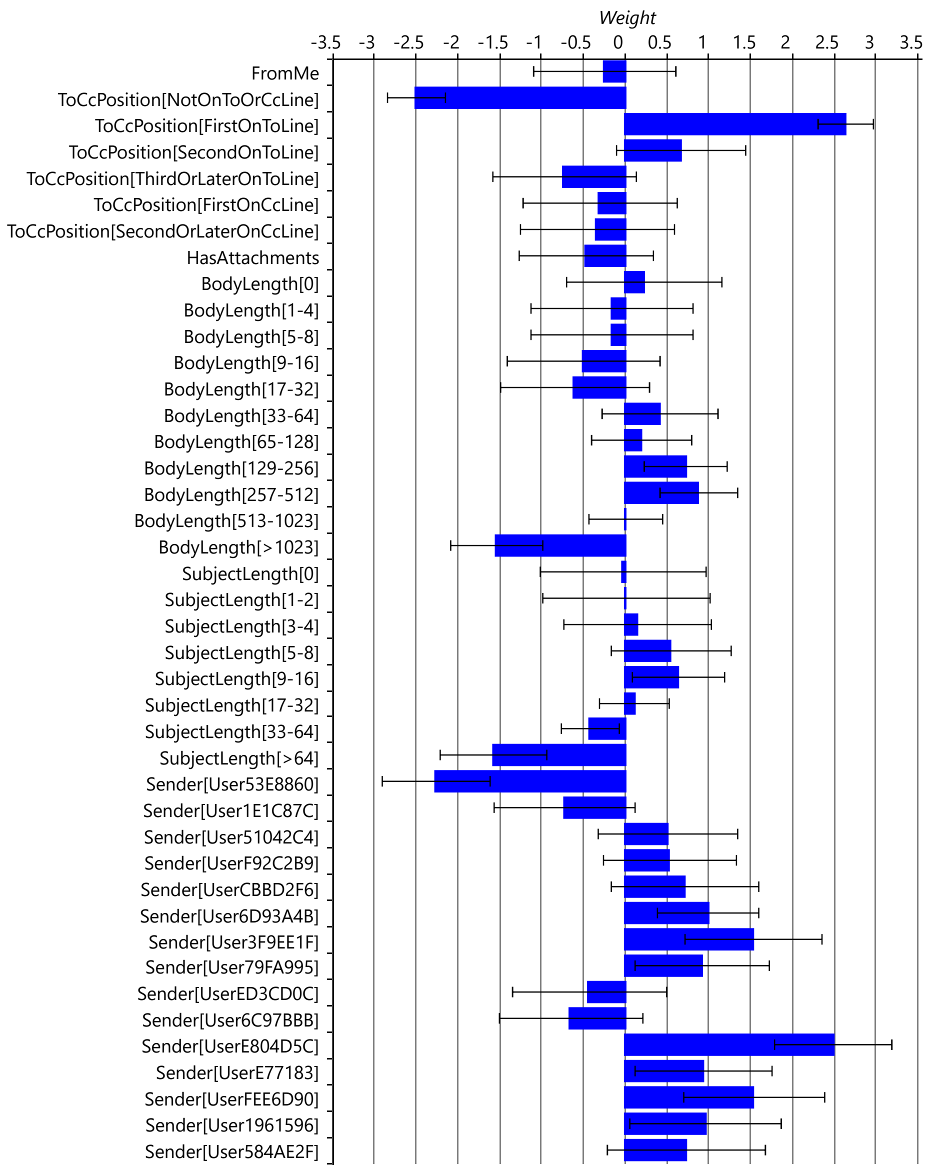


Figure 4.13: Learned Gaussian distributions over the feature bucket weights for User35CB8E5. For each feature bucket, the blue bar indicates the mean of the Gaussian weight distribution showing how much the system expects the feature bucket to increase or decrease the score for an email. The error bars indicate the uncertainty in this learned value by showing plus/minus one standard deviation around the mean.

to 0.0 and whose standard deviation is close to 1.0. So, overall, manual inspection of the learned weights is consistent with what we might expect. Inspecting the learned weights of other users also show plausible weight distributions.

Had we found some unexpected weight values here, the most likely explanation would be a bug in the feature calculation. However, unexpected weight values can also uncover faulty intuitions about the kinds of email a user is likely to reply to, or even allow us to discover new types of email reply behaviour that we might not have guessed at.

4.5.3 Evaluating reply prediction

Using the trained model for each user, we can now predict a reply probability for each email in the user's validation set. As we saw in chapter 2, we can plot an ROC curve to assess the accuracy of these predictions. Doing this for each user, gives the plots in Figure 4.14.

These curves look very promising – there is some variation from user to user, but all the curves are all up in the top left of the ROC plot where we want them to be. But do these plots tell us what we need to know? Given that our aim is to identify emails with particular actions (or lack of actions), we need to know two things:

1. *Out of all replied-to emails, what fraction do we predict will be replied to?*

This is the true positive rate, which the ROC curve is already giving us on its y-axis. In this context, the true positive rate is also referred to as the **recall** since it measures how many of the replied to emails were successfully 'recalled' by the system.

2. *Out of emails that we predict will be replied to, what fraction actually are?*

This is a new quantity called the **precision** and is *not* shown on the ROC curve. Note that this is a different meaning of the word *precision* to its use as a parameter describing the inverse variance of a Gaussian – it is usually clear from the context which meaning is intended. To visualise the precision we must instead use a **precision-recall curve** (P-R curve) which is a plot of precision on the y-axis against recall on the x-axis. Figure 4.15 shows precision-recall curves for exactly the same prediction results as for the ROC curves in Figure 4.14. To get a summary accuracy number for a precision-recall curve, similar to the area under an ROC curve, we can compute the **average precision** (AP) across a range of recalls – these are shown in the legend of Figure 4.15. Precision-recall curves tend to be very noisy at the left hand end since at this point the precisions are being computed from a very small number of emails – for this reason, we compute the average precision between recalls of 0.1 and 0.9 to give a more stable and reliable accuracy metric. Omitting the right hand end of the plot as well helps correct for the reduction in average precision caused by ignoring the left hand end of the plot.

Compare the ROC and precision-recall curves – once again we can see the value of using more than one evaluation metric: the precision-recall curves tell

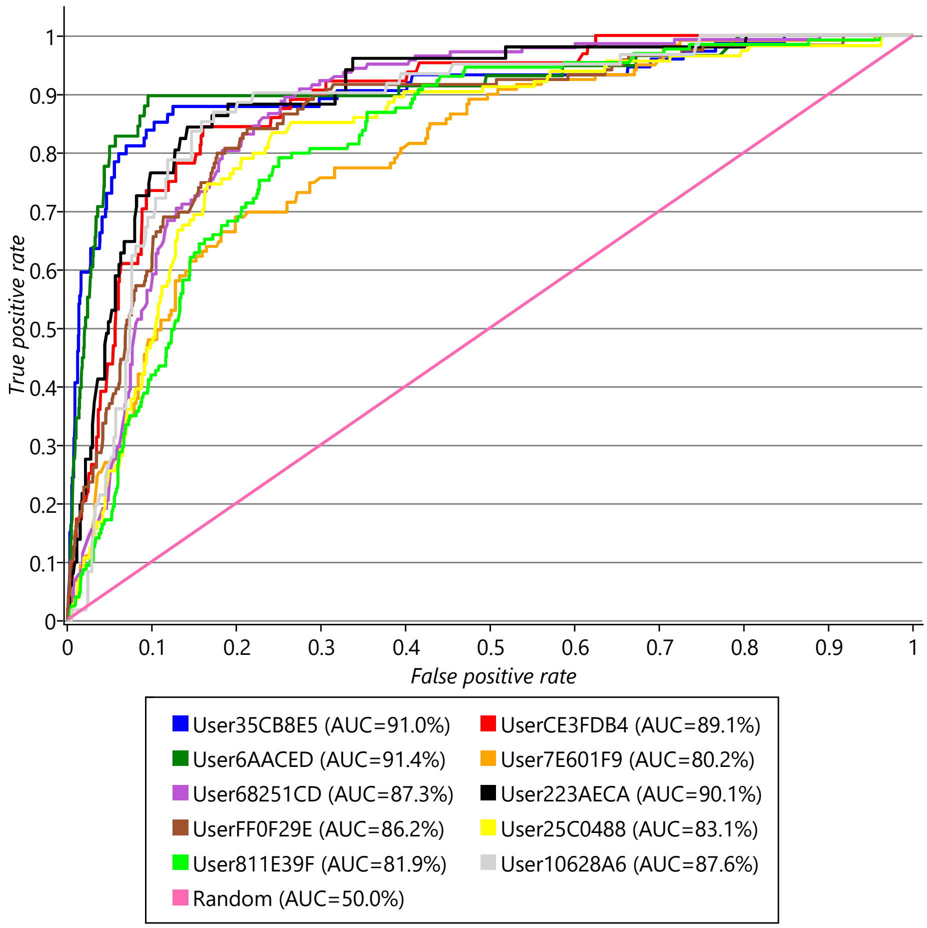


Figure 4.14: ROC curves for each user in our data set computed using predictions on the user's validation set. The legend gives the area under the curve (AUC) for each user.

a very different story! They show that there is quite a wide variability in the precision we are achieving for different users, and also that the users with the highest precision-recall curves (such as User68251CD) are not the same users that have the highest ROC curves (such as User6AACED). So what's going on?

To help understand the difference, consider a classifier that predicts reply or no-reply at random. The ROC curve for such a classifier is the diagonal line labelled 'Random' in Figure 4.14. To plot the P-R curve for a random classifier, we need to consider that it will classify some random subset of emails as being positives, so the fraction of these that are true positives (the precision) is just the fraction of emails that the user replies to in general. So if a user replies to 20% of their emails, we would expect a random classifier to have a precision of

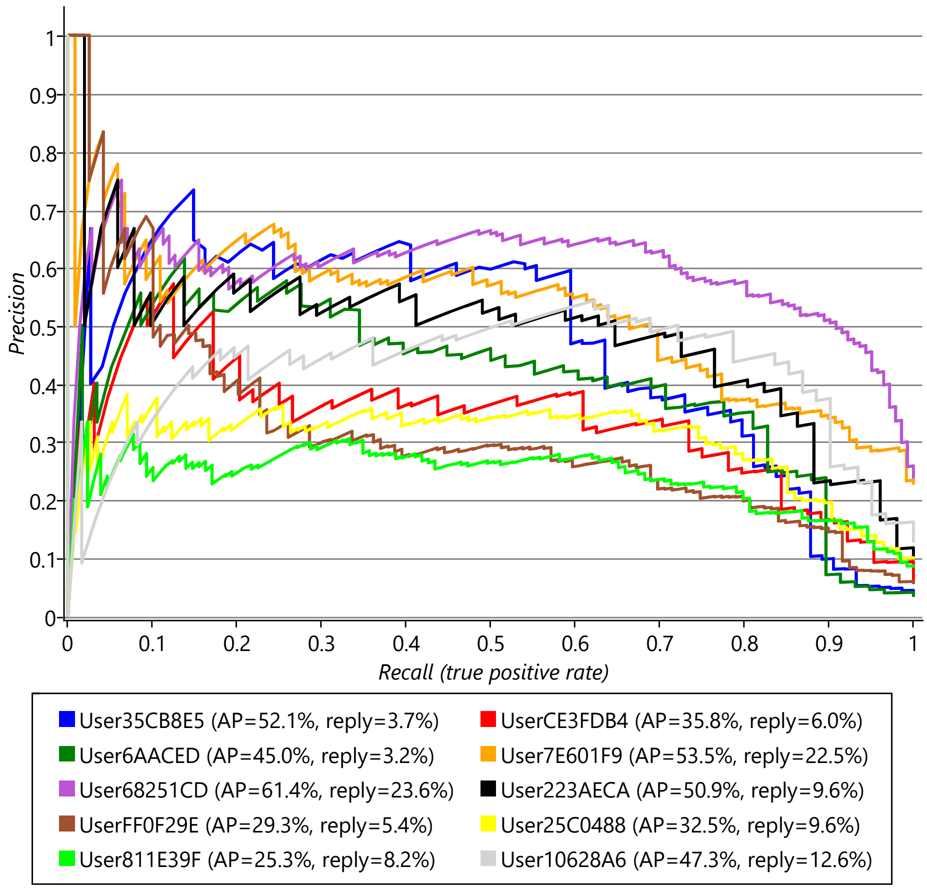


Figure 4.15: Precision-recall curves for the same prediction results as the ROC curves of Figure 4.14. The legend gives the average precision (AP) for each user, along with the percentage of validation set emails that were replied to by that user.

20%. If another user replies to 2% of their emails, we may expect a random classifier to have a precision of 2%. The fraction of emails that each of our users replies to is given in the legend of Figure 4.15, following the average precision. User68251CD replies to the highest percentage of emails 23.6% which means we might expect it to be easier to get higher precisions for that user – and indeed that user has the highest average precision, despite having an intermediate ROC curve. Conversely, User6AACED, who has one of the highest ROC curves, has only a middling P-R curve, because this user only replies to 3.2% of their email. Given that our two error metrics are giving us different information, how can we use them to assess success? How can we set target values for these metrics? The answer lies in remembering that we use metrics like AP and AUC only as a proxy for the things that we really care about – user happiness and productivity. So we need to understand how the values of our metrics map into the users' experience of the system.

4.5.4 Understanding the user's experience

Once the system is being beta tested by large numbers of users, we can use explicit feedback (for example, questionnaires) or implicit feedback (for example, how quickly people process their email or how many people turn off the feature) to assess how happy/productive users are for particular values of the evaluation metrics. During the early stages of developing the system, however, we must use our own judgement of how well the system is working on our own emails.

To understand how our evaluation metrics map into a real user's experience, it is *essential* to get some users using the system as soon as possible, even if these users are just team members. To do this, we need a working end-to-end system, including a user interface, that can be used to evaluate qualitatively how well the system is performing. Having a working user interface is particularly important since the choice of user interface imposes requirements on the underlying machine learning system. For example, if emails are to be removed from a user's inbox without giving any visual indication, then a very high precision is essential. Conversely, if emails are just to be gently de-emphasised but left in place, then a lower precision can be tolerated, which allows for a higher recall. These examples show that the user interface and the machine learning system need to be well matched to each other. The user interface should be designed carefully to tolerate any errors made by the machine learning component, whilst maximising its value to the user (see Patil [2012]). A well-designed user interface can easily make the difference between users adopting a particular machine learning system or not.

For our purposes, we need a user interface that emulates an email client but which also displays the reply prediction probability in some visual way. Figure 4.16 shows a suitable user interface created as an evaluation and debugging tool.

The tool has a cut-off reply probability threshold which can be adjusted by a slider – emails with predicted reply probabilities above this threshold are predicted to be replied to and all other emails are predicted as not being replied to. The tool also marks which emails were correctly classified and which were false positives or false negatives, given this cut-off threshold. The use of a threshold on the predicted probability again emphasises the importance of good calibration. If the calibration of the system is poor, or varies from user to user, then it makes it much harder to find a cut-off threshold that gives a good experience. The calibration of our predictions can be plotted and evaluated, as described in Panel 4.3.

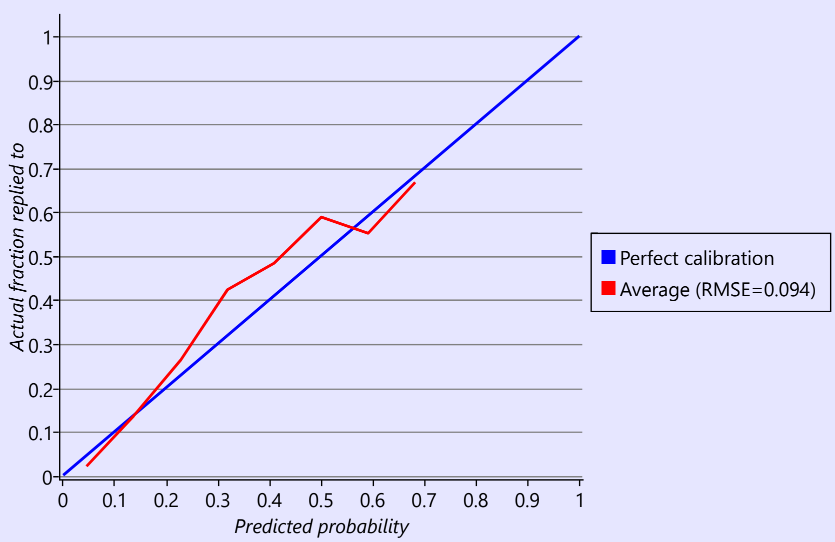
For debugging purposes, the tool shows the feature buckets that are active

Panel 4.3 – Calibration

A machine learning system is well-calibrated if the predicted probabilities it gives are accurate. For example, if a well-calibrated system predicts an event with a probability of 90%, then we should expect this event to happen 90% of the time. It is important to evaluate the calibration of any machine learning system because:

- We often need to be able to trust the probabilities coming from the system. For example, they may be used to drive a user interface which varies with the probability of the prediction (such as only marking emails above a certain probability). Accurate probabilities are especially important if they are to be used as input to another machine learning system.
- If a machine learning system is poorly calibrated then it suggests a problem either in the model (such as an overly restrictive assumption) or in the approximate inference. Fixing this problem will not only improve calibration but also usually improve prediction accuracy as well.

We can use a calibration plot to evaluate how well-calibrated our email model is. To do this we take all the validation set predictions made for each user and divide them into bins according to the predicted probability of reply (0-10%,11-20% and so on). For each bin, we then compute the fraction of emails that were actually replied to (we discard bins with too few emails, since then this fraction would be very noisy). Finally, we plot the average of this fraction across users against the predicted probability, as shown below.



The plot also shows the line for a perfectly calibrated system, which is a diagonal line. Our system is reasonably well-calibrated (within about 0.1 of this diagonal). We can get an overall calibration metric by measuring how far we are from this diagonal using – for example, using a root-mean-squared-error (RMSE) difference, which for our system gives 0.094.

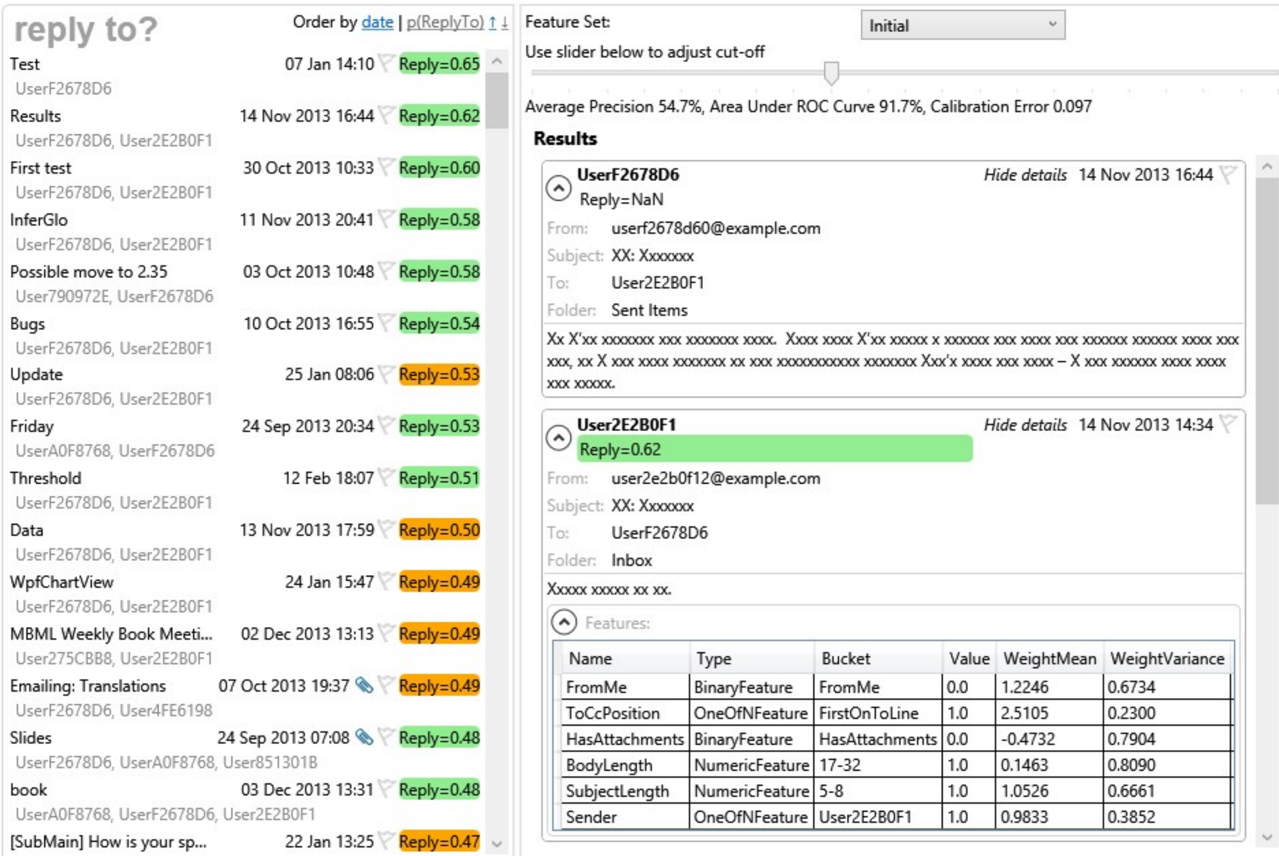


Figure 4.16: Screenshot of the user interface of the evaluation and debugging tool which allows the accuracy of the system to be assessed on real emails. The tool also exposes the calculated features, learned weights and predicted reply probability for each email, which makes it easier to debug the system. The coloured background of the reply probabilities indicates whether the prediction is a true positive (green), false positive (orange) or true negative or false negative for the current cut-off threshold. To preserve the privacy of the user whose emails are shown here, the content of the emails have been hidden and the identities of all senders and recipients have been anonymised.

for each email along with the corresponding feature value and learned weight distribution. This is extremely helpful for checking that the feature computation is correct, since the original email and computed features are displayed right next to each other.

Using this tool, we can assess qualitatively how well the system is working for a particular threshold on the reply probability. Looking at a lot of different emails, we find that the system seems to be working very well, despite the apparently moderate precision. This is because a proportion of the apparent incorrect predictions are actually reasonable, such as:

- False positives where the user "responded" to the email, but not by directly replying. This could be because they responded to the sender without using email, (for example: in person, on the phone or via instant messaging) or responding by writing a fresh email to the sender or by replying to a different email.

- False positives where the user intended to reply, but forgot to or didn't have time.

- False negatives where a user replied to an email, as a means of replying to an email earlier in the conversation thread.

- False negatives where a user replied to an email and deleted the contents/subject as a way of starting a new email to the sender.

In all four of these cases the prediction is effectively correct: in the first two cases this *is* an email that the user would want to reply to and in the last two it is not. The issue is that the 'ground truth' label that we have for the item is not correct, since whether or not a user wanted to reply to an email is assumed to be the same as whether they actually did. But in these four cases, it is not. Later in the chapter we will look at how to deal with such noisy ground truth labels.

Since the ground truth labels are used to evaluate the system, such incorrect labels can have a big detrimental effect on the measured accuracy. For example, if 25% of positive emails are incorrectly labelled as negatives, then the measured precision of a perfect classifier would be only 75% rather than 100%. If 5% of negative emails are also incorrectly labelled as positive then, for a user who replies to 10% of their emails, the recall of a perfect classifier would be just 62.5%! To see where this number came from, consider 1000 emails received by the user. The user would reply to 100 of these emails (10%) and so would not reply to 900 emails. Of the replied-to emails, only 75% (=75 emails) would be labelled positive and of the not-replied-to emails, 5% of 900 = 45 emails would be incorrectly labelled positive. So a perfect classifier would make positive predictions on 75 of the 75+45=120 emails that were labelled as positive, meaning that the measured recall would be $\frac{75}{120} = 62.5\%$.

However, even taking into account noisy ground truth labels, there are still a number of incorrect predictions that are genuinely wrong. Examples of these are:

1. False negatives where the email is a reply to an email that the user sent, but the sender is new or not normally replied to.

2. False negatives where the email is a forward, but the sender is new or not normally replied to.

3. False negatives for emails to a distribution list that the user owns or manages and so is likely to reply to.

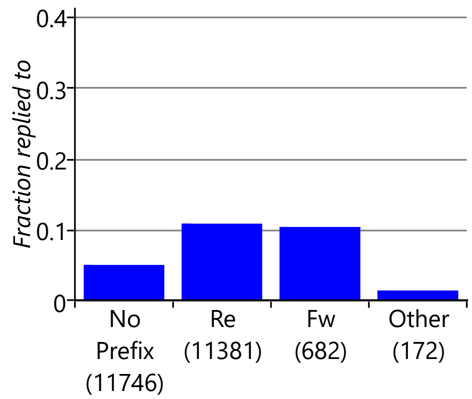


Figure 4.17: Fraction of emails that were replied to where the email had different subject prefixes (re,fw/fwd), an unknown prefix (other) or no prefix at all.

4. False positives for newsletter/marketing/social network emails (sometimes known as 'graymail') sent directly to the user, particularly where the sender is new.

We will now look at how to modify the feature set to address some of these incorrect predictions.

4.5.5 Improving the feature set

The first two kinds of incorrect prediction are false negative predictions where the email is a reply to an email from the user or a forward of an email to the user. These mistakes occur because no existing feature distinguishes between these cases and a fresh email coming from the same sender – yet if the email is a reply or forward, there is likely to be a very different reply probability. This violates Assumption 7, that is, whether the user will reply or not depends only on the feature values. To fix this issue, we need to introduce a new feature to distinguish these cases. We can detect replies and forwards, by inspecting the prefix on the subject line – whether it is "re:", "fw:", "fwd:" and so on. Figure 4.17 shows the fraction of emails replied to in the training and validation sets for known prefixes, an unknown prefix (other) or no prefix at all. The plot shows that, indeed, users are more likely to reply to messages which are replies or forwards and a *SubjectPrefix* feature might therefore be informative. What this plot does not tell us is whether this new feature gives additional information over the features we already have in our feature set. To check whether it does, we need to evaluate the feature set with and without this new feature. Figure 4.18 gives the area under the ROC curve and the average precision for each user and averaged, for our feature set with and without the *SubjectPrefix* feature.

What these results show is that the new feature sometimes increases accuracy and sometimes reduces accuracy depending on the user (whichever metric you look at). However, on average the accuracy is improved with the feature, which

UserName	AveragePrecision	AreaUnderCurve
User35CB8E5	52.1%	91.0%
UserCE3FDB4	35.8%	89.1%
User6AACED	45.0%	91.4%
User7E601F9	53.5%	80.2%
User68251CD	61.4%	87.3%
User223AECA	50.9%	90.1%
UserFF0F29E	29.3%	86.2%
User25C0488	32.5%	83.1%
User811E39F	25.3%	81.9%
User10628A6	47.3%	87.6%
Average	43.3%	86.8%

(a) Initial results

UserName	AveragePrecision	AreaUnderCurve
User35CB8E5	54.8%	91.0%
UserCE3FDB4	34.4%	89.1%
User6AACED	46.4%	91.2%
User7E601F9	53.2%	79.9%
User68251CD	62.8%	87.3%
User223AECA	50.2%	89.8%
UserFF0F29E	30.9%	87.2%
User25C0488	31.2%	82.2%
User811E39F	26.4%	82.2%
User10628A6	48.6%	88.6%
Average	43.9%	86.9%

(b) With *SubjectPrefix* feature

Figure 4.18: Evaluation results for each user and overall, for the previous feature set and a feature set with the new *SubjectPrefix* feature added. On average, both the area under the curve and the average precision are slightly improved by adding the *SubjectPrefix* feature.

suggests that we should retain it in the feature set. Notice that the average precision is a more sensitive metric than the area under the curve – so it is more helpful when judging a feature's usefulness. It is also worth bearing in mind that either evaluation metric only gives an overall picture. Whilst headline accuracy numbers like these are useful, it is important to always look at the underlying predictions as well. To do this we can go back to the tool and check that adding in this feature has reduced the number of false negatives for reply/forward emails. Using the tool, we find that this is indeed the case, but also that we are now slightly more likely to get false positives for the last email of a conversation. This is because the only difference between the last email of a conversation and the previous ones is the message content, which we have limited access to through our feature set. Although incorrect, such false positives can be quite acceptable to the user, since the user interface will bring the conversation to the user's attention, allowing them to decide whether to continue the conversation or not. So we have removed some false negatives that were quite jarring to the user at the cost of adding a smaller number of false positives that are acceptable to the user. This is a good trade-off – and also demonstrates the risk of paying too much attention to overall evaluation metrics. Here, a small increase in the evaluation metric (or even no increase at all for some users) corresponds to an improvement in user satisfaction.

The next kind of error we found were false negatives for emails received via distribution lists. In these situations, a user is likely to reply to emails received on certain distribution lists, but not on others. The challenge we face with this kind of error is that emails often have multiple recipients and, if the user is not explicitly named, it can be impossible to tell which recipients are distribution lists and which of these distribution lists contain the user. For example, if an email is sent to three different distribution lists and the user is on one of these, it may not be possible to tell which one.

To get around this problem, we can add a *Recipients* feature that captures all of the recipients of the email, on the grounds that one of them (at least) will correspond to the user. Again, this is helping to conform to Assumption 7 since we will no longer be ignoring a relevant signal: the identities of the email recipients. We can design this feature similarly to the *Sender* feature, except that multiple buckets of the feature will have non-zero values at once, one for each recipient. We have to be very careful when doing this to ensure that our new *Recipients* feature matches the assumptions of our model. A key assumption is the contribution of a single feature to the overall score is normally in the range -1.0 to 1.0, since the weight for a bucket normally takes values in the range and we have always used feature values of 1.0. But now if we have an email with twenty recipients, then we have twenty buckets active – if each bucket has a feature value of 1.0, then the *Recipients* feature would normally contribute between -20.0 to 20.0 to the overall score. To put it another way, the influence of the *Recipients* feature on the final prediction would be twenty times greater for an email with twenty recipients than for an email with one recipient. Intuitively this does not make sense since we really only care about the single recipient that caused the user to receive the email. Practically this would lead to the feature either dominating all the other features or being ignored depending on the number of recipients – very undesirable behaviour in either case. To rectify this situation, we can simply ensure that, no matter how many buckets of the feature are active, the sum of their feature values is always 1.0. So for an email with five recipients, five buckets are active, each with a feature value of 0.2. This solution is not perfect since there is really only one recipient that we care about and the signal from this recipient will be diluted by the presence of other recipients. A better solution would be to add in a variable to the model to identify the relevant recipient. To keep things simple, and to demonstrate the kind of compromises that arise when designing a feature set with a fixed model, we will keep the model the same and use a feature-based solution. As before, we can evaluate our system with and without this new *Recipients* feature.

The comparative results in Figure 4.19 are more clear-cut than the previous ones: in most cases the accuracy metrics increase with the *Recipients* feature added. Even where a metric does not increase, it rarely decreases by very much. On average, we are seeing a 0.2% increase in AUC and a 0.8% increase in AP. These may seem like small increases in these metrics, but they are in fact quite significant. Using the interactive tool tells us that a 1% increase in average precision gives a very noticeable improvement in the perceived accuracy of the system, especially if the change corrects particularly jarring incorrect predictions. For example, suppose a user owns a particular distribution list and replies to posts on the list frequently. Without the *Recipients* feature the

UserName	AveragePrecision	AreaUnderCurve
User35CB8E5	54.8%	91.0%
UserCE3FDB4	34.4%	89.1%
User6AACED	46.4%	91.2%
User7E601F9	53.2%	79.9%
User68251CD	62.8%	87.3%
User223AECA	50.2%	89.8%
UserFF0F29E	30.9%	87.2%
User25C0488	31.2%	82.2%
User811E39F	26.4%	82.2%
User10628A6	48.6%	88.6%
Average	43.9%	86.9%

(a) Without *Recipients* feature

UserName	AveragePrecision	AreaUnderCurve
User35CB8E5	57.6%	91.7%
UserCE3FDB4	33.9%	89.0%
User6AACED	46.7%	91.1%
User7E601F9	54.5%	80.2%
User68251CD	63.8%	87.7%
User223AECA	51.5%	89.2%
UserFF0F29E	30.6%	87.2%
User25C0488	32.1%	83.3%
User811E39F	26.4%	82.3%
User10628A6	50.0%	88.9%
Average	44.7%	87.1%

(b) With *Recipients* feature

Figure 4.19: Evaluation results for the previous feature set without the *Recipients* feature and for a feature set with the *Recipients* feature included.

system would likely make incorrect predictions on such emails which would be quite jarring to the user, as the owner of the distribution list. Fixing this problem by adding in the *Recipients* feature would substantially improve the user's experience despite leading to only a tiny improvement in the headline AUC and AP accuracy numbers.

We are now free to go to the next problem on the list and modify the feature set to try to address it. For example, addressing the issue of 'graymail' emails would require a feature that looked at the content of the email – in fact a word feature works well for this task. For the project with the Exchange team, we continued to add to and refine the feature set, ensuring at each stage that the evaluation metrics were improving and that mistakes on real emails were being fixed, using the tool. Ultimately we reached the stage where the accuracy metrics were very good and the qualitative accuracy was also good. At this point you might think we were ready to deploy the system for some beta testers – but in real machine learning systems things are never that easy. . .

Review of concepts introduced in this section

recall Another term for the true positive rate, often used when we are trying to find rare positive items in a large data set. The recall is the proportion of these items successfully found ('recalled') and is therefore equal to the true positive rate.

precision The fraction of positive predictions that are correct. Precision is generally complementary to recall in that higher precision means lower recall and vice versa. Precision is often used as an evaluation metric in applications where the focus is on the accuracy of positive predictions. For example, in a search engine the focus is on the accuracy of the documents that are retrieved as results and so a precision metric might be used to evaluate this accuracy.

This kind of precision should not be confused with the inverse variance of a Gaussian which is also known as the precision. In practice, the two terms are used in very different contexts so confusion between the two is rare.

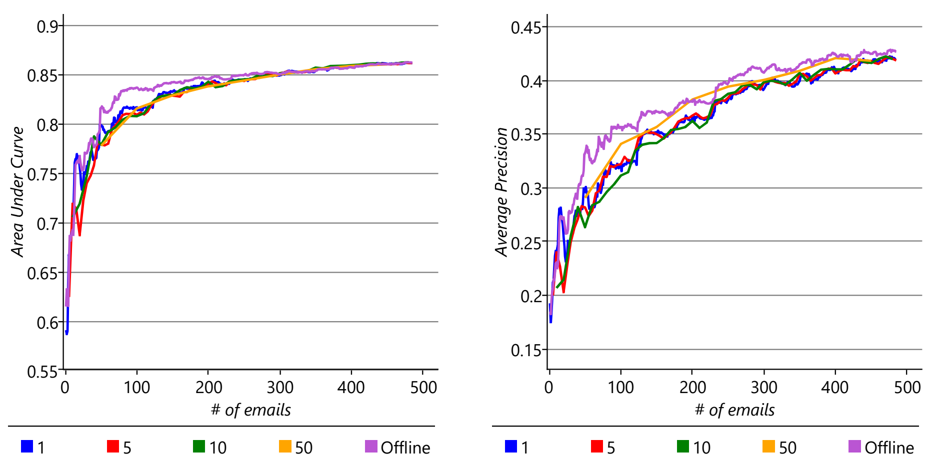
precision-recall curve A plot of precision against recall for a machine learning system as some parameter of the system is varied (such as the threshold on a predicted probability). Precision-recall curves are useful for assessing prediction accuracy when the probability of a positive prediction is relatively low.

average precision The average precision across a range of recalls in the precision-recall curve, used as a quantitative evaluation metric. This is effectively the area under the P-R curve if the full range of recalls is used. However, the very left hand end of the curve is often excluded from this average since the precision measurements are inaccurate, due to being computed from a very small number of data items.

4.6 Learning as emails arrive

So far we've been able to train our model on a large number of emails at once. But for our application we need to be able to learn from a new email as soon as a user replies to it, or as soon as it becomes clear that the user is not going to reply to it. We cannot wait until we have received a large number of emails, then train on them once and use the trained model forever. Instead, we have to keep training the model as new emails come in and always use the latest trained model to make predictions.

As we saw in section 3.3 in the previous chapter, we can use online learning to continually update our model as we receive new training data. In our model online learning is straightforward: for each batch of emails that have arrived since we last trained, we use the previous posterior distributions on `weight` and `threshold` as the priors for training. Once training on the batch is complete, the new posterior distributions over `weight` and `threshold` can be used for making predictions. Later when the next batch of emails is trained on, these posterior distributions will act as the new priors. We can check how well this procedure works by dividing our training data into batches and running online learning as each batch comes in. We can then evaluate this method in comparison to offline training, where all the training data seen up to that point is presented at once. Figure 4.20 shows the AUC and AP averaged across all 10 users using either offline training or online training with different batch sizes.



(a) Area Under Curve (b) Average Precision

Figure 4.20: Prediction accuracy as more and more training emails become available, averaged over all 10 users. For each metric, the offline curve shows the accuracy if we retrain the model from scratch on all emails received up to that point. The four other curves show the accuracy if we instead do online training to update the model incrementally after every 1, 5, 10 or 50 emails.

These results show that online learning gives an accuracy similar to, but slightly lower than offline training, with larger batch sizes giving generally better accuracy. The plots also show that the difference in accuracy decreases as more emails are received. So it seems like online learning could be a suitable solution, once sufficient emails have been received. But this brings us to another problem: it takes around 400 to 500 emails for the average precision to get close to a stable value. For a time before that number is reached, and particularly when relatively few emails have been trained on, the accuracy of the classifier is low. This means that the experience for new users would be poor. Of course, we could wait until the user has received and acted on sufficient emails, but for some users this could take weeks or months. It would be much better if we could give them a good experience straight away. The challenge of making good predictions for new users where there is not yet any training data is known as a **cold start problem**.

4.6.1 Modelling a community of users

We've already shown that we can solve certain prediction problems by changing the feature set. But in this case, there is no change to the feature set that can help us – we cannot even compute feature values until we have seen at least one email! But since we have a classification model rather than a fixed classification algorithm, we have an additional option available to us: to change the model.

How can we change our model to solve the cold start problem? We can exploit the fact that different users tend to reply to the same kinds of emails. For example, users tend to be more likely to reply to emails where they are first on the To line or where the email is forwarded to them. This suggests that we might expect the learned weights to be similar across users, at least for those feature buckets that capture behaviours common amongst users. However, there may also be other feature buckets which capture differences in the behaviour from user to user, where we may expect the learned weights to differ between users. To investigate which feature buckets are similar across users, we can plot the learned weights for the first five of our users, for all feature buckets that they have in common (that is, all buckets except those of the *Sender* and *Recipients* features). The resulting plot is shown in Figure 4.21.

Learning from many users will help us to make better predictions for a new user.

As you can see, for many feature buckets, the weights are similar for all five users and even for buckets where there is more variability across users the weights tend to be all positive or all negative. But in a few cases, such as the *FromMe* feature, there is more variability from user to user. This variability suggests that these features capture differences in behaviour between users, such as whether a particular user sends emails to themselves as reminders. Overall

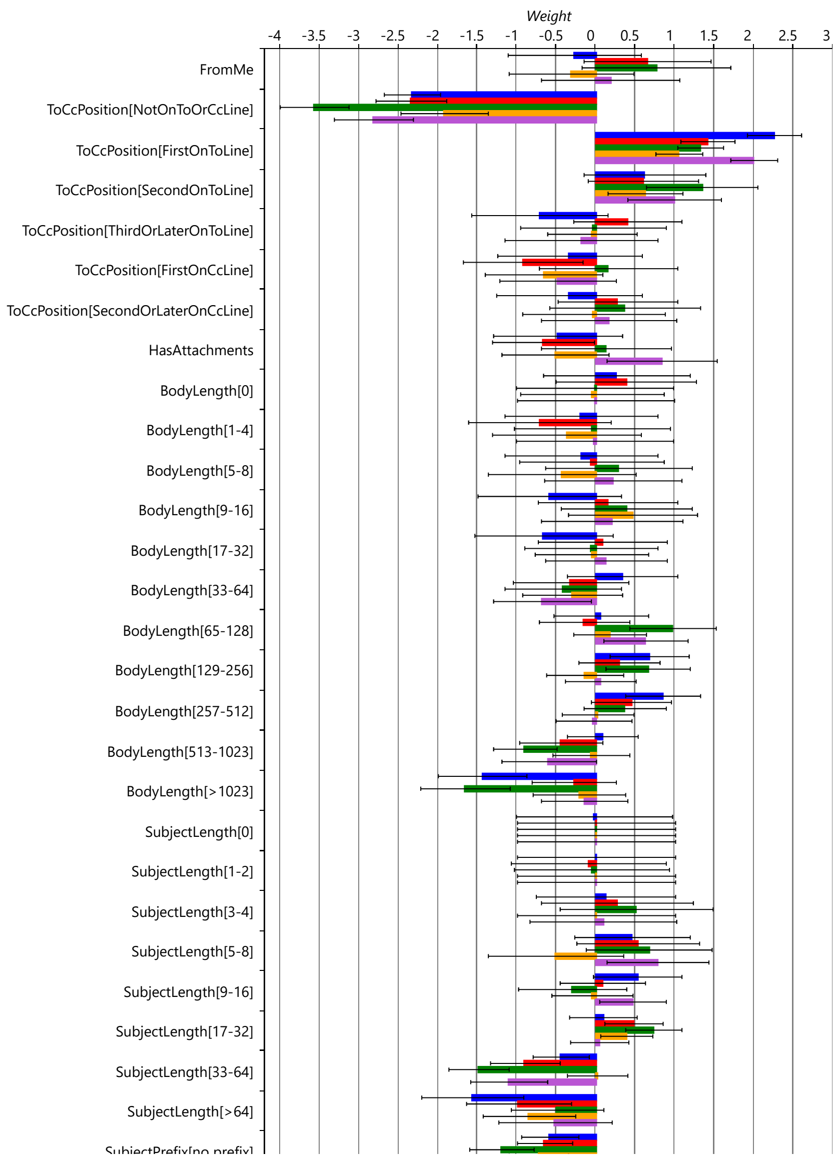


Figure 4.21: Learned Gaussian distributions for the weights for each feature bucket for the first five users in our data set. For most feature buckets the learned weights are similar across users, demonstrating that they reply to emails with similar characteristics.

it seems like there is enough similarity between users that we could exploit this similarity to make predictions for a completely new user. To do this, we need to make a new modelling assumption about how the weights vary across multiple users:

⑧ Across many users the variability in the weight for a feature bucket can be captured by a Gaussian distribution.

This assumptions says that we can represent how a weight varies across users by an average weight (the mean of the Gaussian distribution) and a measure of how much a typical user's weight deviates from this average (the standard deviation of the Gaussian distribution).

Let's change our model to add in this assumption. Since we are now modelling multiple users, we need to add a plate across users and put our entire existing model inside it. The only variables outside of this new plate will be two new variables per feature bucket: `weightMean` to capture the average weight across users and `weightPrecision` to capture the precision (inverse variance) across users. We then replace the *Gaussian*(0,1) factor inside the plate (that we used to use as a prior) by a Gaussian factor connected to `weightMean` and `weightPrecision`. The resulting factor graph is shown in Figure 4.22.

You'll notice that we have used precision (inverse variance) rather than variance to capture the variability in weights across users. A high `weightPrecision` for a bucket means that its weight tends to be very similar from user to user, whilst a low `weightPrecision` means the bucket weight tends to vary a lot from user to user. We choose to use precision because we are now trying to learn this variability and it turns out to be much easier to do this using a precision rather than a variance. This choice allows us to use a **gamma distribution** to represent the uncertainty in the `weightPrecision` variable, either when setting its prior distribution or when inferring its posterior distribution. The gamma distribution is a distribution over continuous positive values (that is, values greater than zero). We need to use a new distribution because precisions can only be positive – we cannot use a Gaussian distribution since it allows negative values, and we cannot use a beta distribution since it only allows values between zero and one. The gamma distribution also has the advantage that it is the conjugate distribution for the precision of a Gaussian (see Panel 3.3 and Bishop [2006]).

The gamma distribution has the following density function:

$$Gamma(x; k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\theta^k \, \Gamma(k)} \tag{4.1}$$

where $\Gamma()$ is the gamma function, used to ensure the area under the density function is 1.0. The gamma distribution has two parameters: the *shape* parameter k and the *scale* parameter θ – example gamma distributions with different values of these parameters are shown in Figure 4.23a. Confusingly, the gamma distribution is sometimes parameterised by the shape and the *inverse* of the scale, called the *rate*. Since both versions are common it is important to check which is being used – in this book, we will always use shape and scale parameters.

Since we have relatively few users, we will need to be careful in our choice of gamma prior for `weightPrecision` since it will have a lot of influence on how the model behaves. Usually we expect the precision to be higher than 1.0, since we expect most weights to be similar across users. However, we also need to allow the precision to be around 1.0 for those rarer weights that vary substantially across users. Figure 4.23b shows a *Gamma*(4,0.5) distribution that meets both of these requirements.

There is one more point to discuss about the model in Figure 4.22, before we try it out. If you are very observant, you will notice that the `threshold` variable has been fixed to zero. This is because we want to use our communal `weightMean` and `weightPrecision` to learn about how the threshold varies across users as well as how the weights vary. To do this, we can use a common trick which is to fix the threshold to zero and create a new feature which is always on for all

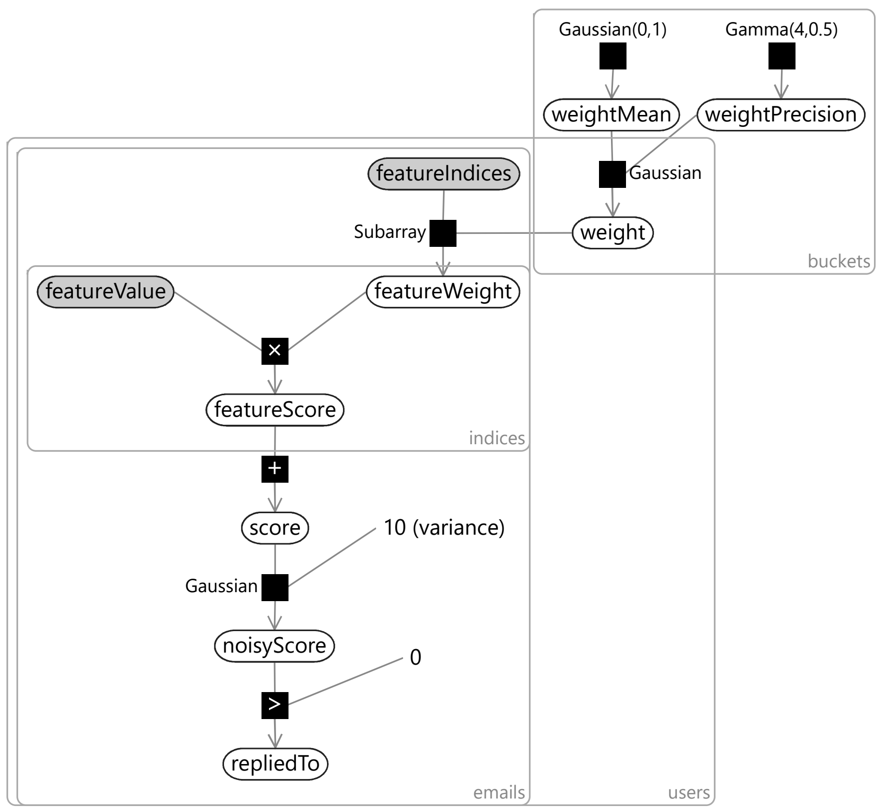


Figure 4.22: Model for jointly classifying emails of multiple users. Our classification model is duplicated for each user by placing it inside a `users` plate. We then introduce two shared variables for each feature bucket: `weightMean` captures the typical (average) weight for that bucket across users and `weightPrecision` captures how much the weight tends to vary across users.

emails – this is known as the **bias**. The idea is that changing the score by a fixed value for all emails is equivalent to changing the threshold by the same value. So we can use the bias feature to effectively set the threshold, whilst leaving the actual threshold fixed at 0. Since feature weights have a $Gaussian(0,1)$ prior but the threshold has a $Gaussian(0,10)$ prior, we need to set the value of this new bias feature to be $\sqrt{10}$, in order to leave the model unchanged – if we have a variable whose uncertainty is $Gaussian(0,1)$ and we multiply it by $\sqrt{10}$, we get a variable whose uncertainty is $Gaussian(0,10)$, as required.

4.6.2 Solving the cold start problem

We can now train our communal model on the first five users (the users whose weights were plotted in Figure 4.21). Even though we have substantially changed the model, we are still able to use expectation propagation to do inference tasks like training or prediction. So we do not need to invent a new algorithm to do joint training on multiple users – we can just run the familiar EP algorithm on our extended model.

A hands-on solution to the cold start problem

Figure 4.24 shows the community weight distributions learned: each bar shows the mean of the posterior over `weightMean` and the error bars show a standard deviation given by the mean value of `weightPrecision`. Note the different use of error bars – to show `weightPrecision` (the learned variability across users) rather than the uncertainty in `weightMean` itself. If you compare the distributions of Figure 4.24 with the individual weights of Figure 4.21, you can see how the

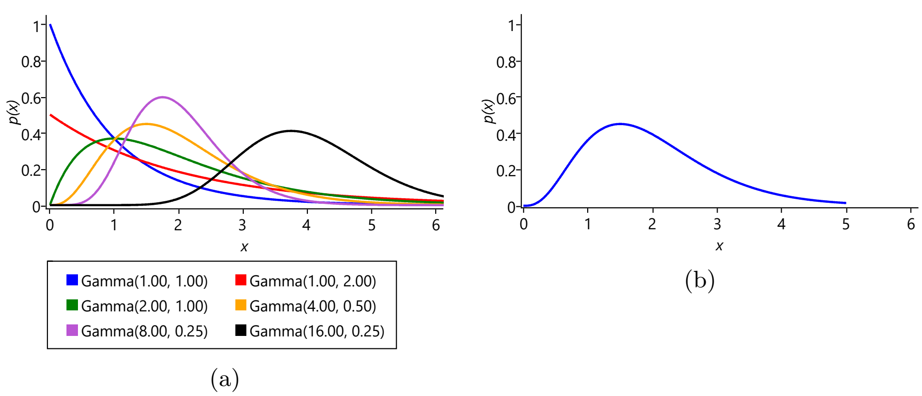


Figure 4.23: (a) Example gamma distributions for different values of the shape and scale parameters. (b) The $Gamma(4,\ 0.5)$ distribution which we use as a prior for the precision of the weights.

learned distributions have nicely captured the variability in weights across users.

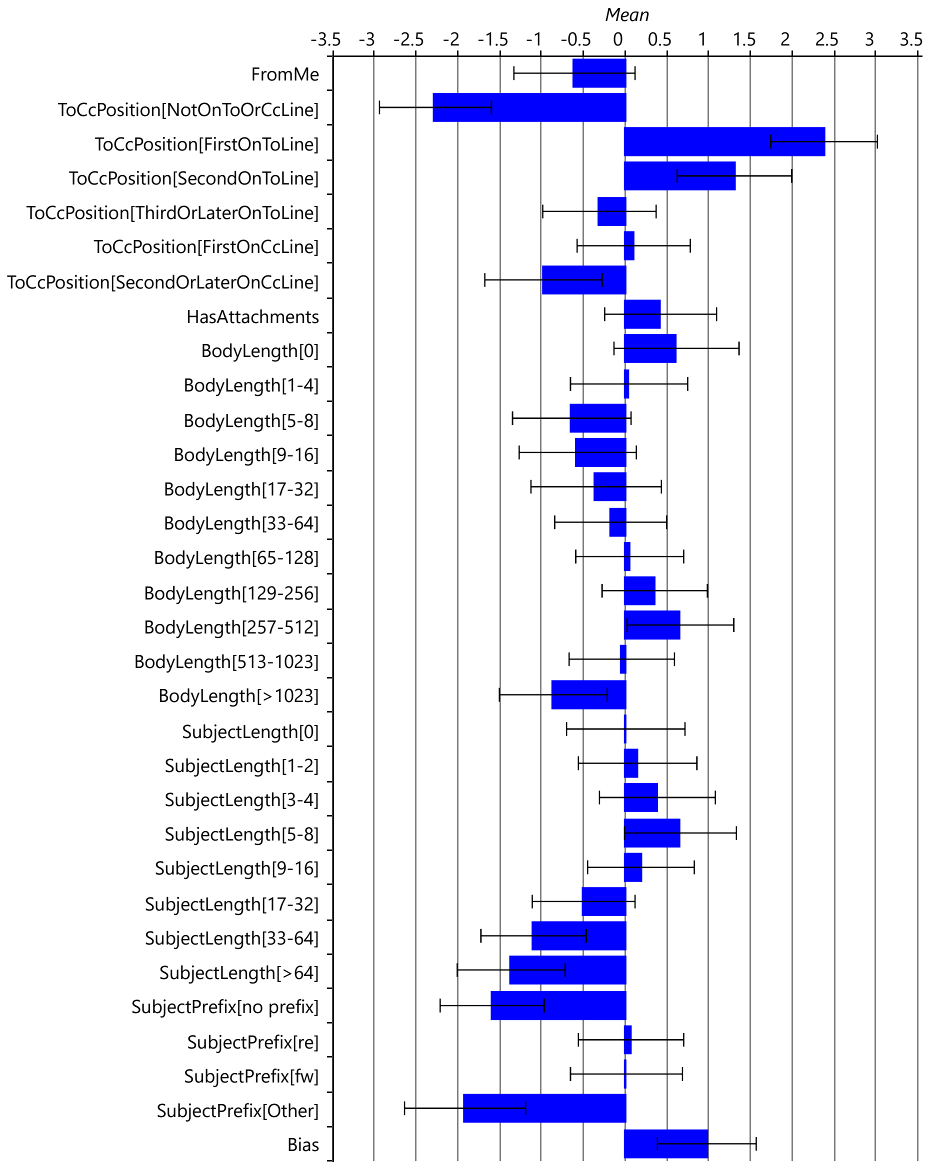


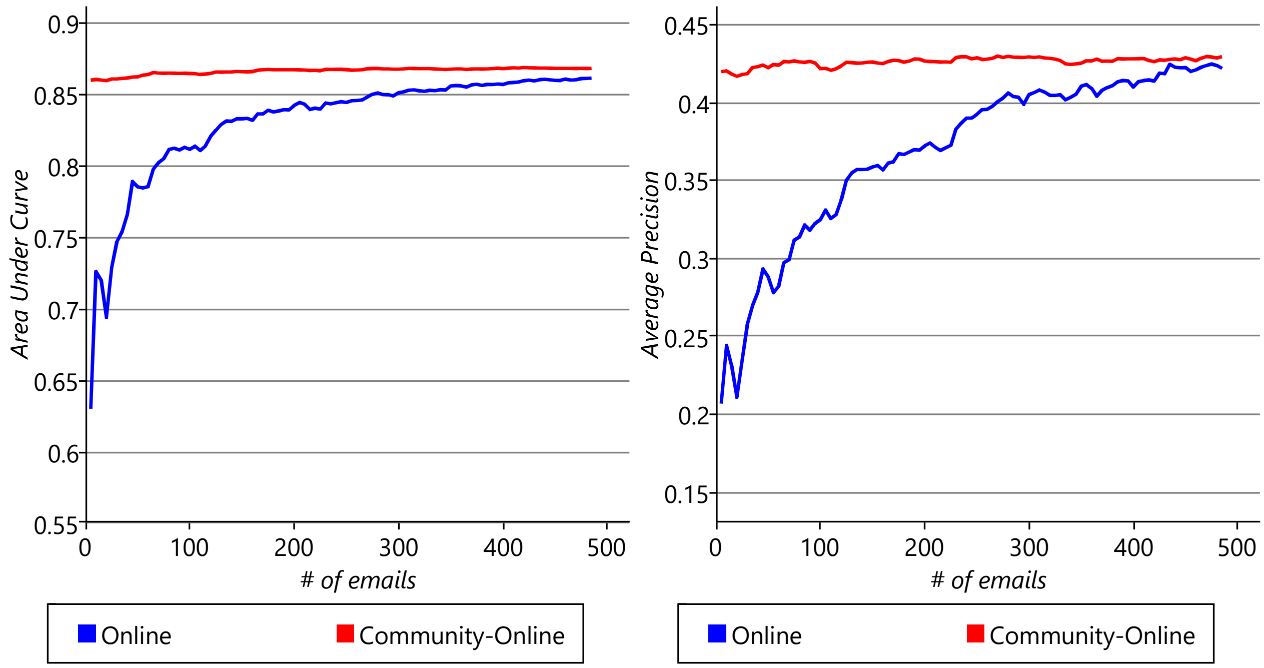
Figure 4.24: Community weight distributions learned from the first five users in our data set. The blue bar shows the expected value of `weightMean` and the errors bars show one standard deviation either side of this corresponding to the expected value of `weightPrecision`. Comparing to Figure 4.21 shows that the learned weight distributions are consistent with the weights learned individually for each user.

To apply our learned community weight distributions for a new user, we can use the same model configured for a single user with the priors over `weightMean` and `weightPrecision` replaced by the Gaussian and gamma posteriors learned from the first five users. We can use this model to make predictions even when we have not seen any emails for the new user. But we can also use the model to do online training, as we receive emails for a new user. As we do online training using the community model, we can smoothly evolve from making generic predictions that may apply to any user to making personalised predictions specific to the new user. This evolution happens entirely automatically through doing inference in our model – there is no need for us to specify an ad-hoc procedure for switching from community to personalised predictions.

Figure 4.25 shows the accuracy of predictions made using online training in the community model compared to the individual model (using a batch size of 5) for varying amounts of training data. For this plot we again average across all ten users – we make prediction results for the first five users using a separate community model trained on the last five users. The results are very satisfactory – the initial accuracy is high (an average AP of 41.8%) and then it continues to rise smoothly until it reaches an average AP of 43.2% after 500 emails have been trained on. As we might have hoped, our community model is making good predictions from the start, which then become even better as the model personalizes to the individual user. The cold start problem is solved!

In the production system used by Exchange, we had a much larger number of users to learn community weights from. In this case, the posteriors over `weightMean` and `weightPrecision` became very narrow. When these posteriors are used as priors, the values of `weightMean` and `weightPrecision` are effectively fixed. This allows us to make a helpful simplification to our system: once we have used the multi-user model to learn community weight distributions, we can go back to the single user model to do online training and make predictions. All we need to do is replace the *Gaussian*(0,1) prior in the single user model with a Gaussian prior whose mean and precision are given by the expected values of the narrow `weightMean` and `weightPrecision` distributions. So, in production, the multi-user model is trained once offline on a large number of users and the learned community weight distributions are then used to do training and prediction separately for each user. This separation makes it easier to deploy, manage and debug the behaviour of the system since each user can be considered separately.

There is one final thing to do before we deploy our system to some beta testers. Remember the test sets of email data that we put to one side at the start of the chapter? Now is the time to break them out and see if we get results on the test sets that are comparable to the results we have seen on our validation sets. Comparative results for the validation and test sets are shown in Table 4.5.



(a) Area Under Curve (b) Average Precision

Figure 4.25: Prediction accuracy against amount of training data using individual models or the community model. In both cases training is done online with batches of 5 emails. Results are averaged over all 10 users – for the first five users prediction uses a community model trained on the second five users, and vice versa for the second five users.

UserName	AveragePrecisionValidation	AveragePrecisionTest	AreaUnderCurveValidation	AreaUnderCurveTest	ValidationReplyCount	TestReplyCount
User35CB8E5	57.6%	90.6%	91.7%	92.3%	74	10
UserCE3FDB4	33.9%	38.5%	89.0%	88.2%	64	21
User6AACED	46.7%	46.0%	91.1%	91.7%	58	16
User7E601F9	54.5%	54.2%	80.2%	84.3%	119	36
User68251CD	63.8%	78.8%	87.7%	89.3%	142	62
User223AECA	51.5%	24.3%	89.2%	82.6%	51	12
UserFF0F29E	30.6%	24.3%	87.2%	85.5%	119	40
User25C0488	32.1%	39.4%	83.3%	86.1%	114	44
User811E39F	26.4%	36.9%	82.3%	82.6%	129	64
User10628A6	50.0%	55.5%	88.9%	90.3%	61	24
Average	44.7%	48.9%	87.1%	87.3%	93.1	32.9

Table 4.5: Final accuracy results for the validation and test sets for each user and overall. The right-hand columns show the number of replied to emails in each data set, which gives an indication of the reliability of the corresponding average precision metric.

The table shows that the AUC measurements for the users' test sets are generally quite similar to those of the validation sets, with no obvious bias favouring one or the other. This suggests that in designing our model and feature set we have not overfit to the validation data. The AP measurements are more different, particularly for some users – this is because the test sets are quite small and some contain only a few replied-to emails. In such situations, AP measurements become quite noisy and unreliable. However, even if we focus on those users with more replied to emails, it does not appear that the test AP is consistently lower than the validation AP. So both evaluation metrics suggest that there is no fundamental difference between test and validation set accuracies and so we should expect to achieve similar prediction accuracy for real users.

4.6.3 Final testing and changes

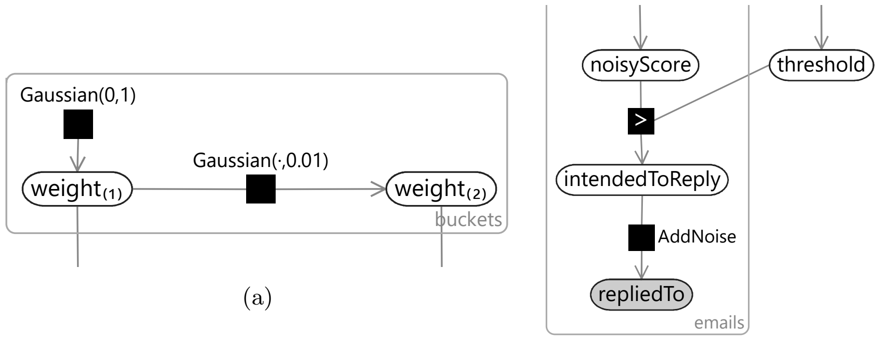
At this point, the prediction system was deployed to beta testers for further real-world testing. Questionnaires were used to get feedback on how well the system was working for users. This testing and feedback highlighted two additional issues:

- The predictions appeared to get less accurate over time, as the user's behaviour evolved, for example, when they changed projects or changed teams the clutter predictions did not seem to change quickly enough to match the updated behaviour.

- The calibration of the system, although correct on average, was incorrect for individual users. The predicted probabilities were too high for some users and too low for others.

Investigation of the first issue identified a similar problem to the one we diagnosed in chapter 3. We have assumed that the weights in the model are fixed across time for a particular user. This assumption does not allow for user behaviour to change. The solution was to change the model to allow the weights to change over time, just as we allowed the skills to change over time in the TrueSkill system. The modified model has random variables for each bucket weight for each period of time, such as a variable per week. Figure 4.26a shows an example model segment that contains weights for two consecutive weeks $\texttt{weight}_{(1)}$ and $\texttt{weight}_{(2)}$. To allow the weights to change over time, the weight for the second week is allowed to vary slightly from the weight for the first week, through adding Gaussian noise with very low variance. As with the TrueSkill system, this change allows the system to track slowly-changing user behaviours.

The second issue was harder to diagnose. Investigation of the issue found that the too-high predicted probabilities occurred for users that had a low volume of clutter and the too-low predicted probabilities occurred for users that had a high volume of clutter. It turned out that the problem was the noisy ground truth labels that we encountered in section 4.5 – for users with a high



(a) (b)

Figure 4.26: Modifications to the model to fix issues found by beta testers (a) Allowing the weights to change over time addresses the issue that action predictions do not evolve as user behaviour changes (b) Explicitly modelling the difference between the intended action label and the actual action label addresses poor calibration that occurs when the intended and actual labels do not match.

volume of clutter, a lot of clutter items were incorrectly labelled as not clutter and vice versa for users with a low volume of clutter. Training with these incorrect labels introduced a corresponding bias into the predicted probability of clutter. The solution here is to change the model to represent label noise explicitly. For example, for reply prediction, we can create a new variable in the model `intendedToReply` representing the true label of whether the user truly intended to reply to the message. We then define the observed label `repliedTo` to be a noisy version of this variable, using a factor like the *AddNoise* factor that we used back in chapter 2. Figure 4.26a shows the relevant piece of a modified model with this change in place. Following this change, the calibration was found to be much closer to ideal across all users and the systematic calibration variation for users with high or low clutter volume disappeared.

In addressing each of these issues we needed to make changes to the model, something that would be impossible with a black box classification algorithm, but which is central to the model-based machine learning approach. With these model changes in place, the Clutter prediction system is now deployed as part of Office365, helping to remove clutter emails from peoples' inboxes. Figure 4.27 shows a screenshot of the system in action, all using model-based machine learning!

Review of concepts introduced in this section

cold start problem The problem of making good predictions for a new entity (for example, a new user) when there is very little (or no) training data

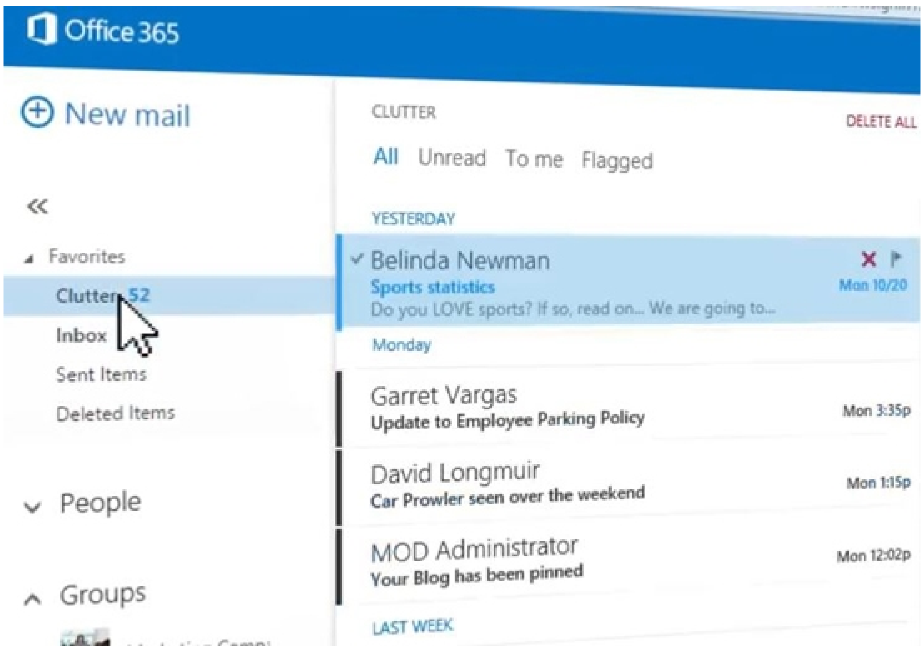


Figure 4.27: The clutter system in action in Office 365.

available that is specific to that entity. In general, a cold start problem can occur in any system where new entities are being introduced – for example, in a recommendation system, a cold start problem occurs when trying to predict whether someone will like a newly released movie that has not yet received any ratings.

gamma distribution A probability distribution over a positive continuous random variable whose probability density function is

$$Gamma(x; k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\theta^k \, \Gamma(k)} \tag{4.2}$$

where $\Gamma()$ is the gamma function, used to ensure the area under the density function is 1.0. The gamma distribution has two parameters *shape* parameter k and the *scale* parameter θ.

bias A feature which is always on for all data items. Since the bias feature is always on, its weight encodes the prior probability of the label. For example, the bias weight might encode probability that a user will reply to an email, before we look at any characteristics of that particular email. Equivalently, use of a bias features allows the `threshold` variable to be fixed to zero, since it is no longer required to represent the prior label probability.

Chapter 5

Making Recommendations

Whether you're into music, books, films or video games, a good recommendation can be a real joy – and can help less well known works get into the spotlight. But what one person considers a new classic, another will write off as a dud. Can a model be used to understand what someone likes and dislikes well enough to provide tailored recommendations?

Retailers of all kinds are keen to make accurate, personalized recommendations to their customers. But developing an automatic recommendation system requires expertise and investment beyond the means of many retailers, especially smaller ones. Instead, such retailers can turn to the cloud and make use of online recommendation services.

In Microsoft, the Azure Machine Learning team wanted to make it easy for developers and data scientists to embed predictive analytics and machine learning into their applications. The team's solution was a cloud-based platform for building and exploring analytics pipelines, constructed from a number of machine learning building blocks (Figure 5.1). Crucially, the platform also lets these pipelines be deployed as web services which can then be accessed from within an application. With high demand for automated recommendation, the Azure ML team wanted to have building blocks for making recommender systems, flexible enough to meet the needs of different customers.

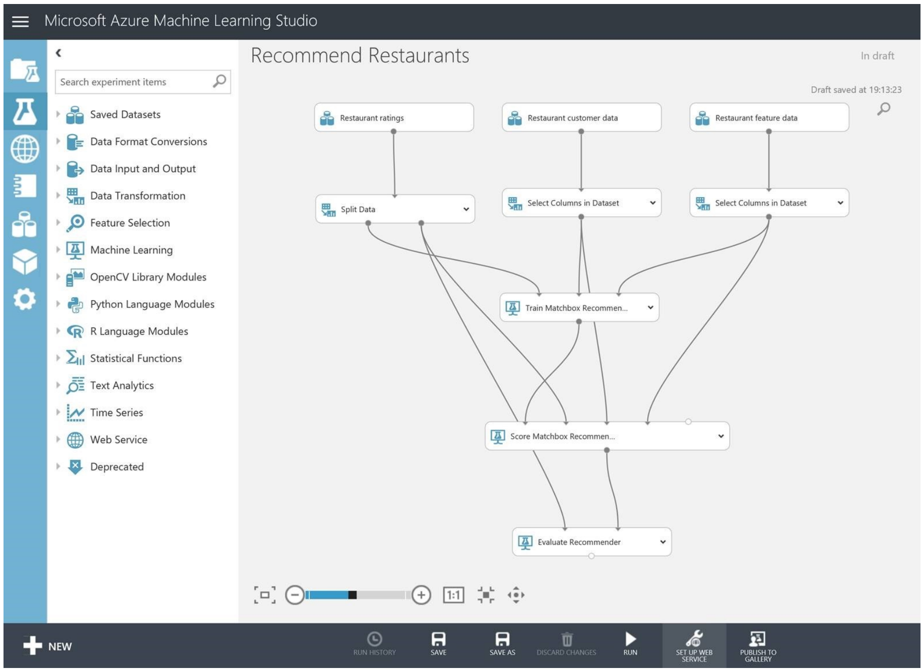


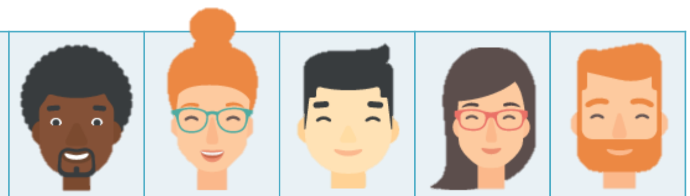
Figure 5.1: The goal: make it possible to construct customized recommendation services in Azure Machine Learning.

Potential customers had varying requirements that a recommender system needed to fulfill. Some wanted to make recommendations based solely on other items that a user has liked or disliked. Some had extra information about each item (such as the genre of a movie) that they wanted the system to take into account. Similarly, some had additional data about their users (such as age or gender) that they wanted to use to improve recommendations. Furthermore, while some user feedback came in the form of star ratings, other feedback systems only allowed users to like or dislike items. In addition, the items being recommended varied from traditional retail products like books and films, to restaurants and online services.

We needed to construct a model that could meet all of these requirements. In this chapter, we'll show how to develop such a flexible model and how to use it to make personalised recommendations. As an example, we will be using movies as the items to make recommendations for, since these have been very well explored and there are freely available data sets of movie ratings. We will start with an initial model that can predict like or dislike and then extend it to meet the additional customer requirements mentioned above. The model that we will develop in this chapter is closely based on the Matchbox model of Stern et al. [2009].

5.1 Learning about people and movies

The goal of this chapter is to make personalized movie recommendations to particular people. One way to think about this problem is to imagine a table where the rows are movies and the columns are people. The cells of the table show whether the person likes or dislikes the movie – for example, as shown in Table 5.1. This table is an illustration of the kind of data we might have to train a recommender system, where we have asked a number of people to say whether they like or dislike particular movies.



Movie					
The Lion King	👍			👎	
Lethal Weapon	👎	👍	👍	👍	
The Sound of Music		👍			👎
Amadeus	👍	👎		👍	
When Harry Met Sally	👍	👍		👎	👍

Table 5.1: A table showing the kind of data used to train a recommender system. Each row is a movie and each column is a person. Filled cells show where a person has said that they liked or disliked a movie. Empty cells show where we do not have any information about whether the person liked the movie, and so are where we could make a like/dislike prediction. Making such a prediction for every empty cell in a person's column would allow us to make a movie recommendation for that person – for example, by recommending the movie with the highest probability that the person would like it.

The empty cells in Table 5.1 show where we do not know whether the person likes the movie or not. There are bound to be such empty cells – we cannot ask every person about every movie and, even if we did, there will be movies that a person has not seen. The goal of our recommender system can be thought of as filling in these empty cells. In other words, given a person and a movie, predict whether they will like or dislike that movie. So how can we go about making such a prediction?

5.1.1 Characterizing movies

Let's start by considering how to characterize a movie. Intuitively, we can assume that each movie has some traits, such as whether it is an escapist or realistic, action or emotional, funny or serious. If we consider a particular trait as a line, we can imagine placing movies on that line, like this:

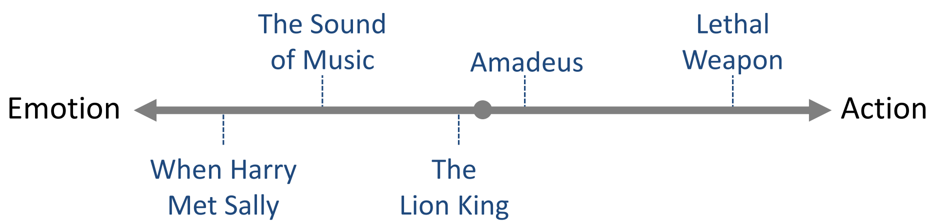


Figure 5.2: Movies placed on a line representing how much each movie is an emotional movie or as an action movie (or neither).

Movies towards the left of the line are emotional movies, like romantic comedies. Movies towards the right of the line are action movies. Movies near the middle of the line are neutral – neither action movies nor emotional movies. Notice that, in defining this trait, we have made the assumption that action and emotional are opposites.

Now let's consider people. A particular person might like emotional movies and dislike action movies. We could place that person towards the left of the line (Figure 5.3). We would expect such a person to like movies on the left-hand end of the line and dislike movies on the right-hand end of the line.

Figure 5.3: A person placed on the left of the line would be expected to like emotional movies and dislike action movies.

Another person may have the opposite tastes: disliking emotional movies and loving action movies. We can place this person towards the right of the line (Figure 5.4). We would expect such a person to dislike movies on the left-hand end of the line and like movies on the right-hand end of the line.

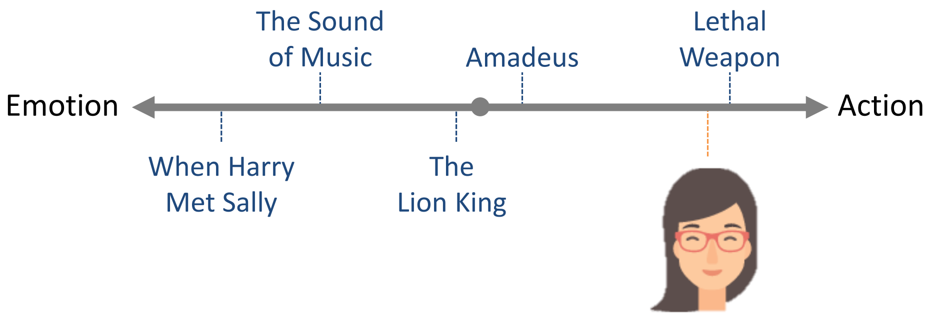


Figure 5.4: A person placed on the right of the line would be expected to like action movies and dislike emotional movies.

It is also perfectly possible a person to like (or dislike) both action and emotional movies. We could consider such a person to be neutral to the action/emotion trait and place them in the middle of the line (Figure 5.5). We would expect that such a person might like or dislike movies anywhere on the line.

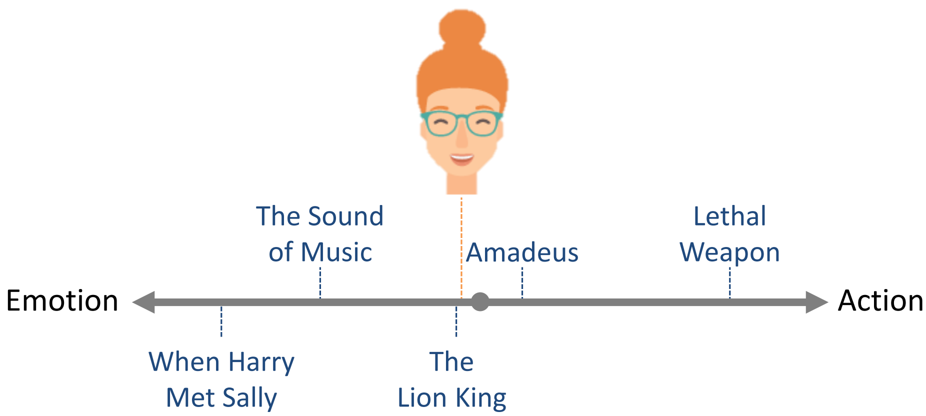


Figure 5.5: A person placed in the middle of the line, would be expected to not care whether a movie was an action movie or an emotional one.

We'd like to use an approach like this to make personalized recommendations. The problem is that we do not know where the movies lie on the line *or* where the people lie on the line. Luckily, we can use model-based machine learning to infer both of these using an appropriate model.

5.1.2 A model of a trait

Let's build a model for the action/emotion trait we just described. First, let's state some assumptions that follow from the description above:

① Each movie can be characterized by its position on the trait line, represented as a continuous number.

② A person's preferences can be characterized by a position on the trait line, again represented as a continuous number.

In our model, we will use a `trait` variable to represent the position of each movie on the trait line. Because it is duplicated across movies, this variable will need to lie inside a `movies` plate. We also need a variable for the position of the person on the line, which we will call `preference` since it encodes the person's preferences with respect to the trait. To make predictions, we need a variable showing how much the person is expected to like each movie. We will call this the `affinity` variable and assume that a positive value of this variable means that we expect the person to like the movie and a negative value means that we expect the person to dislike the movie.

We need a way to combine the `trait` and the `preference` to give the behaviour described in the previous section. That is, a person with a negative (left-hand end) `preference` should prefer movies with negative (left-hand end) `trait` values. A person with a positive (right-hand end) `preference` should prefer movies with positive (right-hand end) `trait` values. Finally, a neutral person with a `preference` near zero should not favour any movies, whatever their `trait` values. This behaviour can be summarised as an assumption:

③ A positive preference value means that a person prefers movies with positive values of the trait (and vice versa for negative values). The absolute size of the preference value indicates the strength of preference, where zero means indifference.

This behaviour assumption can be encoded in our model by defining `affinity` to be the product of the `trait` and the `preference`. So we can connect these variables using a product factor, giving the factor graph of Figure 5.6.

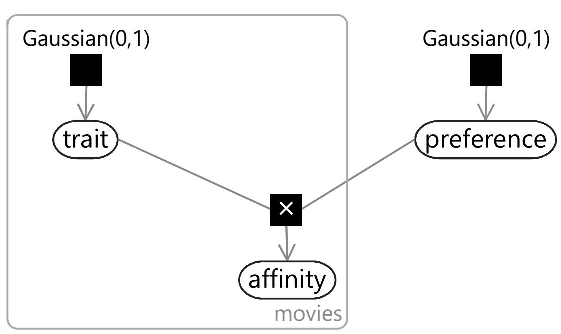


Figure 5.6: Factor graph for a single trait. Each movie has a `trait` value which is multiplied by the person's `preference` to give their `affinity` for that movie. More positive `affinity` values mean that the person is more likely to like the movie.

If you have a very good memory, you might notice that this factor graph is nearly identical to the one for a one-feature classifier (Figure 4.1) from the previous chapter. The only difference is that we have an unobserved `trait` variable where before we had an observed `featureValue`. As we construct our recommendation model, you will see that it is similar in many ways to the classification model from chapter 4.

Given this factor graph, we want to infer both the movies' `trait` values and the person's `preference` from data about the person's movie likes and dislikes. To do any kind of learning we need to have some variable in the model that we can observe – more specifically, we need a binary variable that can take one of two values (like or dislike). Right now we only have a continuous `affinity` variable rather than a binary one. Sounds familiar? Yes! We encountered exactly this problem back in section 4.2 of the previous chapter, where we wanted to convert a continuous score into a binary reply prediction. Our solution then was to add Gaussian noise and then threshold the result to give a binary variable. We can use exactly the same solution here by making a noisy version of the affinity (called `noisyAffinity`) and then thresholding this to give a binary `likesMovie` variable. The end result is the factor graph of Figure 5.7 (which closely resembles Figure 4.4 from the last chapter).

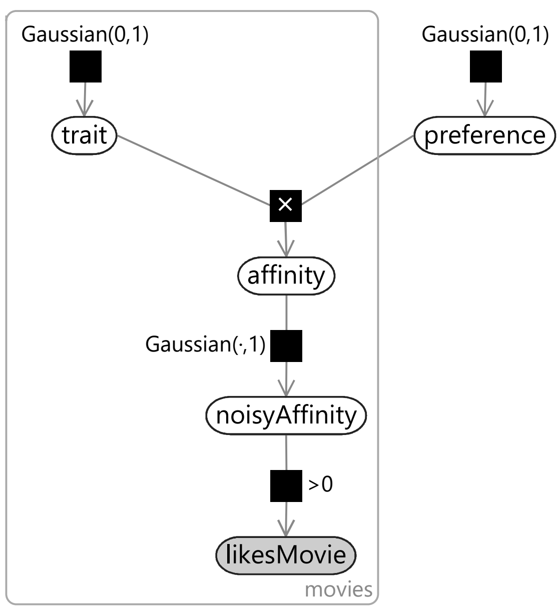
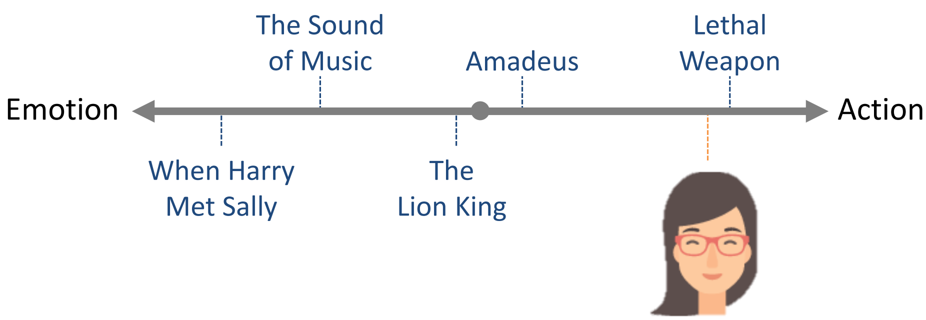


Figure 5.7: Extended factor graph that converts the continuous `affinity` into a binary `likesMovie` variable, which can be observed to train the model.

We could start using this model with one trait and one person, but that wouldn't get us very far – we would only learn about the movies that the person has already rated and so would only be able to recommend movies that they have already seen. In the next section, we will extend our model to handle multiple traits and multiple people so that we can characterise movies more accurately and use information from many peoples' ratings pooled together, to provide better recommendations for everyone.

5.2 Multiple traits and multiple people

Our model with just one trait is not going to allow us to characterize movies very well. To see this, take another look at Figure 5.4:



Using just the action/emotion trait, we can hardly distinguish between *The Lion King* and *Amadeus* since these have very similar positions on this trait line. So for the woman in this figure, we would not be able to recommend films like *Amadeus* (which she likes) without also recommending films like *The Lion King* (which she doesn't like).

We can address this problem by using additional traits. If we include a second trait representing how escapist or realist the film is, then each movie will now have a position on this second trait line as well as on the original trait line. This second trait value allows us to distinguish between these two movies. To see this, we can show the movies on a two-dimensional plot where the escapist/realist trait position is on the vertical axis, as shown in Figure 5.8.

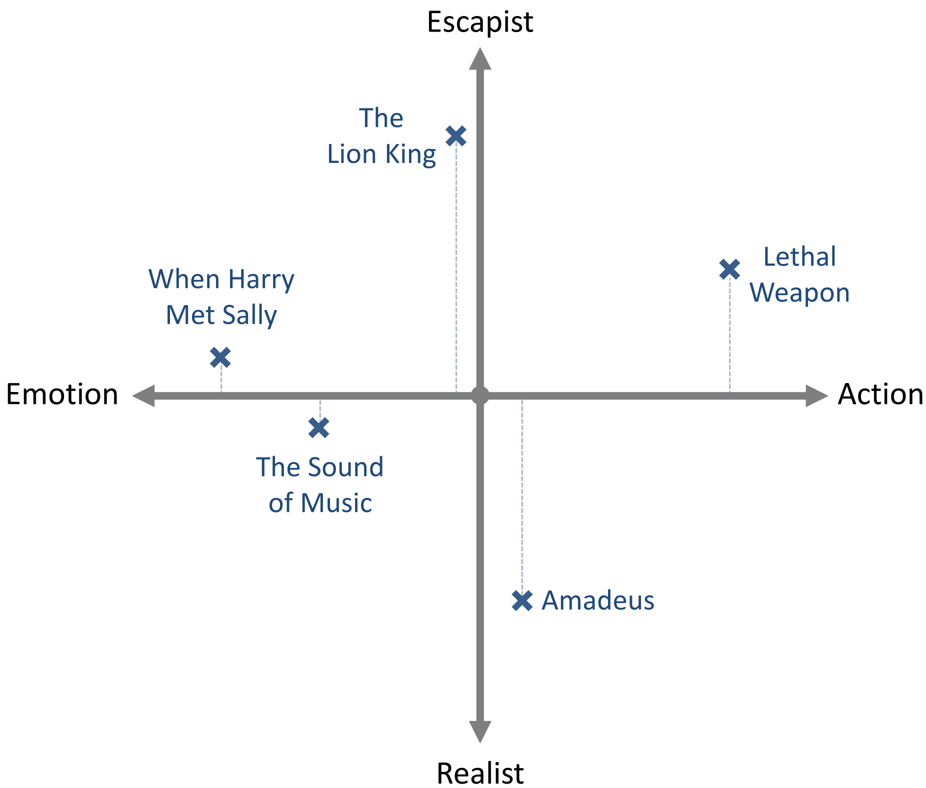


Figure 5.8: Two-dimensional plot where the new vertical axis shows how escapist or realist a movie is. Dotted lines show that the horizontal position of the movies has not changed.

In Figure 5.8, the more escapist movies have moved above the emotion/action line and the more realist movies have moved below. The left/right position of these movies has not changed from before (as shown by the dotted lines). This two-dimensional space allows *Amadeus* to be move far away from the *The Lion King* which means that the two movies can now be distinguished from each other.

Given this two dimensional plot, we can indicate each person's preference for more escapist or realist movies by positioning them appropriately above or below the emotion/action line, as shown in Figure 5.9. Looking at this figure, you can see that the woman from Figure 5.4 has now moved below the emotion/action line, since she has a preference for more realistic movies. Her preference point is now much closer to *Amadeus* than to *The Lion King* – which means it is now possible for our system to recommend *Amadeus* without also recommending *The Lion King*.

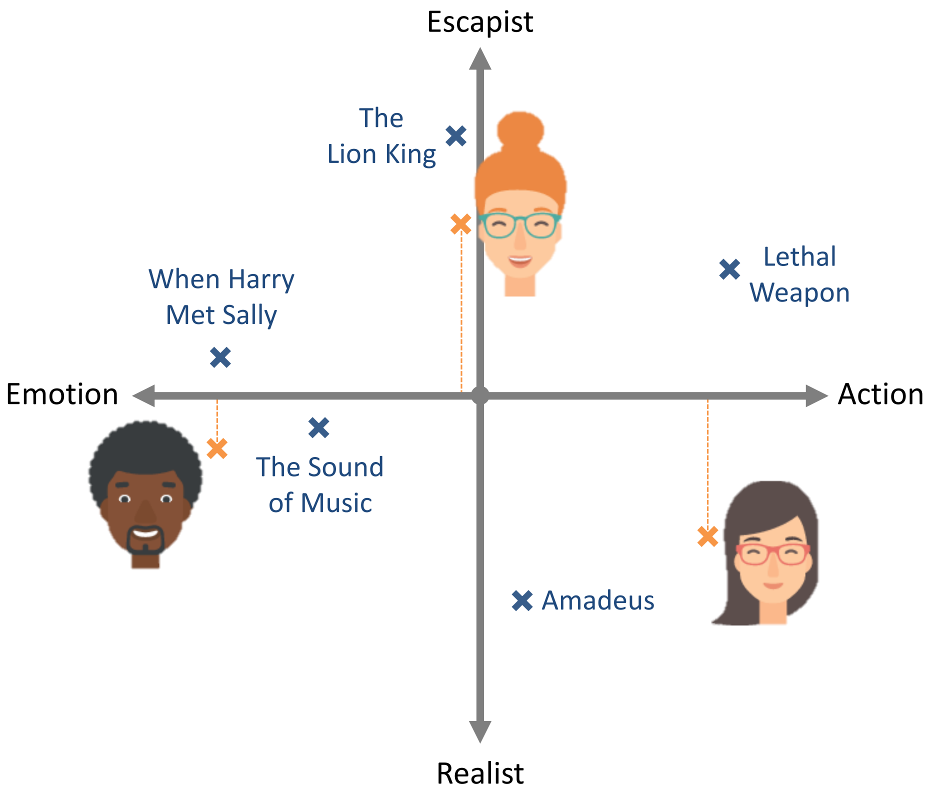


Figure 5.9: Placing people on the two-dimension plot allows us to capture their preferences for escapist/realist movies, whilst still representing their preferences for emotional/action movies.

We have now placed movies and people in a two-dimensional space, which we will call **trait space**. If we have three traits then trait space will be 3-dimensional, and so on for higher numbers of traits. We can use the concept of trait space to update our first two assumptions to allow for multiple traits:

1. Each movie can be characterized by its position ~~on the trait line~~ in trait space, represented as a continuous number for each trait.

2. A person's preferences can be characterized by a position ~~on the trait line~~ in trait space, again represented as a continuous number for each trait.

Assumption 3 does not need to be changed since we are combining each `trait` and `preference` exactly as we did when there was just one trait. However, we do need to make an additional assumption about how a person's preferences for different traits combine together to make an overall affinity.

4. The effect of one trait value on whether a person likes or dislikes a movie is the same, no matter what other trait values that movie has.

We can encode this assumption in our model by computing a separate affinity for each trait (which we will call the `traitAffinity`) and then just add them together to give an overall `affinity`. Figure 5.10 gives the factor graph for this model with a new plate over traits that contains the `trait` value for each movie, the `preference` for each person and the `traitAffinity`, indicating that all of these variables are duplicated per trait.

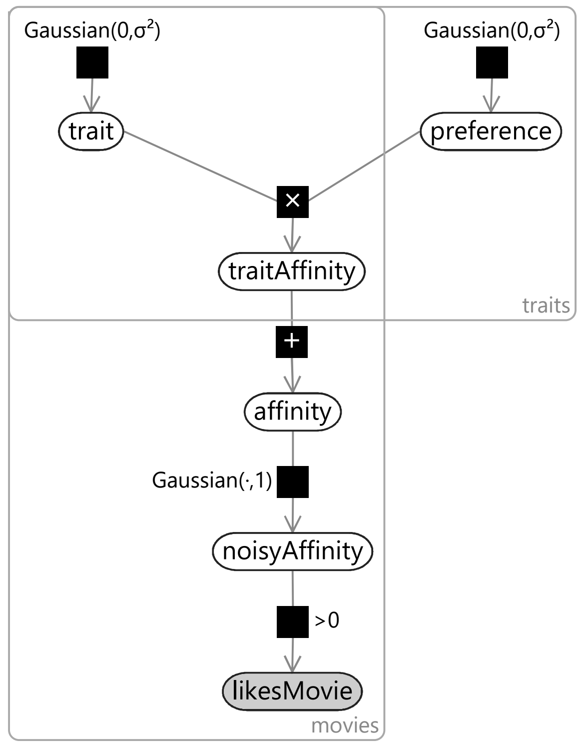


Figure 5.10: Factor graph for combining together multiple traits.

This model combines together traits in exactly the same way that we combined together features in the previous chapter. Once again, it leads to a very similar factor graph – to see this, compare Figure 5.10 to Figure 4.5. The main difference again is that we now have an unobserved `trait` variable where before we had an observed `featureValue`. This may seem like a small difference, but the implications of having this variable unobserved are huge. Rather than using features which are hand-designed and provide given values for each item, we are now asking our model to learn the traits and the trait values for itself! Think about this for a moment – we are effectively asking our system to create its own feature set and assign values for those features to each movie – all by just using movie ratings! The fact that this is even possible may seem like magic – but it arises from having a clearly defined model combined with a powerful inference algorithm.

One new complexity arises in this model around the choice of the prior variance σ^2 for the `trait` and `preference` variables. Because we are now adding together several trait affinities, we risk changing the range of values that the `affinity` can take as we vary the number of traits. To keep this range approximately fixed, we set $\sigma^2 = 1/\sqrt{T}$ where T is the number of traits. The intuition behind this choice of variance is that we would then expect the trait affinity to have a variance of approximately $1/\sqrt{T} \times 1/\sqrt{T} = 1/T$. The sum of T of these would have variance of approximately 1, which is the same as the single trait model.

5.2.1 Learning from many people at once

If we try to use this model to infer traits and preferences given data for just one person, we will only be able to learn about movies which that person has rated – probably not very many. We can do much better if we pool together the data from many people, since this is likely to give a lot of data for popular movies and at least a little data for the vast majority of movies. This approach is called **collaborative filtering** – a term coined by the developers of Tapestry, the first ever recommender system. In Tapestry, collaborative filtering was proposed for handling email documents, where "people collaborate to help one another perform filtering by recording their reactions to documents they read" [Goldberg et al., 1992]. In our application we want to filter movies by recording the ratings (that is, reactions) that other people have to the movies they watch – a different application, but the underlying principle is the same.

To extend our factor graph to handle multiple people, we add a new plate over people and put all variables inside it except the `trait` variable, (which is shared across people). The resulting factor graph is shown in Figure 5.11. Looking at this factor graph, you can see that it is symmetric between people and movies. In other words, we could swap over people and movies and we would end up with exactly the same model!

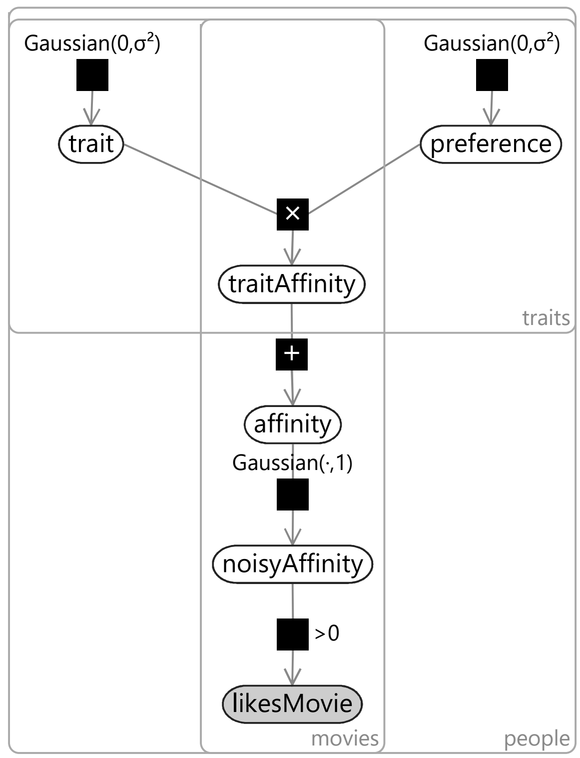


Figure 5.11: Factor graph for a recommender model which can learn from like/dislike data pooled across many people.

In this model we have chosen to threshold the `noisyAffinity` at zero, roughly corresponding to the assumption that half the ratings will be 'like' and half will be 'dislike'. This is quite a strong assumption to be making, so we could instead learn this threshold value as we did for the classifier model. Instead we will do something better – we will make a change that effectively allows different thresholds to be learned for each movie and for each person. We will add a bias variable per movie and a bias variable per user and include these two variables in the sum when we compute the total `affinity`. We can actually achieve this without changing the factor graph from the one in Figure 5.11 – all we do is use a traits plate that is two bigger than the desired number of traits and fix the first `preference` value and the second `trait` value to be exactly 1.0. If we use the model in this way, the first `trait` value will be the bias for a movie and the second `preference` value will be the bias for a person. Introducing biases in this way allows the model to capture the general popularity of a movie and the degree to which each person likes movies in general. We use this trick to include biases is all models in this chapter, but they will not be shown explicitly in the factor graphs, to keep them uncluttered.

Our final assumption is that we do not need any more variables in our model

– or to put it another way:

(5) Whether a person will like or dislike a movie depends only on the movie's traits and not on *anything* else.

We will assess the validity of this assumption shortly, but first let's put all of our assumptions together in one place so that we can review them all (Table 5.2).

(1) Each movie can be characterized by its position in trait space, represented as a continuous number for each trait.
(2) A person's preferences can be characterized by a position in trait space, again represented as a continuous number for each trait.
(3) A positive preference value means that a person prefers movies with positive values of the trait (and vice versa for negative values). The absolute size of the preference value indicates the strength of preference, where zero means indifference.
(4) The effect of one trait value on whether a person likes or dislikes a movie is the same, no matter what other trait values that movie has.
(5) Whether a person will like or dislike a movie depends only on the movie's traits and not on *anything* else.

Table 5.2: The assumptions encoded in our recommender model.

Assumption (1) seems reasonable since we can theoretically make trait space as large as we like, in order to completely characterize any movie – for smaller numbers of traits this assumption will hold less well, but still hopefully be a good enough assumption for practical purposes. Assumption (2) assumes that a person's tastes can be well represented by a single point in trait space. Quite possibly, people could occupy multiple points in trait space, for example a person may like both children's cartoons and very violent movies, but nothing in between. However, it may be reasonable to assume that such people are rare and so a person occupying a single point is a decent assumption in most cases.

Assumption (3) and Assumption (4) relate to how movie and person traits combine together to give an affinity. Perhaps the most questionable assumption here is Assumption (4) which says that the effect of each trait does not depend on the other traits. In practice, we might expect some traits to override others or to combine in unusual ways. For example, if someone only likes action movies that star Arnold Schwarzenegger, but dislikes all the other kinds of movies that he appears in – then this would be poorly modelled by these assumptions because the 'stars Arnold Schwarzenegger' trait would have a positive effect in some cases and a negative effect in others.

Finally, we have Assumption 5 which says that whether someone likes or dislikes a movie will depend only on the movie's traits – in fact it may depend on many other things. For example, the time of year may be a factor – someone may love Christmas movies in December but loathe them in January. Another factor could be the other people that are watching the movie – whether someone enjoys a movie could well depend on who is watching it with them. Following this line of thought, we could imagine a recommendation system that recommends movies for groups of people – this has in fact been explored by, for example, Zhang et al. [2015]. Other things that could influence a person's enjoyment could include: the time of day or time of week, their emotional state (do they want a happy movie or a sad one? do they want to be distracted from real life or challenged?) and so on. In short, there is plenty to question about Assumption 5 – but it's fine to stick with it for now and then consider extending the model to capture additional cues later on.

A person may only like some movies at particular times of year

So let's keep the model as it is and use it to make some recommendations!

Review of concepts introduced in this section

trait space A multi-dimensional space where each point in the space corresponds to an item with a particular set of trait values. Nearby points will correspond to items with similar traits, whereas points that are further apart represent items with less in common. A trait space is useful for identifying similar items and also for making item recommendations. See Figure 5.9 for a visualisation of a two-dimensional trait space.

collaborative filtering A means of filtering items for one user of a system based on the implicit or explicit rating of items by other users of that system. For example, filtering emails based on others' responses to the same emails or recommending movies based on others' ratings of those movies.

5.3 Training our recommender

Before we can train our model, we need some data to train it on. The good news here is that there are some high quality public data sets which can be used for training recommender models. We will use a data set from the excellent MovieLens site by GroupLens Research at the University of Minnesota. The particular data set we will use has been made freely available for education and development purposes - thank you MovieLens!

5.3.1 Getting to know our data

As with any new data set, our first task is to get to know the data. First of all, here is a sample of 10 ratings from the data set:

User	Movie	Rating
1	Willow (1988)	2
1	Antz (1998)	2
1	Fly, The (1986)	2.5
1	Time Bandits (1981)	1
1	Blazing Saddles (1974)	3
2	GoldenEye (1995)	4
2	Sense and Sensibility (1995)	5
2	Clueless (1995)	5
2	Seven (a.k.a. Se7en) (1995)	4
2	Usual Suspects, The (1995)	4

Table 5.3: A sample of ratings from the MovieLens data set.

The sample shows that each rating gives the ID of the person providing the rating, the movie being rated, and the number of stars that the person gave the movie. In addition to ratings, the data set also contains some information about each movie – we'll look at this later on, in section 5.6.

It's a good idea to view a new data set in many different ways, to get a deeper understanding of the data and to identify any possible data issues as early as possible. As an example, let's make a plot to understand what kind of ratings people are giving. The above sample suggests that ratings go up to 5 stars and that half stars are allowed. To confirm this and to understand how frequently each rating is given, we can plot a histogram of all the ratings in the data set.

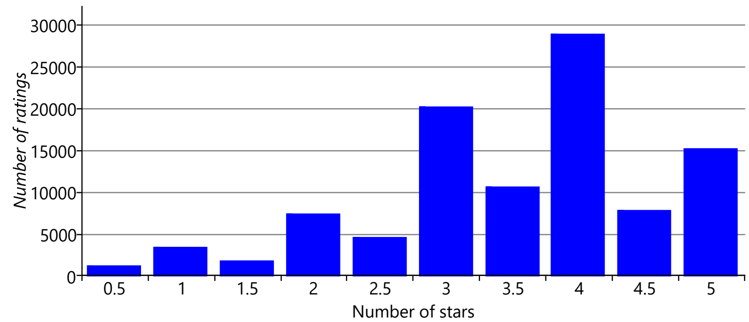


Figure 5.12: The number of ratings given for each possible number of stars (from half a star up to five stars).

We can learn a few things about the ratings from Figure 5.12. The first is that whole star ratings are given more than nearby ratings with half stars. Secondly, the plot is biased to the right, showing that people are much more likely to give a rating above three stars than below. This could perhaps be because people are generous to the movies and try to give them decent ratings. Another possibility is that people only rate movies that they watch and they only watch movies that they expect to like. For example, someone might hate horrors movies and so would never watch them, and so never rate them. If they were forced to watch the movie, they would likely give it a very low rating. Since people are not usually forced to watch movies, such ratings would not appear in the data set, leading to the kind of rightward bias shown in Figure 5.12.

5.3.2 Training on MovieLens data

The model we have developed allows for two possible ratings: ‘like’ or ‘dislike’. If we want to use the MovieLens data set with this model, we need a way to convert each star rating into a like or a dislike. Guided by Figure 5.12, we will assume that 3 or more stars means that a person liked the movie, and that 2.5 or fewer stars means they did not like the movie. Applying the transformation gives us a new data set of like/dislike ratings.

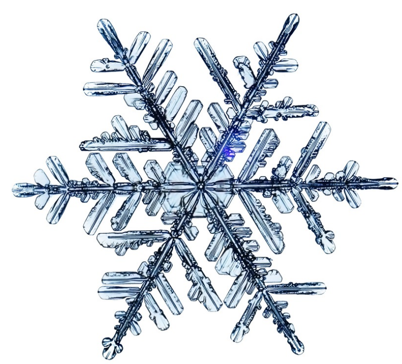
We need to split this like/dislike data into a training set for training our model, and a validation set to evaluate recommendations coming from the model. For each person we will use 70% of their likes/dislikes to train on and leave 30% to use for validation. We also remove ratings from the validation set for any movies that do not appear anywhere in the training set (since the trait position for these movies cannot be learned). The result of this process is:

- a training set of 69,983 ratings (57,383 likes/12,600 dislikes) covering 8,032 movies,

- a validation set of 28,831 ratings (23,952 likes/4,879 dislikes) covering 4,761 movies.

Both data sets contain ratings from 671 different people.

To train the model, we attach the training set data to the `likesMovie` variable and once again use expectation propagation to infer the `trait` values for each movie and the `preference` values for each person. However, when we try to do this, the posterior distributions for these variables remain broad and centered at zero. What is going on here?



Symmetries can cause inference problems

To understand the cause of this problem, let's look again at the picture of trait space from Figure 5.9, which we've repeated in Figure 5.13a. The choice of having emotion on the left and action on the right was completely arbitrary. We could flip these over so that action is on the left and emotion is on the right, whilst also flipping the positions of all the people and movies correspondingly, as shown in Figure 5.13b. The result is a flipped trait space that gives exactly the same predictions. We could also swap the action/emotion trait with the escapist/realist trait, as shown in Figure 5.13c. Again the result would give exactly the same predictions. Notice that Figure 5.13c is also the same as Figure 5.13b rotated by 90-degrees to the left. We can also apply other rotations so that the axes of the plot no longer lined up with our original traits (Figure 5.13d) and we *still* get the same predictions! When a model's variables can be systematically transformed without changing the resulting predictions, the model is said to contain **symmetries**. During inference, these symmetries cause the posterior distributions to get very broad, as they try to capture all rotations and flips of trait space simultaneously. Not helpful!

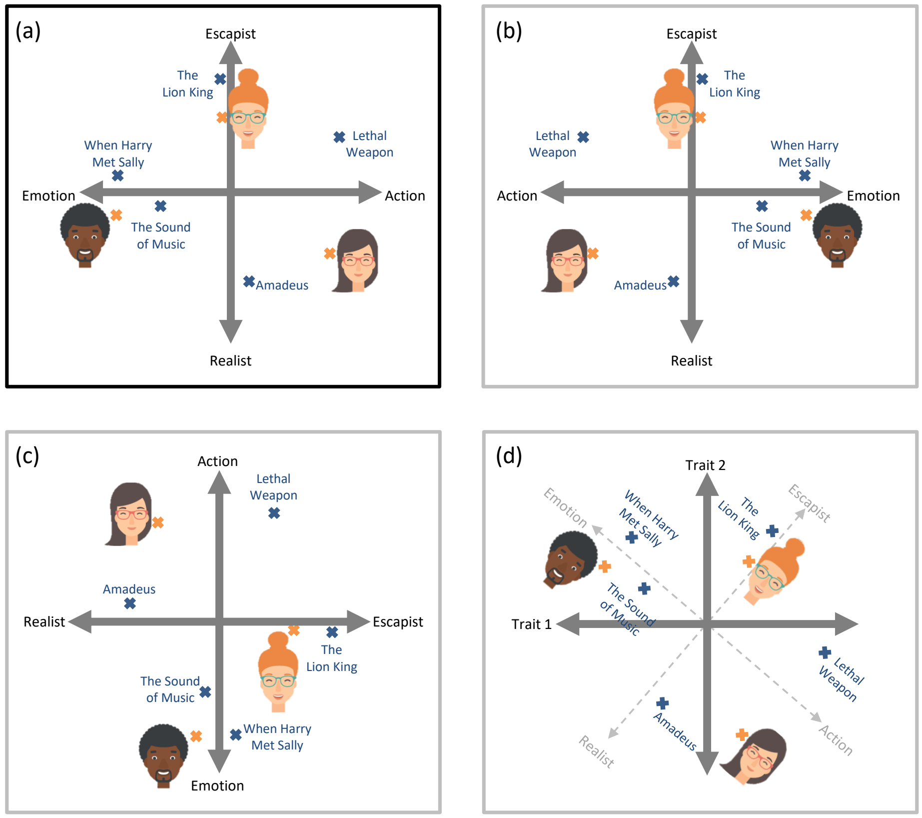


Figure 5.13: Examples of symmetries in our recommender model. (a) Original trait space (b) A left-right flip symmetry (c) A flip symmetry caused by swapping the axes (d) A rotational symmetry.

To solve this inference problem, we need to do some kind of **symmetry breaking**. Symmetry breaking is any modification to the model or inference algorithm with the aim of removing symmetries from the posterior distributions of interest. For a two-trait version of our model, we can break symmetry by fixing the position of two points in trait space – for example, fixing the positions of the first two movies in the training set. We choose to fix the first movie to (1,0) and the second to (0,1). These two points mean that rotations and flips of the trait space now lead to different results, since these two movies cannot be rotated/flipped correspondingly – and so we have removed the symmetries from our model.

With symmetry breaking in place, EP now converges to a meaningful result. However, the EP message passing algorithm runs extremely slowly due to the high cost of computing messages relating to the product ($\times$) factor. In Stern et al. [2009] a variation of the EP message calculation is used for these messages, as shown in equation (6) in the paper), which has the effect of speeding up the message calculation dramatically.

This faster inference algorithm gives posteriors over the position in trait space for each movie and each person. In many cases, these posteriors are quite broad because there were not enough ratings to place the movie or person accurately in trait space. In Figure 5.14, we plot the inferred positions of those movies where the posterior was narrow enough to locate the movie reasonably precisely. Specifically, we plot a point at the posterior mean for each movie where the posterior variance is less than 0.2 in each dimension – this means that points are plotted for only 158 of our 8,032 movies. The learned positions of people in trait space are distributed in broadly similar fashion to the positions of movies, and so we will not show a plot of their positions.

This plot shows that our model has been able to learn two traits and assign values for these traits to some movies, entirely using ratings – a pretty incredible achievement! We can see that the learned trait values have some reassuring characteristics – for example, movies in the same series have been placed near each other (such as the two *Lord of the Rings* movies or the two *Ace Venture* movies). This alone is pretty incredible – our system had no idea that these movies were from the same series, since it was not given the names of the movies. Just using the like/dislike ratings alone, it has placed these movies close together in trait space! Beyond these characteristics, it is hard to interpret much about the traits themselves at this stage. Instead, we'll just have to see how useful they are when it comes to making recommendations.

Review of concepts introduced in this section

symmetries A symmetry in a model is where parts of the model are interchangeable or can act as equivalent to each other. When a model contains symmetries, this means there are multiple configurations of the models variables that give rise to the same data. During inference, such symmetries cause problems, since the posterior distributions will try to capture all these equivalent configurations simultaneously, usually with unhelpful results. When a model contains symmetries, it is usually necessary to do some kind of symmetry breaking.

symmetry breaking Modifications to a model or inference algorithm that allow symmetries to be removed, leading to more useful posterior distributions. A typical method of symmetry breaking involves adding perturbations to the initial messages in a message passing algorithms. Other approaches involve making changes to the model to remove the symmetries, such as fixing the values of certain latent variables or adding ordering constraints.

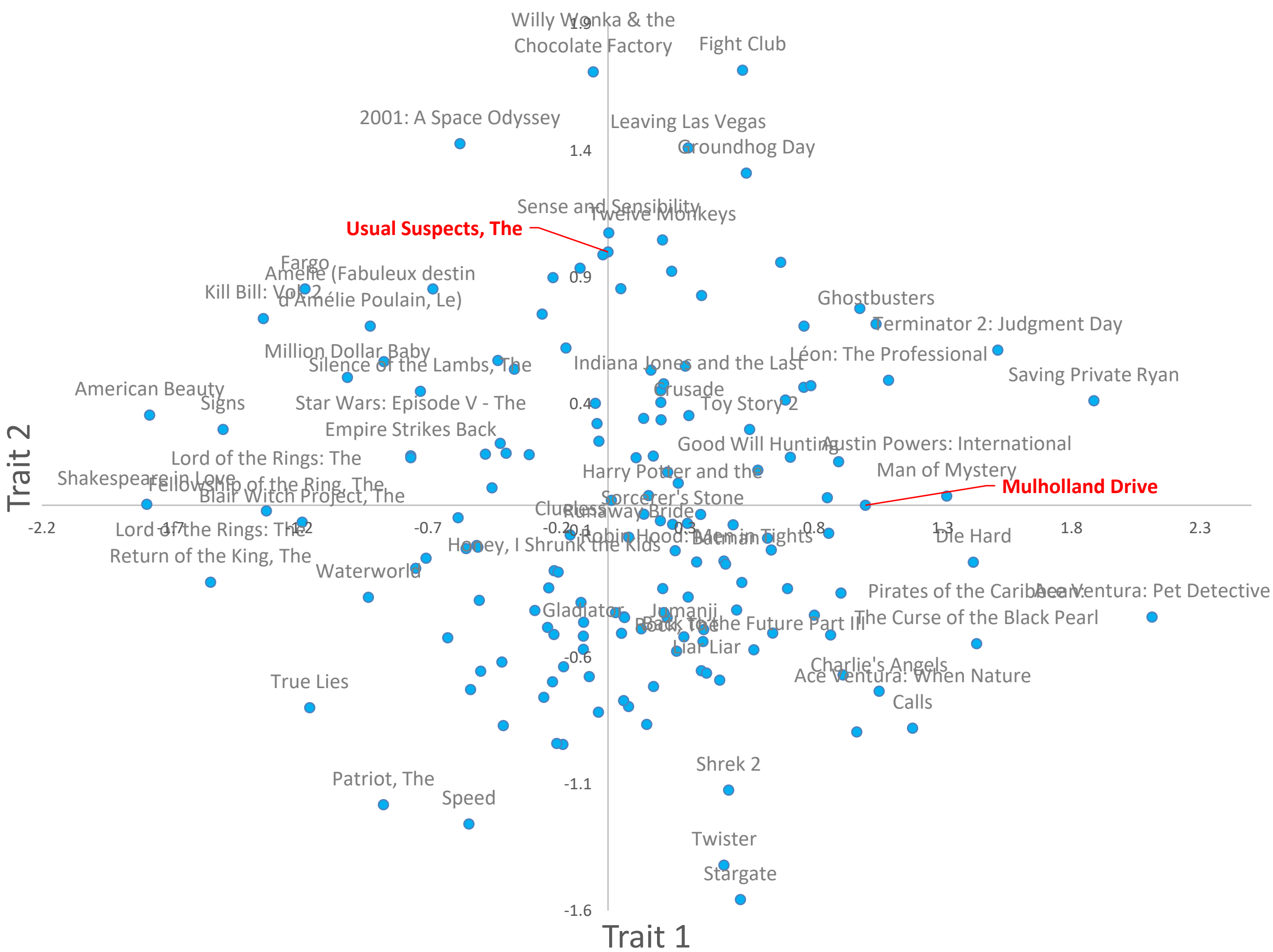
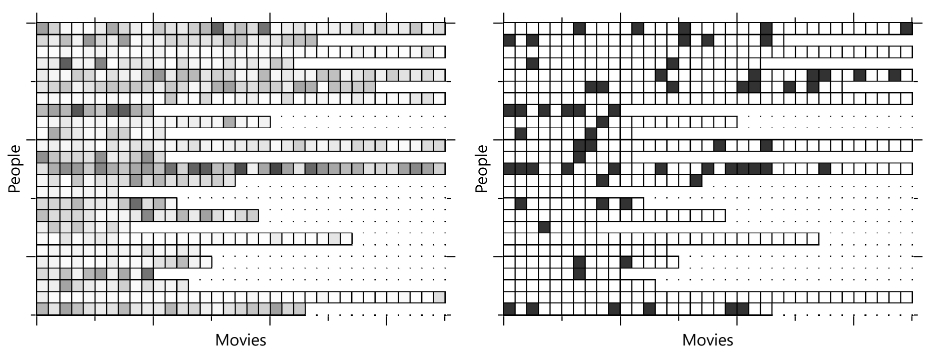


Figure 5.14: Learned positions of movies in trait space. For readability, only a subset of points have been labelled with the name of the movie (centered on the corresponding point). The two 'anchor' movies, *The Usual Suspects* and *Mulholland Drive* are shown in red at (0,1) and (1,0).

5.4 Our first recommendations

With our trained two-trait model in hand, we are now ready to make some recommendations! During training we learned the (uncertain) position of each movie and each person in trait space. We can now make a prediction for each of the held out ratings in our validation set. We do this one rating at a time – that is, for one person and one movie at a time. First, we set the priors for the movie `trait` and the person `preference` to the posteriors learned during training. Then we run expectation propagation to infer the posterior distribution over `likesMovie` to compute the probability that the person would like the movie. Repeating this over all ratings in the validation set gives a probability of 'like' for each rating, which we can compare with the ground truth like/dislike label. Figure 5.15 shows the predicted like probability and the ground truth for the ratings from the first 25 people in the validation set with more than five ratings.



(a) Inferred probability of like (b) Ground truth like/dislike

Figure 5.15: Initial results of our recommender model. (a) Computed probability of each person liking each movie. White squares correspond to probability 1.0, black to probability 0.0 and shades of grey indicate intermediate probability values. (b) Ground truth – where white indicates that the person liked the movie, black indicates they disliked it.

The first thing that stands out from Figure 5.15b is that people mostly like movies, rather than dislike them. In a sense then, the task that we have set our recommender is to try and work out which are the few movies that a person does not like. Looking at the predicted probabilities in Figure 5.15a, we can see some success in this task – because some of the darker squares do correctly align with black squares in the ground truth. In addition, some rows are generally darker or lighter than average indicating that we are able to learn how likely each person is to like or dislike movies in general. However, the predictions are not perfect – there are many disliked movies that are missed and some predictions of dislike that are incorrect. But before we make any improvements to the model, we need to decide which evaluation metrics we will use to measure and track these improvements.

5.4.1 Evaluating our predictions

In order to evaluate these predictions, we need to decide on some evaluation metrics. As discussed in chapter 2, it makes sense to consider multiple metrics to avoid falling into the trap described by Goodhart's law. For the first metric, we will just use the fraction of correct predictions, when we predict the most probable value of `likesMovie`. For the two-trait experiment above, we see that we get 84.8% of predictions correct. This metric is helpful for tracking the raw accuracy of our recommender but it does not directly tell us how good our recommendation experience will be for users. To do this, we will need a second metric more focused on how the recommender will actually be used.

The most common use of a recommender system is to provide an ordered list of recommendations to the user. We can use our predicted probabilities of 'like' to make such a list by putting the movie with the highest probability first, then the one with the second highest probability and so on. In this scenario, a reasonable assumption is that the user will scan through the list looking for a recommendation that appeals – but that they may give up at some point during this scan. It follows that it is most important that the first item in the list is correct, then the second, then the third and so on through to the end of the list. We would like to use an evaluation metric which rewards correct predictions at the start of the list more than at the end (and penalises mistakes at the start of the list more than mistakes at the end).

A metric that has this behaviour is **Discounted Cumulative Gain** (DCG) which is defined as the sum of scores for individual recommendations, each weighted by a discount function that depends on the position of the recommendation in the list. Figure 5.16 shows the calculation of DCG for a list of five recommendations. In this figure, the discount function used is $\frac{1}{\log_2(position+1)}$ where *position* the position in the list, starting at 1. This function is often used because it smoothly decreases with list position, as shown by the blue bars in the figure. The score that we will use for a recommendation is the ground truth number of stars that the person gave that movie. So if they gave three stars then the score will be 3. Since we are calculating DCG for a list of five recommendations, we sometimes write this as DCG@5.

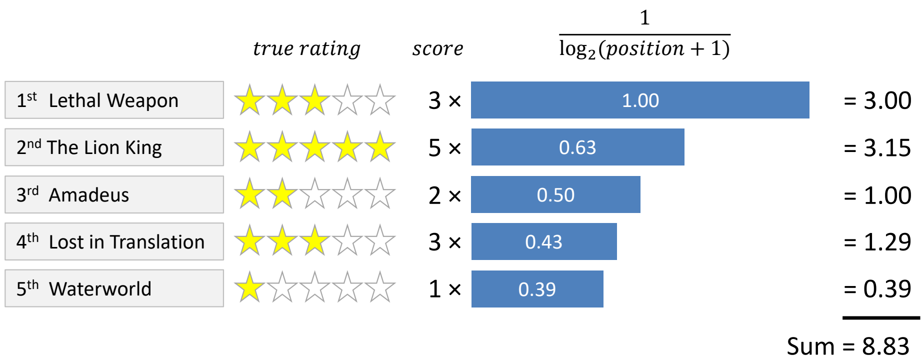


Figure 5.16: Calculation of Discounted Cumulative Gain (DCG) for a list of five movie recommendations.

We can only evaluate a recommendation when we know the person's actual rating for the movie being recommended. For our data set, this means that we will only be able to make recommendations for movies from the 30% of ratings in the validation set. Effectively we will be ordering these from 'most likely to like the movie' to 'least likely to like the movie', taking the top 5 and using DCG to evaluate this ordering.

One problem with DCG is that the maximum achievable value varies depending on the ratings that the person gave to the validation set movies. If there are 5 high ratings then the maximum achievable DCG@5 will be high. But if there are only 2 high ratings then the maximum achievable DCG@5 will be lower. To interpret the metric, all we really want to know is how close we got to the maximum achievable DCG. We can achieve this by computing the maximum DCG (as shown in Figure 5.17) and then dividing our DCG value by this maximum possible value. This gives a new metric called the **Normalized Discounted Cumulative Gain** (NDCG). An NDCG of 1.0 always means that the best possible set of recommendations were made. Using the maximum value from Figure 5.17, the NDCG for the recommendations in Figure 5.16 is equal to $8.83/9.64 = 0.916$.

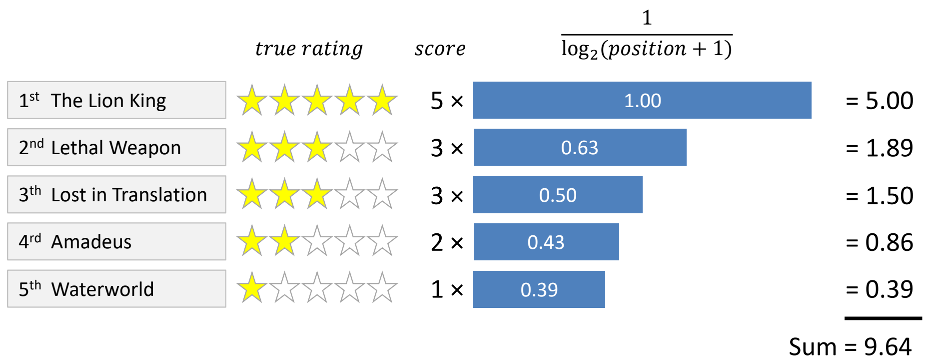


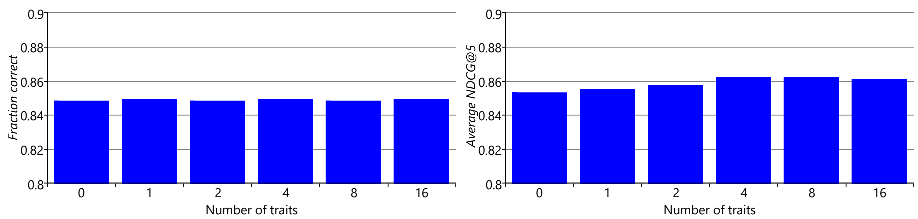
Figure 5.17: Calculation of the maximum possible DCG for the five movies from Figure 5.16. The maximum DCG is for the movies in decreasing order of the number of stars in the ground truth rating.

We produce a list of recommendations for each person in our validation set, and so can compute an NDCG for each of these lists. To summarise these in a single metric, we then take an average of all the individual NDCG values. For the experiment we just ran, this gives an average NDCG@5 of 0.857.

5.4.2 How many traits should we use?

The metrics computed above are for a model with two traits. In practice, we will want to use the number of traits that gives the best recommendations according to our metrics. We can run the model with 1, 2, 4, 8, and 16 traits to see how changing the number of traits affects the accuracy of our recommendations. We can also run the model with zero traits, meaning that it gives the same recommendations to everyone – this provides a useful baseline and indicates how much we are gaining by using traits to personalise our recommendations to individual people. Note that when using zero traits, we do still include the movie and user biases in the model.

Figure 5.18 shows how our two metrics vary as we change the number of traits. Looking at the like/dislike accuracy in Figure 5.18a, shows that the accuracy is essentially unchanged as we change the number of traits. But the NDCG in Figure 5.18b tells a very different story , with noticeable gains in NDCG@5 as we increase the number of traits up to around 4 or 8. Beyond this point adding additional traits does not seem to help (and maybe even reduces the accuracy slightly). The overall gain is relatively small, which shows that though personalized recommendations are better than non-personalized recommendations, they do not give as much improvement as we might expect.



(a) Fraction of predictions correct (b) Average NDCG@5

Figure 5.18: Accuracy and NDCG metrics computed for different numbers of traits. The metrics for a random recommender are also shown for comparison. To make the change in metrics visible in these bar charts, we have had to start the y-axis at 0.8 rather than zero. In general, this practice should be avoided since it falsely exaggerates the differences between the bars. Since we have chosen to use it here and in some later charts, please do bear in mind that the actual differences are smaller than the charts might suggest.

You may be wondering why we see an increase in average NDCG when there is no increase in prediction accuracy. The answer is that NDCG is a more sensitive metric because it makes use of the original ground truth star ratings, rather than these ratings converted into likes/dislikes. This sensitivity suggests that we would benefit by training our model on star ratings rather than just on a binary like or dislike. In the next section, we will see what changes our model needs in order to work with the full range of star ratings.

Review of concepts introduced in this section

Discounted Cumulative Gain A metric for a list of recommendations that is defined as the sum of scores for each individual recommendation, weighted by a discount function that depends on the position of that recommendation in the list. The discount function is selected to give higher weights to recommendations at the start of the list and lower weights towards the end. Therefore, the DCG is higher when good recommendations are put at the start of the list than when the list is reordered to put them at the end. See Figure 5.16 for a visual example of calculating DCG.

Normalized Discounted Cumulative Gain A scaled version of the Discounted Cumulative Gain, where the scaling makes the maximum possible value equal to 1. This scaling is achieved by dividing by the actual DCG by the maximum possible DCG. See Figure 5.16 and Figure 5.17 for visual examples of calculating a DCG and a maximum possible DCG.

5.5 Modelling star ratings

Our model turns the full range of star ratings into a simple like or dislike, which means it is throwing away a lot of useful information. There is a world of difference between rating a movie at 3 stars and rating it at 5 stars, yet we are treating both of these cases the same. In order to make use of the difference between different star ratings, we need to change our model to work with the full range of ratings rather than a binary like/dislike. Not only will this let us train on star ratings, but we will also be able to predict star ratings – a double benefit!

We can make this change by building on the binary like/dislike model that we have already designed. Inside this model we have an `affinity` variable which is a continuous number representing how much a person likes a movie. We currently threshold this `affinity` at zero and say that values above zero mean the person likes the movie and values below zero mean that they do not like the movie. To model different star ratings, we can assume that a higher affinity means that a person will give a higher star rating. More precisely, rather than thresholding only at zero, we can now introduce thresholds for each star rating. If a person's affinity for a movie is above the threshold for a particular number of stars, then we expect them to give the movie at least that number of stars.

To add these thresholds into our model, we need to make one additional assumption. We need to decide whether the same thresholds should be used for everyone, or whether different people can have different thresholds. Allowing different thresholds might be useful – for example, it is possible that some people give a really bad movie a rating of two stars, while other people give a really bad movie a rating of one star or even half a star. If we want to model these different behaviours, we would need to allow different people to have different thresholds. This can be done but it would introduce problems of data scarcity since some people might not have any ratings for particular thresholds. Rather than tackle these problems, we will make the simplifying assumption that the thresholds are the same for everyone. We can express this assumption precisely, like so:

6. When two people have the same affinity for a movie, they will give it the same number of stars.

Figure 5.19 shows the factor graph for an extended model that encodes this assumption. In this model, we have added a new variable `starThreshold` which is inside a `stars` plate, meaning that there is a threshold for each number of stars.

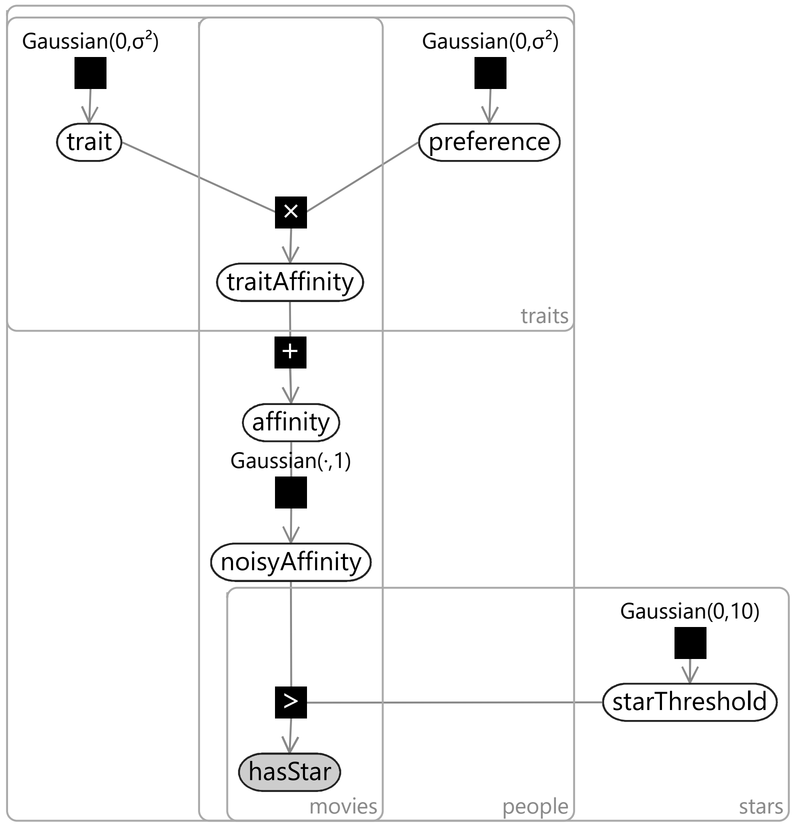


Figure 5.19: Factor graph for a recommender model that can consume and predict star ratings. Ratings are indirectly represented using binary values of the variable `hasStar` as discussed in the text.

For each movie and person, the observed variable in this graph is now called `hasStar`. This variable lies inside the `stars` plate and so has a value for each number of stars. In other words, each single star rating is represented as a set of binary variables. The binary variable for a particular number of stars is `true` if the rating has *at least* that number of stars. As an example, a rating of three stars means that the first three binary variables are `true` and the other two are `false`. Figure 5.20 shows the relationship between the star rating and the binary values used for the observation of `hasStar`.

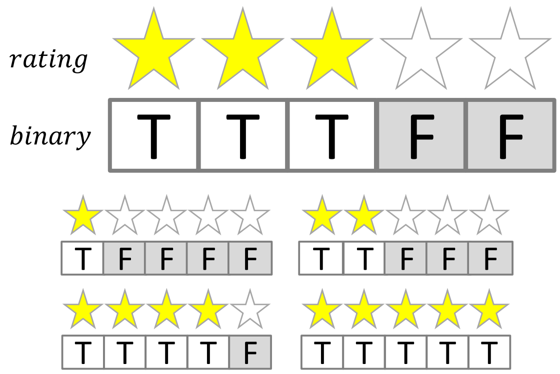


Figure 5.20: Relationship between different star ratings and the binary values used for the `hasStar` variable in the factor graph of Figure 5.19.

When we train this model, we set `hasStar` to the observed values given in Figure 5.20 for the corresponding rating. When using the model to make a recommendation, we get back a posterior probability of each binary variable being true. These can be converted into the probability of having a particular number of stars using subtraction. For example, if we predict the probability of having 3 or more stars is 70% and the probability of having 4 or more stars is 60%, then the probability of having exactly 3 stars must be $70\% - 60\% = 10\%$. Using this trick, we can convert the individual binary probabilities back into separate probabilities for each star rating.

There are a few more details we need to work out before we can train this model. First, in our data set we need to be able to work with half-star ratings, such as $3\frac{1}{2}$ stars. We can handle these by doubling the number of thresholds, so that there are thresholds for both whole and half star ratings. Second, there is a symmetry between the star thresholds and the biases – adding a constant value to all user or movie biases and subtracting that value off all thresholds leads to the same predictions. This can be solved by fixing one of the thresholds to be zero – for our experiments we choose to fix the three star threshold to be zero. Finally, if you look at Figure 5.20, you will note that the first binary value is always `true`. This means that the affinity must always be greater than the lowest threshold, so we can simply remove it from the model. In our case, that means there will be no threshold for a $\frac{1}{2}$ star and so the lowest threshold will be for 1 star. With these changes in place, we are now ready to train!

5.5.1 Results with star ratings

Now that we can train on star ratings, we can use the same training data as before (section 5.3) but without converting ratings to like/dislike. When we do this training, we expect that the extra information coming from the star ratings will allow us to locate movies more precisely in trait space. Back in Figure 5.14 we found that, after training on like/dislike, 158 of the movies had a posterior variance of less than 0.2 in each dimension of trait space. After training on star ratings, the number of movies with such low posterior variance increases to 539, showing that we have indeed managed to locate movies more precisely.

As part of training the model, we also learn Gaussian posterior thresholds for each star rating – these are shown in Figure 5.21.

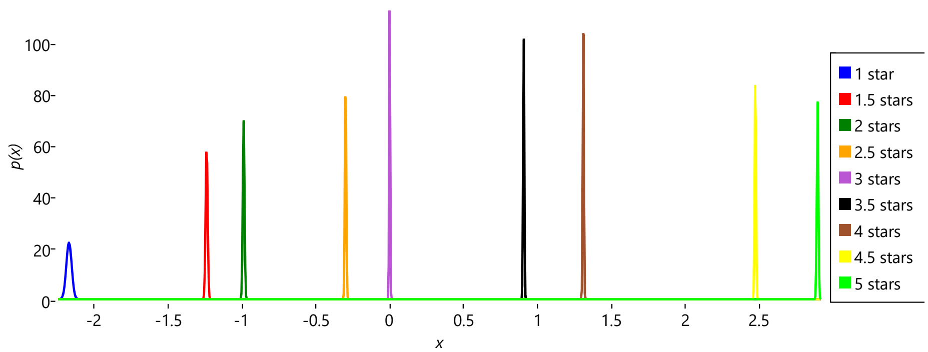
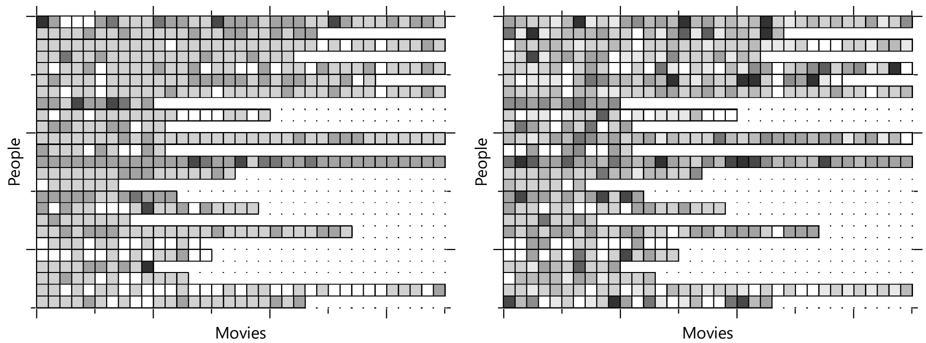


Figure 5.21: Posterior distributions for star ratings thresholds from 1 star to 5 stars. The threshold for three stars is fixed to be exactly zero – all other thresholds have been learned.

These threshold posteriors are worth looking at. The first thing to note is that the thresholds are ordered correctly from 1 star through to 5 stars, as we would expect. This ordering was not enforced directly in the model since the priors for all the thresholds were the same – instead, the ordering has arisen from the way the model has been trained. Another thing to note is that the posterior distribution for 1 star is much broader than for other thresholds. This is because there are very few half stars and one stars in the training set (to confirm this look back at Figure 5.12). It is these ratings which are used to learn the 1 star threshold and so their relative scarcity leads to higher uncertainty in the threshold location. A final note is that the half star thresholds are generally closer to the star rating above than the one below. For example, the $3\frac{1}{2}$ star threshold is much closer to the 4 star threshold than to the 3 star threshold. This implies that when a person gives $3\frac{1}{2}$ stars to a movie, in their minds they consider that to be almost a 4 star movie, rather than just better than a 3 star movie. Another explanation is that some people may never use half stars (which would explain why they are relatively scarcer than the surrounding whole stars), which would introduce some bias in the inferred thresholds. It is an interesting exercise to think about how the model could be changed to reflect the fact that some people never use half stars.

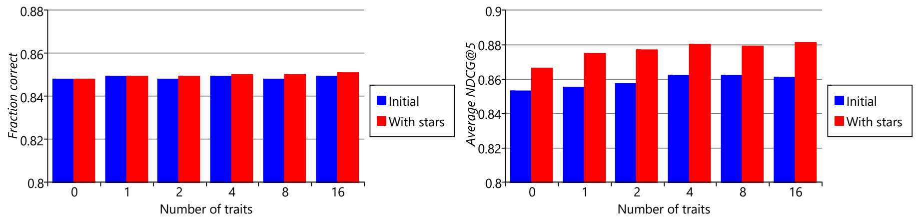
Using our newly trained model, we can make predictions for exactly the same people and movies as we did in section 5.4. Now our model is predicting star ratings, we can plot the most probable star rating, instead of posterior probabilities of like.



(a) Inferred most probable number of stars (b) Ground truth number of stars

Figure 5.22: Results of our recommender model with star ratings. (a) Predicted most probable ratings, where white squares correspond to five stars, black to half a star and shades of grey represent intermediate numbers of stars. (b) Ground truth ratings using the same colour key.

Figure 5.22a shows nicely that we are now able to predict numbers of stars, rather than just like or dislike. Comparing the two plots, we can see that there are sometimes darker or lighter regions in our predictions corresponding to those in the ground truth – but that equally often there are not. It is almost impossible to look at Figure 5.22 and say whether the new model is making better recommendations than the old one. Instead we need to make a quantitative comparison, by re-computing the same metrics as before and comparing the results. For NDCG, we can rank our recommendations by star rating and compute the metric exactly as before. For like/dislike accuracy, we need to convert our star predictions back into binary like/dislike predictions. We can do this by summing up the probabilities of all ratings of 3 stars or higher – if this sum is greater than 0.5, then we predict that the person will like the movie, otherwise that they will dislike it. Figure 5.23 shows that our new model has a significantly improved NDCG than the previous model, demonstrating the value of using the full star ratings. The improvement even shows up in our relatively insensitive fraction-correct metric, although the change is much smaller.



(a) Fraction of predictions correct (b) Average NDCG@5

Figure 5.23: Comparison of two metrics for the old like/dislike model and the new model with star ratings. The star ratings model gives a significant boost to NDCG, and even shows a small improvement in like/dislike accuracy.

Because we add together probabilities of different star ratings when computing that the like/dislike accuracy metric, we are throwing away information about our recommendations. For example, we are throwing away whether we predicted 3, 4 or 5 stars. The result will be to make the metric less sensitive to improvements in accuracy. We only computed it for Figure 5.23 so that we could compare to the results of the initial model. Now that we have predictions of star ratings, we need to replace this metric with a new one that can make use of ratings. For this new metric, we could look at the fraction of times that the predicted rating correctly matched the ground truth rating. However, this would mean that a prediction that is half a star out would be treated the same as one that is four stars out. Instead, we can look at how far the predicted number of stars was from the actual number of stars, so that the error is:

$$\text{Error} = |\text{Predicted star rating} - \text{Ground truth star rating}|. \tag{5.1}$$

In equation (5.1), the vertical bars mean that we take the absolute size of the difference. For example, if the prediction is two stars and the ground truth is five stars, the error will be 3.0. The error will also be 3.0 if we swap these over so that the prediction is five stars and the ground truth is two stars. Because we use this absolute size, we call this error the **absolute error**. To compute a metric over all predictions, we average the absolute errors of each prediction, giving a metric called the **mean absolute error** (MAE).

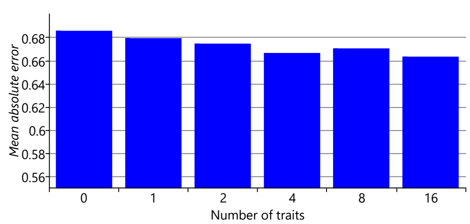


Figure 5.24: Mean absolute error for different numbers of traits in our new star rating model. The MAE generally decreases slightly as we increase the number of traits.

Figure 5.24 shows this metric computed for varying numbers of traits in our new model. Taking all three metrics together, having more traits generally seems to give better quality recommendations. So we can choose to use the 16-trait version of our latest model which gives an NDCG@5 of 0.881 and an MAE of 0.663. While this gives us our best performing recommender system yet, it would still be good to make further improvements. In the next section we'll diagnose where we are still making mistakes and look at one way to further improve our recommendation accuracy.

Review of concepts introduced in this section

absolute error The difference between a predicted value and the corresponding ground truth value, ignoring the sign of the result. The absolute error between 2 stars and 5 stars is 3. The absolute error between 5 stars and 2 stars is also 3. Because we ignore the sign, the absolute error is always positive (or zero).

mean absolute error The average (mean) of the absolute error between a predicted value and the ground truth value, across all predictions. The best possible value for this metric is 0. All other values will be positive numbers, with smaller values considered better than larger ones.

5.6 Another cold start problem

When we plotted the position of movies in trait space (Figure 5.14), we showed only those movies where the position was known reasonably accurately (that is, where the posterior variance was low). It follows that there are many movies where the posterior variance is larger, possibly much larger. This means that in some cases we essentially do not know where the movie is in trait space. We might expect this to be the case for movies which do not have very many ratings. It follows that if we do not know where a movie is in trait space, then we might expect the accuracy of recommendations relating to the movie to be low. How can we diagnose if this is the case?

First, it would be useful to understand how many ratings each movie typically has. Figure 5.25 shows the number of ratings for each movie in the data set as a whole, with the movies ordered from most ratings on the left to least ratings on the right.

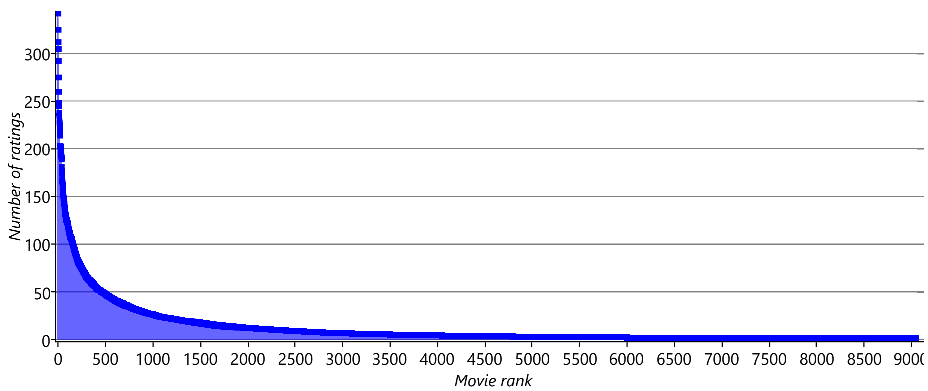


Figure 5.25: The number of ratings given for each movie in the data set as a whole. The movies are ordered from most ratings on the left to least ratings on the right.

From Figure 5.25, we can see that only about 500 of the 9000 movies have more than 50 ratings. Looking more closely, only around 2000 movies have more than 10 ratings. This leaves us with 7000 movies that have 10 or fewer ratings – of which about 3000 have only a single rating! It would not be surprising if such movies cannot be placed accurately in trait space, using rating information alone. As a result, we might expect that our prediction accuracy would be lower for those movies with few ratings than for those with many.

To confirm this hypothesis, we can plot the mean absolute error across the movies divided into groups according to the number of ratings they have in the training set. This plot is shown in Figure 5.26 for an experiment with 16 traits. For this experiment, we added into the validation set the movies that do not have any ratings in the training set (the left-hand bar in Figure 5.26). This provides a useful reference since it shows what the MAE is for movies with no ratings at all. The plot shows that when we have just one rating (second bar), we do not actually reduce the MAE much compared to having zero ratings (first bar). For movies with more and more ratings, the mean absolute error drops significantly, as shown by the third and fourth bars in Figure 5.26. Overall, this figure shows clearly that we are doing better at predicting ratings for movies that have more ratings – and very badly for those movies with just one.

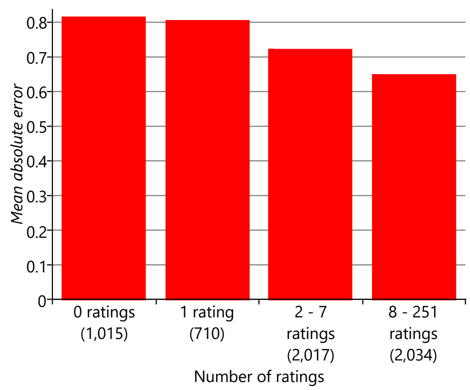


Figure 5.26: Mean absolute error for movies with different numbers of ratings in the training set, for a model with 16 traits. Each bar is labelled with the range of ratings and, in brackets, the number of movies that fall into that range. For example, the left-hand bar gives the MAE for movies with no ratings in the training set, of which there are 1,015. Comparing the four bars shows that movies with many ratings have substantially lower prediction errors than those with few or zero ratings.

Figure 5.26 confirms that we have an accuracy problem for movies with few ratings. This is particularly troubling in practice since newly released movies are likely to be the most useful recommendations but are also likely to have relatively few ratings. So how can we solve this problem? Recalling section 4.6 from the previous chapter, we can think of this as another cold start problem. We need to be able to make recommendations about a movie even though we have few or even zero ratings for that movie.

Apart from ratings, what other information do we have that could be used to improve our recommendations? Looking at our data set, we see that it also includes the year of release and the genres that each movie belongs to. A sample of this additional information is shown in Table 5.4.

Id	Name	Year	Genres
10	GoldenEye	1,995	{Action, Adventure, Thriller}
17	Sense and Sensibility	1,995	{Drama, Romance}
39	Clueless	1,995	{Comedy, Romance}
47	Seven (a.k.a. Se7en)	1,995	{Mystery, Thriller}
50	Usual Suspects, The	1,995	{Crime, Mystery, Thriller}
2,193	Willow	1,988	{Action, Adventure, Fantasy}
2,294	Antz	1,998	{Adventure, Animation, Children, Comedy, Fantasy}
2,455	Fly, The	1,986	{Drama, Horror, Sci-Fi, Thriller}
2,968	Time Bandits	1,981	{Adventure, Comedy, Fantasy, Sci-Fi}
3,671	Blazing Saddles	1,974	{Comedy, Western}

Table 5.4: A sample of the additional information available for each movie.

If we could use this information to place our movies more accurately in trait space, perhaps that would improve our recommendations for movies where we only have a few ratings. We can try this out by adding this information to our model using features, just like we did in the previous chapter.

5.6.1 Adding features to our model

To add features to our recommender model, we can re-use a chunk of the classification model from section 4.3. Specifically, we will introduce variables for the `featureValue` for each movie and feature, along with a `weight` for each feature and trait. As before, the product of these will give a `featureScore`. The sum of these feature scores will now be used as the mean for the trait prior – which we shall call `traitMean`. It follows that the prior position of the movie in trait space can now change, depending on the feature values, before any ratings have been seen! The resulting factor graph is shown in Figure 5.27 – the unchanged part of the graph has been faded out to make the newly-added part stand out.

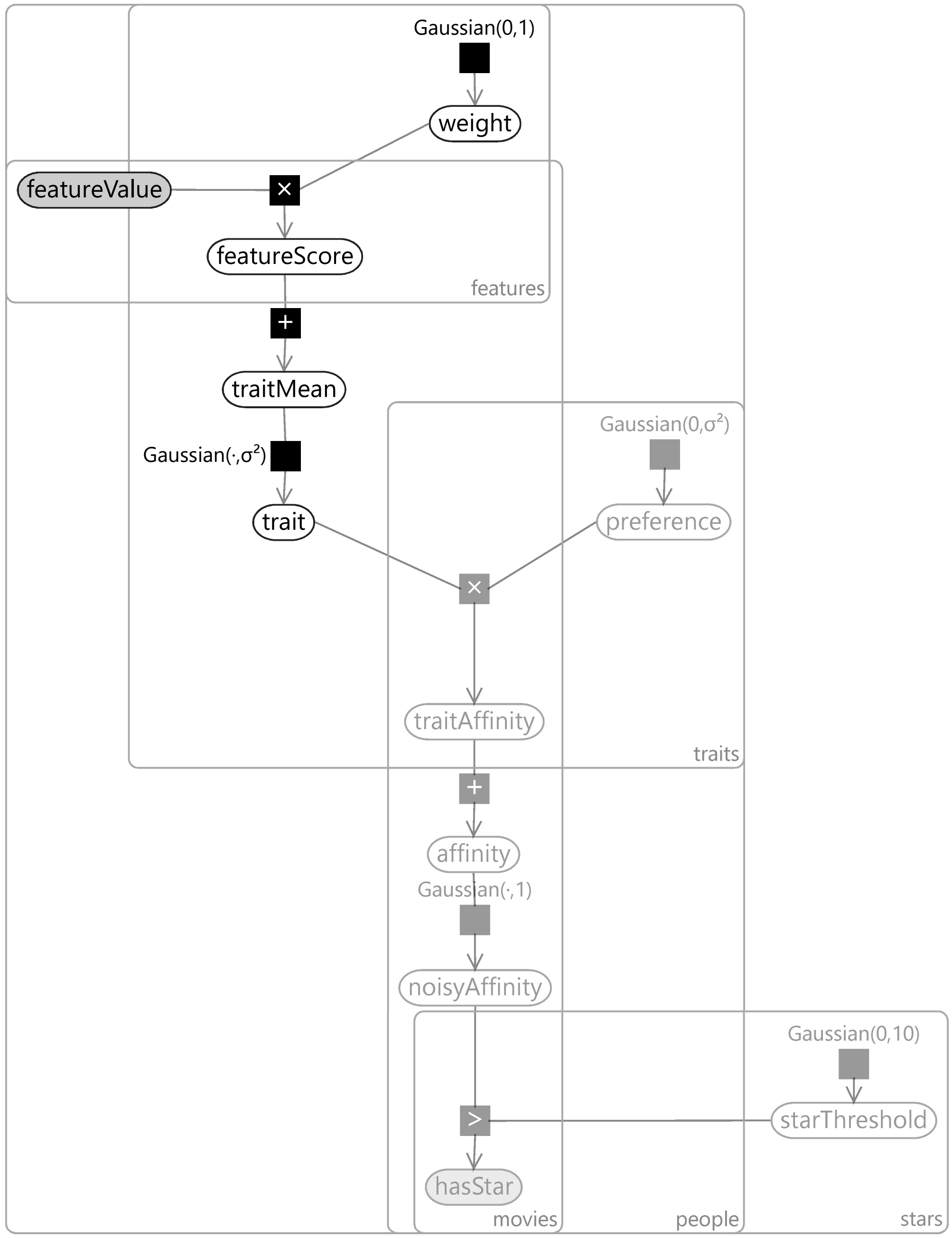


Figure 5.27: Factor graph for a recommender model that can consume feature values for individual movies. To emphasize the variables and factors which have been added, the remaining parts of the graph have been faded out.

In taking this chunk of model from the previous chapter, we must remember that we have also inherited the corresponding assumptions. Translated into the language of our model, these are:

(7) The feature values can always be calculated, for any movie.

(8) If a movie's feature value changes by x, then each trait mean will move by $weight \times x$ for some fixed, continuous, trait-specific weight.

(9) The weight for a feature and trait is equally likely to be positive or negative.

(10) A single feature normally has a small effect on a trait mean, sometimes has an intermediate effect and occasionally has a large effect.

(11) A particular change in one feature's value will cause the same change in each trait mean, no matter what the values of the other features are.

We explored these assumptions extensively in the previous chapter, so will not discuss them again here. However, it would be a worthwhile exercise to spend some time reflecting on how each assumption will affect the behaviour of our recommender system.

As in the previous chapter, we need to decide how to represent our movie information as features. The features that we will use are:

1. A constant feature set to 1.0 for all movies, used to capture any fixed bias.

2. A *ReleaseYear* feature which is represented using buckets, much like the *BodyLength* feature we designed in section 4.4. We choose the buckets to be every ten years until 1980 and then every five years after that – giving 17 buckets in total.

3. A *Genres* features which has the same design as the *Recipients* feature from section 4.5. That is, a total feature value of 1.0 is split evenly among the genres that a movie has. So if a movie is a Drama and a Romance, the Drama bucket will have a value of 0.5 and the Romance bucket will also have a value of 0.5.

This data set contains additional information about the movies but not about the people giving the ratings (such as age or gender). If we had such additional information we could incorporate it into our model using features, just as we did for movies. All we would need to do is add a features model for the mean of the `preference` prior of the same form as the one used for the `trait` prior in Figure 5.27. The resulting model would then be symmetrical between the movies/traits and people/preferences.

5.6.2 Results with features

Let's see what effect using movie features has on our accuracy metrics. Figure 5.28 shows the mean absolute error for models with and without features, for groups of movies with different numbers of ratings. We can see that adding features has improved accuracy for all four groups, with the biggest improvements in the groups with zero ratings. While there is still better accuracy for movies with more ratings, using features has helped narrow the gap between these movies and movies where few ratings are available.

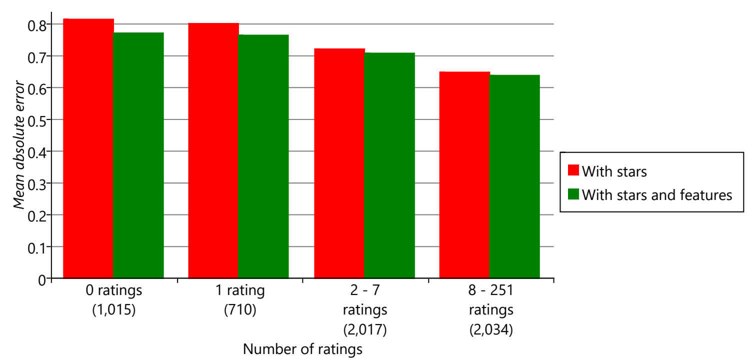
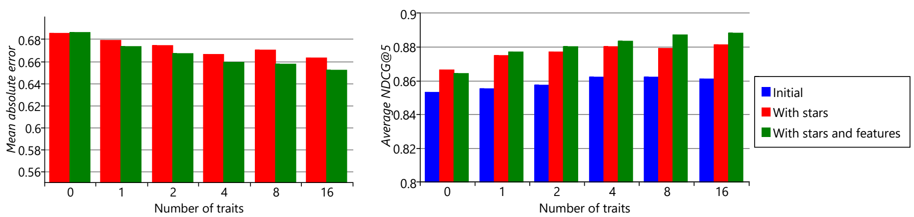


Figure 5.28: Including feature information in our model has reduced the prediction error, particularly for movies with only no ratings in the training set.

We can also look at the effect of using features on our overall metrics. These are shown for different numbers of traits in Figure 5.29. For comparison with previous results, we once again exclude ratings for movies that do not occur in the training set (that is, the left-hand bar of Figure 5.28). The chart shows that features increase accuracy whichever metric we look at. Interestingly, this increase is greater when more traits are used. The explanation for this effect is that we are not directly using features to make recommendations but instead we are using them indirectly to position movies in trait space. Using more traits helps us to capture the feature information more precisely, since a position in trait space conveys more information when there are more traits.



(a) Mean absolute error (MAE) (b) Average NDCG@5

Figure 5.29: Comparison of MAE and NDCG metrics for each of our models (note that MAE cannot be calculated for the initial model because it does not predict star ratings). According to these metrics, feature increases accuracy for any model with at least one trait, with the increase being larger as more traits are used.

Overall, using features has provided a good increase in accuracy, particularly for items with few ratings. This means that our model should now do a much better job of making recommendations, particularly for new movies – which is a very desirable characteristic indeed!

5.6.3 Final thoughts

In this chapter, we have developed a flexible recommender model that can consume like/dislike labels or full star ratings. In addition, the model can make use of additional information about either the items being recommended or the people for whom recommendations are being made. This model is already enough to be valuable for many customers of Azure machine learning – and indeed is very close to the one that was actually used in Azure ML. The main difference is that the Azure ML model can also learn personalised star ratings thresholds – this was achieved by moving the `starThreshold` variable inside the people plate and giving each threshold a suitably informative prior, to allow for data scarcity.

In developing our model, we have assumed that good recommendations are ones where the user will rate the item highly, but in fact this may not be the case. For a science fiction fan it may be likely that they would rate Star Wars highly, but it would be a poor recommendation because they would probably have seen it already. In other words, a good recommendation is for a movie that you are likely to enjoy but not to have already seen. Real recommendation systems keep a record of what movies a person has seen through the system and these are automatically removed from any list of recommendations. But such systems have no knowledge of what movies have been watched outside of the system. We could modify our model to predict both whether someone would like a movie and whether they are likely to have seen it. Using both of these predictions together could lead to much more valuable recommendations.

Similar items are nearby in trait space.

By learning the positions of items in trait space, we have also learned which items are similar since these will be close to each other in trait space. Given a target item, we can work out which items are similar to it by finding nearby items in trait space. More precisely, we do this by making recommendations for an imaginary person located at the same position in trait space as the target item. The result of this process is useful for making item-specific recommendations, such as "people who liked this movie, also liked". Item relatedness can also be used to improve the diversity of a set of recommendations. For example, we might not want to have two very similar movies in a list of recommendations (such as two movies in the same series). We could use the distance between the movies in trait space to remove such similar movies and so create a more diverse list of recommendations.

There are further model extensions that could usefully be made. One would be to make use of *implicit* feedback about an item. For example, many people never rate any movie, but instead just watch them. Even in this case, there is still useful information about the movies that the person likes. We may assume that they watch movies that they expect to like – so watching a movie is an implicit signal that the person liked the movie. It is harder to get an implicit signal that a person did not like a movie, so often when using implicit feedback there is positive-only data. In other words we have only the good ratings and none of the bad ones. Having a model that can cope with such positive-only data would be very useful – the most common approach today is to treat a random sample of unrated movies as if they were negatively rated.

Even when we do have ratings, the information about which ratings we have and which we do not have is very valuable. Having a rating is a bit like watching a movie – it provides a positive signal about liking the movie. The best performing recommender systems make use of the fact that missing ratings provide information about what a person likes or dislikes. With any piece of data that can be missing, we can model whether or not it is missing, as well as modelling the data itself. In the next chapter, we will discuss different kinds of missing data and how to handle them – while building models for understanding childhood asthma.

Chapter 6

Understanding Asthma

Asthma is the most common chronic disease of childhood and can have serious outcomes for those who suffer from it. Studies have shown that children with allergies are generally more likely to develop asthma. A better understanding of the relationship between allergies and asthma could improve detection, diagnosis and treatment of childhood asthma. Can model-based machine learning help provide this deeper understanding?

Asthma is a very common disease which affects around 5% of people in the UK [Ross Anderson et al., 2007] and about 7% in the US [Fanta, 2009]. Globally around 250,000 people die each year from asthma (Global Initiative for Asthma, 2011). If we could better understand what causes people to develop asthma, it would have a hugely beneficial impact on asthma detection, diagnosis and treatment. One known risk factor for asthma is if a person has allergies, but the relationship between developing allergies and developing asthma is not well understood. An improved understanding of this relationship could potentially allow early detection of the kind of severe asthma that can lead to hospitalisation or worse.

The Manchester Asthma and Allergy Study (MAAS) is a study designed to help understand the causes of childhood asthma and allergies. In particular, the study aims to understand why some children with allergies develop asthma while others do not. MAAS is a birth cohort study – in other words, people were re-

cruited into the study at birth – and consists of
around 1,000 people. The study began in 1995 and continues to this day, collecting ongoing data about the study participants, who are now young adults. As you might imagine, a huge amount of dedication and commitment is required of these participants and their families – we and the study team are immensely grateful to them all!

In this chapter, we will look at how to apply model-based machine learning to data collected in this study, to model the onset of childhood allergies and see how this relates to the development of asthma. This kind of machine learning application is different to those we have looked at in previous chapters, because we are interested in improving understanding as a primary goal of the project, rather than predicting who will develop asthma without any understanding of why. It's worth looking at these two contrasting goals in a bit more detail:

- **Predictive machine learning** – the goal is to make predictions, without requiring an explanation of the predictions. This kind of goal is common when building automated systems where explanations are not needed.
- **Explanatory machine learning** – the goal is to explain or understand patterns in the data. This kind of goal is common when doing scientific or medical research, where there is a human in the loop who wishes to understand the processes that give rise to the data.

Often there are elements of both of these goals in a particular machine learning project. For example, when doing predictions it may be useful to provide some explanation of those predictions. And even when the primary goal is improved understanding, such as in this asthma project, it may still be useful to apply that understanding to make predictions, such as predicting whether a child will develop asthma.

The model developed in this chapter was created as part of a collaboration with the MAAS team, particularly Professors Adnan Custovic and Angela Simpson, as described in Simpson et al. [2010] and Lazic et al. [2013].

6.1 A model of allergies

Our primary goal is to improve our understanding of allergy development, as it relates to childhood asthma, by looking for patterns in the MAAS data. To understand the relevant data in the study, we need to learn a little bit about diagnosing allergies. The doctors in the study used two types of test to try to detect if a person is allergic to a specific **allergen**, such as cat hair or peanuts. The two types of test were:

- A **skin prick test** where a drop of allergen solution is placed on the patient's skin (see image) which is then pricked with a needle. If the skin shows an immune response in the form of a red bump of a certain size, then the test is positive, otherwise it is negative.

- An allergen-specific **IgE test** – this is a blood test that looks for a kind of antibody called Immunoglobulin E (IgE) that specifically targets a particular allergen. The presence of this antibody is an indicator that the patient is allergic to that allergen. If this antibody is present in sufficient quantities the test is positive, otherwise negative.

If a child has a positive skin prick test or IgE test for an allergen, then they are said to be *sensitized* to that allergen.

For the children taking part in this study, both of these tests were performed for eight allergens: dust mite, cat, dog, pollen, mould, milk, egg and peanut. So that the development of allergies could be tracked over time, the tests were repeated at different ages (1, 3, 5 and 8). Therefore, the available data points are the two test results for each allergen, for each child, at each of the four ages.

The clinicians on the study believe that different patterns of allergies make children susceptible to different diseases, some of which may have significant impact on the child's health (such as severe asthma) and some of which may be more benign (such as mild hayfever). The goal of the project is to identify such patterns and see if they are indicative of developing particular diseases and of the severity of the disease. Our task is to develop a model of the allergen data set that can achieve this.

6.1.1 Modelling test results

To start with, let's consider a model of a child's test results for one allergen at one point in time. First, we need variables for the results of each test –

we will call these `skinTest` and `igeTest`. These variables will be `true` if the corresponding test is positive and `false` if the test is negative.

Remember that the purpose of these tests is to try and detect whether a child is actually sensitized (allergic) to a particular allergen. However, the tests are not perfectly consistent – for example, it is not unusual for a child to have a positive IgE test but a negative skin test. To cope with such inconsistencies, we can have a variable representing whether the child is truly sensitized to the allergen, which we will call `sensitized`. This variable will be `true` if the child is actually sensitized to the allergen and false if they are not sensitized. We then allow for the results of the tests to occasionally disagree with the value of this variable. In other words, we assume that each test can give a false positive (where the test is positive but the child is not sensitized) or a false negative (where the test is negative but the child is sensitized).

If a child is sensitized to a particular allergen (`sensitized`=`true`), then a skin prick test will be positive (`skinTest`=`true`) with some probability, which we will call `probSkinIfSens`. Since we expect the test to be mostly correct we would expect this probability to be high but less than one, since a skin prick test can give false negatives. Conversely, even if a child is not sensitized to a particular allergen (`sensitized`=`false`), then we might occasionally expect a skin prick test to be positive, but with some low probability `probSkinIfNotSens`. Although this probability is low, we still expect it to be greater than zero because a skin prick test can give false positives.

These two probabilities together define a conditional probability table for `skinTest` conditioned on `sensitized`.

sensitized	skinTest=true (positive)	skinTest=false (negative)
true	probSkinIfSens	1 - probSkinIfSens
false	probSkinIfNotSens	1 - probSkinIfNotSens

Table 6.1: The conditional probability table for $P($`skinTest`$|$`sensitized`$)$. Table columns correspond to values of the conditioned variable `skinTest`, rows correspond to values of the conditioning variable `sensitized`, and table cells contain the conditional probability values.

We have introduced these two probabilities as random variables in our model because we will want to learn them from data, in order to determine the false positive and false negative rates for the skin prick test. In order to learn their values, we must provide suitable prior distributions for each variable, that encode our assumptions about them. Let's write down those assumptions:

1. If a child is sensitized to a particular allergen, there is a high probability that they will get a positive test.

2. If a child is NOT sensitized to a particular allergen, there is a low probability that they will get a positive test.

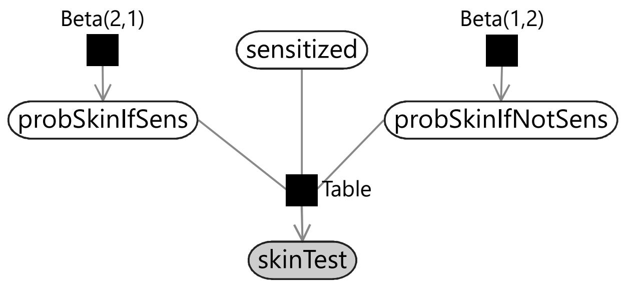


Figure 6.1: A model relating the result of a skin prick test (`skinTest`) to the underlying allergic sensitization state (`sensitized`). The `skinTest` variable is observed to equal the actual outcome of the test and so is shown shaded.

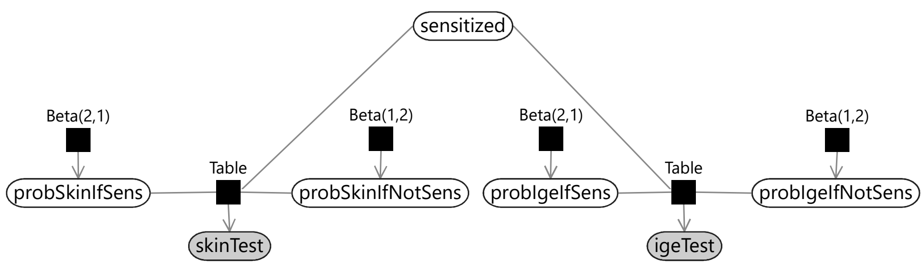


Figure 6.2: A model relating the results of both kinds of allergy test to the underlying allergic sensitization state. Each type of test has its own probability variables which means that each test can have different false positive and false negative rates. The test results are observed and so are shown shaded.

As in section 2.6, we can use beta distributions as prior distributions over probabilities that can represent these assumptions. Assumption 1 says that we expect `probSkinIfSens` to be high so we can use a *Beta*(2,1) prior which favours higher probability values. Assumption 2 says that we expect `probSkinIfNotSens` to be low so we can use a *Beta*(1,2) prior which favours low probability values. Armed with these prior probabilities, we can now draw a factor graph for a skin test, using the *Table* factor that we introduced back in section 2.6.

Now that we have a model for a skin test, we can add in the corresponding model for an IgE test. We again need probability variables for the probability of a positive test if sensitized `probIgeIfSens` and if not sensitized `probIgeIfNotSens` with the corresponding beta distribution priors. The `sensitized` variable is shared between the two tests, because both tests are attempting to detect the same underlying sensitization. The resulting factor graph for both tests is shown in Figure 6.2.

Inference in this model enables us to fuse the outcomes of both tests into a single underlying sensitization state. Learning the probabilities of true and false positives will let the model learn which test to pay most attention to. For example, if a test has a high false positive probability, then a positive outcome would influence the inference of the sensitization state less than a positive outcome for a test with a low false positive probability.

6.1.2 Modelling tests through time

For each child, we have test measurements at multiple points in time – ages 1, 3, 5 and 8. Such a collection of measurements is known as a **time series**, and analysis of such data is known as **time series analysis**. To understand the development of allergies, we need to build a model of a time series of allergy test results.

We could start building a time series model by duplicating the factor graph of Figure 6.2 at each time point. This would introduce a separate `sensitized` variable at each age, which we could call `sensitized1`, `sensitized3`, `sensitized5` and `sensitized8`. It would also introduce separate test result variables at each age, which we could similarly call `skinTest1`, `igeTest1`, `skinTest3`, `igeTest3` and so on. However, directly duplicating the factor graph would also mean having separate variables at each time point for the probability of a positive test given sensitized/not sensitized. Do we really expect the false positive and false negative rates for the tests to change over time? If exactly the same tests were done at each age, it would be reasonable to assume that the false positive and false negative rates did not change over time. Let's write down this assumption:

③ For each type of test, the false positive and false negative rates are the same for all such tests carried out in the study.

The consequence of this assumption is that the skin test probability variables (`probSkinIfSens`, `probSkinIfNotSens`) and the IgE test probability variables (`probIgeIfSens`, `probIgeIfNotSens`) will be shared across all time points. The result of this sharing is the factor graph of Figure 6.3.

You might wonder why we have drawn out the variables for each time point, rather than use a plate to collapse them all together. This is because, when modelling time series, we expect variables later in time to depend on the values of variables earlier in time. By drawing out all variables, we can now add factors connecting variables across time. But what should these factors be?

At age 1, there is a certain initial probability that a child will already be sensitized to a particular allergen – let's call this `probSens1`. Now, suppose the child is not sensitized at age 1 (`sensitized1`=`false`), there is some probability that they will become sensitized by age 3 – let's call this `probGain3`. Conversely, if the child is sensitized at age 1 (`sensitized1`=`true`), there is some probability that they retain that sensitization to age 3 – let's call this `probRetain3`. We can model this using a *Table* factor, just as we did for modelling the skin and IgE tests.

When we consider age 5, we need to ask ourselves a question: do we think that the sensitization at age 5 depends on both previous sensitizations (at ages 1 and 3), or just the most recent one (at age 3). Similarly, do we think that sensitization at age 8 depends on all three previous sensitizations (at ages 1, 3

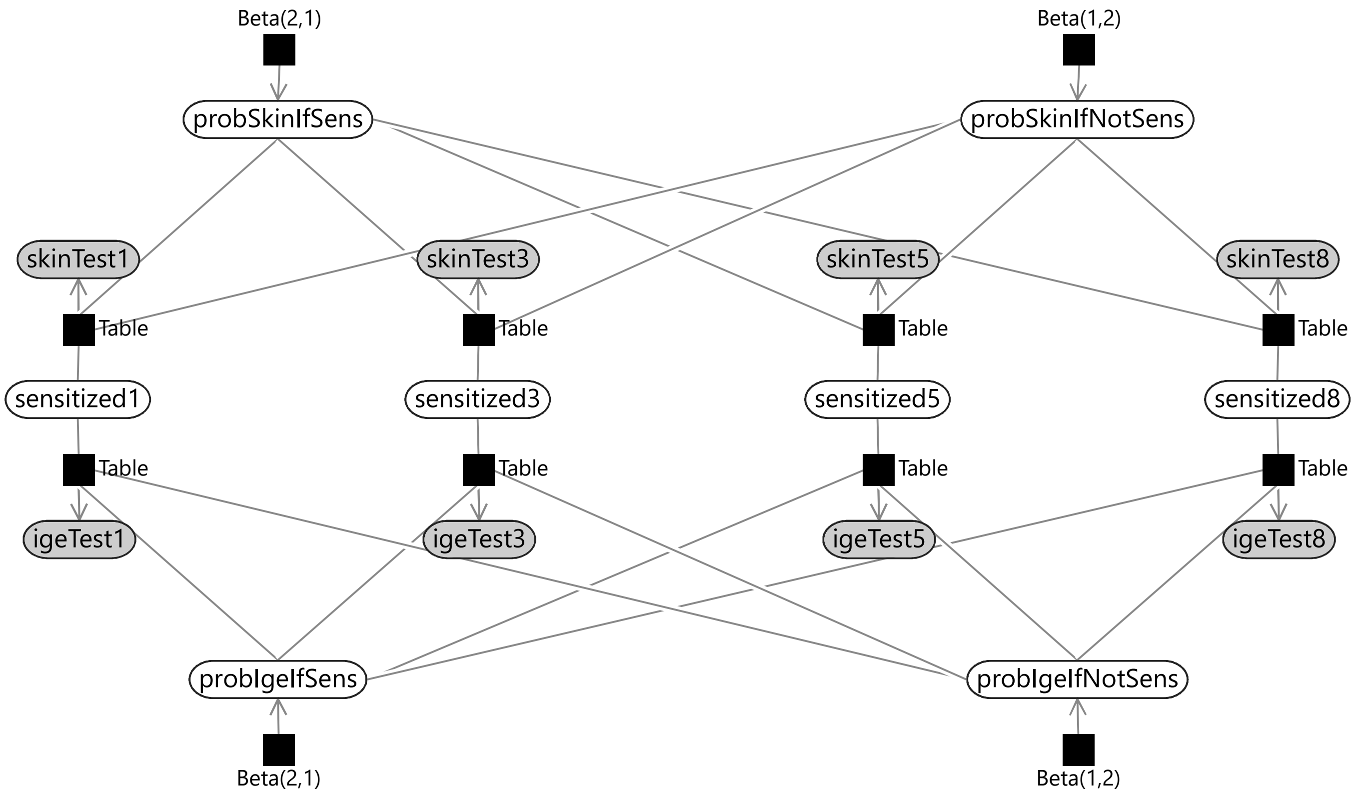


Figure 6.3: An initial model of a time series of allergy test results, which are explained by a series of underlying sensitizations. The false positive/false negative probability variables for each test are shared across all time points.

and 5) or just the most recent one (at age 5). Either of these assumptions might be reasonable, depending on the details of how the immune system functions. For now, we will assume that just the most recent sensitization is relevant, since that simplifies the model the most:

4. Whether a child is sensitized to an allergen at a particular time point depends only on whether they were sensitized to that allergen at the previous time point.

This kind of assumption is so common in time series modelling that it even has a name – it is called a **Markov assumption** after the Russian mathematician Andrey Markov. Our Markov assumption means that we can model sensitization at ages 5 and 8 just like we did at age 3. So for age 5, we have variables `probGain5` and `probRetain5` for the probabilities of gaining or retaining sensitization between the ages of 3 and 5. Similarly, for age 8, we have variables `probGain8` and `probRetain8` for the probabilities of gaining or retaining sensi-

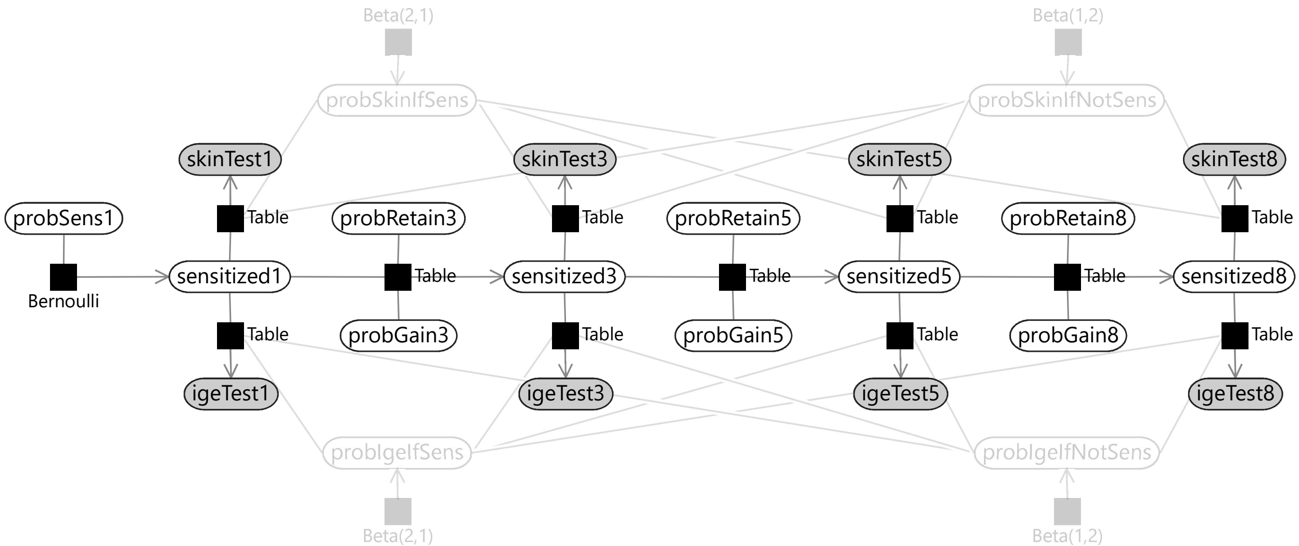


Figure 6.4: An improved time series model where the allergic sensitization at each point in time, depends on the sensitization at the previous point in time. The variables and factors relating to the test false positive/false negative rates have been dimmed, to emphasize the new factors added in the model.

tization between the ages of 5 and 8. As for age 3, we can model sensitivity at ages 5 and 8 using a *Table* factor, giving the factor graph of Figure 6.4.

Looking at Figure 6.4, you can see the chain of factors connecting the sensitization variables through time, from `sensitized1` through to `sensitized8`. This kind of chain structure is a common feature of time series model that make Markov assumptions, and so is called a **Markov chain**.

6.1.3 Completing the model

To complete our time series model, we need to extend it to cover multiple allergens and multiple children. We can add plates for allergens and children and place the sensitization and skin/IgE test variables inside both plates, since there are tests and sensitization states for every child and allergen. Assumption 3 says that the false positive and false negative rates of our tests are the same throughout the study, and so the variables `probSkinIfSens`, `probIgeIfSens`, `probSkinIfNotSens` and `probIgeIfNotSens` lie outside both plates. This leaves only the variables relating to the probability of initial having, gaining and retaining sensitization. We want these variables to be able to vary between allergens, so we can learn if different allergies are gained or lost at different points in time. So these variables must lie *inside* the `allergens` plate. But if we are trying to learn patterns of gaining or losing sensitization that are common to multiple children, we must have these probability variables shared across children. Right now, the only way of doing this is to place them outside the `children` plate.

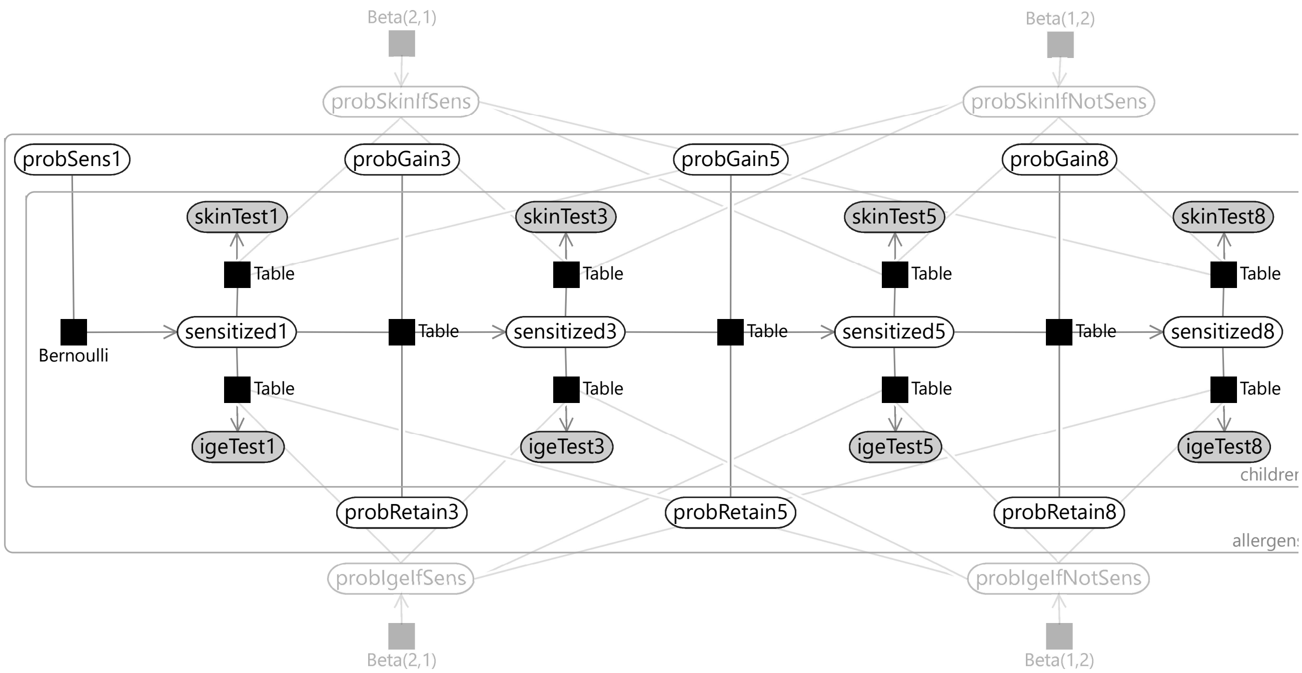


Figure 6.5: A complete model of a set of allergy tests for multiple children and multiple allergens. Plates are used to duplicate certain variables across children and allergens (see text for discussion). As in Figure 6.4, the variables and factors relating to the test false positive/false negative rates have been dimmed, to make the factor graph easier to read and to emphasise the Markov chain.

This corresponds to the following assumption, which is the final assumption of the model:

5 The probabilities relating to initially having, gaining or retaining sensitization to a particular allergen are the same for all children.

Given this assumption, we can now draw the factor graph with plates, where the variables have been appropriately placed inside or outside each plate (see Figure 6.5).

Reviewing Figure 6.5, you can see that:

- the test false positive/false negative probabilities are outside both plates and so are shared across all children and allergens;
- the probabilities of initially having, gaining and retaining sensitization are inside the allergens plate but outside the children plate, so are shared across children but can differ across allergens;
- the test results and sensitization are inside both plates, since there are tests and sensitization states for each child and allergen.

Given these plates, we now have a complete model that we can use with our data set of skin and IgE test results.

6.1.4 Reviewing our assumptions

As in previous chapters, we should take a moment to review our modelling assumptions. They are shown all together in Table 6.2.

① If a child is sensitized to a particular allergen, there is a high probability that they will get a positive test.
② If a child is NOT sensitized to a particular allergen, there is a low probability that they will get a positive test.
③ For each type of test, the false positive and false negative rates are the same for all such tests carried out in the study.
④ Whether a child is sensitized to an allergen at a particular time point depends only on whether they were sensitized to that allergen at the previous time point.
⑤ The probabilities relating to initially having, gaining or retaining sensitization to a particular allergen are the same for all children.

Table 6.2: The five assumptions encoded in our allergy model.

Assumption ① and Assumption ② seem to be safe assumptions – doctors would not use these tests if they were not correct most of the time. Assumption ③ seems like a plausible assumption, but we might worry that the tests have different false positive/false negative rates for different allergens. It might also be possible that the test was improved or updated during the study and so that the rates would change over time. To check this out we consulted with the MAAS clinicians and they confirmed that the tests were performed exactly the same way throughout the study – the same test methodology, the same allergen solutions, even the same person doing the tests! So it seems like this assumption is a relatively safe one.

Assumption ④ is our Markov assumption – this is a common simplifying assumption but is also commonly criticised as being too simplistic. For example, in our case, it says that the probability of gaining/retaining sensitization depends only the sensitization state at the previous time point and not, for example, on how long the child has had the sensitization (or lack of sensitization). Nonetheless, this assumption keeps the model simple and so we will stick with it.

Finally, Assumption ⑤ says that all children have the same patterns of gaining and losing sensitization. This assumption goes against the very purpose of the project, which is to identify how these patterns vary between children.

We will spend much of the rest of this chapter looking at how to improve on this assumption, but it is useful to keep it in place for now so we explore the behaviour of our new model.

Review of concepts introduced in this section

allergen A substance which someone can be allergic to, such as cat hair or peanuts.

skin prick test A test where a drop of allergen solution is placed on the patient's skin, which is then pricked with a needle. If the skin shows an immune response in the form of a red bump of a certain size, then the test is positive, otherwise it is negative.

IgE test A blood test that looks for a kind of antibody called Immunoglobulin E (IgE) that specifically targets a particular allergen. If this antibody is present in sufficient quantities the test is positive, otherwise negative.

time series A series of data points, listed in time order, that represent the measurement of some quantity over time – such as a stock price, blood pressure or population counts.

time series analysis Analysis of a time series, so as to understand the time-varying process underlying the time series data.

Markov assumption The assumption that a state of a process depends only on the previous state of that process, and not any earlier states. Named after the Russian mathematician Andrey Markov.

Markov chain A random process such that the probability distribution of the next state depends only on the previous state and not on any earlier state. In a factor graph, a Markov chain appears as a chain of time series variables with adjacent variables connected by factors.

6.2 Trying out the model

Now that we have a complete model, we are ready to try it out on some study data. As we've emphasised many times before in this book, when using a real data set, it is *essential* to look carefully at the data set to make sure that it is complete, correct and has the form that you expect. Remember that many common machine learning problems are caused by problems with data (such as those listed in section 2.5). A good way to check your data set is to construct visualisations that let you to see at a glance what it looks like. In this case, we need to create visualisations of the test results for each child, allergen and time point. However, this study data set contains private medical data and so we cannot share the data publicly in this book, even in the form of a visualisation. The most important thing that we learned from doing this visualisation is that there are a lot of test results missing from the data set.

When there are **missing data**, it is always worth analysing to understand why they are missing. In Figure 6.6, we plot the number of test results in the data set (whether positive or negative) for each age and type of test.

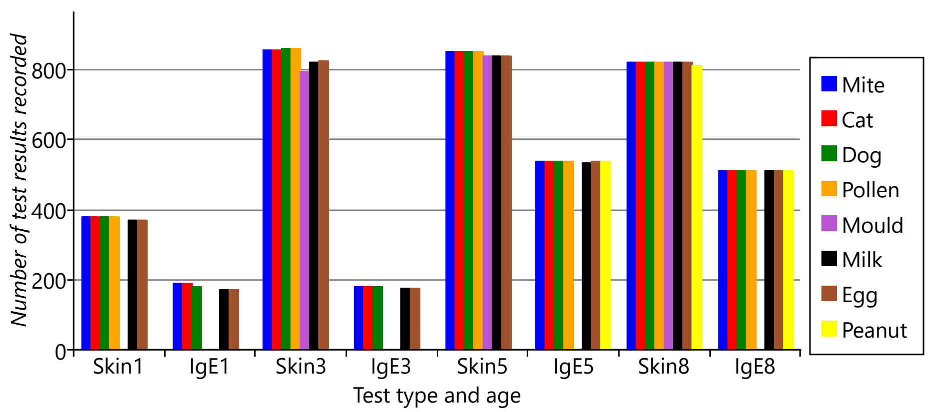


Figure 6.6: The test results recorded for each of the two types of tests, split by age of child.

You can see several different patterns of missing data in Figure 6.6. First, the plot shows that there are ages and test types that have no data for particular allergens. For example, peanut has no results at all for ages 1 and 3, and only IgE results at age 5. Mould has no IgE results at all, and no skin test results at age 1. Second, there is a lot more missing data at early ages, particularly age 1. Third, the plot shows that there is a lot more missing data overall for IgE tests than skin tests. We need to take into consideration the effect of all these missing data points.

6.2.1 Working with missing data

Missing data can obscure or distort the patterns in a data set

Missing data can introduce bias into the posterior distributions computed by running inference on a model, leading to incorrect or misleading results. Whether or not this effect will occur, and how big the bias will be, depends on why the data points are missing in the first place. In statistics, it is common to consider three kinds of missingness, which are referred to using the following (quite confusing!) terms:

- **missing completely at random** (MCAR) – where the missing data points occur entirely at random. In other words, the fact that the data is missing is independent of the value of the missing data point (the test result that would have been given had the test actually happened).

  When data is MCAR, the remaining, non-missing, data points are effectively just a random subset of the overall data set. In this case, the posterior distributions computed by probabilistic inference will be unbiased by the missing data. Unfortunately, in reality, missing data is rarely missing completely at random. However, it may be an acceptable approximation to assume that it is – in which case, this assumption should be made with full understanding of the possibility of introducing biases.

- **missing at random** (MAR) – where the missingness is not random, but where other known data values fully account for the fact that the data is missing. For example, suppose that boys are more likely to refuse an IgE test than girls. Considering the fact that boys are more likely to have allergies, this would introduce a bias in our results, since the missing tests would be more likely to be positive than the non-missing tests.

  When data is MAR, it is possible to correct for the bias, at least to some extent, by changing the model appropriately to account for why the data is missing. This extension requires creating a new variable in the model for each data point, which is `true` if the data point is missing and `false` otherwise, and then building a suitable sub model to explain this new variable. For example, if boys are more likely than girls to skip an IgE test, then to correct for bias we would need to extend our model to represent this effect, such as by adding a new `gender` variable connected to the missingness variable. We would also need to allow this `gender` variable to affect the probability of sensitization in an appropriate way. The degree to which this approach corrects the bias introduced by missing data, depends on how good the model of missingness is. As ever, a better model will give better results.

- **missing not at random** (MNAR) – where the missingness is not either MCAR or MAR. In this case, the fact that a data point is missing depends on the value of that data point. For example, this would occur if children with lots of allergies were more likely to skip a skin prick test because of concerns about the discomfort involved in having a positive test. Or such children might be more used to medical interventions and so may be less likely to skip a blood test due to fear of needles.

  When data is MNAR, it is not possible to correct for the bias without making modelling assumptions about the nature of the bias (which could be dangerous as there would be no data to verify such assumptions). One possible approach would be to try and collect additional information relevant to why the data is missing, in the hope that this would now make it missing at random (MAR).

For our study, we need to find out why the various patterns of missing data arose. Consulting again with the MAAS team, we find that:

1. The clinicians chose to omit mould tests at age 1, since this is a rare allergy and there was a desire to minimise the number of tests performed on babies. Similarly, a decision was made half way through the study to add in peanut tests.

2. The reduced number of tests at age 1 are due to manpower limitations as the study was ramped up – not all children could be brought in for testing by age 1.

3. The greater number of missing IgE tests are due to children not wanting to give blood, or parents not wanting babies or young children to have blood taken.

For 1, we know why the data is missing - because the clinicians chose not to do certain tests. Such data can be assumed to be missing completely at random, since the choice of which tests to perform at each age was made independently of any test results. For 2, the study team chose whether to invite a child in for testing by age 1 and so could choose in a way that was not influenced by the child's allergies (such as, at random). So again, we could assume such data to be missing completely at random. For 3, we might be more concerned, as now it is a decision of the child or the parents that is influencing whether the test is performed. This is more likely to be affected by the child's allergies, as we discussed above, and so it is possible that such missing data is not missing completely at random. For the sake of simplicity, we will assume that it is – this is such an important assumption that we should record it:

⑥ Missing test results are missing completely at random.

Having made this assumption, we should bear in mind that our inference results may contain biases. One reassuring point is that where we do not have an IgE test result, we often have a skin test result. This means that we still have some information about the underlying sensitization state even when an IgE test result is missing, which is likely to diminish any bias caused by its missingness.

There is another impact of missing data. Even when missing data is not introducing bias, if there is a lot of missing data it can lead to uncertainty, in the form of very broad posterior distributions. For example, at several time points we have no data for mould or peanut and so the gain/retain probabilities for those ages would be very uncertain, and so have broad posterior distributions. When included in results plots, such broad distributions can distract from the remaining meaningful results. To keep our plots as clear as possible, we will simply drop the mould and peanut allergens from our data set and consider only the remaining six allergens.

6.2.2 Some initial results

Having decided to treat our missing data as missing completely at random, we are now in a position to apply expectation propagation to our model and get some results. Where we have a missing data point, we simply do not observe the value of the corresponding random variable.

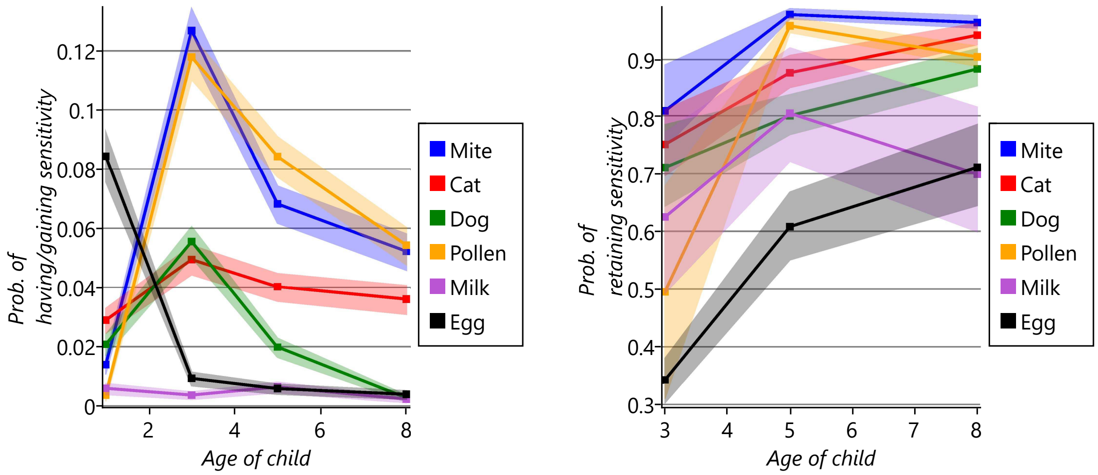
Having run our inference algorithm, the first posterior distributions we will look at are those for `probSkinIfSens`, `probSkinIfNotSens`, `probIgeIfSens` and `probIgeIfNotSens`. These posteriors are beta distributions, which we can summarise using a mean plus or minus a value indicating the width of the beta distribution, as shown in Table 6.3.

	If Sensitized	If Not Sensitized
Prob. of Pos. Skin Test	79.0%±0.7%	0.5%±0.04%
Prob. of Pos. IgE Test	93.0%±0.6%	3.7%±0.1%

Table 6.3: The probability of a positive test for each test type and for each sensitization state. The plus/minus values indicate the uncertainty in the probability given by the posterior beta distributions. The table shows that the skin test has a low false positive probability, but also a lower true positive probability. Conversely, the IgE test has a higher false positive probability, but a very high true positive probability. These results show that, taken together, the tests have complementary strengths and weaknesses.

The results in Table 6.3 show that the two types of test are complementary: the skin prick test has a very low false positive rate (¡1%) but as a result has a reduced true positive rate (79%); in contrast, the IgE test has a high true positive rate (93%) but as a result has a higher false positive rate (4%). The complementary nature of the two tests show why they are both used together – each test brings additional information about the underlying sensitization state of the child. During inference, our model will automatically take these true and false positive rates into account when inferring the sensitization state at each time point, so it will gain the advantage of the strengths of both tests, whilst being able to minimise the weaknesses.

Next let's look at the inferred probabilities of initially having, gaining and retaining sensitization for each allergen. Figure 6.7a shows the probability of initially having a sensitization (age 1) and then the probability of gaining sensitization (ages 3, 5, 8). Similarly, Figure 6.7b shows the probability of retaining sensitization since the previous time point (for ages 3, 5 and 8 only). Since each probability has a beta posterior distribution, the charts show the uncertainty associated with the probability values, using the lower and upper quartiles of each beta distribution.



(a) The probability of having sensitivity (age 1) or subsequently gaining sensitivity (ages 3, 5 and 8).

(b) The probability of retaining sensitivity since the previous time point at ages 3, 5 and 8.

Figure 6.7: Plots showing the probabilities for (a) having/gaining and (b) retaining sensitization for each time point and allergen.

Looking at Figure 6.7a and Figure 6.7b together, we can see that different allergens have different patterns of onset and loss of sensitization. For example, there is a high initial probability of sensitivity to egg but, after that, a very low probability of gaining sensitivity. Egg also has the lowest probability of retaining sensitization, meaning that children tend to have egg sensitivity very early in life and then rapidly lose it. As another example, mite and pollen have very low initial probabilities of sensitization, but then very high probabilities of gaining sensitization by age 3. Following sensitization to mite or pollen, the probability of retaining that sensitization is very high. In other words, children who gain sensitization to mite or pollen are most likely to do so between ages 1 and 3 and will then likely retain that sensitization (at least to age 8). Cat and dog have similar patterns of gain and loss to each other, but both have a higher initial probability of sensitization and a lower peak than mite and pollen. Milk shows the lowest probabilities of sensitization, meaning that it is a rare allergy in this cohort of children. As a result, the probability of retaining a milk sensitization is more uncertain, since it is learned from relatively few children. This uncertainty is shown by the broad shaded region for milk in Figure 6.7b.

Another way of visualizaing these results, is to look at the inferred sensitizations. We have inferred the posterior probability of each child having a sensitization to each allergen at each time point. We can then count the number of children who are more likely to be sensitized than not sensitized (that is, where the probability is ¿50%). Plotting this count of sensitizations for each allergen and age gives Figure 6.8.

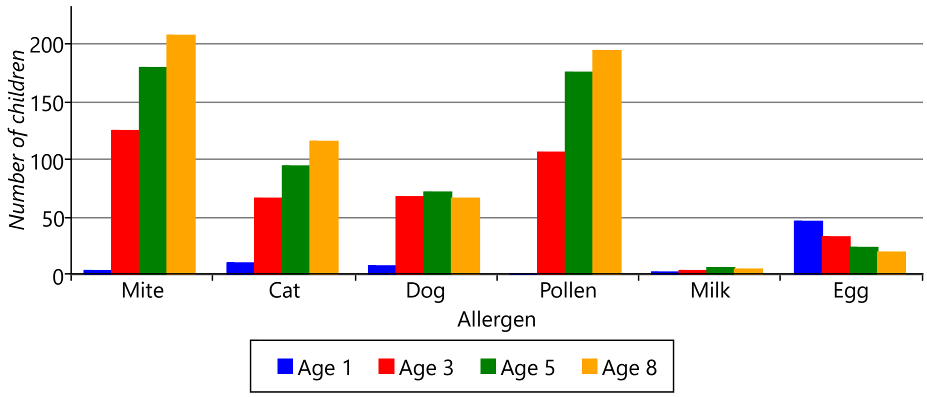


Figure 6.8: The number of children with inferred sensitizations for each allergen, at each point in time.

Figure 6.8 shows the patterns of gaining and losing sensitization in a different way, by showing the count of sensitized children. The chart shows that egg allergies start off common and disappear over time. The chart also shows that mite and pollen allergies start between ages 1 and 3 and the total number of allergic children only increases with age. In many ways, this chart is easier to read than the line charts of Figure 6.7a and Figure 6.7b because it looks directly at the counts of sensitizations rather than at changes in sensitizations. Also, all the information appears on one chart rather than two. For this reason, we will use this kind of chart to present results as we evolve the model later in the chapter.

To summarize, we have built a model that can learn about the patterns of gaining and losing allergic sensitization. The patterns that we have found apply to the entire cohort of children – effectively they are patterns for the population as a whole. What the model does not tell us is whether there are groups of children within the cohort that have different patterns of allergic sensitization, which might give rise to different diseases. By looking at all children together, this information is lost. Reviewing our assumptions, the problematic assumption is this one:

5 The probabilities relating to initially having, gaining or retaining sensitization to a particular allergen are the same for all children.

We'd really like to change the assumption to allow children to be in different groups, where each group of children can have different patterns of sensitization. Let's call these groups 'sensitization classes'. The assumption would then be:

5 The probabilities relating to initially having, gaining or retaining sensitization to a particular allergen are the same for all children in each sensitization class.

The problem is that we do not know which child is in which sensitization class. We need a model that can represent alternative processes for gaining and losing sensitization, and which can determine which process took place for each individual child. In other words, we need to be able to compare alternative models for each child's data and determine which is likely to be the one that gave rise to the data. To achieve this will require some new tools for modelling and inference, which we will introduce in the next section.

Review of concepts introduced in this section

missing data In a data set, a missing data point is one where no value is available for a variable in an observation. The reason for the value being missing is important and can affect the validity of probabilistic inference using the remaining non-missing values. See subsection 6.2.1.

missing completely at random Where missing data points occur entirely at random. In other words, the fact that the data is missing is independent of the value of the missing data point.

missing at random Where missing data points do not occur at random, but where other known data values fully account for the fact that the data is missing.

missing not at random Where missing data is neither missing completely at random (MCAR) not missing at random (MAR). In this case, the fact that a data point is missing depends on the value of that data point. Where data is missing not at random, it is very difficult to avoid biases in the results of inference.

6.3 Comparing alternative models

In all the previous chapters, we have assumed that the data arose from a single underlying process. But now we can no longer presume this, since we expect there to be different processes for children who do develop allergies and asthma and for those who do not. To handle these kinds of alternative processes, we need to introduce a new modelling technique.

This technique will allow us to:

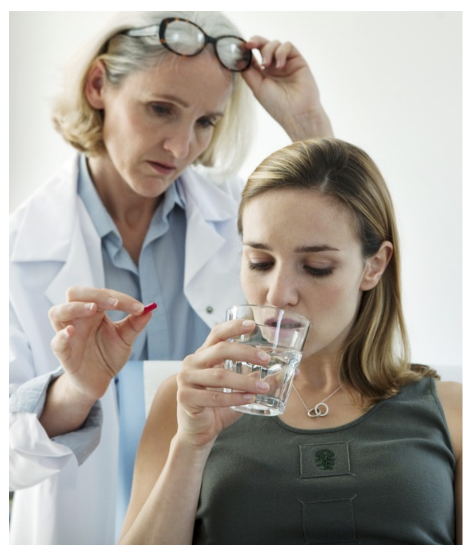
- Represent multiple alternative processes within a single model;
- Evaluate the probability that each alternative process gave rise to a particular data item (such as the data for a particular child);
- Compare two or more different models to see which best explains some data.

To introduce this new technique, we will need to put the asthma project to one side for now and instead look at a simple example of a two-process scenario (if you'd prefer to stay focused on the asthma project, skip ahead to section 6.5). Since we are in the medical domain, there is a perfect two-process scenario available: the **randomised controlled trial**. A randomised controlled trial is a kind of clinical trial commonly used for testing the effectiveness of various types of medical intervention, such as new drugs. In such a trial, each subject is randomly assigned into either a treated group (which receives the experimental intervention) or a control group (which does not receive the intervention). The purpose of the trial is to determine whether the experiment intervention has an effect on one or more outcomes of interest, and to understand the nature of that effect.

Let's consider a simple trial to test the effectiveness of a new drug on treating a particular illness. We will use one outcome of interest – whether the patient made a full recovery from the illness. In modelling terms, the purpose of this trial is to determine which of the following two processes occurred:

1. A process where the drug <u>had no effect</u> on whether the patient recovered.
2. A process where the drug <u>did have an effect</u> on whether the patient recovered.

To determine which process took place, we need to build a model of each process and then compare them to see which best fits the data. In both models, the data is the same: whether or not each subject recovered. We can attach the



The goal of our randomized controlled trial will be to find out if a new drug is effective.

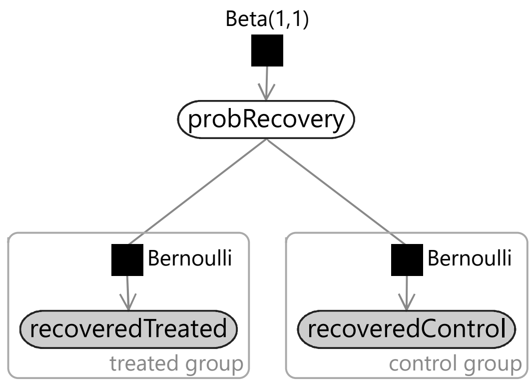


Figure 6.9: Factor graph for a process where the experimental drug has no effect. In this case, the probability of recovery is the same for the treated and control groups.

data to each model using binary variables which are `true` if that subject recovered and `false` otherwise. We'll put these binary variables into two arrays: `recoveredControl` contains the variables for each subject in the control group and `recoveredTreated` similarly contains the variables for each subject in the treated group.

Model where the drug had no effect

Let's start with a model of the first process, where the drug had no effect. In this case, because the drug had no effect, there is no difference between the treated group and the control group. So we can use an assumption like this one:

1. The (unknown) probability of recovery is the same for subjects in the treated and control groups.

It is perfectly possible that a subject could recover from the illness without any medical intervention (or with a medical intervention that does nothing). In this model, we assume that the drug has no effect and therefore all recoveries are of this kind. We do not know what the probability of such a spontaneous recovery is and so we can introduce a random variable `probRecovery` to represent it, with a uniform *Beta*(1,1) prior. Then for each variable in the `recoveredControl` and `recoveredTreated` arrays, we assume that they were drawn from a Bernoulli distribution whose parameter is `probRecovery`. The resulting model is shown as a factor graph in Figure 6.9 – for a refresher on Beta-Bernoulli models like this one, take a look back at chapter 2.

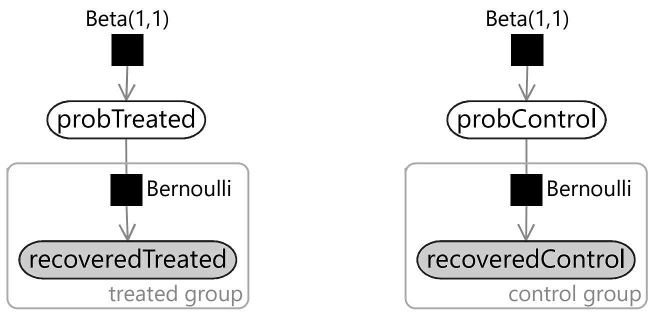


Figure 6.10: Factor graph for a process where the experimental drug does have an effect, and so the probability of recovery is different for the treated group and for the control group.

Model where the drug did have an effect

Now let's turn to the second process, where the drug did have an effect on whether the patient recovered. In this case, we need to assume that there is a different probability of recovery for the treated group and for the control group. We hope that there is a higher probability of recovery for the treated group, but we are not going to assume this. We are only going to assume that the probability of recovery changes if the drug is taken.

② The probability of recovery is different for subjects in the treated group and for subjects in the control group.

To encode this assumption in a factor graph, we need two variables: `probTreated` which is the probability of recovery for subjects who were given the drug and `probControl` which is the probability of recovery for subjects in the control group who were not given the drug. Once again, we choose uniform $Beta(1,1)$ priors over each of these variables. Then for each variable in the `recoveredControl` array we assume that they were drawn from a Bernoulli distribution whose parameter is `probControl`. Conversely, for each variable in the `recoveredTreated` array we assume that they were drawn from a Bernoulli distribution whose parameter is `probTreated`. The resulting model is shown in Figure 6.10.

Compare the models of the two different processes given in Figure 6.9 and Figure 6.10. You can see that the factor graphs are pretty similar. The only difference is that the 'no effect' model has a single shared probability of recovery whilst the 'has effect' model has different probabilities of recovery for the treated and control groups.

Selecting between the two models

We now need to decide which of these two models gave rise to the actual outcomes measured in the trial. The task of choosing which of several models best fits a particular data set is called **model selection**. In model-based machine learning, if we want to know the value of an unknown quantity, we introduce a random variable for that quantity and infer a posterior distribution over the value of the variable. We can use exactly this approach to do model selection. Let's consider a random variable called `model` which has two possible values `NoEffect` if the 'no effect' model gave rise to the data and `HasEffect` if the 'has effect' model gave rise to the data. Notice the implicit assumption here:

③ Either the 'no effect' model or the 'has effect' model gave rise to the data. No other model will be considered.

For brevity, let's use `data` to refer to all our observed data, in other words, the two arrays `recoveredTreated` and `recoveredControl`. We can then use Bayes' rule (Panel 1.1) to infer a posterior distribution over `model` given the `data`.

$$P(\texttt{model}|\texttt{data}) = \frac{P(\texttt{model})P(\texttt{data}|\texttt{model})}{P(\texttt{data})}. \tag{6.1}$$

Models can be compared using model evidence, in a process called Bayesian model selection.

Unsurprisingly, this technique of using Bayes's rule to do model selection is called **Bayesian model selection**. In equation (6.1), the left hand side is the posterior distribution over models that we want to compute. On the right hand side, $P(\texttt{model})$ encodes our prior belief about which model is more probable – usually, this prior is chosen to be uniform so as not to favour any one model over another. Also on the right hand side, $P(\texttt{data}|\texttt{model})$ gives the probability of the data conditioned on the choice of model. This is the data-dependent term that varies from model to model and so provides the evidence for or against each model. For this reason, this quantity is known as the **model evidence** or sometimes just as the **evidence**.

With a uniform prior over models, the result is that the posterior distribution over `model` is equal to the model evidence values normalised to add up to 1. In other words, the posterior probability of a model is proportional to the model evidence for that model. For this reason, when comparing two models, it is common to look at the ratio of their model evidences – a quantity known as a **Bayes factor**. For example, the Bayes factor comparing the 'has effect' model evidence to the 'no effect' model evidence is:

$$\text{Bayes factor} = \frac{P(\texttt{data}|\texttt{model} = \texttt{HasEffect})}{P(\texttt{data}|\texttt{model} = \texttt{NoEffect})} \tag{6.2}$$

The higher the Bayes factor, the stronger the evidence that the top model (in this case the 'has effect' model) is a better model than the bottom model (the 'no effect' model). For example, Kass and Raftery [1995] suggest that a Bayes factor between 3-20 is positive evidence for the top model, a Bayes factor between 20-150 is strong evidence, and a Bayes factor above 150 is very strong evidence. However, it is important to bear in mind that this evidence is only *relative* evidence that the top model is better than the bottom one – it is not evidence that this is the true model of the data or even that it is a good model of the data.

You might worry that the 'has effect' model will *always* be favoured over the 'no effect' model, because the 'has effect' model includes the 'no effect' model as a special case (when `probTreated` is equal to `probControl`). This means that the 'has effect' model can always fit any data generated by the 'no effect' model. So, even if the drug has no effect, the 'has effect' model will still fit the data well. As we will see when we start computing Bayes factors, if the drug has no effect the Bayes factor will correctly favour the 'no effect' model.

So why is the 'no effect' model favoured in this case? It is because of a principle known as **Occam's razor** (named after William of Ockham who popularized it) which can be expressed as "where multiple explanations fit equally well with a set of observations, favour the simplest". Bayesian model selection applies Occam's razor automatically by favouring simple models (generally those with fewer variables) over complex ones. This arises because a more complex model can generate more different data sets than a simpler model, and so will place lower probability on any particular data set. It follows that, where a data set could have been generated by either model, it will have higher probability under the simpler model – and so a higher model evidence. We will see this effect in action in the next section, where we show how to compute model evidences and Bayes factors for different trial outcomes.

6.3.1 Comparing the two models using Bayesian model selection

INFERENCE

Inference deep-dive

In this optional section, we show the inference calculations needed to do Bayesian model selection for the two models we just described. If you want to focus on modelling, feel free to skip this section.

Next we can look at how to perform Bayesian model selection between the two models in our randomised controlled trial. As an example, we will consider a trial with 40 people: 20 in the control group and 20 in the treated group. In this example trial, we found that 13 out of 20 people recovered in the treated group compared to just 8 out of 20 in the control group. To do model selection for this trial, we will need to compute the model evidence for each of our two models.

Computing the evidence for the 'no effect' model

Let's first compute the evidence for the 'no effect' model, which is given by $P(\texttt{data}|\texttt{model} = \texttt{NoEffect})$. Remembering that `data` refers to the two arrays `recoveredTreated` and `recoveredControl`, we can write this more precisely as $P(\texttt{recoveredTreated}, \texttt{recoveredControl}|\texttt{model} = \texttt{NoEffect})$.

If we write down the joint probability for the 'no effect' model, it looks like this:

$$
\begin{aligned}
P(\texttt{recoveredTreated}, &\texttt{recoveredControl}, \texttt{probRecovery}|\texttt{model} = \texttt{NoEffect}) \\
&= \mathit{Beta}(\texttt{probRecovery}; 1, 1) \\
&\times \prod_{i \in \text{treated}} \mathit{Bernoulli}(\texttt{recoveredTreated}[i]|\texttt{probRecovery}) \\
&\times \prod_{i \in \text{control}} \mathit{Bernoulli}(\texttt{recoveredControl}[i]|\texttt{probRecovery})
\end{aligned}
\tag{6.3}
$$

In equation (6.3), the notation $\prod_{i \in \text{treated}}$ means a product of all the contained terms where i varies over all the people in the treated group. Notice that there is a term in the joint probability for each factor in the factor graph of Figure 6.9, as we learned back in section 2.1. Also notice that when working with multiple models, we write the joint probability conditioned on the choice of model, in this case $\texttt{model} = \texttt{NoEffect}$. This conditioning makes it clear which model we are writing the joint probability for.

We can simplify this joint probability quite a bit. First, we can note that $\mathit{Beta}(\texttt{probRecovery}; 1, 1)$ is a uniform distribution and so we can remove it (because multiplying by a uniform distribution has no effect). Second, we can use the fact that `recoveredTreated` and `recoveredControl` are both observed variables, so we can replace the Bernoulli terms by `probRecovery` for each subject that recovered and by $(1-\texttt{probRecovery})$ for each subject that did not recover. It is helpful at this point to define some counts of subjects. Let's call the number of treated group subjects that recovered T_T and the number which did not recover T_F. Similarly, let's call the number of control group subjects that recovered C_T and the number which did not recover C_F.

$$
\begin{aligned}
&P(\texttt{recoveredTreated}, \texttt{recoveredControl}, \texttt{probRecovery}|\texttt{model} = \texttt{NoEffect}) \\
&\quad = \texttt{probRecovery}^{T_T}(1 - \texttt{probRecovery})^{T_F} \times \texttt{probRecovery}^{C_T}(1 - \texttt{probRecovery})^{C_F} \\
&\quad = \texttt{probRecovery}^{(T_T + C_T)}(1 - \texttt{probRecovery})^{(T_F + C_F)}
\end{aligned}
\tag{6.4}
$$

This joint probability $P(\texttt{recoveredTreated}, \texttt{recoveredControl}, \texttt{probRecovery}|\texttt{model} = \texttt{NoEffect})$ is quite similar to the model evidence that we are trying to compute $P(\texttt{recoveredTreated}, \texttt{recoveredControl}|\texttt{model} = \texttt{NoEffect})$. The difference is that the joint probability includes the `probRecovery` variable. In order to compute the model evidence, we need to remove this variable by marginalising (integrating) it out.

$$
\begin{aligned}
&P(\texttt{recoveredTreated}, \texttt{recoveredControl}|\texttt{model} = \texttt{NoEffect}) \\
&= \int P(\texttt{recoveredTreated}, \texttt{recoveredControl}, \texttt{probRecovery}|\texttt{model} = \texttt{NoEffect}) \; d\texttt{probRecovery} \\
&= \int \texttt{probRecovery}^{(T_T + C_T)}(1 - \texttt{probRecovery})^{(T_F + C_F)} \; d\texttt{probRecovery}
\end{aligned}
\tag{6.5}
$$

To evaluate this integral, we can compare it to the probability density function of the beta distribution, that we introduced back in equation (2.18):

$$Beta(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha, \beta)} \tag{6.6}$$

We know that the integral of this density function is 1, because the area under any probability density function must be 1. Our model evidence in equation (6.5) looks like the integral of a beta distribution with $\alpha = T_T + C_T + 1$ and $\beta = T_F + C_F + 1$, except that it is not being divided by the normalising beta function $\mathrm{B}(\alpha, \beta)$. If we did divide by $\mathrm{B}(\alpha, \beta)$, the integral would be 1. Since we are not, the integral must equal $\mathrm{B}(\alpha, \beta)$ for the above values of α and β. In other words, the model evidence is equal to $\mathrm{B}(T_T + C_T + 1, T_F + C_F + 1)$.

For the counts in our example, this model evidence is $\mathrm{B}(13+8+1, 7+12+1)$, which equals $\mathrm{B}(22, 20)$.

Computing the evidence for the 'has effect' model

The computation of the model evidence for the 'has effect' model is actually quite similar. Again, we write down the joint distribution

$$\begin{aligned}
P(&\texttt{recoveredTreated}, \texttt{recoveredControl}, \texttt{probTreated}, \texttt{probControl} | \texttt{model} = \texttt{HasEffect}) \\
&= Beta(\texttt{probTreated}; 1, 1) \\
&\times Beta(\texttt{probControl}; 1, 1) \\
&\times \prod_{i \in \text{treated}} Bernoulli(\texttt{recoveredTreated}[i] | \texttt{probTreated}) \\
&\times \prod_{i \in \text{control}} Bernoulli(\texttt{recoveredControl}[i] | \texttt{probControl})
\end{aligned} \tag{6.7}$$

We now condition the joint distribution on $\texttt{model} = \texttt{HasEffect}$, which shows that this is the joint distribution for the 'has effect' model. We can simplify this expression by removing the uniform beta distributions and again using the counts of recovered/not recovered subjects in each group:

$$\begin{aligned}
P(&\texttt{recoveredTreated}, \texttt{recoveredControl}, \texttt{probTreated}, \texttt{probControl} | \texttt{model} = \texttt{HasEffect}) \\
&= \texttt{probTreated}^{T_T} (1 - \texttt{probTreated})^{T_F} \times \texttt{probControl}^{C_T} (1 - \texttt{probControl})^{C_F}
\end{aligned} \tag{6.8}$$

Notice that in this model we have two extra variables that we need to get rid of by marginalisation: `probTreated` and `probControl`. To integrate this expression over these extra variables, we can use the same trick as before except that now we have two beta densities: one over `probTreated` and one over `probControl`. The resulting model evidence is:

$$\begin{aligned}
P(&\texttt{recoveredTreated}, \texttt{recoveredControl} | \texttt{model} = \texttt{HasEffect}) \\
&= \mathrm{B}(T_T + 1, T_F + 1) \times \mathrm{B}(C_T + 1, C_F + 1)
\end{aligned} \tag{6.9}$$

For the counts in our example, this model evidence is $\mathrm{B}(13+1, 7+1)\mathrm{B}(8+1, 12+1)$, which simplifies to $\mathrm{B}(14, 8)\mathrm{B}(9, 13)$.

Computing the Bayes factor for the 'has effect' model over the 'no effect' model

We now have the model evidence for each of our two models:

- $P(\texttt{data}|\texttt{model} = \texttt{NoEffect}) = \mathrm{B}(T_T + C_T + 1, T_F + C_F + 1)$
- $P(\texttt{data}|\texttt{model} = \texttt{HasEffect}) = \mathrm{B}(T_T + 1, T_F + 1) \times \mathrm{B}(C_T + 1, C_F + 1)$

These model evidence values can be plugged into equation (6.1) to compute a posterior distribution over the `model` variable.

Let's compute the Bayes factor for our example trial, where 8/20 of the control group recovered, compared to 13/20 of the treated group:

$$\text{Bayes factor} = \frac{P(\texttt{model})P(\texttt{data}|\texttt{model})}{P(\texttt{data})} = \frac{\mathrm{B}(14, 8)\mathrm{B}(9, 13)}{\mathrm{B}(22, 20)} = 1.25 \tag{6.10}$$

A Bayes factor of just 1.25 shows that the 'has effect' model is very slightly favoured over the 'no effect' model but that the evidence is very weak. Note that this does not mean that the drug has no effect, but that we have not yet shown reliably that it does have an effect. The root problem is that the trial is just too small to provide strong evidence for the effect of the drug. We'll explore the effect on the Bayes factor of increasing the size of the trial in the next section.

Earlier, we claimed that the Bayes factor will correctly favour the 'no effect' model in the case where the drug really has no effect. To prove this, let's consider a trial where the drug does indeed have no effect, which leads to an outcome of 8/20 recovering in both the control and treated groups. In this case, the Bayes factor is given by:

$$\text{Bayes factor} = \frac{P(\texttt{model})P(\texttt{data}|\texttt{model})}{P(\texttt{data})} = \frac{\mathrm{B}(9, 13)\mathrm{B}(9, 13)}{\mathrm{B}(17, 25)} = 0.37 \tag{6.11}$$

Now we have a Bayes factor of less than 1 which means that the 'no effect' model has been favoured over the 'has effect' model, despite them both fitting the data equally well. This tendency of Bayesian model selection to favour simpler models is crucial to selecting the correct model in real applications. As this example shows, without it, we would not be able to tell that a drug doesn't work!

The model evidence calculations we have just seen have a familiar form. We introduced a random variable called `model` and then used Bayes' rule to infer the posterior distribution over that random variable. However, the random variable `model` did not appear in any factor graph and we manually computed its posterior distribution, rather than using a general-purpose message passing algorithm. It would be simpler, easier and more consistent if the posterior distribution could be calculated by defining a model containing the `model` variable and running a standard inference algorithm on that model. In the next section, we show that this can be achieved using a modelling structure called a *gate*.

Review of concepts introduced in this section

randomised controlled trial A randomised controlled trial is a kind of clinical trial commonly used for testing the effectiveness of various types of medical intervention, such as new drugs. In such a trial, each subject is randomly assigned into either a treated group (which receives the experimental intervention) or a control group (which does not receive the intervention). The purpose of the trial is to determine whether the experimental intervention has an effect or not on one or more outcomes of interest, and to understand the nature of that effect.

model selection The task of choosing which of several models best fits a particular data set. Model selection is helpful not only because it allows the best model to be used, but also because identifying the best model helps to understand the processes that gave rise to the data set.

Bayesian model selection The process of doing model selection by computing a posterior distribution over the choice of model conditioned on a given data set. Rather than given a single 'best' model, Bayesian model selection returns a probability for each model and the relative size of these probabilities can be used to assess the relative quality of fit of each model.

model evidence The probability of the data conditioned on the choice of model, in other words $P(\texttt{data}|\texttt{model})$. This conditional probability provides evidence for or against each model being the one that gave rise to the data set, thus the name 'model evidence'. Comparing model evidence values for different models allows for Bayesian model selection. Because it is a frequently used concept, model evidence is often called just the 'evidence'.

Bayes factor The ratio of the model evidence for a particular model of interest to the model evidence for another model, usually a baseline or 'null' model. The higher the Bayes factor, the greater the support for the proposed model relative to the a baseline model.

Occam's razor Where multiple explanations fit equally well with a set of observations, favour the simplest. It is named after William of Ockham who used it in his philosophical arguments. He did not invent the concept, however, there are references to it as early as Aristotle (384-322 BC).

6.4 Modelling with gates

In the previous section, we saw how to compare alternative processes by manually inferring the posterior distribution over a random variable that selects between them. What we will now see is how to do the same calculation by defining an appropriate model and performing inference within that model. To do this, we need a new modelling structure that allows alternatives to be represented within a model. The modelling structure that we can use to do this is called a **gate**, as described in Minka and Winn [2009].

A gate allows part of a factor graph to be turned on or off.

A gate encloses part of a factor graph and switches it on or off depending on the state of a random variable called the **selector variable**. The gate is on when the selector variable has a particular value, called the *key*, and off for all other values. An example gate is shown in the factor graph of Figure 6.11. The gate is shown as a dashed rectangle with the key value (`true`) in the top left corner. The selector variable `selector` has an edge connecting it to the gate – the arrow on the edge shows that the gate is considered to be a child of the selector variable. When `selector` equals `true`, the gate is on and so `x` has a *Bernoulli*(0.2) distribution. Otherwise, the gate is off and `x` has a uniform distribution, since it is not connected to any factors.

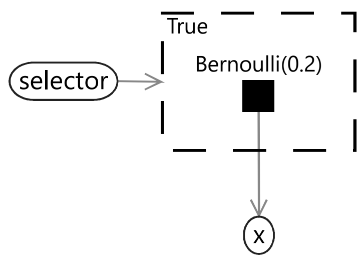


Figure 6.11: An example of a factor graph which contains a gate, shown as a dashed rectangle. When `selector` equals the key value `true` (shown in the top left of the gate), the gate is on and the variable `x` has a *Bernoulli*(0.2) distribution. When `selector` is `false`, the gate is off and `x` has a uniform distribution since it is not connected to any factors.

When writing the joint distribution for a factor graph with a gate, all terms relating to the part of the graph inside the gate need to be switched on or off according to whether the selector variable takes the key value or not. Such terms can be turned off by raising them to the power zero and left turned on by raising to the power one. For example, the joint distribution for Figure 6.11 is

$$P(\texttt{selector}, \texttt{x}) \propto \mathit{Bernoulli}(x; 0.2)^{\delta(\texttt{selector=true})} \tag{6.12}$$

where the function $\delta()$ equals one if the expression in brackets is true and zero

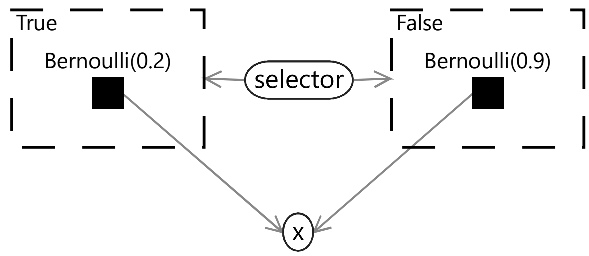


Figure 6.12: An example of a factor graph which contains a gate block. When `selector` equals `true`, the left gate is on and the right gate is off and so `x` has a *Bernoulli*(0.2) distribution. When `selector` equals `false`, the left gate is off and the right gate is on and so `x` has a *Bernoulli*(0.9) distribution.

otherwise. If `selector` is not `true` the $Bernoulli(x; 0.2)$ term will be raised to the power zero, making the term equal to one – equivalent to removing it from the product (i.e. turning it off).

When using gates inside a model, it is common to have a gate for each value of the selector variable. In this case, the resulting set of gates is called a **gate block**. Because the selector variable can only have one value, only one gate in a gate block can be on at once. An example gate block is shown in the factor graph of Figure 6.12. In this example, the selector variable is binary and so there are two gates in the gate block, one with the key value `true` and one with the key value `false`. It is also possible to have selector variables with any number of values, leading to gate blocks containing the corresponding number of gates.

The joint probability distribution for this factor graph is

$$P(\texttt{selector}, \texttt{x}) \propto Bernoulli(x; 0.2)^{\delta(\texttt{selector}=\texttt{true})}\ Bernoulli(x; 0.9)^{\delta(\texttt{selector}=\texttt{false})}. \tag{6.13}$$

Looking at this joint probability, you might be able to spot that the gate block between `selector` and `x` represents a conditional probability table, like so:

selector	x=true	x=false
true	0.200	0.800
false	0.900	0.100

Table 6.4: The conditional probability table represented by the gate block in Figure 6.12.

As another example, we can represent the conditional probability table for the skin test (Figure 6.1) using gates like this:

Representing this conditional probability table using a gate block is less compact than using a *Table* factor (as we did in Figure 6.1) but has the advantage of making the relationship between the parent variable and child variable more

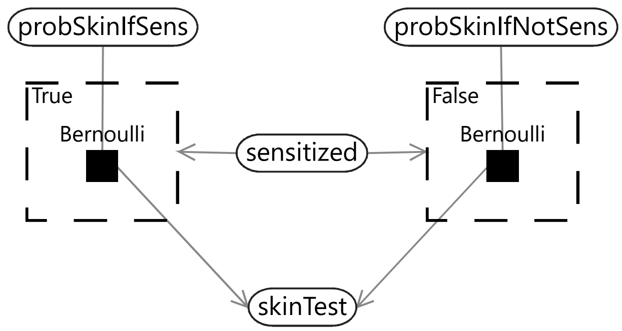


Figure 6.13: The conditional probability table for the skin test (Figure 6.1) represented using a gate block. If `sensitized` is `true`, the left hand gate is on and the right hand gate is off. The skin test result `skinTest` then has a Bernoulli distribution with the probability of true given by `probSkinIfSens`. If `sensitized` is `false`, then `skinTest` has a Bernoulli distribution with the probability of true given by `probSkinIfNotSens`.

clear and precise. When a variable has multiple parents, using a gate block to represent a conditional probability table can also lead to more accurate or more efficient inference.

6.4.1 Using gates for model selection

Representing a conditional probability table is just the start of what can be achieved using gates. For example, they can also be used to do model selection. To see how, let's return to our model selection problem from the previous section. Remember that we wanted to select between a 'has effect' model and a 'no effect' model, by inferring the posterior distribution of a random variable called `model`. Using gates, we can represent this model selection problem as a single large factor graph, using a gate block where the selector variable is `model`. We then place the entire 'no effect' model inside a gate whose key value is `NoEffect` and the entire 'has effect' model inside the other gate of the block whose key value is `HasEffect`. The observed variables are left outside of both gates because they are common to both models and so are always on. The result is the factor graph in Figure 6.14.

This factor graph may look a bit scary, but it can be interpreted in pieces. The top gate contains exactly the model from Figure 6.10 with the observed variables outside the gate. The bottom gate contains exactly the model from Figure 6.9 drawn upside down and sharing the same observed variables. Finally we have one new variable which is our `model` variable used to do model selection.

Given this factor graph, we just need to run expectation propagation to infer the posterior distribution over `model`. Right? Well, almost – it turns out that first we need to make some extensions to expectation propagation to be able to handle gates. The good news is that these modifications allow expectation

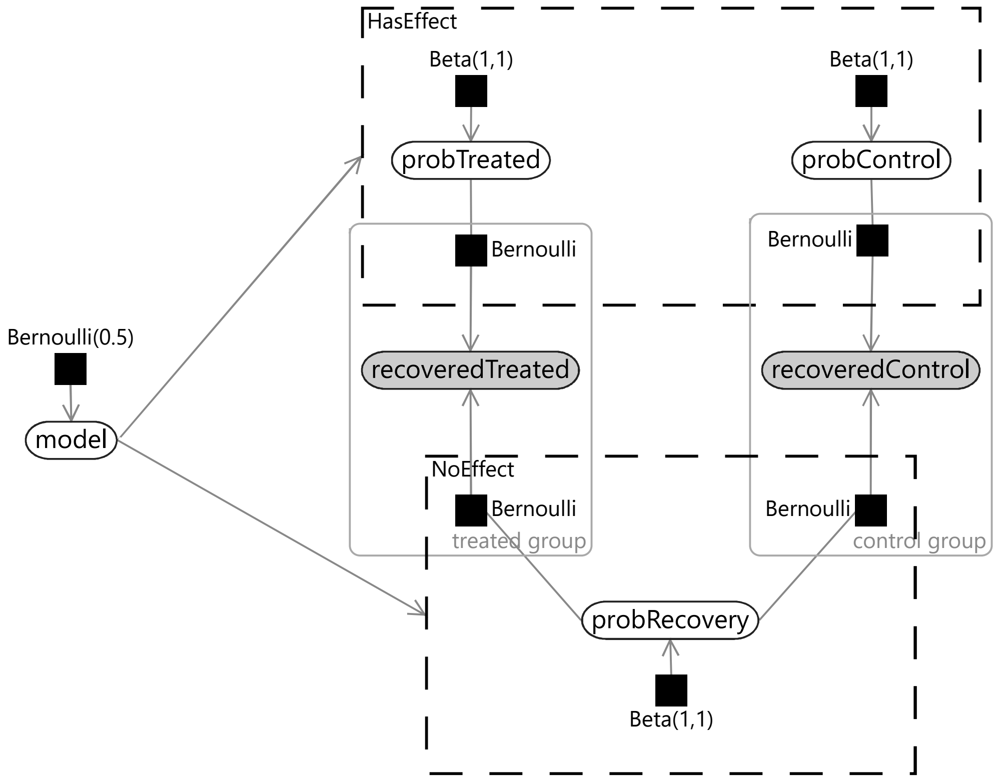


Figure 6.14: A factor graph which uses gates to do model selection between two models. The 'has effect' model is in the top gate and the 'no effect' mode is in the bottom gate. The observed data variables lie outside both gates, since they are common to both models. When the selector variable `model` has the value `HasEffect` the top gate is on and the bottom gate is off and so the 'has effect' model applies. When the selector variable `model` has the value `NoEffect` the top gate is off and the bottom gate is on and so the 'no effect' model applies. Because `model` is a random variable with unknown value, inferring its posterior distribution is equivalent to doing Bayesian model selection between the two models.

propagation to be applied to any factor graph containing gates.

INFERENCE

6.4.2 Expectation propagation in factor graphs with gates

Inference deep-dive
In this optional section, we see how to use expectation propagation to compute model evidence and then how to extend expectation propagation to work on graphs containing gates. If you want to focus on modelling, feel free to skip this section.

To run expectation propagation in a factor graph which contains gates, we first need to be able to compute the model evidence for a factor graph without gates. It turns out that we can compute an approximation to the model evidence by using existing EP messages to compute evidence contributions for each variable and factor individually, and then multiplying them together. For example, the evidence contribution for a variable `x` is given by:

$$\text{evidence}_x = \sum_x \text{product of all messages into x} \tag{6.14}$$

This equation states that to compute the evidence for a variable `x`, first take the product of all incoming messages on edges connected to the variable, then sum the result over the values that `x` can take (this is what the notation $\sum_x$ means). Because of this sum the result is a single number rather than a distribution – this number is the local contribution to the model evidence.

The evidence contribution for a factor f connected to multiple variables `Y` is given by:

$$\text{evidence}_f = \frac{\sum_Y f(Y) \times \text{product of all messages into } f}{\sum_Y \text{product of all messages into or out of } f} \tag{6.15}$$

In this equation, the notation $\sum_Y$ means the sum over all joint configurations of the connected variables `Y`.

We can use equations (6.14) and (6.15) to calculate evidence contributions for every variable and factor in the factor graph. The product of all these contributions gives the EP approximation to the model evidence. For a model `M`, this gives:

$$\text{evidence}_M = \prod_{x \text{ in } M} \text{evidence}_x \times \prod_{f \text{ in } M} \text{evidence}_f \tag{6.16}$$

In equation (6.16), the first team means the product of the evidence contributions from every variable in model `M` and the second term means the product of evidence contributions from every factor in model `M`.

Adding in gates

If we now turn to factor graphs which contains gates, there is a new kind of evidence contribution that comes from any edge that crosses over a gate boundary. If such an edge connects a variable `x` to a factor f, then the evidence contribution is:

$$\text{evidence}_{fx} = \sum_x \text{message from } \mathtt{x} \text{ to } f \times \text{message from } f \text{ to } \mathtt{x} \tag{6.17}$$

In other words, we take the product of the two messages passing in each direction over the edge and then sum the result over the values of the variable `x`.

The advantage of computing evidence contributions locally on parts of the factor graph is that, as well as computing evidence for the model as a whole, we can also compute evidence for any particular gate. The evidence for a gate is the product of the evidence contributions for all variables and factors inside the gate, along with the contributions from any edges crossing the gate boundary. For a gate g, this product is given by:

$$\text{evidence}_g = \prod_{x \text{ in } g} \text{evidence}_x \times \prod_{f \text{ in } g} \text{evidence}_f \times \prod_{fx \text{ crossing } g} \text{evidence}_{fx} \quad (6.18)$$

If there are no edges crossing the gate boundary – in other words, the gate contains an entire model disconnected from the rest of the graph – then this equation reduces to the model evidence equation (6.16) above, and so gives the evidence for the contained model.

Given these evidence contributions, we can now define an extended version of expectation propagation which works for factor graphs that contain gates. The algorithm requires that gates only occur in gate blocks and that any variable connecting to a factor in one gate of a gate block, also connects to factors in all other gates of the gate block. This 'gate balancing' can be achieved by connecting the variable to uniform factors in any gate where it does not already connect to a factor. We need this gate balancing because messages will be defined as going to or from gate blocks, rather than to or from individual gates.

When sending messages from a factor f inside a gate g to a variable $\mathtt{x}$ outside the gate, we will need to weight the message appropriately, using a weight defined as:

$$\text{weight}_{gfx} = \frac{\text{evidence}_g}{\text{evidence}_{fx}} \times \text{message from the selector variable[key]} \quad (6.19)$$

where the notation [key] indicates that we are evaluating the probability of the gate's key value under the distribution given by the message from the selector variable. Using these weights, we can define our extended expectation propagation algorithm as shown in algorithm 6.1.

Algorithm 6.1: Expectation Propagation with Gates

Input: factor graph with gate blocks, list of target variables to compute marginals for, message-passing schedule, initial message values (optional), choice of approximating distributions for each edge.
Output: marginal distributions for target variables.

Initialise all messages to uniform (or initial values, if provided).
repeat
  foreach *edge in the message-passing schedule* **do**
    Send the appropriate message below:
    - Selector variable to gate block: the product of all messages received on the other edges connected to the selector variable;
    - Gate block to selector variable: a distribution over the selector variable where the probability of each value is proportional to the evidence for the gate with that key value;
    - Factors in gate block to variable outside gate block: Compute weighted sum of messages from the factor in each gate using weights given by (6.19). Multiply by the context message (the message coming from the variable to the gate block). Project into the desired distribution type using moment matching. Divide out the context message.
    - All other messages: the normal EP message (defined in algorithm 3.1);
  end
until *all messages have converged*
Compute marginal distributions as the product of all incoming messages at each target variable node.

The full derivation of this algorithm is given in Minka and Winn [2009], along with some additional details that we have omitted here (such as how to handle nested gates).

Now that we have a general-purpose inference algorithm for gated graphs, we can use it to do Bayesian model selection and to infer posterior distributions over variables of interest, both at the same time! For example, recall the example trial from section 6.3. In this trial, 13 out of 20 people in the treated group recovered compared to 8 out of 20 in the control group. Attaching this data to the gated factor graph of Figure 6.14, we can apply expectation propagation to compute posteriors over the model selection variable `model` and also over other variables such as `probTreated` and `probControl`. The results are shown in Figure 6.15.

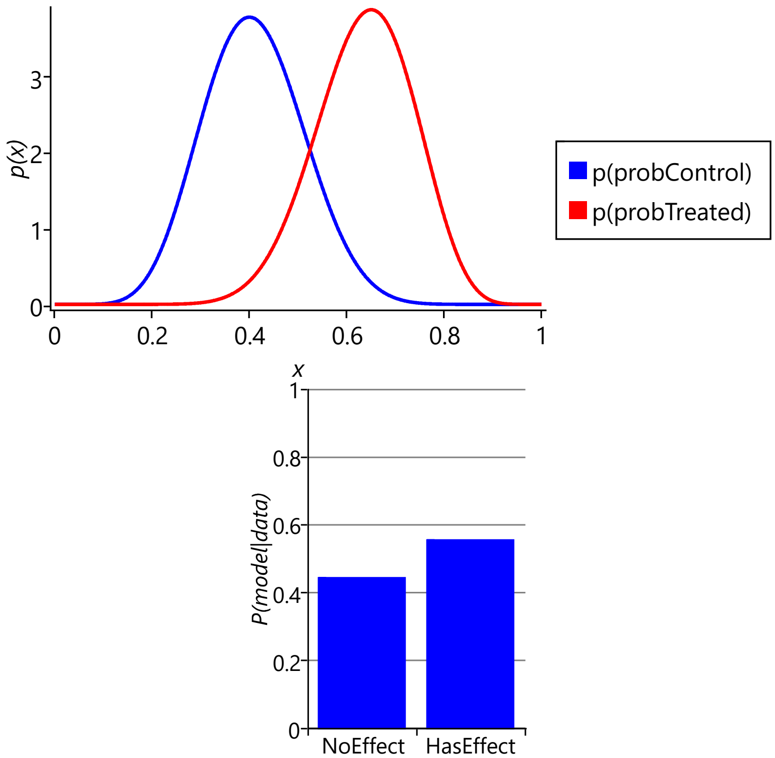


Figure 6.15: Inferred posterior distributions for the example trial with 20 people in each group. The left plot shows posteriors over `probControl` and `probTreated` in the `HasEffect` model. The right plot shows the posterior distribution over the `model` variable.

Figure 6.15 shows that the posterior distribution over `model` puts slightly higher probability on the 'has effect' model than on the 'no effect' model. The exact values are 0.5555 for `model=HasEffect` and 0.4445 for `model=NoEffect`. The ratio of these probabilities is the Bayes factor, which in this case is 1.25. This is the same value that we computed manually in section 6.3, showing that for this model the expectation propagation posterior is exact. The posterior distributions over `probControl` and `probTreated` give an indication of why the Bayes factor is so small. The plots show that there is a lot of overlap between the two distributions, meaning that is possible that both probabilities are the same value, in other words, that the 'no effect' model applies.

Let's see what happens when we increase the size of the trial, but leave the proportions of people who recovered the same in each group. For a trial of three times the size, this would see 39 out of 60 recovered in the treated group compared to 24 out of 60 in the control group. Plugging this new data into our model, gives the results shown in Figure 6.16.

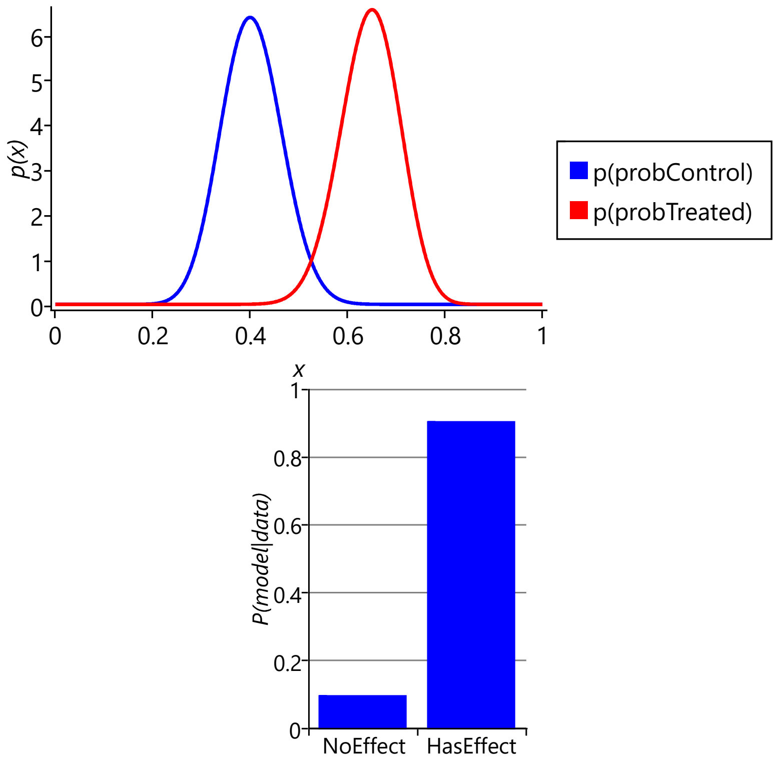


Figure 6.16: Inferred posterior distributions for the example trial with 60 people in each group. The left plot shows posteriors over `probControl` and `probTreated` in the `HasEffect` model. The right plot shows the posterior distribution over the `model` variable.

Figure 6.16 shows that, after tripling the size of the trial, the 'has effect' model has a much higher probability of 0.904, giving a Bayes factor of 9.41. Since this factor lies in the range 3-20, the outcome of this trial can now be considered positive evidence in favour of the 'has effect' model. The posterior distributions over `probControl` and `probTreated` shows why the Bayes factor is now much larger: the two curves have much less overlap, meaning that the chances of the two probabilities being the same is much reduced. We can take this further and increase the trial size again so that it is five times the size of the original trial. In this larger trial, 65 out of 100 recovered in the treated group compared to 40 out of 100 in the control group, giving the results shown in Figure 6.17.

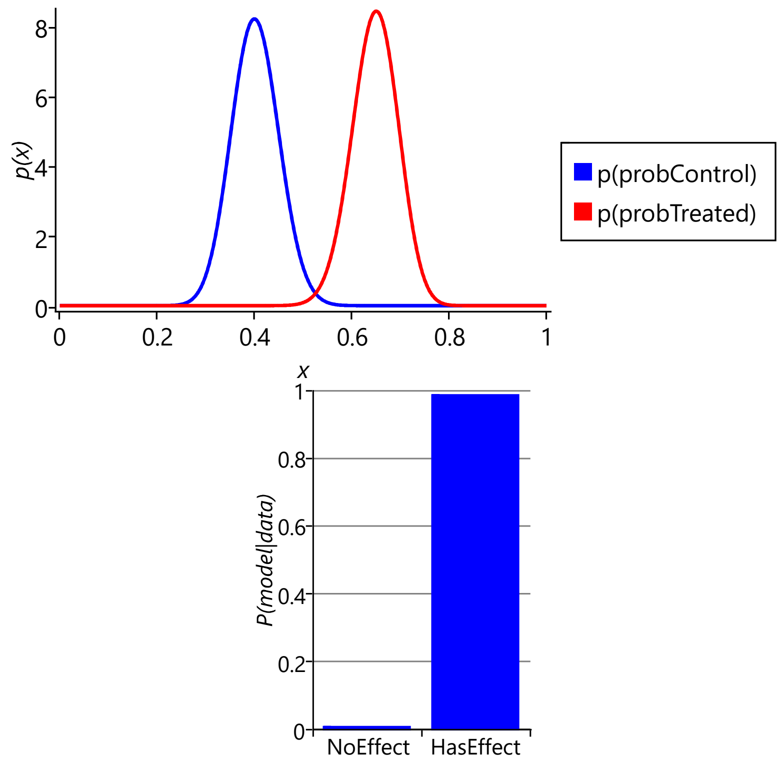


Figure 6.17: Inferred posterior distributions for the example trial with 100 people in each group. The left plot shows posteriors over `probControl` and `probTreated` in the `HasEffect` model. The right plot shows the posterior distribution over the `model` variable.

In Figure 6.17, the posterior distributions over `probControl` and `probTreated` hardly overlap at all. As a result, the 'has effect' model now has a probability of 0.989, giving a Bayes factor of 92.4. Since this factor lies in the range 20-150, the outcome of this trial can now be considered strong evidence in favour of the 'has effect' model. These results show the importance of running a large enough clinical trial if you want to prove the effectiveness of your new drug!

Now that we understand how gates can be used to model alternatives in our randomised controlled trial model, we are ready to use gates to model alternative sensitization classes in our allergy model, as we will see in the next section.

Review of concepts introduced in this section

gate A container in a factor graph that allows the contained piece of the graph to be turned on or off, according to the value of another random variable in the graph (known as the selector variable). Gates can be used to create alternatives within a model and also to do model selection. More details of gates can be found in Minka and Winn [2009] or in the expanded version Minka and Winn [2008].

selector variable A random variable that controls whether a gate is on or off. The gate will specify a particular key value – when the selector variable has that value then the gate is on; for any other value it is off. For an example of a selector variable, see Figure 6.11.

gate block A set of gates each with a different key value corresponding to the possible values of a selector variable. For any value of the selector variable, one gate in the gate block will be on and all the other gates will be off. An example gate block is shown in the factor graph of Figure 6.12.

6.5 Discovering sensitization classes

Now that we have gates in our modelling toolbox, we can extend our allergy model so that different children can have different patterns of allergy gain and loss. As you may recall from section 6.2, the model change that we want to make is to encode this modified assumption:

5. The probabilities relating to initially having, gaining or retaining sensitization to a particular allergen are the same for all children in each sensitization class.

This assumption requires that each child belongs to some sensitization class, but we do not know which class each child belongs to. We can represent this unknown class membership using a `sensClass` random variable for each child, which takes a value in $0, 1, 2, \ldots$ depending on whether the child is in class 0, class 1 and so on. Because this variable can take more than two values, we cannot use a *Bernoulli* distribution to represent its uncertain value. Instead we need a **discrete distribution**, which is a generalisation of a Bernoulli distribution to variables with more than two values.

Our aim is to do unsupervised learning of this `sensClass` variable – in other words, we want to learn which class each child is in, even though we have no idea what the classes are and we have no labelled examples of which child is in which class. Grouping data items together using unsupervised learning is sometimes called **clustering**. The term clustering can be misleading, because it suggests that data items naturally sit together in unique clusters and we just need to use machine learning to reveal these clusters. Instead, data items can usually be grouped together in many different ways, and we choose a particular kind of grouping to meet the needs of our application. For example, in this asthma project, we want to group together children that have similar patterns of allergic sensitization. But for another project, we could group those same children in a different way, such as by their genetics, by their physiology and so on. For this reason, we will avoid using the terms 'clustering' and 'clusters' and use the more precise term 'sensitization class'.

Each sensitization class needs to have its own patterns of gaining and losing allergic sensitizations, with the corresponding probabilities for gaining and losing sensitizations at each time point. For example, each class should have its own value of `probSens1` which gives the probability of sensitization at age 1 for children in that particular sensitization class. To achieve this in our model, we need the sensitization state at age 1 (`sensitized1`) to be connected to the appropriate `probSens1` corresponding to the sensitization class of the child. We can achieve this by replicating the connecting *Bernoulli* factor for each sensitization class, and then using a gate block to ensure that only one of these factors is turned on, as shown in Figure 6.18.

In Figure 6.18, we have assumed that there are four sensitization classes and duplicated `probSens1` into separate probabilities for each class ($\texttt{probSens1}_0$, $\texttt{probSens1}_1 \ldots$). There is a gate for each class, keyed by the number of the

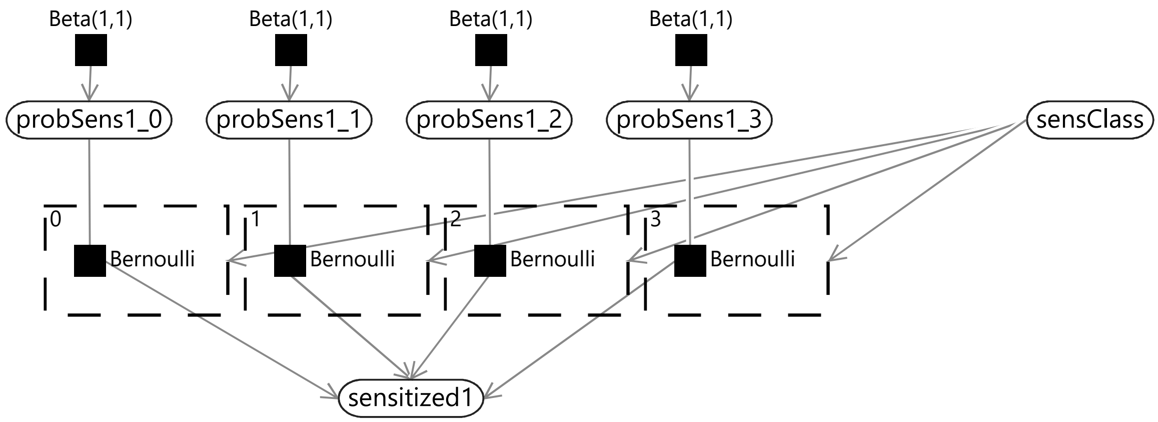


Figure 6.18: A factor graph with four different probabilities of sensitization at age 1, where the appropriate probability is selected according to the value of the `sensClass` variable (0, 1, 2 or 3). For any value of `sensClass`, one gate is on and all other gates are off.

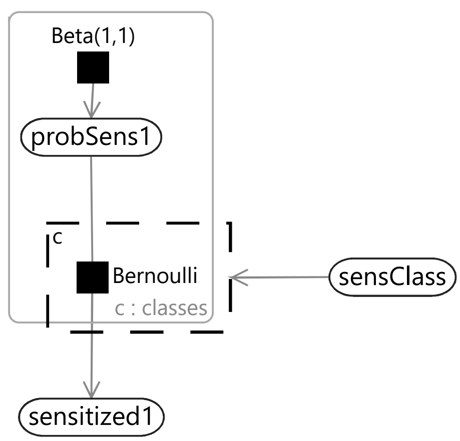


Figure 6.19: The same model as Figure 6.18, shown more compactly by using a plate across sensitization classes. The initial sensitization probabilities, gates and corresponding factors are duplicated for each sensitization class.

class (0,1,2 or 3). Because each key is different, any value of `sensClass` leads to one gate being on and all the other gates being off. In this way, the value of `sensClass` determines which of the four initial sensitization probabilities to use.

The factor graph of Figure 6.18 is quite cluttered because of the repeated factors and variables for each sensitization class. We can represent the same model more compactly if we introduce a plate across the sensitization classes and put the repeated elements inside the plate, as shown in Figure 6.19.

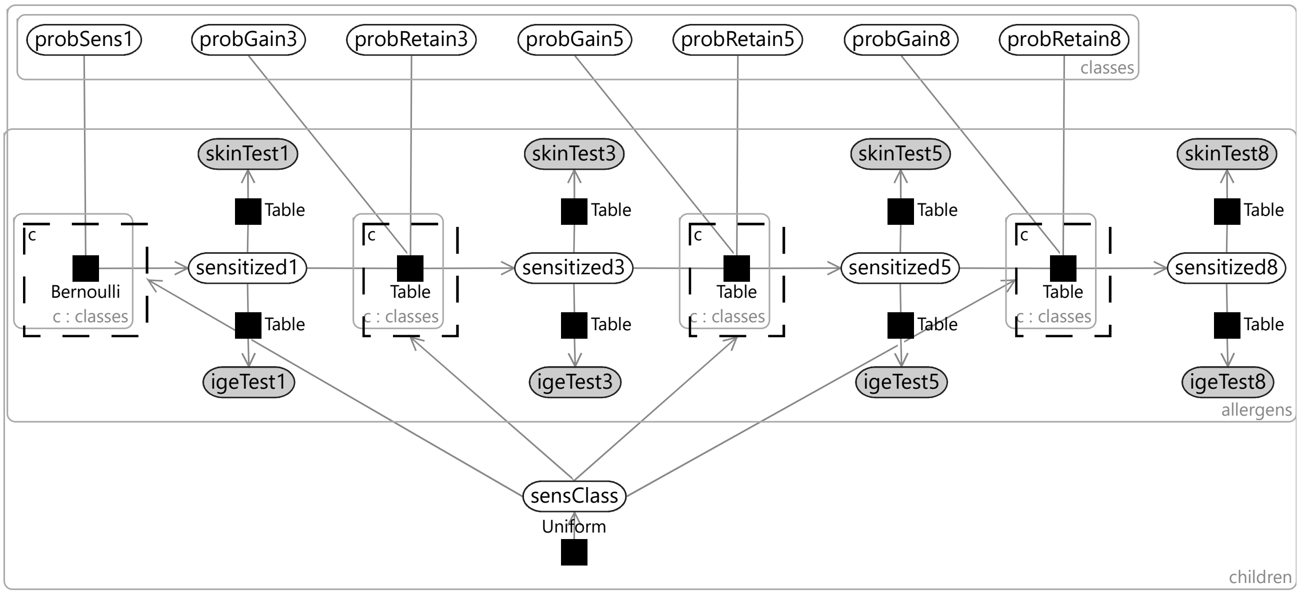


Figure 6.20: Modified factor graph which has different probabilities of having, gaining and retaining sensitization for each sensitization class. The random variables for these probabilities are duplicated by a `classes` plate at the top of the factor graph. These probabilities are then connected into the rest of the model by factors each contained in a gate and a plate. The `sensClass` variable is connected to all gates and switches between the different sets of probabilities, according to the sensitization class of the child. In this figure, the probability variables relating to skin and IgE tests have been omitted for clarity.

Using the compact notation of Figure 6.19, we can modify our allergy model of Figure 6.5 to have different probabilities for each sensitization class. We take all our probability variables `probSens1`, `probGain3` and so on, and duplicate them across classes using a plate. We then place each factor in the Markov chain inside a gate and plate, where the gates are all connected to a `sensClass` selector variable. Finally, we choose a uniform prior over `sensClass`, giving the factor graph of Figure 6.20.

6.5.1 Testing the model with two classes

To test out our model in its simplest form, we can set the number of sensitization classes to two. With just two classes, we would expect the model to divide the children into a group which have no sensitizations and a second group that contains those children with sensitizations. However, when we run expectation propagation in the model, we get an unexpected result. The posterior distributions over the sensitization class are all uniform, for every child! In addition, when we look at the learned probabilities of gaining/retaining sensitizations, they are also all the same for each class – and look just like the one-class probabilities shown in Figure 6.7. What has happened here?

The issue is that our model defines every sensitization class in exactly the same way – each class has the same set of variables which all have exactly the same priors. We could reorder the sensitization classes in any order and the model would be unchanged. This self-similarity is a symmetry of the model, very similar to the symmetry we encountered in section 5.3 in the previous chapter. During inference, this symmetry causes problems because the posterior distributions will not favour any particular ordering of classes and so will end up giving an average of all classes – in other words, the same results as the one-class model. Not helpful!

As in the previous chapter, we need to apply some kind of symmetry breaking to get useful inference results. In this case, we can break symmetry by providing initial messages to our model, such that the messages differ from class to class. A simple approach is to provide an initial message into each `sensClass` variable which is a point mass at a randomly selected value. The effect of these initial messages is to randomly assign children to sensitization classes for the first iteration of expectation propagation. This randomization affects the messages going to the class-specific variables (such as `probSens1`) in the first iteration, which in turn means that the messages to each `sensClass` variable are non-uniform in the next iteration and so on. The end result is that the class-specific variables eventually converge to describe different underlying sensitization classes and the `sensClass` variables converge to assign children to these different classes.

With symmetry breaking in place, we can now run inference successfully in a two-class model. We can visualize the results using a chart like Figure 6.8 for each class. To do this, we assign each child to the sensitization class with the highest posterior probability, giving the plots of Figure 6.21 for the two classes. The figure shows that the model has picked up on a large class of 757 children who have virtually no sensitizations and a smaller class of 296 children who do have sensitizations. In other words, the two-class model has behaved as expected and separated out the children who have sensitizations from those who do not.

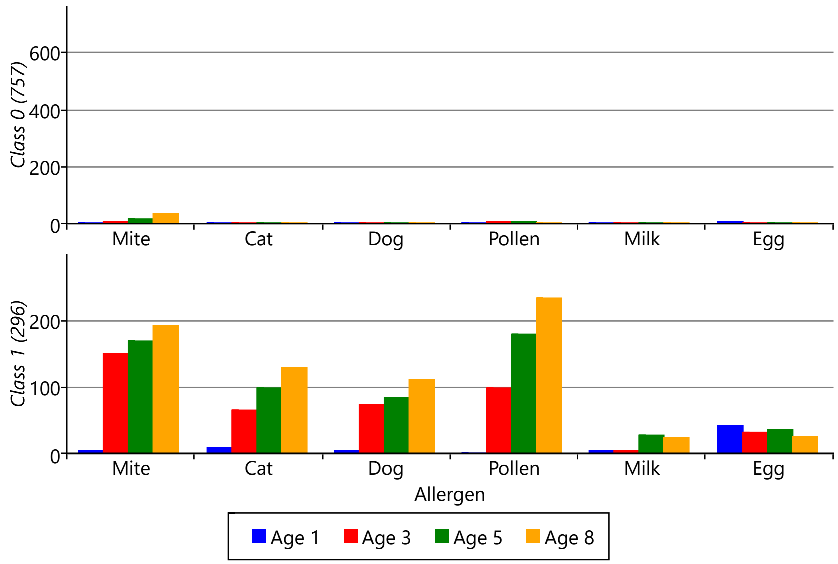


Figure 6.21: Plots for each class showing the number of children with inferred sensitizations for each allergen/time. The first class contains roughly three-quarters of the children who have almost no sensitizations. The remaining children in the second class are those with sensitizations.

6.5.2 Exploring more sensitization classes

The results for two classes provide a useful sanity check that the model is doing something reasonable. However, we are really interested in what happens when we have more than two classes, since we hope additional classes would uncover new patterns of sensitization. Let's consider running the model with five possible classes. We say five 'possible' classes, because there is no guarantee that all classes will be used. That is, it is possible to run the inference algorithm and find that there are classes with no children assigned to them. With our model and data set, we find that it is common when running with five classes, that only four of them are actually in use. Effectively the number of classes in the model defines a maximum on the number of classes found – which allows for the number of classes itself to be learned. Different random initialisations give slightly different sensitization classes, but often these contain very similar looking classes. Figure 6.22 shows some typical results for the four classes found when up to five were allowed in the model.

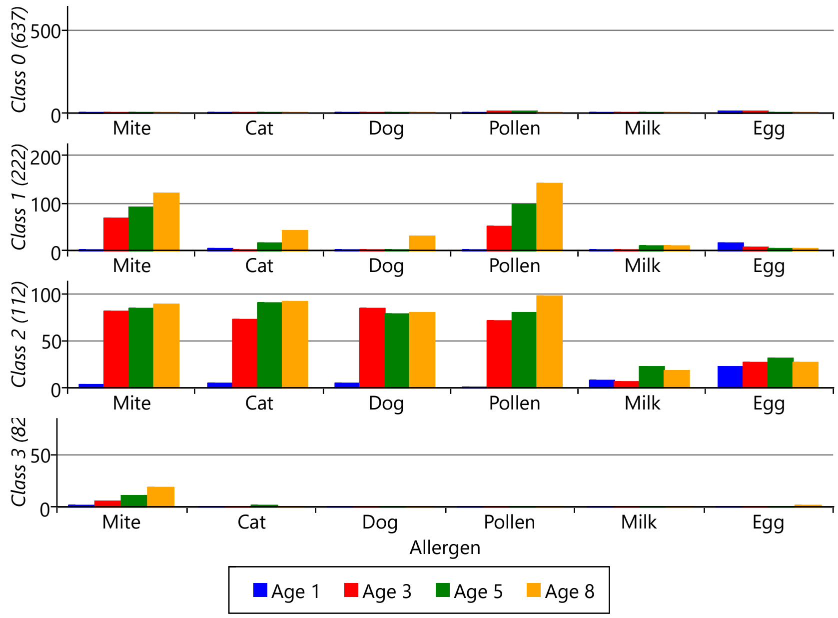
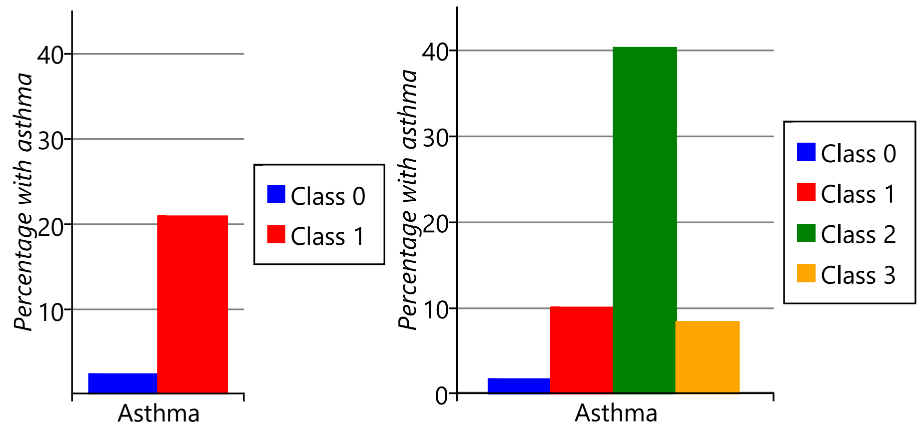


Figure 6.22: Plots for each of four classes showing the number of children with inferred sensitizations for each allergen/time. The first class contains roughly three-quarters of the children who have almost no sensitizations. The remaining children, with sensitizations, are divided into three classes according to which sensitizations they have and when they acquired them, as discussed in the text.

As you can see from Figure 6.22, model has divided the children with sensitizations into three separate classes. The largest of these, Class 1, contains 222 children who predominantly have mite and pollen allergies, but have few other allergies. In contrast, Class 2 contains 112 children who have allergies to cat and dog as well as mite and pollen. This class also contains those children who have milk and egg allergies. It is also worth noting that the children in this class acquire their allergies early in life – in most cases by age 3. The final class, Class 3 is relatively small and contains 82 children who predominantly have mite allergies.

These results demonstrate the strength of unsupervised learning – it can discover patterns in the data that you did not expect in advance. Here we have uncovered three different patterns of sensitization that we were not previously aware of. The next question to ask is "how does this new knowledge help our understanding of asthma?". To answer this question, we can see if there is any link between which sensitization class a child belongs to and whether they went on to develop asthma.

For each child, our data set contains a measurement of whether they had developed asthma by age 8. For each of the two class and four class models, we can use these measurements to plot the percentage of children in each sensitization class that went on to develop asthma. The results are shown in Figure 6.23.



(a) (b)

Figure 6.23: Percentage of children in each class who developed asthma by age 8, for (a) the two class model (b) the four class model. In the four class model, class 2 has a much higher percentage of children with asthma than any other class, in either model.

Let's start by looking at plots for the two class model. As we might expect, the percentage of children with asthma is higher in the class with sensitizations (class 1), than the class without sensitizations (class 0). Indeed, the presence of allergic sensitizations is used as a predictor of developing asthma. But when we look at the results for the four class model, we see a very interesting result – whilst all the classes with sensitizations show an increased percentage of children developing asthma, class 2 shows a *much* higher percentage than any other class. It seems that children who have the broad set of allergies characterised by class 2 are more than four times as likely to develop asthma than children who have other patterns of allergies! This is a very exciting and clinically useful result. Indeed, when we looked further we found that this pattern of allergies also led to an increased chance of severe asthma with an associated increased risk of hospital admission [Simpson et al., 2010]. Being able to detect such severe asthma early in life, could help prevent such life-threatening episodes from occurring.

In summary, in this chapter, we have seen how unsupervised learning discovered new patterns of allergic sensitization in our data set. In this case, these patterns have led to a new understanding of childhood asthma with the potential of significant clinical impact. Although, in general, unsupervised learning can be more challenging than supervised learning, the value of the new understanding that it delivers frequently justifies the extra effort involved.

Review of concepts introduced in this section

discrete distribution A probability distribution over a many-valued random variable which assigns a probability to each possible value. The parameters of the distribution are these probabilities, constrained to add up to 1 across all possible values. This distribution is also known as a categorical distribution.

An example of a discrete distribution is the outcome of rolling a fair dice, which can be written as $Discrete(\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6})$. The Bernoulli distribution is actually a special case of a discrete distribution for when there are only two possible values.

clustering A form of unsupervised learning where data items are automatically collected into a number of groups, which are known as clusters. Each cluster is then assumed to contain items which are in some way similar.

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