Machine learning in science and society

From automated science to beneficial artificial intelligence

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Chapter 1

Introduction

1.1 Introduction to machine learning

What are the central problems in machine learning?

Problems in machine learning are similar to problems in science. Scientists must plan experiments intelligently and collect data. The must be able to use the data to verify a different hypothesis. More generally, they must be able to make decisions under uncertainty (Without uncertainty, there would be no need to gather more data). Similar problems appear in more mundane tasks, like learning to drive a car.

For that reason, science is a very natural application area for machine learning. We can model the effects of climate change and how to mitigate it; discover structure in social networks; map the existence of dark matter in the universe by intelligently shifting through weak gravitational lens data, and not only study the mechanisms of protein folding, but discover methods to synthesize new drugs.

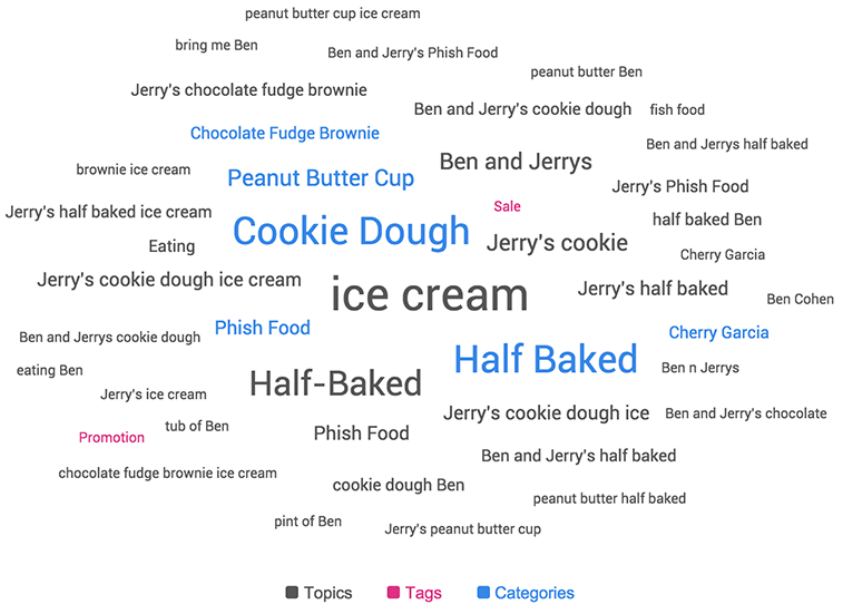
We must be careful, however. In many cases we need to be able to interpret what our model tells us. We also must make sure that the any results we obtain are reproducible. This is something that we shall emphasize in this course.

While machine learning models in science are typically carefully handcrafted by scientists and experts in machine learning and statistics, this is not typically the case in everyday applications. Nevertheless, well-known or home-grown machine learning models are being deployed across the application spectrum. This involve home assistants that try and get you want, web advertising, which tries to find new things for you to want, lending, which tries to optimally lend you money so that you buy what you didn't need before. We also have autonomous vehicles, which take you were you want to go, and ridesharing services, which do the same thing, but use humans instead. Finally, there are many applications in public policy, such as crime prevention, justice, and disease control which use machine learning. In all those cases, we have to worry about a great many things that are outside the scope of the machine learning problems itself. These are (a) privacy: you don't want your data used in ways that you have not consented to (b) fairness: you don't want minorities to be disadvantaged and (c) safety: you don't want your car to crash.

1.1.1 Data analysis, learning and planning

To make the above more concrete, let's have a look at a number of problems in machine learning. These involve learning from and analysing data, including inferring decision rules, and constructing complex plans using the evidence gleaned from the data. Machine learning problems are commonly separated in three different types: supervised, unsupervised and reinforcement learning. Typical supervised learning problems include classification and regression, while unsupervised problems include compression, clustering and topic modelling. Reinforcement learning, on the other hand, is concerned with artificially intelligent agents more generally, with examples including game playing and adaptive control. Their main differences are two. Firstly, the *type* of feedback we have about learning performance. Secondly, and perhaps more importantly, whether or not the problem involves *active data collection*. In this course, we will try and take a global view of these problems in the context of decision theory.

Can machines learn from data?



An unsupervised learning problem: topic modelling

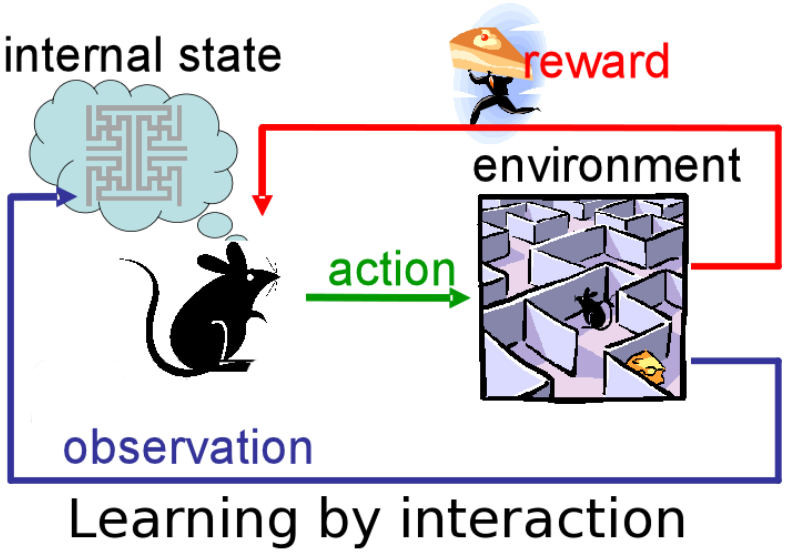
A supervised learning problem: object recognition

You can use machine learning just to analyse, or find structure in the data. This is generally called unsupervised learning. One such example is topic modelling, where you let the algorithm find topics from a corpus of text. These days machines are used to learn from in many applications. These include speech recognition, facial authentication, weather prediction, etc. In general, in these problems we are given a *labelled* dataset with, say, example images from each class. Unfortunately this does not scale very well, because obtaining labels is expensive.

This is partially how science works, because what we need to do is to find a general rule

of nature from data. Starting from some hypothesis and some data, we reach a conclusion. However, many times we may need to actively experiment to obtain more data, perhaps because we found that our model is wrong.

Can machines learn from their mistakes?



Reinforcement learning
Take actions $a_1, \ldots, a_t$, so as to maximise utility $U = \sum_{t=1}^{T} r_t$

So, what happens when we make a mistake? Can we somehow recognise it? Humans and other animals can actually learn from their mistakes. Consider the proverbial rat in the maze. At some intervals, the experimenter places some cheese in there, and the rat must do a series of actions to obtain it, such as navigating the maze and pulling some levers. It doesn't know how to get to the cheese easily, but it slowly learns the layout of the maze through observation, and in the end, through trial-and-error it is able to get to the cheese very efficiently.

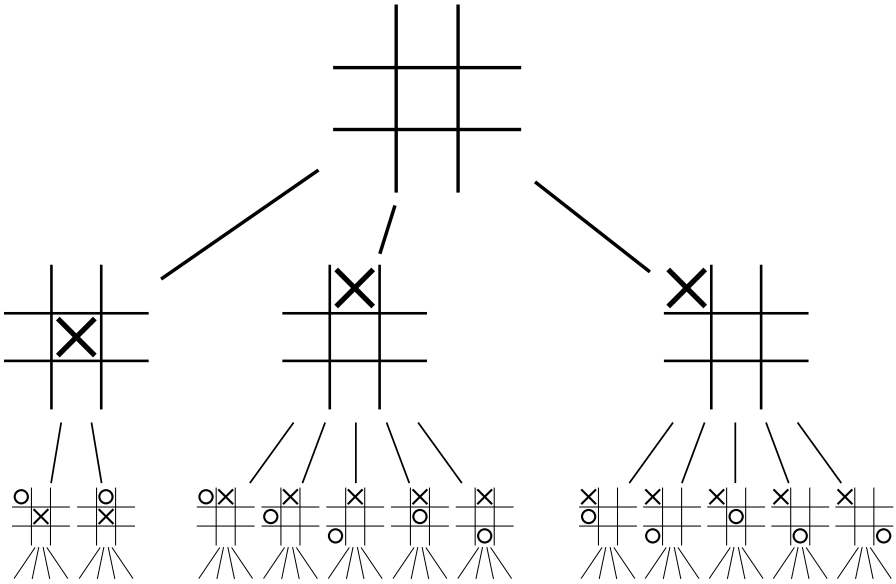
We can formalise this as a reinforcement learning problem, where the rat takes a series of actions; at each step it also obtains a reward, let's say equal to 0 when it has no cheese, and 1 when it eats cheese. Then we can declare that the rat's utility is the sum of all rewards over time, i.e. the total amount of cheese it can eat before it dies. The rat needs to explore the environment in order to be able to get to the cheese.

An example in robotics is trying to teach a robot to flip pancakes. One easy thing we can try is to show the robot how to do it, and then let it just copy the demonstrated movement. However, this doesn't work! The robot needs to explore variations of the movement, until it manages to successfully flip pancakes. Again, we can formulate this as a reinforcement learning problem, with a reward that is high whenever the pancake's position is flipped, and on the pan; and low everywhere else. Then the robot can learn to perform this behaviour through trial and error. It's important to note that in this example, merely demonstration is not enough. Neither is reinforcement learning enough. The same thing is true for the recent success of AlphaGo in beating a master human: apart from planning, they used both demonstration data and self-play, so that it could learn through trial and error.

Can machines make complex plans?

I suppose the first question is whether machines can plan ahead. Indeed, even for large problems, such as Go, machines can now perform at least as well as top-rated humans. How is this achieved?

Machines can make complex plans!

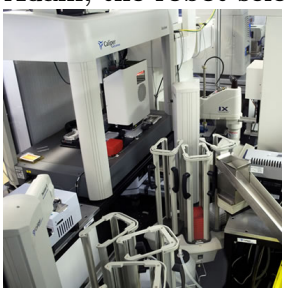


The basic construction is the planning tree. This is an enumeration of all possible future events. If a complete enumeration is impossible, a partial tree is constructed. However this requires evaluating non-terminal game positions. In the old times, this was done with heuristics, but now this is data-driven, both through the use of expert databases, and through self-play and reinforcement learning.

1.1.2 Experiment design

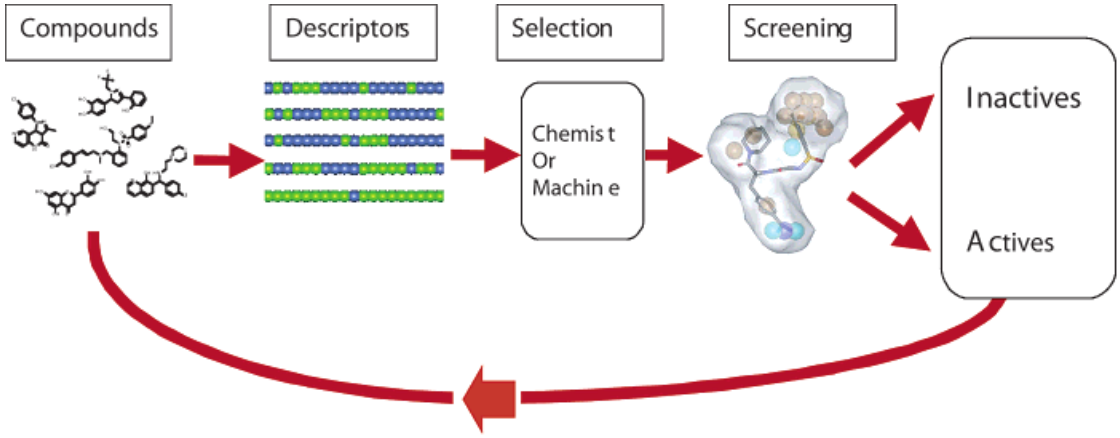
An example that typifies trial and error learning are bandit problems. Imagine that you are in a Casino and you wish to maximise the amount of money you make during the night. There are a lot of machines to play. If you knew which one was the best, then you'd just play it all night long. However, you must also spend time trying out different machines, in order to get an estimate of how much money each one gives out. The trade off between trying out different machines and playing the one you currently think is best is called the exploration-exploitation trade-off and it appears in many problems of experiment design for science.

Adam, the robot scientist



Let's say we want to build a robot scientist and tell it to discover a cure for cancer. What does the scientist do and how can the robot replicate it??

Drug discovery



Simplifying the problem a bit, consider that you have a large number of drug candidates for cancer and you wish to discover those that are active against it. The ideas is that you select some of them, then screen them, to sort them into active and inactive. However, there are too many drugs to screen, so the process is interactive. At each cycle, we select some drugs to screen, classify them, and then use this information to select more drugs to screen. This cycle, consequently has two parts: 1. Selecting some drugs given our current knowledge. 2. Updating our knowledge given new evidence.

Drawing conclusions from results

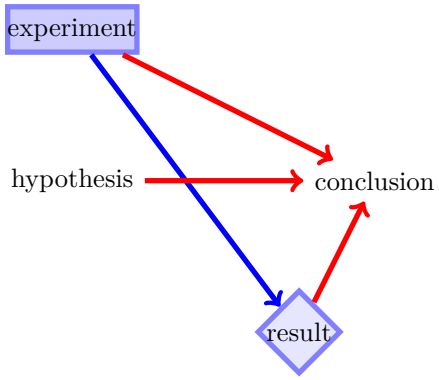


Figure 1.1: Dependence diagram between selection of an experiment, formulation of a hypothesis, and drawing of a conclusion. The result depends only on the experiment. However, the conclusion depends on the experiment, hypothesis and the obtained result. The red lines indicate computational dependencies, while the blue lines indicate physical dependencies.

In general, we would like to have some method which can draw conclusions from results. This involves starting with a hypothesis, performing an experiment to verify or refute it, obtain some experimental result; and then concluding for or against the hypothesis. Here the arrows show dependencies between these variables. So what do we mean by ”hypothesis” in this case?

1.1.3 Bayesian inference.

Tycho Brahe’s minute eye measurements

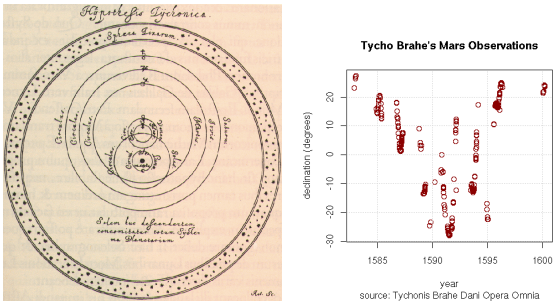
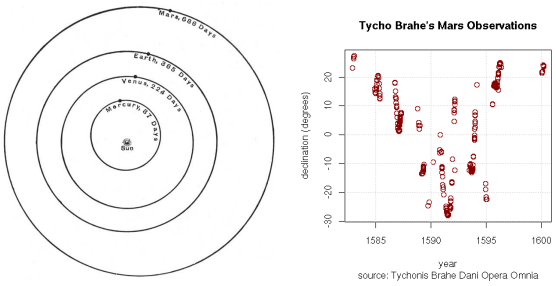


Figure 1.2: Tycho's measurements of the orbit of Mars and the conclusion about the actual orbits, under the assumption of an earth-centric universe with circular orbits.

- Hypothesis: Earth-centric, Circular orbits
- Conclusion: *Specific* circular orbits

Let's take the example of planetary orbits. Here Tycho famously spent 20 years experimentally measuring the location of Mars. He had a hypothesis: that planetary orbits were circular, but he didn't know which were the right orbits. When he tried to fit his data to this hypothesis, he concluded a specific circular orbit for Mars …around Earth.

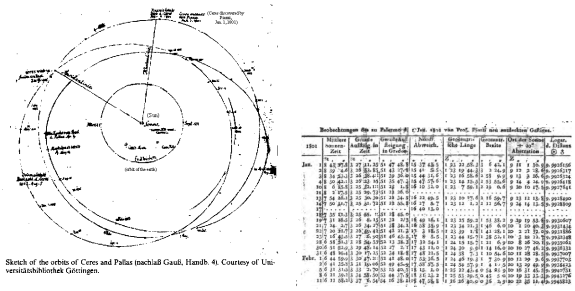
Johannes Kepler's alternative hypothesis



- Hypothesis: Circular *or* elliptic orbits
- Conclusion: Specific *elliptic* orbits

Kepler had a more general hypothesis: that orbits could be circular or elliptic, and he actually accepted that the planets orbited the sun. This led him to the broadly correct model of all planets being in elliptical orbits around the sun. However, the actual verification that all things do not revolve around earth, requires different experiments.

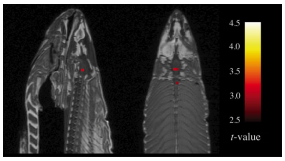
200 years later, Gauss formalised this statistically



Sketch of the orbits of Ceres and Pallas (nach:aß Gauß, Handb. 4). Courtesy of Universitätsbibliothek Göttingen.

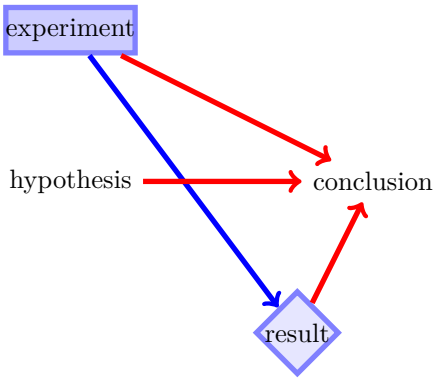
Later on, Gauss collected even more experimental data to calculate the orbit of Ceres. He did this using one of the first formal statistical methods; this allowed him to avoid cheating (like Kepler did, to accentuate his finding that orbits were elliptical).

A warning: The dead salmon mirage



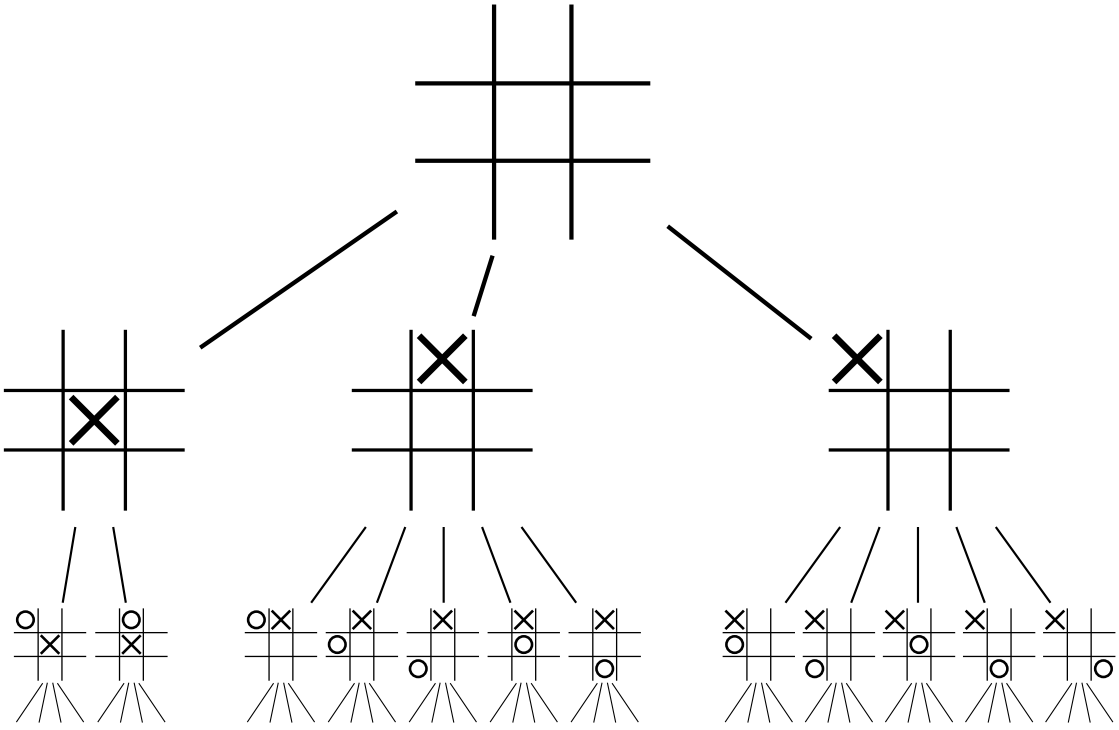
It is quite easy to draw the wrong conclusions from applying machine learning / statistics to your data. For example, it was fashionable to perform fMRI studies in humans to see whether some neurons have a particular functional role. There were even articles saying that "we found the neurons encoding for Angelina Jolie". So some scientists tried to replicate those results. They took a dead salmon, and put it an fMRI scanner. They checked its brain activity when it was shown images of happy or sad people. Perhaps surprisingly, they found an area of the brain that was correlated with the pictures - so it seemed, as though the dead salmon could distinguish photos of happy people from sad ones. However, this was all due to a misapplication of statistics. In this course, we will try and teach you to avoid such mistakes.

Planning future experiments



I mentioned before that we must decide what experiment to do. This is indeed difficult, especially in setting such as drug discovery where the number of experiments is huge. However, conceptually, there is a simple and elegant solution to this problem.

Planning experiments is like Tic-Tac-Toe



The basic idea is to think of experiment design as a game between the scientist and Nature. At every step, the scientist plays an X to denote an experiment. Then Nature responds with an Observation. The main difference from a game is that Nature is (probably) not adversarial. We can also generalise this idea to problems in robotics, etc.

These kinds of techniques, coming from the reinforcement learning literature have been successfully used at the university of Manchester to create a robot, called Eve, that recently (re)-discovered a malaria drug.

1.1.4 Course overview

Machine learning in practice

Avoiding pitfalls

- Choosing hypotheses.
- Correctly interpreting conclusions.
- Using a good testing methodology.

Machine learning in society

- Privacy — Credit risk.
- Fairness — Job market.
- Safety — Medicine.

One of the things we want to do in this course is teach you to avoid common pitfalls.

Now I want to get into a different track. So far everything has been about pure research, but now machine learning is pervasive: Our phones, cars, watches, bathrooms, kettles are connected to the internet and send a continuous stream of data to companies. In addition, many companies and government actors use machine learning algorithms to make or support decisions. This creates a number of problems in privacy, fairness and safety.

Technical topics

Machine learning problems

- Unsupervised learning. Loosely speaking, this is simply the problem of estimating some structure from data. In statistical terms, it is usually the problem of estimating some joint distribution of random variables under some model assumptions. Problems in unsupervised learning include clustering, anomaly detection, compression.
- Supervised learning. In this setting data can be split in two groups of variables. One group that is always available, and another group that must be predicted. A special case of the problem is when we wish to estimate some function $f : \mathcal{X} \to \mathcal{Y}$ from data. Classical problems in this setting are classification and regression.
- Reinforcement learning. This is a very general sequential decision problem, where an agent must learn how to behave optimally in an unknown environment only by limited feedback and reinforcement. The standard setting involves the agent trying to maximise its (expected) cumulative reward over time.

Algorithms and models

- Bayesian inference and graphical models.
- Stochastic optimisation and neural networks.
- Backwards induction and Markov decision processes.

Course structure

Module structure

- *Activity*-based, hands-on.
- Mini-lectures with short exercises in each class.
- Technical tutorials and labs in alternate week.

Modules

Three mini-projects.

- Simple decision problems: Credit risk.
- Structured problems: Fake news.
- Sequential problems: Medical diagnostics and treatment.

Chapter 2

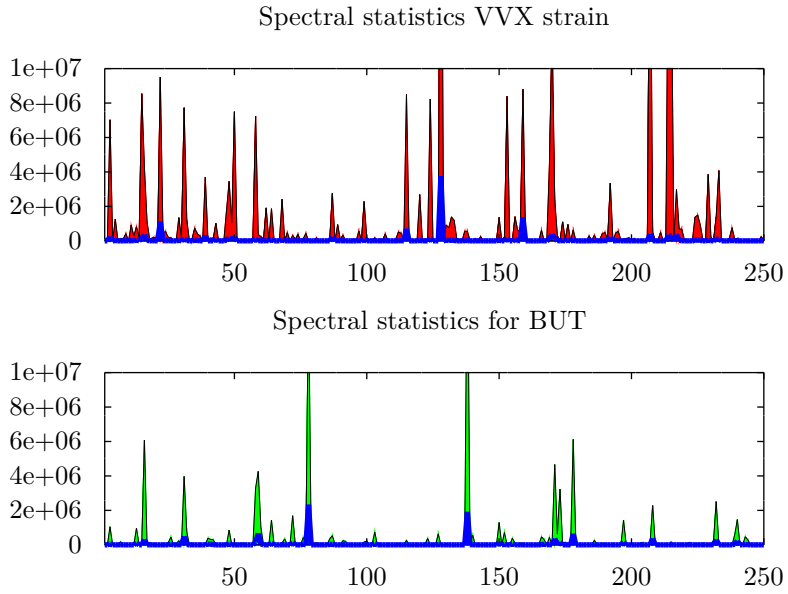
Simple decision problems

This chapter deals with simple decision problems, whereby a decision maker (DM) makes a simple choice among many. In some of this problems the DM has to make a decision after first observing some side-information. Then the DM uses a *decision rule* to assign a probability to each possible decision for each possible side-information. However, designing the decision rule is not trivial, as it relies on previously collected data. A higher-level decision includes choosing the decision rule itself. The problems of classification and regression fall within this framework. While most steps in the process can be automated and formalised, a lot of decisions are actual design choices made by humans. This creates scope for errors and misinterpretation of results.

In this chapter, we shall formalise all these simple decision problems from the point of view of statistical decision theory. The first question is, given a real world application, what type of decision problem does it map to? Then, what kind of machine learning algorithms can we use to solve it? What are the underlying assumptions and how valid are our conclusions?

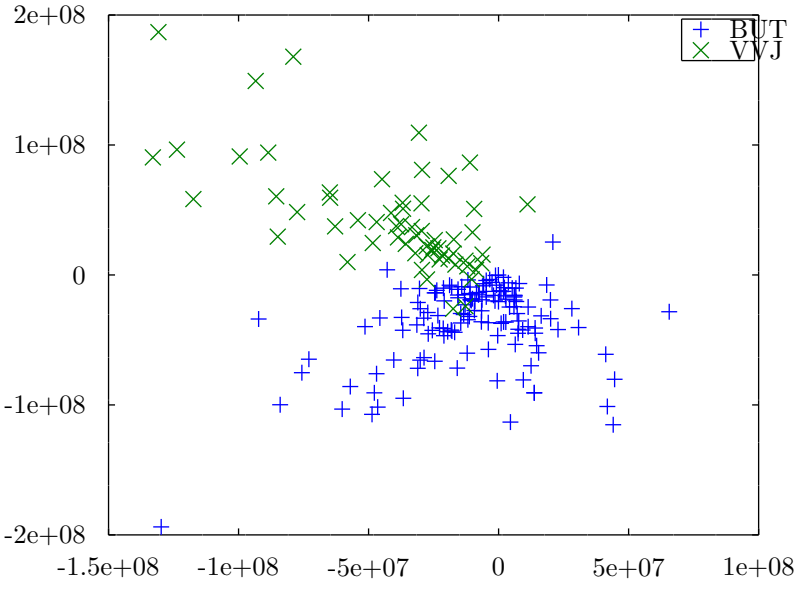
2.1 Nearest neighbours

Discriminating between diseases



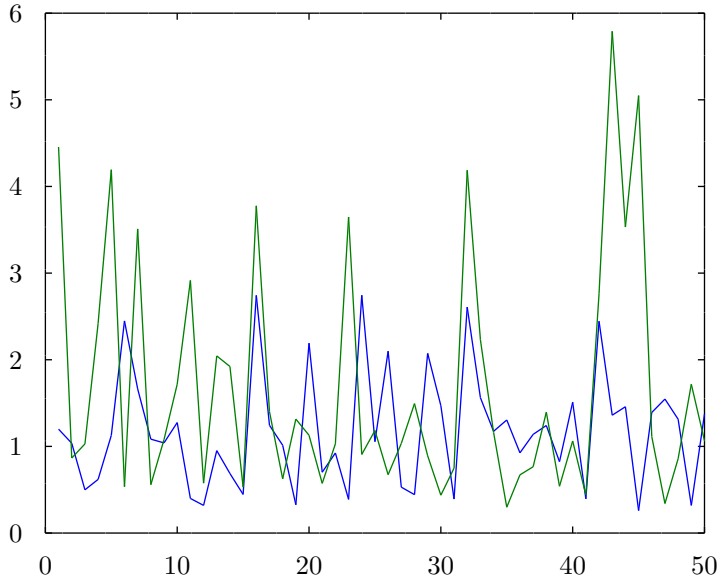
Let's tackle the problem of discriminating between different disease vectors. Ideally, we'd like to have a simple test that tells us what ails us. One kind of test is mass spectrometry. This graph shows spectrometry results for two types of bacteria. There is plenty of variation within each type, both due to measurement error and due to changes in the bacterial strains. Here, we plot the average and maximum energies measured for about 100 different examples from each strain.

Nearest neighbour: the hidden secret of machine learning



Now, is it possible to identify an unknown strain based on this data? Actually, this is possible. Sometimes, very simple algorithms work very well. One of the simplest one involves just measuring the distance between the decsription of a new unknown strain and known ones. In this visualisation, I projected the 1300-dimensional data into a 2-dimensional space. Here you can clearly see that it is possible to separate the two strains. We can use the distance to examples VVT and BUT in order to decide the type of an unknown strain.

Comparing spectral data



The choice of distance in this kind of algorithm is important, particularly for very high dimensions. For something like a spectrogram, one idea is look at the total area of the difference between two spectral lines.

The nearest neighbour algorithm

The nearest neighbour algorithm for classification (Alg. 1) does not include any complicated learning. Given a training dataset D, it returns a classification decision for any new point x by simply comparing it to its closest k neighbours in the dataset. It then estimates the probability p_y of each class y by calculating the average number of times the neighbours take the class y.

Algorithm 1 K-NN Classify

1: **Input** Data $D = \{(x_1, y_1), \ldots, (x_T, y_T)\}$, $k \geq 1$, $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$, new point $x \in \mathcal{X}$
2: $D = \texttt{Sort}(D, d)$ % Sort D so that $d(x, x_i) \leq d(x, x_{i+1})$.
3: $p_y = \sum_{i=1}^{k} \mathbb{I}\{y_i = y\} / k$ for $y \in \mathcal{Y}$.
4: **Return** $\boldsymbol{p} \triangleq (p_1, \ldots, p_k)$

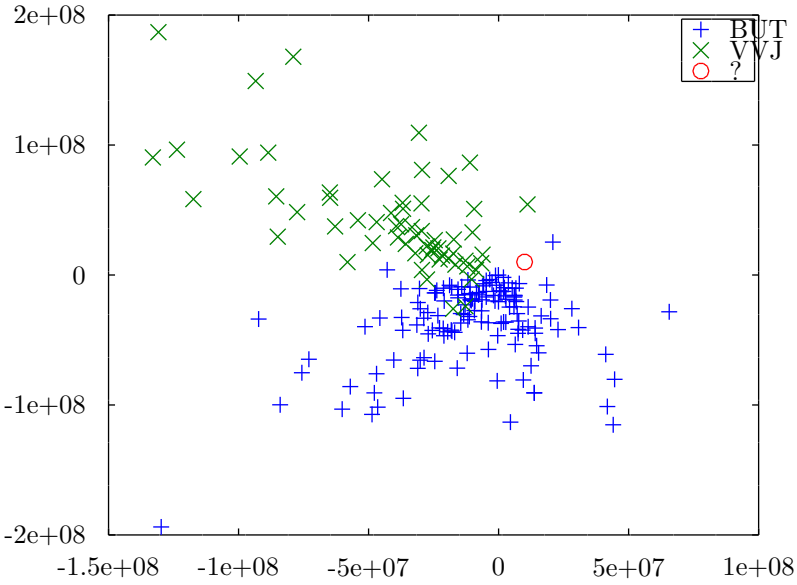
Algorithm parameters

In order to use the algorithm, we must specify some parameters, namely.

- Neighbourhood $k \geq 1$. The number of neighbours to consider.
- Distance $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$. The function we use to determine what is a neighbour.

Figure 2.1: The nearest neighbours algorithm was introduced by Fix and Hodges Jr[3], who also proved consistency properties.

Nearest neighbour: What type is the new bacterium?



Given that the + points represent the BUT type, and the × points the VVJ type, what type of bacterium could the circle point be?

Separating the model from the classification policy

- The K-NN algorithm returns a model giving class probabilities for new data points.

- It is up to us to decide how to use this model to decide upon a given class. A typical decision making rule can be in the form of a policy π that depends on what the model says. However, the simplest decision rule is to take the most likely class:

$$\pi(a \mid x) = \mathbb{I}\left\{p_a \geq p_y \forall y\right\}, \qquad \boldsymbol{p} = \text{K-NN}(D, k, d, x)$$

Discussion: Shortcomings of k-nearest neighbour

- Choice of k The larger k is, the more data you take into account when making your decision. This means that you expect your classes to be more spread out.
- Choice of metric d. The metric d encodes prior information you have about the structure of the data.
- Representation of uncertainty. The predictions of kNN models are simply based on distances and counting. This might not be a very good way to represent uncertainty about class label. In particular, label probabilities should be more uncertain when we have less data.
- Scaling with large amounts of data. A naive implementation of kNN requires the algorithm to shift through all the training data to find the k nearest neighbours, suggesting a super-linear computation time. However, advanced data structures such as Cover Trees (or even KD-trees in low dimensional spaces) can be used to find the neighbours in polylog time.
- Meaning of label probabilities. It is best to think of K-NN as a *model* for predicting the class of a new example from a finite set of existing classes. The model itself might be incorrect, but this should nevertheless be OK for our purposes. In particular, we might later use the model in order to derive classification rules.

Learning outcomes

Understanding

- How kNN works
- The effect of hyperameters k, d for nearest neighbour.
- The use of kNN to classify new data.

Skills

- Use a standard kNN class in python
- Optimise kNN hyperparameters in an unbiased manner.
- Calculate probabilities of class labels using kNN.

Reflection

- When is kNN a good model?
- How can we deal with large amounts of data?
- How can we best represent uncertainty?

2.2 Reproducibility

One of the main problems in science is reproducibility: when we are trying to draw conclusions from one specific data set, it is easy to make a mistake. For that reason, the scientific process requires us to use our conclusions to make testable predictions, and then test those predictions with new experiments. These new experiments should bear out the results of the previous experiments. In more detail, reproducibility can be thought of as two different aspects of answering the question "can this research be replicated?"

Computational reproducibility: Can the study be repeated?
Can we, from the available information and data, exactly reproduce the reported methods and results?

This is something that is useful to be able to even to the original authors of a study. The standard method for achieving this is using version control tools so that the exact version of algorithms, text and data used to write up the study is appropriately labelled. Ideally, any other researcher should be able to run a single script to reproduce all of the study and its computations. The following tools are going to be used in this course:

- `jupyter` notebooks for interactive note taking.
- `svn`, `git` or `mercurial` version control systems for tracking versions, changes and collaborating with others.

Scientific reproducibility: Is the conclusion correct?
Can we, from the available information and a *new* set of data, reproduce the conclusions of the original study?

Here followup research may involve using exactly the same methods. In AI research would mean for example testing whether an algorithm is really performing as well as it is claimed, by testing it in new problems. This can involve a re-implementation. In more general scientific research, it might be the case that the methodology proposed by an original study is flawed, and so a better method should be used to draw better conclusions. Or it might simply be that more data is needed.

When publishing results about a *new method*, computational reproducibility is essential for

scientific reproducibility.

A simple example is the 2016 election. While we can make models about people's opinions regarding candidates in order to predict voting totals, the test of these models comes in the actual election. Unfortunately the only way we have of tuning our models is on previous elections, which are not that frequent, and on the results of previous polls. In addition, predicting the winner of an election is slightly different from predicting how many people are prepared to vote for them across the country. This, together with other factors such as shifting opinions, motivation and how close the sampling distribution is to the voting distribution have a significant effect on accuracy.

The same thing can be done in when dealing purely with data, by making sure we use some

of the data as input to the algorithm, and other data to measure the quality of the algorithm itself. In the following, we assume we have some algorithm $\lambda : \mathcal{D} \to \Pi$, where $\mathcal{D}$ is the universe of possible input data and Π the possible outputs, e.g. all possible classification policies. We also assume the existence of some quality measure U. How should we measure the quality of our algorithmic choices?

Take classification as an example. For a given training set, simply memorising all the labels of each example gives us perfect performance on the training set. Intuitively, this is not a good measure of performance, as we'd probably get poor results on a freshly sampled set. We can think of the training data as input to an algorithm, and the resulting classifier as the algorithm output. The evaluation function also requires some data in order to measure the performance of the policy. This can be expressed into the following principle.

The principle of independent evaluation

Data used for estimation cannot be used for evaluation.

This applies both to computer-implemented and human-implemented algorithms.

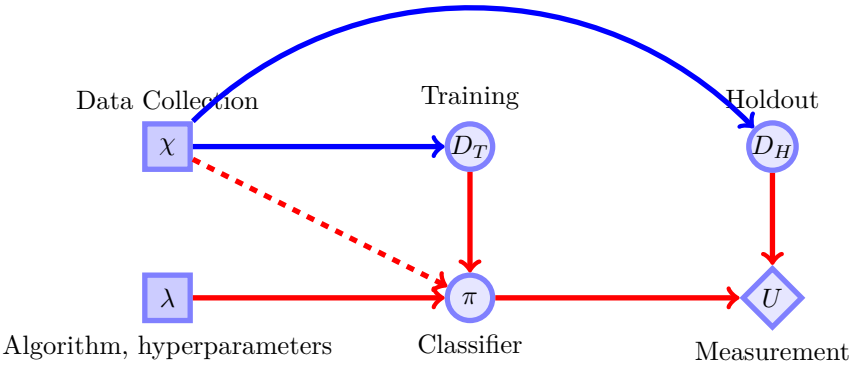


Figure 2.2: The decision process in classification.

One can think of the decision process in classification as follows. First, we decide to collect some data according to some experimental protocol χ. We also decide to use some algorithm (with associated hyperparameters) λ together with data D_T we will obtain from our data collection in order to obtain a classification policy π. Typically, we need to measure the quality of a policy according to how well it classifies on unknown data. This is because our policy has been generated using D_T, and so any measurement of its quality is going to be biased.

For classification problems, there is a natural metric U to measure. The classification accuracy of the classifier. If the classification decisions are stochastic, then the classifier assigns probability $\pi(a \mid x)$ to each possible label a, and our utility is simply the identity function $U(a, y) \triangleq \mathbb{I}\{a = y\}$.

Classification accuracy

$$\mathbb{E}_\chi[U(\pi)] = \sum_{x,y} \underbrace{\mathbb{P}_\chi(x,y)}_{\text{Data probability}} \overbrace{\pi(a = y \mid x)}^{\text{Decision probability}}$$

The classification accuracy of policy π under χ is the expected number of times the policy decides π chooses the correct class. However, when approximating χ with a sample D_H, we instead obtain the empirical estimate:

$$\mathbb{E}_{D_H} U(\pi) = \sum_{(x,y)\in D_H} \pi(a = y \mid x)/|D_H|.$$

Of course, there is no reason to limit ourselves to the identity function. The utility could very well be such that some errors are penalised more than other errors. Consider for example an intrusion detection scenario: it is probably more important to correctly classify intrusions.

2.2.1 The human as an algorithm

The human as an algorithm.

The same way with which an algorithm creates a model from some prior assumptions and data, so can a human select an algorithm and associated hyperparamters by executing an algorithm herself. This involves trying different algorithms and hyperparametrs on the same training data D_T and then measuring their performance in the holdout set D_H.

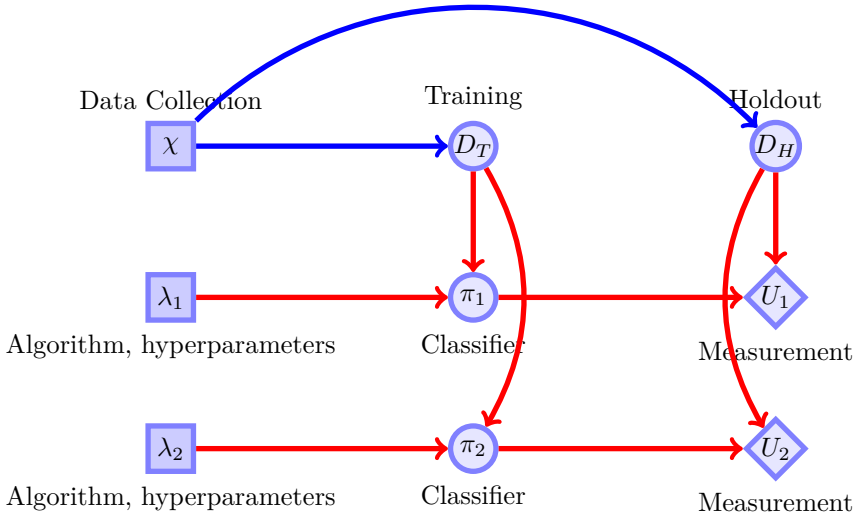


Figure 2.3: Selecting algorithms and hyperparameters through holdouts

Holdout sets

To summarise, holdout sets are used in order to be able to evaluate the performance of specific algorithms, or hyparameter selection.

- Original data D, e.g. $D = (x_1, \ldots, x_T)$.
- Training data $D_T \subset D$, e.g. $D_T = x_1, \ldots, x_n$, $n < T$.
- Holdout data $D_H = D \setminus D_T$, used to measure the quality of the result.
- Algorithm λ with hyperparametrs ϕ.
- Get algorithm output $\pi = \lambda(D_T, \phi)$.
- Calculate quality of output $U(\pi, D_H)$

We start with some original data D, e.g. $D = (x_1, \ldots, x_T)$. We then split this into a training data set $D_T \subset D$, e.g. $D_T = x_1, \ldots, x_n$, $n < T$ and holdout dataset $D_H = D \setminus D_T$. This is used to measure the quality of selected algorithms λ and hyperparameters ϕ. We run an algorithm/hyperparameter combination on the training data and obtain a result $\pi = \lambda(D_T, \phi)$. [1] We then calculate the quality of the output $U(\pi, D_H)$ on the holdout set. Unfortunately, the combination that appears the best due to the holdout result may look inferior in a fresh sample. Following the principle of "data used for evaluation cannot be used for estimation", we must measure performance on another sample. This ensures that we are not biased in our decision about what is the best algorithm.

Holdout and test sets for unbiased algorithm comparison

Consider the problem of comparing a number of different algorithms in Λ. Each algorithm λ has a different set of hyperparameters Φ_λ. The problem is to choose the best parameters for each algorithm, and then to test them independently. A simple meta-algorithm for doing this is based on the use of a *holdout* set for choosing hyperparameters for each algorithm, and a *test* set to measure algorithmic performance.

Algorithm 2 Unbiased adaptive evaluation through data partitioning

```
Partition data into D_T, D_H, D*.
for λ ∈ Λ do
    for φ ∈ Φ_λ do
        π_{φ,λ} = λ(D_T, φ).
    end for
    Get π*_λ maximising U(π_{φ,λ}, D_H).
    u_λ = U(π*_λ, D*).
end for
λ* = arg max_λ u_λ.
```

[1] As typically algorithms are maximising the quality metric on the training data,

$$\lambda(D_T) = \arg\max_y U(y, D_T)$$

we typically obtain a biased estimate, which depends both on the algorithm itself and the training data. For K-NN in particular, when we measure accuracy on the training data, we can nearly always obtain near-perfect accuracy, but not always perfect. Can you explain why?

Final performance measurement

When comparing many algorithms, where we must select a hyperparameter for each one, then we can use one dataset as input to the algorithms, and another for selecting hyperparameters. That means that we must use another dataset to measure performance. This is called the testing set. Figure 2.4 illustrates this.

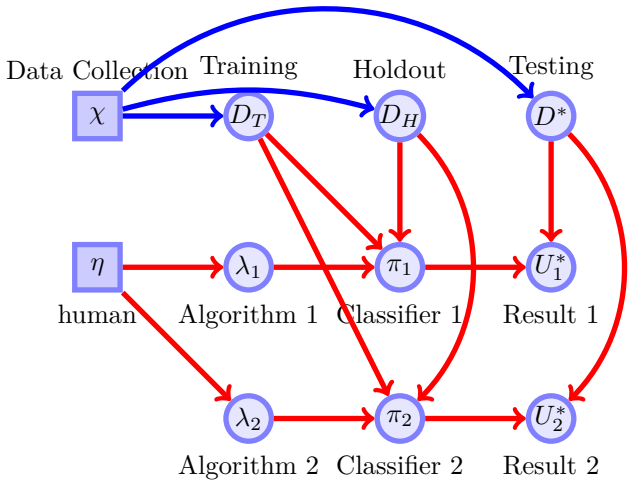


Figure 2.4: Simplified dependency graph for selecting hyperparameters for different algorithms, and comparing them on an independent test set. For the i-th algorithm, the classifier model is

2.2.2 Algorithmic sensitivity

The algorithm's output does have a dependence on its input, obviously. So, how sensitive is the algorithm to the input?

Independent data sets

One simple idea is to just collect independent datasets and see how the output of the algorithm changes when the data changes. However, this is quite expensive, as it not might be easy to collect data in the first place.

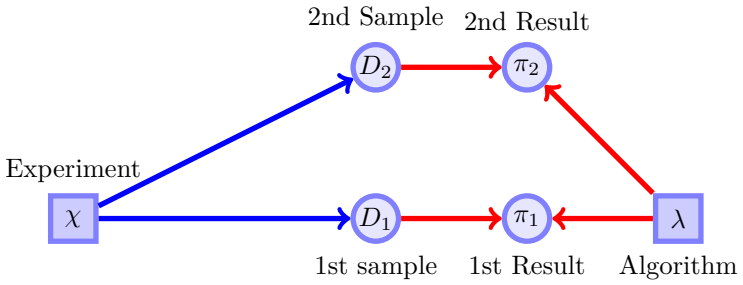


Figure 2.5: Multiple samples

Bootstrap samples

A more efficient idea is to only collect one dataset, but then use it to generate more datasets. The simplest way to do that is by sampling with replacement from the original dataset, new datasets of the same size as the original. Then the original dataset is sufficiently large, this is approximately the same as sampling independent datasets. As usual, we can evaluate our algorithm on an independent data set.

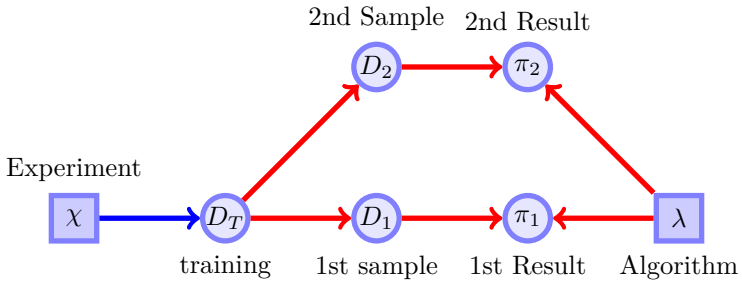


Figure 2.6: Bootstrap replicates of a single sample

Bootstrapping

Bootstrapping is a general technique that can be used to:

- Estimate the sensitivity of λ to the data x.
- Obtain a distribution of estimates π from λ and the data x.
- When estimating the performance of an algorithm on a small dataset D^*, use bootstrap samples of D^*. This allows us to take into account the inherent uncertainty in measured performance. It is very useful to use bootstrapping with pairwise comparisons.

Bootstrapping

1. **Input** Training data D, number of samples k.
2. **For** $i = 1, \ldots, k$
3. $D^{(i)} = \text{Bootstrap}(D)$
4. **return** $\left\{ D^{(i)} \;\middle|\; i = 1, \ldots, k \right\}$.

where Bootstrap(D) samples with replacement $|D|$ points from D_T.

In more detail, remember that even though the test score is an *independent* measurement of an algorithm's performance, it is *not* the actual expected performance. At best, it's an unbiased estimate of performance. Hence, we'd like to have some way to calculate a likely performance range from the test data. Bootstrapping can help: by taking multiple samples of the test set and calculating performance on each one, we obtain an empirical distribution of scores.

Secondly, we can use it to tell us something about the sensitivity of our algorithm. In particular, by taking multiple samples from the training data, we can end up with multiple

models. If the models are only slightly different, then the algorithm is more stable and we can be more confident in its predictions.

Finally, bagging also allows us to generate probabilistic predictions from deterministic classification algorithms, by simply averaging predictions from multiple bootstrapped predictors. This is called *bagging predictors*[1].

Cross-validation

While we typically use a single training, hold-out and test set, it might be useful to do this multiple times in order to obtain more robust performance estimates. In the simplest case, cross-validation can be used to obtain multiple training and hold-out sets from a single dataset. This works by simply partitioning the data in k *folds* and then using one of the folds as a holdout and the remaining $k-1$ as training data. This is repeated k times. When k is the same size as the original training data, then the method is called *leave-one-out cross-validation.*

k-fold Cross-Validation

1. **Input** Training data D_T, number of folds k, algorithm λ, measurement function U
2. Create the partition $D^{(1)} \ldots, D^{(k)}$ so that $\bigcup_{i=1}^{k} D^{(k)} = D$.
3. Define $D_T^{(i)} = D \setminus D^{(i)}$
4. $\pi_i = \lambda(D_T^{(i)})$
5. **For** $i = 1, \ldots, k$:
6. $\pi_i = \lambda(D^{(i)})$
7. $u_i = U(\pi_i)$
8. **return** $\{y_1, \ldots, y_i\}$.

Independent replication

The gold standard for reproducibility is independent replication. Simply have another team try and reproduce the results you obtained, using completely new data. If the replication is successful, then you can be pretty sure there was no flaw in your original analysis.

Replication study

1. Reinterpret the original hypothesis and experiment.
2. Collect data according to the original protocol, *unless flawed*. It is possible that the original experimental protocol had flaws. Then the new study should try and address this through an improved data collection process. For example, the original study might not have been double-blind. The new study can replicate the results in a double-blind regime.

3. Run the analysis again, *unless flawed*. It is possible that the original analysis had flaws. For example, possible correlations may not have been taken into account.
4. See if the conclusions are in agreement.

Learning outcomes

Understanding

- What is a hold-out set, cross-validation and bootstrapping.
- The idea of not reusing data input to an algorithm to evaluate it.
- The fact that algorithms can be implemented by both humans and machines.

Skills

- Use git and notebooks to document your work.
- Use hold-out sets or cross-validation to compare parameters/algorithms in Python.
- Use bootstrapping to get estimates of uncertainty in Python.

Reflection

- What is a good use case for cross-validation over hold-out sets?
- When is it a good idea to use bootstrapping?
- How can we use the above techniques to avoid the false discovery problem?
- Can these techniques fully replace independent replication?

EXERCISE 1. Work in teams of 2-3 students.

Select an arbitrary classification dataset from `https://archive.ics.uci.edu/ml/datasets.html?task=cla`.

Select any arbitrary machine learning algorithm for classification from `scikitlearn` that can be used with this dataset, and identify its main hyperparameters.

Varying at least one hyperparameter, use bootstrapping and/or cross-validation to find the optimal value for that hyperparameter, and report its performance. How close to the reported accuracy do you expect its performance to be in reality? What are the factors that might cause it to deviate?

Write a short report summarising both your methodology and your results. Exchange this report with another group of students. See whether you can reproduce exactly what they have done.

2.3 Beliefs and probabilities

Probability can be used to describe purely chance events, as in for example quantum physics. However, it is mostly used to describe uncertain events, such as the outcome of a dice roll or a coin flip, which only appear random. In fact, one can take it even further than that, and use it to model subjective uncertainty about any arbitrary event. Although probabilities are not the only way in which we can quantify uncertainty, it is a simple enough model, and with a rich enough history in mathematics, statistics, computer science and engineering that it is the most useful.

Uncertainty

- We cannot perfectly predict the future.
- We cannot know for sure what happened in the past.
- How can we quantify this uncertainty?
- Probabilities!

Axioms of probability
For any probability measure[2] P on (Ω, Σ),

1. The probability of the certain event is $P(\Omega) = 1$
2. The probability of the impossible event is $P(\emptyset) = 0$
3. The probability of any event $A \in \Sigma$ is $0 \leq P(A) \leq 1$.
4. If A, B are disjoint, i.e. $A \cap B = \emptyset$, meaning that they cannot happen at the same time, then
$$P(A \cup B) = P(A) + P(B)$$

Sometimes we would like to calculate the probability of some event A happening given that we know that some other event B has happened. For this we need to first define the idea of conditional probability.

Definition 2.3.1 (Conditional probability)**.** The probability of A happening if we know that B has happened is defined to be:
$$P(A \mid B) \triangleq \frac{P(A \cap B)}{P(B)}.$$

Conditional probabilities obey the same rules as probabilities. Here, the probability measure of any event A given B is defined to be the probability of the intersection of of the events divided by the second event. We can rewrite this definition as follows, by using the definition for $P(B \mid A)$

Bayes's theorem
For $P(A_1 \cup A_2) = 1$, $A_1 \cap A_2 = \emptyset$,
$$P(A_i \mid B) = \frac{P(B \mid A_i)P(A_i)}{P(B)} = \frac{P(B \mid A_i)P(A_i)}{P(B \mid A_1)P(A_1) + P(B \mid A_2)P(A_2)}$$

EXAMPLE 1 (probability of rain). What is the probability of rain given a forecast x_1 or x_2?

ω_1: rain	$P(\omega_1) = 80\%$
ω_2: dry	$P(\omega_2) = 20\%$

Table 2.1: Prior probability of rain tomorrow

x_1: rain	$P(x_1 \mid \omega_1) = 90\%$
x_2: dry	$P(x_2 \mid \omega_2) = 50\%$

Table 2.2: Probability the forecast is correct

$P(\omega_1 \mid x_1) = 87.8\%$
$P(\omega_1 \mid x_2) = 44.4\%$

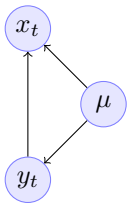
Table 2.3: Probability that it will rain given the forecast

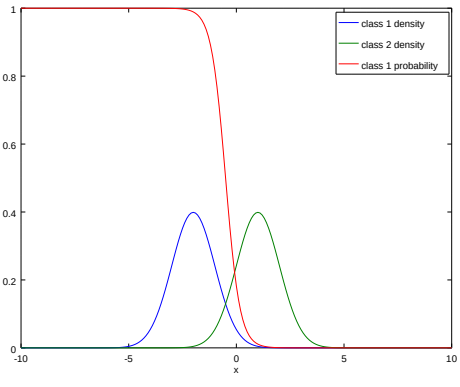
Classification in terms of conditional probabilities

Conditional probability naturally appears in classification problems. Given a new example vector of data $x_t \in \mathcal{X}$, we would like to calculate the probability of different classes $c \in \mathcal{Y}$ given the data, $P_\mu(y_t = c \mid x_t)$. If we somehow obtained the distribution of data $P_\mu(x_t \mid y_t)$ for each possible class, as well as the prior class probability $P_\mu(y_t = c)$, from Bayes's theorem, we see that we can obtain the probability of the class:

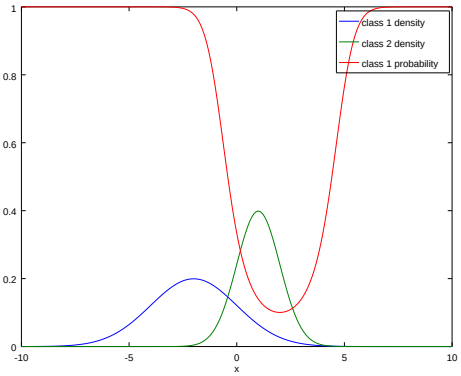
$$P_\mu(y_t = c \mid x_t) = \frac{P_\mu(x_t \mid y_t = c)P_\mu(y_t = c)}{\sum_{c' \in \mathcal{Y}} P_\mu(x_t \mid y_t = c')P_\mu(y_t = c')}$$

for any class c. This directly gives us a method for classifying new data, as long as we have a way to obtain $P_\mu(x_t \mid y_t)$ and $P_\mu(y_t)$.

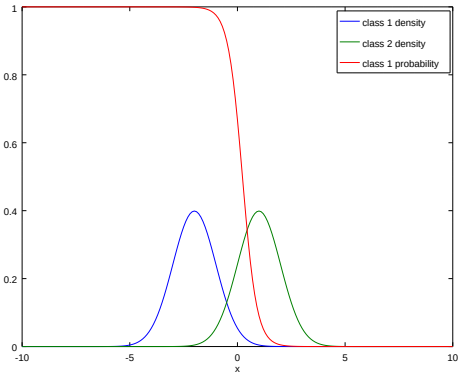




EXAMPLE 2 (Normal distribution). Equal prior and



variance



Unequal variance

prior

But how can we get a probability model in the first place?

Subjective probability

While probabilities apply to truly random events, they are also useful for representing subjective uncertainty. In this course, we will use a special symbol for subjective probability, ξ.

Subjective probability measure ξ

- If we think event A is more likely than B, then $\xi(A) > \xi(B)$.
- Usual rules of probability apply:
  1. $\xi(A) \in [0, 1]$.
  2. $\xi(\emptyset) = 0$.
  3. If $A \cap B = \emptyset$, then $\xi(A \cup B) = \xi(A) + \xi(B)$.

Bayesian inference illustration

Use a subjective belief $\xi(\mu)$ on $\mathcal{M}$

- *Prior* belief $\xi(\mu)$ represents our initial uncertainty.
- We *observe history* h.
- Each possible μ assigns a *probability* $P_\mu(h)$ to h.
- We can use this to *update* our belief via Bayes' theorem to obtain the *posterior* belief:

$$\xi(\mu \mid h) \propto P_\mu(h)\xi(\mu) \qquad \text{(conclusion} = \text{evidence} \times \text{prior)}$$

2.3.1 Probability and Bayesian inference

One of the most important methods in machine learning and statistics is that of Bayesian inference. This is the most fundamental method of drawing conclusions from data and explicit prior assumptions. In Bayesian inference, prior assumptions are represented as a probabilities on a space of hypotheses. Each hypothesis is seen as a probabilistic model of all possible data that we can see.

Frequently, we want to draw conclusions from data. However, the conclusions are never solely inferred from data, but also depend on prior assumptions about reality.

Some examples

EXAMPLE 3. John claims to be a medium. He throws a coin n times and predicts its value always correctly. Should we believe that he is a medium?

- μ_1: John is a medium.
- μ_0: John is not a medium.

The answer depends on what we *expect* a medium to be able to do, and how likely we thought he'd be a medium in the first place.

EXAMPLE 4. Traces of DNA are found at a murder scene. We perform a DNA test against a database of 10^4 citizens registered to be living in the area. We know that the probability of a false positive (that is, the test finding a match by mistake) is 10^{-6}. If there is a match in the database, does that mean that the citizen was at the scene of the crime?

Bayesian inference

Now let us apply this idea to our specific problem. We already have the probability of the observation for each model, but we just need to define a *prior probability* for each model. Since this is usually completely subjective, we give it another symbol.

Prior probability
The prior probability ξ on a set of models $\mathcal{M}$ specifies our subjective belief $\xi(\mu)$ that each model is true.[3]

This allows us to calculate the probability of John being a medium, given the data:

$$\xi(\mu_1 \mid \mathbf{x}) = \frac{\mathbb{P}(\mathbf{x} \mid \mu_1)\xi(\mu_1)}{\mathbb{P}_\xi(\mathbf{x})},$$

where

$$\mathbb{P}_\xi(\mathbf{x}) \triangleq \mathbb{P}(\mathbf{x} \mid \mu_1)\xi(\mu_1) + \mathbb{P}(\mathbf{x} \mid \mu_0)\xi(\mu_0).$$

The only thing left to specify is $\xi(\mu_1)$, the probability that John is a medium before seeing the data. This is our subjective prior belief that mediums exist and that John is one of them. More generally, we can think of Bayesian inference as follows:

- We start with a set of mutually exclusive models $\mathcal{M} = \{\mu_1, \dots, \mu_k\}$.
- Each model μ is represented by a specific probabilistic model for any possible data x, that is $P_\mu(x) \equiv \mathbb{P}(x \mid \mu)$.
- For each model, we have a prior probability $\xi(\mu)$ that it is correct.
- After observing the data, we can calculate a posterior probability that the model is correct:

$$\xi(\mu \mid x) = \frac{\mathbb{P}(x \mid \mu)\xi(\mu)}{\sum_{\mu' \in \mathcal{M}} \mathbb{P}(x \mid \mu')\xi(\mu')} = \frac{P_\mu(x)\xi(\mu)}{\sum_{\mu' \in \mathcal{M}} P_{\mu'}(x)\xi(\mu')}.$$

Interpretation

- $\mathcal{M}$: Set of all possible models that could describe the data.
- $P_\mu(x)$: Probability of x under model μ.
- Alternative notation $\mathbb{P}(x \mid \mu)$: Probability of x given that model μ is correct.
- $\xi(\mu)$: Our belief, before seeing the data, that μ is correct.
- $\xi(\mu \mid x)$: Our belief, aftering seeing the data, that μ is correct.

It must be emphasized that $P_\mu(x) = \mathbb{P}(x \mid \mu)$ as they are simply two different notations for the same thing. In words the first can be seen as the probability that model μ assigns to data x, while the second as the probability of x if μ is the true model. Combining the prior belief with evidence is key in this procedure. Our posterior belief can then be used as a new prior belief when we get more evidence.

Exercise 2 (Continued example for medium). Now let us apply this idea to our specific problem. We first make an independence assumption. In particular, we can assume that success and failure comes from a Bernoulli distribution with a parameter depending on the model.

$$P_\mu(x) = \prod_{t=1}^{n} P_\mu(x_t). \qquad \text{(independence property)}$$

We first need to specify how well a medium could predict. Let's assume that a true medium would be able to predict perfectly, and that a non-medium would only predict randomly. This leads to the following models:

$$P_{\mu_1}(x_t = 1) = 1, \qquad P_{\mu_1}(x_t = 0) = 0. \qquad \text{(true medium model)}$$
$$P_{\mu_0}(x_t = 1) = 1/2, \qquad P_{\mu_0}(x_t = 0) = 1/2. \qquad \text{(non-medium model)}$$

The only thing left to specify is $\xi(\mu_1)$, the probability that John is a medium before seeing the data. This is our subjective prior belief that mediums exist and that John is one of them.

$$\xi(\mu_0) = 1/2, \qquad \xi(\mu_1) = 1/2. \qquad \text{(prior belief)}$$

Combining the prior belief with evidence is key in this procedure. Our posterior belief can then be used as a new prior belief when we get more evidence.

$$\xi(\mu_1 \mid x) = \frac{P_{\mu_1}(x)\xi(\mu_1)}{\mathbb{P}_\xi(x)} \qquad \text{(posterior belief)}$$
$$\mathbb{P}_\xi(x) \triangleq P_{\mu_1}(x)\xi(\mu_1) + P_{\mu_0}(x)\xi(\mu_0). \qquad \text{(marginal distribution)}$$

Throw a coin 4 times, and have a classmate make a prediction. What your belief that your classmate is a medium? Is the prior you used reasonable?

Sequential update of beliefs

Assume you have n meteorologists. At each day t, each meteorologist i gives a probability $p_{t,\mu_i} \triangleq P_{\mu_i}(x_t = \text{rain})$ for rain. Consider the case of there being three meteorologists, and each one making the following prediction for the coming week. Start with a uniform prior $\xi(\mu) = 1/3$ for each model.

	M	T	W	T	F	S	S
CNN	0.5	0.6	0.7	0.9	0.5	0.3	0.1
SMHI	0.3	0.7	0.8	0.9	0.5	0.2	0.1
YR	0.6	0.9	0.8	0.5	0.4	0.1	0.1
Rain?	Y	Y	Y	N	Y	N	N

Table 2.4: Predictions by three different entities for the probability of rain on a particular day, along with whether or not it actually rained.

EXERCISE 3.

- n meteorological stations $\{\mu_i \mid i = 1, \dots, n\}$
- The i-th station predicts rain $P_{\mu_i}(x_t \mid x_1, \dots, x_{t-1})$.
- Let $\xi_t(\mu)$ be our belief at time t. Derive the next-step belief $\xi_{t+1}(\mu) \triangleq \xi_t(\mu|y_t)$ in terms of the current belief ξ_t.
- Write a python function that computes this posterior

$$\xi_{t+1}(\mu) \triangleq \xi_t(\mu|x_t) = \frac{P_\mu(x_t \mid x_1, \dots, x_{t-1})\xi_t(\mu)}{\sum_{\mu'} P_{\mu'}(x_t \mid x_1, \dots, x_{t-1})\xi_t(\mu')}$$

Bayesian inference for Bernoulli distributions

Estimating a coin's bias
A fair coin comes heads 50% of the time. We want to test an unknown coin, which we think may not be completely fair.

For a sequence of throws $x_t \in \{0, 1\}$,

$$P_\theta(x) \propto \prod_t \theta^{x_t}(1-\theta)^{1-x_t} = \theta^{\#\text{Heads}}(1-\theta)^{\#\text{Tails}}$$

Say we throw the coin 100 times and obtain 70 heads. Then we plot the *likelihood* $P_\theta(x)$ of different models. From these, we calculate a *posterior* distribution over the correct models. This represents our conclusion given our prior and the data. If the prior distribution is described by the so-called Beta density

$$f(\theta \mid \alpha, \beta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$$

where α, β describe the shape of the Beta distribution.

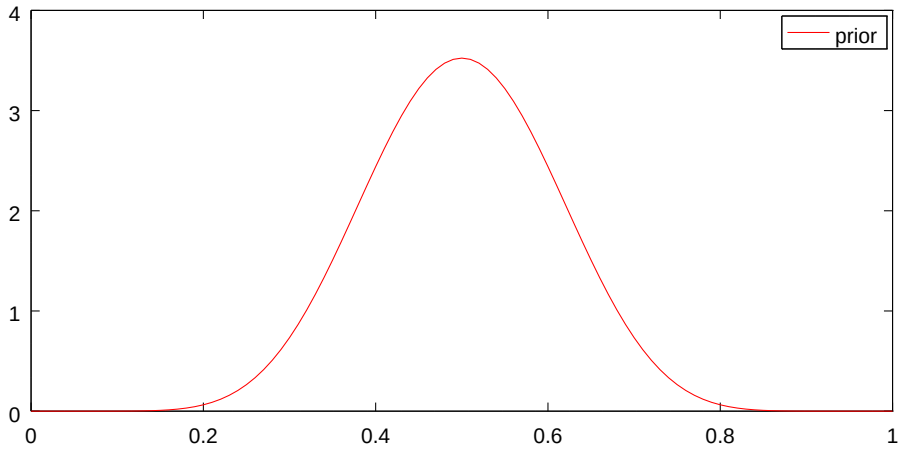


Figure 2.7: Prior belief ξ about the coin bias θ.

Learning outcomes

Understanding

- The axioms of probability, marginals and conditional distributions.
- The philosophical underpinnings of Bayesianism.
- The simple conjugate model for Bernoulli distributions.

Skills

- Be able to calculate with probabilities using the marginal and conditional definitions and Bayes rule.
- Being able to implement a simple Bayesian inference algorithm in Python.

Reflection

- How useful is the Bayesian representation of uncertainty?
- How restrictive is the need to select a prior distribution?
- Can you think of another way to explicitly represent uncertainty in a way that can incorporate new evidence?

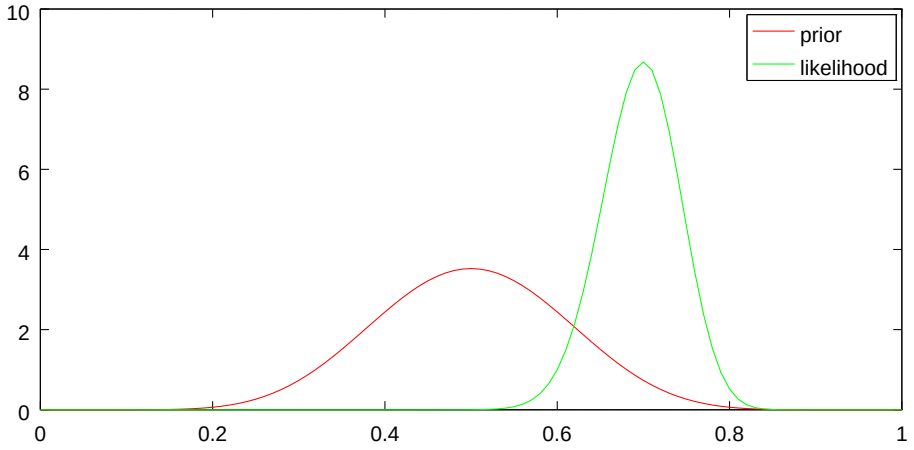


Figure 2.8: Prior belief ξ about the coin bias θ and likelihood of θ for the data.

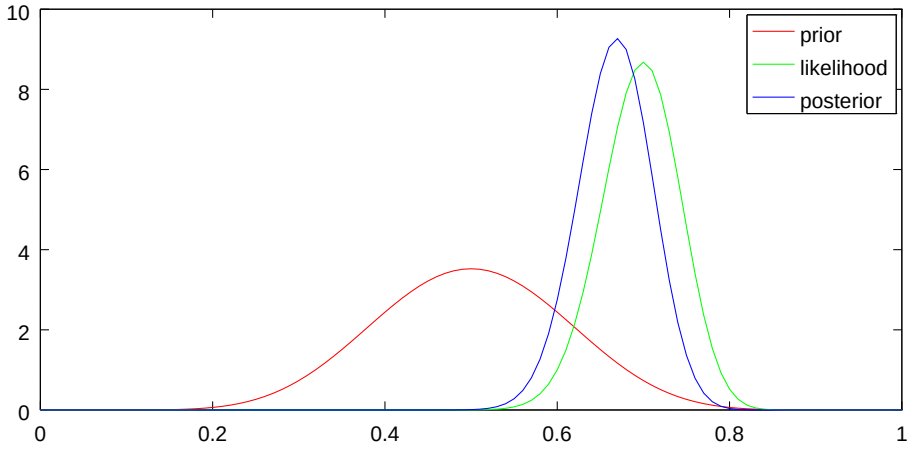


Figure 2.9: Prior belief $\xi(\theta)$ about the coin bias θ, likelihood of θ for the data, and posterior belief $\xi(\theta \mid x)$

2.4 Hierarchies of decision making problems

All machine learning problems are essentially decision problems. This essentially means replacing some human decisions with machine decisions. One of the simplest decision problems is classification, where you want an algorithm to decide the correct class of some data, but even within this simple framework there is a multitude of decisions to be made. The first is how to frame the classification problem the first place. The second is how to collect, process and annotate the data. The third is choosing the type of classification model to use. The fourth is how to use the collected data to find an optimal classifier within the selected type. After all this has been done, there is the problem of classifying new data. In this course, we will take a holistic view of the problem, and consider each problem in turn, starting from the lowest level and working our way up.

2.4.1 Simple decision problems

Preferences

The simplest decision problem involves selecting one item from a set of choices, such as in the following examples

Example 5. **Food**

A McDonald's cheeseburger
B Surstromming
C Oatmeal

Money

A 10,000,000 SEK
B 10,000,000 USD
C 10,000,000 BTC

Entertainment

A Ticket to Liseberg
B Ticket to Rebstar
C Ticket to Nutcracker

Rewards and utilities

In the decision theoretic framework, the things we receive are called rewards, and we assign a utility value to each one of them, showing which one we prefer.

- Each choice is called a *reward* $r \in \mathcal{R}$.
- There is a *utility function* $U : \mathcal{R} \to \mathbb{R}$, assigning values to reward.

- We (weakly) prefer A to B iff $U(A) \geq U(B)$.

In each case, given U the choice between each reward is trivial. We just select the reward:

$$r^* \in \arg\max_r U(r)$$

The main difficult is actually selecting the appropriate utility function. In a behavioural context, we simply assume that humans act with respect to a specific utility function. However, figuring out this function from behavioural data is non trivial. ven when this assumption is correct, individuals do not have a common utility function.

Exercise 4. From your individual preferences, derive a *common utility function* that reflects everybody's preferences in the class for each of the three examples. Is there a simple algorithm for deciding this? Would you consider the outcome fair?

Preferences among random outcomes

Example 6. Would you rather …

A Have 100 EUR now?

B Flip a coin, and get 200 EUR if it comes heads?

The expected utility hypothesis
Rational decision makers prefer choice A to B if

$$\mathbb{E}(U|A) \geq \mathbb{E}(U|B),$$

where the expected utility is

$$\mathbb{E}(U|A) = \sum_r U(r)\, \mathbb{P}(r|A).$$

In the above example, $r \in \{0, 100, 200\}$ and $U(r)$ is increasing, and the coin is fair.

- If U is convex, we prefer B.
- If U is concave, we prefer A.
- If U is linear, we don't care.

Uncertain rewards

However, in real life, there are many cases where we can only choose between uncertain outcomes. The simplest example are lottery tickets, where rewards are essentially random. However, in many cases the rewards are not really random, but simply uncertain. In those cases it is useful to represent our uncertainty with probabilities as well, even though there is nothing really random.

- Decisions $a \in \mathcal{A}$
- Each choice is called a *reward* $r \in \mathcal{R}$.

$\rho(\omega, a)$	a_1	a_2
ω_1	dry, carrying umbrella	wet
ω_2	dry, carrying umbrella	dry
$U[\rho(\omega, a)]$	a_1	a_2
ω_1	0	-10
ω_2	0	1

Table 2.5: Rewards and utilities.

$\rho(\omega, a)$	a_1	a_2
ω_1	dry, carrying umbrella	wet
ω_2	dry, carrying umbrella	dry
$U[\rho(\omega, a)]$	a_1	a_2
ω_1	0	-10
ω_2	0	1
$\mathbb{E}_P(U \mid a)$	0	-1.2

Table 2.6: Rewards, utilities, expected utility for 20% probability of rain.

- There is a *utility function* $U : \mathcal{R} \to \mathbb{R}$, assigning values to reward.
- We (weakly) prefer A to B iff $U(A) \geq U(B)$.

Example 7. You are going to work, and it might rain. What do you do?

- a_1: Take the umbrella.
- a_2: Risk it!
- ω_1: rain
- ω_2: dry

- $\max_a \min_\omega U = 0$
- $\min_\omega \max_a U = 0$

Expected utility

$$\mathbb{E}(U \mid a) = \sum_r U[\rho(\omega, a)] \, \mathbb{P}(\omega \mid a)$$

Example 8. You are going to work, and it might rain. The forecast said that the probability of rain (ω_1) was 20%. What do you do?

- a_1: Take the umbrella.
- a_2: Risk it!

2.4.2 Decision rules

We now move from simple decisions to decisions that depend on some observation. We shall start with a simple problem in applied meteorology. Then we will discuss hypothesis testing as a decision making problem. Finally, we will go through an exercise in Bayesian methods for classification.

Bayes decision rules

Consider the case where outcomes are independent of decisions:

$$U(\xi, a) \triangleq \sum_{\mu} U(\mu, a)\xi(\mu)$$

This corresponds e.g. to the case where $\xi(\mu)$ is the belief about an unknown world.

Definition 2.4.1 (Bayes utility)**.** The maximising decision for ξ has an expected utility equal to:

$$U^*(P) \triangleq \max_{a \in \mathcal{A}} U(\xi, a). \tag{2.4.1}$$

The n-meteorologists problem

Of course, we may not always just be interested in classification performance in terms of predicting the most likely class. It strongly depends on the problem we are actually wanting to solve. In biometric authentication, for example, we want to guard against the unlikely event that an impostor will successfully be authenticated. Even if the decision rule that always says 'OK' has the lowest classification error in practice, the expected cost of impostors means that the optimal decision rule must sometimes say 'Failed' even if this leads to false rejections sometimes.

EXERCISE 5. Assume you have n meteorologists. At each day t, each meteorologist i gives a probability $p_{t,\mu_i} \triangleq P_{\mu_i}(x_t = \text{rain})$ for rain. Consider the case of there being three meteorologists, and each one making the following prediction for the coming week. Start with a uniform prior $\xi(\mu) = 1/3$ for each model.

	M	T	W	T	F	S	S
CNN	0.5	0.6	0.7	0.9	0.5	0.3	0.1
SMHI	0.3	0.7	0.8	0.9	0.5	0.2	0.1
YR	0.6	0.9	0.8	0.5	0.4	0.1	0.1
Rain?	Y	Y	Y	N	Y	N	N

Table 2.7: Predictions by three different entities for the probability of rain on a particular day, along with whether or not it actually rained.

1. What is your belief about the quality of each meteorologist after each day?
2. What is your belief about the probability of rain each day?

$$P_\xi(x_t = \text{rain} \mid x_1, x_2, \dots x_{t-1}) = \sum_{\mu \in \mathcal{M}} P_\mu(x_t = \text{rain} \mid x_1, x_2, \dots x_{t-1})\xi(\mu \mid x_1, x_2, \dots x_{t-1})$$

3. Assume you can decide whether or not to go running each day. If you go running and it does not rain, your utility is 1. If it rains, it's -10. If you don't go running, your utility is 0. What is the decision maximising utility in expectation (with respect to the posterior) each day?

2.4.3 Statistical testing

A common type of decision problem is a statistical test. This arises when we have a set of possible candidate models $\mathcal{M}$ and we need to be able to decide which model to select after we see the evidence. Many times, there is only one model under consideration, μ_0, the so-called *null hypothesis*. Then, our only decision is whether or not to accept or reject this hypothesis.

Simple hypothesis testing

Let us start with the simple case of needing to compare two models.

The simple hypothesis test as a decision problem

- $\mathcal{M} = \{\mu_0, \mu_1\}$
- a_0: Accept model μ_0
- a_1: Accept model μ_1

U	μ_0	μ_1
a_0	1	0
a_1	0	1

Table 2.8: Example utility function for simple hypothesis tests.

There is no reason for us to be restricted to this utility function. As it is diagonal, it effectively treats both types of errors in the same way.

EXAMPLE 9 (Continuation of the medium example).

- μ_1: that John is a medium.
- μ_0: that John is not a medium.

Let x_t be 0 if John makes an incorrect prediction at time t and $x_t = 1$ if he makes a correct prediction. Let us once more assume a Bernoulli model, so that John's claim that he can predict our tosses perfectly means that for a sequence of tosses $\mathbf{x} = x_1, \ldots, x_n$,

$$P_{\mu_1}(\mathbf{x}) = \begin{cases} 1, & x_t = 1 \forall t \in [n] \\ 0, & \exists t \in [n] : x_t = 0. \end{cases}$$

That is, the probability of perfectly correct predictions is 1, and that of one or more incorrect prediction is 0. For the other model, we can assume that all draws are independently and identically distributed from a fair coin. Consequently, no matter what John's predictions are, we have that:

$$P_{\mu_0}(\mathbf{x} = 1 \ldots 1) = 2^{-n}.$$

So, for the given example, as stated, we have the following facts:

- If John makes one or more mistakes, then $\mathbb{P}(\mathbf{x} \mid \mu_1) = 0$ and $\mathbb{P}(\mathbf{x} \mid \mu_0) = 2^{-n}$. Thus, we should perhaps say that then John is not a medium
- If John makes no mistakes at all, then

$$\mathbb{P}(\mathbf{x} = 1, \ldots, 1 \mid \mu_1) = 1, \qquad \mathbb{P}(\mathbf{x} = 1, \ldots, 1 \mid \mu_0) = 2^{-n}. \tag{2.4.2}$$

Now we can calculate the posterior distribution, which is

$$\xi(\mu_1 \mid \mathbf{x} = 1, \ldots, 1) = \frac{1 \times \xi(\mu_1)}{1 \times \xi(model_1) + 2^{-n}(1 - \xi(\mu_1))}.$$

Our expected utility for taking action a_0 is actually

$$\mathbb{E}_\xi(U \mid a_0) = 1 \times \xi(\mu_0 \mid \mathbf{x}) + 0 \times \xi(\mu_1 \mid \mathbf{x}), \qquad \mathbb{E}_\xi(U \mid a_1) = 0 \times \xi(\mu_0 \mid \mathbf{x}) + 1 \times \xi(\mu_1 \mid \mathbf{x})$$

Null hypothesis test

Many times, there is only one model under consideration, μ_0, the so-called *null hypothesis*. This happens when, for example, we have no simple way of defining an appropriate alternative. Consider the example of the medium: How should we expect a medium to predict? Then, our only decision is whether or not to accept or reject this hypothesis.

The null hypothesis test as a decision problem

- a_0: Accept model μ_0
- a_1: Reject model μ_0

Example 10. Construction of the test for the medium

- μ_0 is simply the *Bernoulli*$(1/2)$ model: responses are by chance.
- We need to design a policy $\pi(a \mid \mathbf{x})$ that accepts or rejects depending on the data.
- Since there is no alternative model, we can only construct this policy according to its properties when μ_0 is true.
- In particular, we can fix a policy that only chooses a_1 when μ_0 is true a proportion δ of the time.
- This can be done by construcing a threshold test from the inverse-CDF.

Using p-values to construct statistical tests

Definition 2.4.2 (Null statistical test)**.** A statistical test π is a decision rule for accepting or rejecting a hypothesis on the basis of evidence. A p-value test rejects a hypothesis whenever the value of the statistic $f(x)$ is smaller than a threshold. The statistic $f : \mathcal{X} \to [0, 1]$ is designed to have the property:

$$P_{\mu_0}(\{x \mid f(x) \leq \delta\}) = \delta.$$

If our decision rule is:

$$\pi(a \mid x) = \begin{cases} a_0, & f(x) \leq \delta \\ a_1, & f(x) > \delta, \end{cases}$$

the probability of rejecting the null hypothesis when it is true is exactly δ.

This is because, by definition, $f(x)$ has a uniform distribution under μ_0. Hence the value of $f(x)$ itself is uninformative: high and low values are equally likely. In theory we should simply choose δ before seeing the data and just accept or reject based on whether $f(x) \leq \delta$. However nobody does that in practice, meaning that p-values are used incorrectly. Better not to use them at all, if uncertain about their meaning.

Issues with p-values

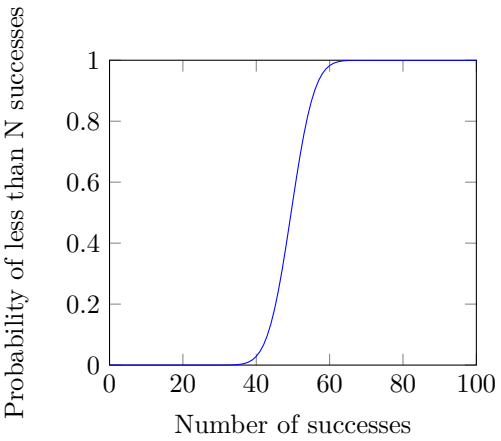
- They only measure quality of fit *on the data*.
- Not robust to model misspecification. For example, zero-mean testing using the χ^2-test has a normality assumption.

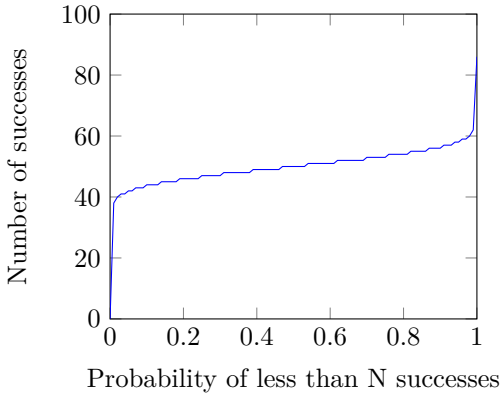
- They ignore effect sizes. For example, a linear analysis may determine that there is a significant deviation from zero-mean, but with only a small effect size of 0.01. Thus, reporting only the p-value is misleading
- They do not consider prior information.
- They do not represent the probability of having made an error. In particular, a p-value of δ does not mean that the probability that the null hypothesis is false given the data x, is δ, i.e. $\delta \neq \mathbb{P}(\neg\mu_0 \mid x)$.
- The null-rejection error probability is the same irrespective of the amount of data (by design).

p-values for the medium example

Let us consider the example of the medium.

- μ_0 is simply the $\mathit{Bernoulli}(1/2)$ model: responses are by chance.
- CDF: $P_{\mu_0}(N \leq n \mid K = 100)$ is the probability of at most N successes if we throw the coin 100 times. This is in fact the cumulative probability function of the binomial distribution. Recall that the binomial represents the distribution for the number of successes of independent experiments, each following a Bernoulli distribution.
- ICDF: the number of successes that will happen with probability at least δ
- e.g. we'll get at most 50 successes a proportion $\delta = 1/2$ of the time.
- Using the (inverse) CDF we can construct a policy π that selects a_1 when μ_0 is true only a δ portion of the time, for any choice of δ.





Building a test

The test statistic

We want the test to reflect that we don't have a significant number of failures.

$$f(x) = 1 - \text{binocdf}(\sum_{t=1}^{n} x_t, n, 0.5)$$

What $f(x)$ is and is not

- It is a **statistic** which is $\leq \delta$ a δ portion of the time when μ_0 is true.
- It is **not** the probability of observing x under μ_0.
- It is **not** the probability of μ_0 given x.

EXERCISE 6.

- Let us throw a coin 8 times, and try and predict the outcome.
- Select a p-value threshold so that $\delta = 0.05$. For 8 throws, this corresponds to > 6 successes or $\geq 87.5\%$ success rate.
- Let's calculate the p-value for each one of you
- What is the rejection performance of the test?

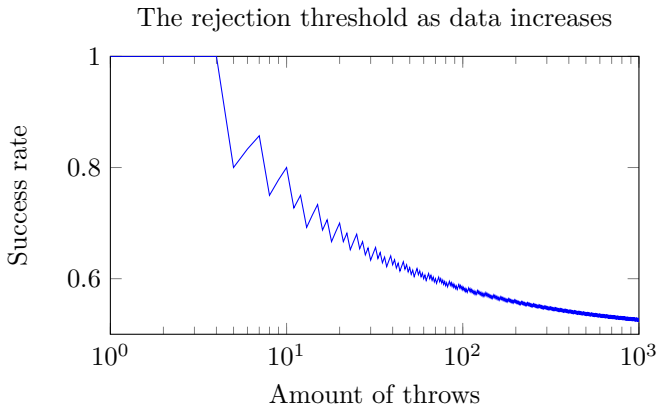


Figure 2.10: Here we see how the rejection threshold, in terms of the success rate, changes with the number of throws to achieve an error rate of $\delta = 0.05$.

As the amount of throws goes to infinity, the threshold converges to 0.5. This means that a statistically significant difference from the null hypothesis can be obtained, even when the actual model from which the data is drawn is only slightly different from 0.5.

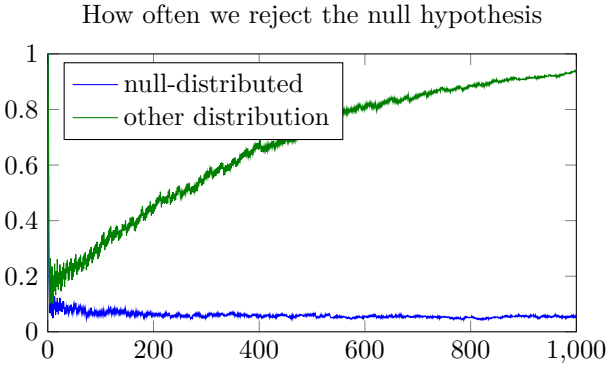


Figure 2.11: Here we see the rejection rate of the null hypothesis (μ_0) for two cases. Firstly, for the case when μ_0 is true. Secondly, when the data is generated from $\mathit{Bernoulli}(0.55)$.

As we see, this method keeps its promise: the null is only rejected 0.05 of the time when it's true. We can also examine how often the null is rejected when it is false... but what should we compare against? Here we are generating data from a $\mathit{Bernoulli}(0.55)$ model, and we can see the rejection of the null increases with the amount of data. This is called the *power* of the test with respect to the $\mathit{Bernoulli}(0.55)$ distribution.

Statistical power and false discovery.

Beyond not rejecting the null when it's true, we also want:

- High power: Rejecting the null when it is false.
- Low false discovery rate: Accepting the null when it is true.

Power
The power depends on what hypothesis we use as an alternative. This implies that we cannot simply consider a plain null hypothesis test, but must formulate a specific alternative hypothesis.

False discovery rate
False discovery depends on how likely it is *a priori* that the null is false. This implies that we need to consider a prior probability for the null hypothesis being true.

Both of these problems suggest that a Bayesian approach might be more suitable. Firstly, it allows us to consider an infinite number of possible alternative models as the alternative hypothesis, through Bayesian model averaging. Secondly, it allows us to specify prior probabilities for each alternative. This is especially important when we consider some effects unlikely.

The Bayesian version of the test

1. Set $U(a_i, \mu_j) = \mathbb{I}\{i = j\}$. This choice makes sense if we care equally about either type of error.

2. Set $\xi(\mu_i) = 1/2$. Here we place an equal probability in both models.

3. μ_0: $\mathit{Bernoulli}(1/2)$. This is the same as the null hypothesis test.

4. μ_1: $\mathit{Bernoulli}(\theta)$, $\theta \sim \mathit{Unif}([0, 1])$. This is an extension of the simple hypothesis test, with an alternative hypothesis that says "the data comes from an arbitrary Bernoulli model".

5. Calculate $\xi(\mu \mid x)$.

6. Choose a_i, where $i = \arg\max_j \xi(\mu_j \mid x)$.

Bayesian model averaging for the alternative model μ_1
In this scenario, μ_0 is a simple point model, e.g. corresponding to a $\mathit{Bernoulli}(1/2)$. However μ_1 is a marginal distribution integrated over many models, e.g. a Beta distribution over Bernoulli parameters.

$$P_{\mu_1}(x) = \int_\Theta B_\theta(x) \, \mathrm{d}\beta(\theta) \tag{2.4.3}$$

$$\xi(\mu_0 \mid x) = \frac{P_{\mu_0}(x)\xi(\mu_0)}{P_{\mu_0}(x)\xi(\mu_0) + P_{\mu_1}(x)\xi(\mu_1)} \tag{2.4.4}$$

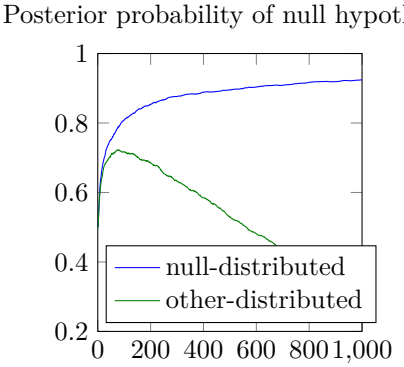


Figure 2.12: Here we see the convergence of the posterior probability.

As can be seen in the figure above, in both cases, the posterior converges to the correct value, so it can be used to indicate our confidence that the null is true.

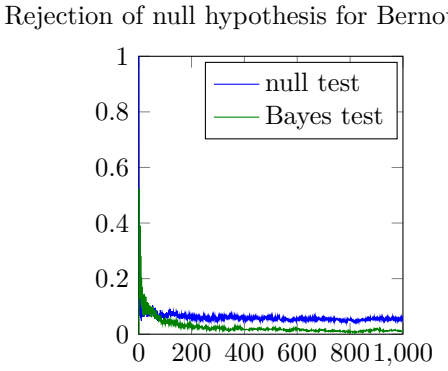


Figure 2.13: Comparison of the rejection probability for the null and the Bayesian test when μ_0 is true.

Now we can use this Bayesian test, with uniform prior, to see how well it performs. While the plain null hypothesis test has a fixed rejection rate of 0.05, the Bayesian test's rejection rate converges to 0 as we collect more data.

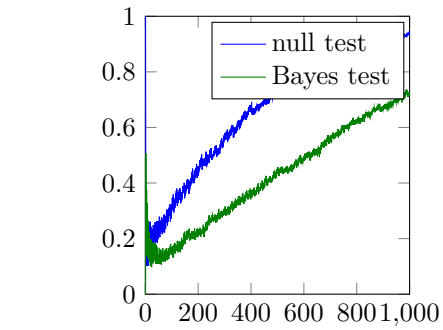


Figure 2.14: Comparison of the rejection probability for the null and the Bayesian test when μ_1 is true.

However, both methods are able to reject the null hypothesis more often when it is false, as long as we have more data.

Further reading

Points of significance (Nature Methods)

- Importance of being uncertain `https://www.nature.com/articles/nmeth.2613`
- Error bars `https://www.nature.com/articles/nmeth.2659`
- P values and the search for significance `https://www.nature.com/articles/nmeth.4120`

- Bayes' theorem `https://www.nature.com/articles/nmeth.3335`
- Sampling distributions and the bootstrap `https://www.nature.com/articles/nmeth.3414`

2.5 Formalising Classification problems

One of the simplest decision problems is classification. At the simplest level, this is the problem of observing some data point $x_t \in \mathcal{X}$ and making a decision about what class $\mathcal{Y}$ it belongs to. Typically, a fixed classifier is defined as a decision rule $\pi(a|x)$ making decisions $a \in \mathcal{A}$, where the decision space includes the class labels, so that if we observe some point x_t and choose $a_t = 1$, we essentially declare that $y_t = 1$.

Typically, we wish to have a classification policy that minimises classification error.

Deciding a class given a model

In the simplest classification problem, we observe some features x_t and want to make a guess a_t about the true class label y_t. Assuming we have some probabilistic model $P_\mu(y_t \mid x_t)$, we want to define a decision rule $\pi(a_t \mid x_t)$ that is optimal, in the sense that it maximises expected utility for P_μ.

- Features $x_t \in \mathcal{X}$.
- Label $y_t \in \mathcal{Y}$.
- Decisions $a_t \in \mathcal{A}$.
- Decision rule $\pi(a_t \mid x_t)$ assigns probabilities to actions.

Standard classification problem

In the simplest case, the set of decisions we make are the same as the set of classes

$$\mathcal{A} = \mathcal{Y}, \qquad U(a, y) = \mathbb{I}\{a = y\}$$

Exercise 7. If we have a model $P_\mu(y_t \mid x_t)$, and a suitable U, what is the optimal decision to make?

Deciding the class given a model family

- Training data $D_T = \{(x_i, y_i) \mid i = 1, \ldots, T\}$
- Models $\{P_\mu \mid \mu \in \mathcal{M}\}$.
- Prior ξ on $\mathcal{M}$.

Similarly to our example with the meteorological stations, we can define a posterior distribution over models.

Posterior over classification models

$$\xi(\mu \mid D_T) = \frac{P_\mu(y_1, \ldots, y_T \mid x_1, \ldots, x_T)\xi(\mu)}{\sum_{\mu' \in \mathcal{M}} P_{\mu'}(y_1, \ldots, y_T \mid x_1, \ldots, x_T)\xi(\mu')}$$

This posterior form can be seen as weighing each model according to how well they can predict the class labels. It is a correct form as long as, for every pair of models μ, μ' we have that $P_\mu(x_1, \ldots, x_T) = P_{\mu'}(x_1, \ldots, x_T)$. This assumption can be easily satisfied without specifying a particular model for the x. If not dealing with time-series data, we assume independence between x_t:

$$P_\mu(y_1, \ldots, y_T \mid x_1, \ldots, x_T) = \prod_{i=1}^{T} P_\mu(y_i \mid x_i)$$

The *Bayes rule* for maximising $\mathbb{E}_\xi(U \mid a, x_t, D_T)$
The decision rule simply chooses the action:

$$a_t \in \arg\max_{a \in \mathcal{A}} \sum_y \sum_{\mu \in \mathcal{M}} P_\mu(y_t = y \mid x_t)\xi(\mu \mid D_T)U(a, y) \tag{2.5.1}$$

$$= \arg\max_{a \in \mathcal{A}} \sum_y \mathbb{P}_{\xi|D_T}(y_t \mid x_t)U(a, y) \tag{2.5.2}$$

We can rewrite this by calculating the posterior marginal marginal label probability

$$\mathbb{P}_{\xi|D_T}(y_t \mid x_t) \triangleq \mathbb{P}_\xi(y_t \mid x_t, D_T) = \sum_{\mu \in \mathcal{M}} P_\mu(y_t \mid x_t)\xi(\mu \mid D_T).$$

Approximating the model

Full Bayesian approach for infinite $\mathcal{M}$
Here ξ can be a probability density function and

$$\xi(\mu \mid D_T) = P_\mu(D_T)\xi(\mu) / \mathbb{P}_\xi(D_T), \qquad \mathbb{P}_\xi(D_T) = \int_{\mathcal{M}} P_\mu(D_T)\xi(\mu)\,\mathrm{d},$$

can be hard to calculate.

Maximum a posteriori model
We only choose a single model through the following optimisation:

$$\mu_{\mathrm{MAP}}(\xi, D_T) = \arg\max_{\mu \in \mathcal{M}} P_\mu(D_T)\xi(\mu) = \arg\max_{\mu \in \mathcal{M}} \overbrace{\ln P_\mu(D_T)}^{\text{goodness of fit}} + \underbrace{\ln \xi(\mu)}_{\text{regulariser}}.$$

You can think of the goodness of fit as how well the model fits the training data, while the regulariser term simply weighs models according to some criterion. Typically, lower weights are used for more complex models.

Learning outcomes

Understanding

- Preferences, utilities and the expected utility principle.
- Hypothesis testing and classification as decision problems.
- How to interpret p-values Bayesian tests.
- The MAP approximation to full Bayesian inference.

Skills

- Being able to implement an optimal decision rule for a given utility and probability.
- Being able to construct a simple null hypothesis test.

Reflection

- When would expected utility maximisation not be a good idea?
- What does a p value represent when you see it in a paper?
- Can we prevent high false discovery rates when using p values?
- When is the MAP approximation good?

2.6 Classification with stochastic gradient descent

Classification as an optimisation problem.

Finding the optimal policy for our belief ξ is not normally very difficult. However, it requires that we maintain the complete distribution ξ and that we also under some probability distribution P. In simple decision problems, e.g. where the set of actions $\mathcal{A}$ is finite, it is possible to do this calculation on-the-fly. However, in some cases we might not have a model.

Recall that we wish to maximise expected utility for some policy under some distribution. In general, this has the form

$$\max_{\pi} \mathbb{E}_{\mu}^{\pi}(U).$$

We also know that any expectation can be approximated by sampling. Let $P_\mu(\omega)$ be the distribution on outcomes defined by our model. Then

$$\mathbb{E}_{\mu}^{\pi}(U) = \sum_{\omega} U(a,\omega) P_\mu(\omega) \approx T^{-1} \sum_{t=1}^{T} U(a,\omega_t), \qquad \omega_t \sim P_\mu(\omega),$$

i.e. when we can replace the explicit summation over all possible outcomes, weighed by their probability through averaging over T outcomes sampled from the correct distribution. In fact this approximation is *unbiased*, as its expectation is equal to the expected utility.

The μ-optimal classifier

Since the performance measure is simply an expectation, it is intuitive to directly optimise the decision rule with respect to an approximation of the expectation

$$\max_{\theta \in \Theta} f(\pi_\theta, \mu, U), \qquad f(\pi_\theta, \mu, U) \triangleq \mathbb{E}_{\mu}^{\pi_\theta}(U) \tag{2.6.1}$$

$$f(\pi_\theta, \mu, U) = \sum_{x,y,a} U(a,y) \pi_\theta(a \mid x) P_\mu(y \mid x) P_\mu(x) \tag{2.6.2}$$

$$\approx \sum_{t=1}^{T} \sum_{a_t} U(a_t, y_t) \pi_{\theta\text{‘‘}232}(a_t \mid x_t), \qquad (x_t, y_t)_{t=1}^{T} \sim P_\mu. \tag{2.6.3}$$

In practice, this is the empirical expectation on the training set $\{(x_t, y_t) \mid t = 1, \dots, T\}$. However, when the amount of data is insufficient, this expectation may be far from reality, and so our classification rule might be far from optimal.

The Bayes-optimal classifier

An alternative idea is to use our uncertainty to create a distribution over models, and then use this distribution to obtain a single classifier that does take the uncertainty into account.

$$\max_{\Theta} f(\pi_\Theta, \xi) \approx \max_{\Theta} N^{-1} \sum_{n=1}^{N} \pi(a_t = y_n \mid x_t = x_n), \qquad (x_n, y_n) \sim P_{\mu_n}, \mu_n \sim \xi.$$

In this case, the integrals are replaced by sampling models μ_n from the belief, and then sampling (x_n, y_n) pairs from P_{μ_n}.

Stochastic gradient methdos

To find the maximum of a differentiable function g, we can use gradient descent

Gradient ascent

$$\theta_{i+1} = \theta_i + \alpha \nabla_\theta g(\theta_i).$$

When f is an expectation, we don't need to calculate the full gradient. In fact, we only need to take one sample from the related distribution.

Stochastic gradient ascent

$$g(\theta) = \int_{\mathcal{M}} f(\theta, \mu) \, \mathrm{d}\xi(\mu)$$
$$\theta_{i+1} = \theta_i + \alpha \nabla_\theta f(\theta_i, \mu_i), \qquad \mu_i \sim \xi.$$

Stochastic gradient methods are commonly employed in neural networks.

2.6.1 Neural network models

Two views of neural networks

In the simplest sense a neural network is simply as parametrised functions f_θ. In classification, neural networks can be used as probabilistic models, so they describes the probability $P_\theta(y|\mathbf{x})$, or as classification policies so that $f_\theta(x, a)$ describes the probability $\pi_\theta(a \mid x)$ of selecting class label a. Let us begin by describing the simplest type of neural network model, the perceptron.

Neural network classification model $P_\theta(\mathbf{y} \mid \mathbf{x}_t)$

Objective: Find the best model for D_T.

Neural network classification policy $\pi(a_t \mid \mathbf{x}_t)$

Objective: Find the best policy for $U(a, \mathbf{x})$.

Difference between the two views

- We can use standard probabilistic methods for P.

- Finding the optimal π is an optimisation problem. However, estimating P can also be formulated as an optimisation.

Linear networks and the perceptron algorithm

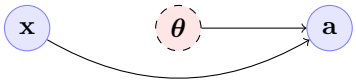


Figure 2.15: Abstract graphical model for a neural network

A neural network as used for modelling classification or regression problems, is simply a parametrised mapping $\mathcal{X} \to \mathcal{Y}$. If we include the network parameters, then it is instead a mapping $\mathcal{X} \times \Theta \to \mathcal{Y}$, as seen in Figure 2.17.

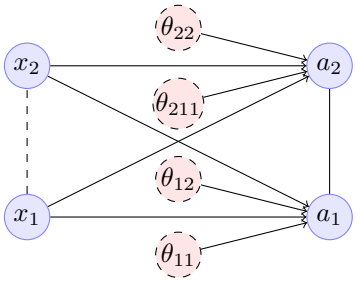


Figure 2.16: Graphical model for a linear neural network.

If we see each possible output as a different random variable, this creates a dependence. After all, we are really splitting one variable into many. In particular, if the network's output is the probability of each action, then we must make sure these sum to 1.

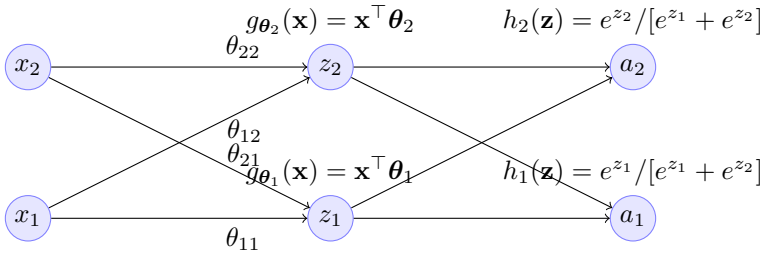


Figure 2.17: Architectural view of a linear neural network.

Definition 2.6.1 (Linear classifier)**.** A linear classifier with N inputs and C outputs is parametrised by

$$\boldsymbol{\Theta} = \begin{bmatrix} \boldsymbol{\theta}_1 & \cdots & \boldsymbol{\theta}_C \end{bmatrix} = \begin{bmatrix} \theta_{1,1} & \cdots & \theta_{1,C} \\ \vdots & \ddots & \vdots \\ \theta_N & \cdots & \theta_{N,C} \end{bmatrix}$$

$$\pi_\Theta(a \mid \mathbf{x}) = \exp\left(\boldsymbol{\theta}_a^\top \mathbf{x}\right) / \sum_{a'} \exp\left(\boldsymbol{\theta}_{a'}^\top \mathbf{x}\right)$$

Even though the classifier has a linear structure, the final non-linearity at the end is there to ensure that it defines a proper probability distribution over decisions. For classification problems, the observations $\mathbf{x}_t$ are features $\mathbf{x}_t = (x_{t,1} \dots, x_{t,n})$ so that $\mathcal{X} \subset \mathbb{R}^N$. It is convenient to consider the network output as a vector on the simplex $\mathbf{y} \in \boldsymbol{\Delta}^A$, i.e. $\sum_{i=1}^C y_{t,i} = 1$, $y_{t,i} \geq 0$. In the neural network model for classification, we typically ignore dependencies between the $x_{t,i}$ features, as we are not very interested in the distribution of $\mathbf{x}$ itself.

Gradient ascent for a matrix U

$$\max_\theta \sum_{t=1}^T \sum_{a_t} U(a_t, y_t) \pi_\theta(a_t \mid x_t) \qquad \text{(objective)}$$

$$\nabla_\theta \sum_{t=1}^T \sum_{a_t} U(a_t, y_t) \pi_\theta(a_t \mid x_t) \qquad \text{(gradient)}$$

$$= \sum_{t=1}^T \sum_{a_t} U(a_t, y_t) \nabla_\theta \pi_\theta(a_t \mid x_t) \qquad (2.6.4)$$

We now need to calculate the gradient of the policy.

Chain Rule of Differentiation

$f(z), z = g(x),$

$$\frac{df}{dx} = \frac{df}{dg}\frac{dg}{dx} \qquad \text{(scalar version)}$$

$$\nabla_\theta \pi = \nabla_g \pi \nabla_\theta g \qquad \text{(vector version)}$$

Learning outcomes

Understanding

- Classification as an optimisation problem.
- (Stochastic) gradient methods and the chain rule.
- Neural networks as probability models or classification policies.
- Linear neural netwoks.
- Nonlinear network architectures.

Skills

- Using a standard NN class in python.

Reflection

- How useful is the ability to have multiple non-linear layers in a neural network.
- How rich is the representational power of neural networks?
- Is there anything special about neural networks other than their allusions to biology?

2.7 Naive Bayes classifiers

One special case of this idea is in classification, when each hypothesis corresponds to a specific class. Then, given a new example vector of data $\mathbf{x}$, we would like to calculate the probability of different classes C given the data, $\mathbb{P}(C \mid \mathbf{x})$. So here, the class is the hypothesis.

From Bayes's theorem, we see that we can write this as

$$\mathbb{P}(C \mid \mathbf{x}) = \frac{\mathbb{P}(\mathbf{x} \mid C)\,\mathbb{P}(C)}{\sum_i \mathbb{P}(\mathbf{x} \mid C_i)\,\mathbb{P}(C_i)}$$

for any class C. This directly gives us a method for classifying new data, as long as we have a way to obtain $\mathbb{P}(\mathbf{x} \mid C)$ and $\mathbb{P}(C)$.

But should we use for the probability model $\mathbb{P}$?

Naive Bayes classifier

Naive Bayes classifiers are one of the simplest classification methods. They can have a full Bayesian interpretation under some assumptions, but otherwise they are too simplistic to be useful.

Calculating the prior probability of classes

A simple method is to simply count the number of times each class appears in the training data $D_T = ((x_t, y_t))_{t=1}^T$. Then we can set

$$\mathbb{P}(C) = 1/T \sum_{t=1}^{T} \mathbb{I}\{y_t = C\}$$

The Naive Bayes classifier uses the following model for observations, where observations are independent of each other given the class. Thus, for example the result of three different tests for lung cancer (stethoscope, radiography and biopsy) only depend on whether you have cancer, and not on each other.

Probability model for observations

$$\mathbb{P}(\mathbf{x} \mid C) = \mathbb{P}(x(1), \ldots, x(n) \mid C) = \prod_{k=1}^{n} \mathbb{P}(x(k) \mid C).$$

There are two different types of models we can have, one of which is mostly useful for continuous attributes and the other for discrete attributes. In the first, we just need to count the number of times each feature takes different values in different classes.

Discrete attribute model.

Here we simply count the average number of times that the attribute k had the value i when the label was C. This is in fact analogous to the conditional probability definition.

$$\mathbb{P}(x(k) = i \mid C) = \frac{\sum_{t=1}^{T} \mathbb{I}\{x_t(k) = i \wedge y_t = C\}}{\sum_{t=1}^{T} \mathbb{I}\{y_t = C\}} = \frac{N_k(i, C)}{N(C)},$$

where $N_k(i, C)$ is the numb l l .er of examples in class C whose k-th attribute has the value i, and $N(C)$ is the number of examples in class C.

Full Bayesian approach versus maximum likelihood

This estimation is simple maximum likelihood, as it does not maintain a distribution over the parameters.

Sometimes we need to be able to deal with cases where there are no examples at all of one class. In that case, that class would have probability zero. To get around this problem, we add "fake observations" to our data. This is called *Laplace smoothing.*

Remark 2.7.1. In Laplace smoothing with constant λ, our probability model is

$$\mathbb{P}(x(k) = i \mid C) = \frac{\sum_{t=1}^{T} \mathbb{I}\{x_t(k) = i \wedge y_t = C\} + \lambda}{\sum_{t=1}^{T} \mathbb{I}\{y_t = C\} + n_k\lambda} = \frac{N_k(i, C) + \lambda}{N(C) + n_k\lambda}.$$

where n_k is the number of values that the k-th attribute can take. This is necessary, because we want $\sum_{i=1}^{n_k} \mathbb{P}(x(k) = i \mid C) = 1$. (You can check that this is indeed the case as a simple exercise).

Remark 2.7.2. In fact, the Laplace smoothing model corresponds to a so-called Dirichelt prior over polynomial parameters with a marginal probability of observation equal to the Laplace smoothing. This is an extension of Beta-Bernoulli example from binary outcomes to multiple outcomes.

Continuous attribute model.
Here we can use a Gaussian model for each continuous dimension.

$$\mathbb{P}(x(k) = v \mid C) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{(v-\mu)^2}{\sigma^2}},$$

where μ and σ are the mean and variance of the Gaussian, typically calculated from the training data as:

$$\mu = \frac{\sum_{t=1}^{T} x_t(k)\, \mathbb{I}\{y_t = C\}}{\sum_{t=1}^{T} \mathbb{I}\{y_t = C\}},$$

i.e. μ is the mean of the k-th attribute when the label is C and

$$\sigma = \frac{\sum_{t=1}^{T} [x_t(k) - \mu]^2\, \mathbb{I}\{y_t = C\}}{\sum_{t=1}^{T} \mathbb{I}\{y_t = C\}},$$

i.e. σ is the variance of the k-th attribute when the label is C. Sometimes we can just fix σ to a constant value, i.e. $\sigma = 1$.

Full Bayesian approach

This estimation is simple maximum likelihood, as it selects a single parameter pair $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$ and $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_n)$ for every class and does not maintain a distribution over the parameters. It also assumes independence between the features. The full Bayesian approach considers an arbitrary covariance matrix $\boldsymbol{\Sigma}$ and maintains a distribution $\xi(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Chapter 3

Privacy

Participating in a study always carries a risk for individuals, namely that of data disclosure. In this chapter, we first explain how simple database query methods, and show even a small number of queries to a database they can compromise the privacy of individuals. We then introduce to formal concepts of privacy protection: k-anonymity and differential privacy. The first is relatively simple to apply and provides some limited resistance to identification of individuals through record linkage attacks. The latter is a more general concept, and can be simple apply in some settings, while it offers information-theoretic protection to individuals. A major problem with any privacy definition and method, however is correct interpretation of the privacy concept used, and correct implementation of the algorithm used.

3.1 Database access models

Databases

ID	Name	Salary	Deposits	Age	Postcode	Profession
1959060783	Mike Pence	150,000	1e6	60	1001	Politician
1946061408	Donald Trump	300,000	-1e9	72	1001	Rentier
2100010101	A. B. Student	10,000	100,000	40	1001	Time Traveller

EXAMPLE 11 (Typical relational database in a tax office).

Database access

- When owning the database: Direct look-up.
- When accessing a server etc: Query model.

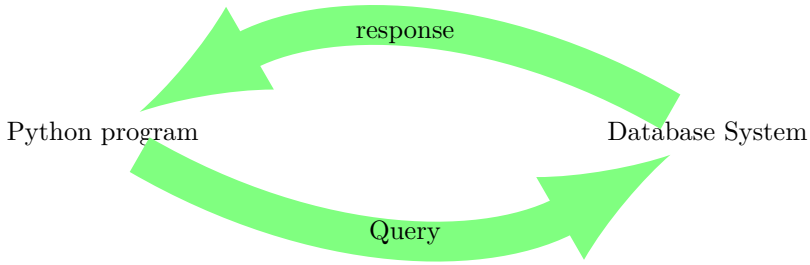


Figure 3.1: Database access model

Queries in SQL

The `SELECT` statement

- `SELECT column1, column2 FROM table;` This selects only some columns from the table
- `SELECT * FROM table;` This selects all the columns from the table

Selecting rows

```
SELECT * FROM table WHERE column = value;
```

Arithmetic queries
Here are some example SQL statements

- `SELECT COUNT(column) FROM table WHERE condition;` This allows you to count the number of rows matching `condition`
- `SELECT AVG(column) FROM table WHERE condition;` This lets you to count the number of rows matching `condition`
- `SELECT SUM(column) FROM table WHERE condition;` This is used to sum up the values in a column.

3.2 Privacy in databases

Anonymisation

If we wish to publish a database, frequently we need to protect identities of people involved. The simplest method for doing that is simply erasing directly identifying information. However, this does not really work most of the time, especially since attackers can have side-information that can reveal the identities of individuals in the original data.

Birthday	Name	Height	Weight	Age	Postcode	Profession
06/07	Li Pu	190	80	60-70	1001	Politician
06/14	Sara Lee	185	110	70+	1001	Rentier
01/01	A. B. Student	170	70	40-60	6732	Time Traveller

Example 12 (Typical relational database in Tinder).

The simple act of hiding or using random identifiers is called anonymisation. However this is generally insufficient as other identifying information may be used to re-identify individuals in the data.

Record linkage

In particular, anonymisation is not enough as record linkage can allow you to still extract information using data from another database through *quasi-identifiers*.

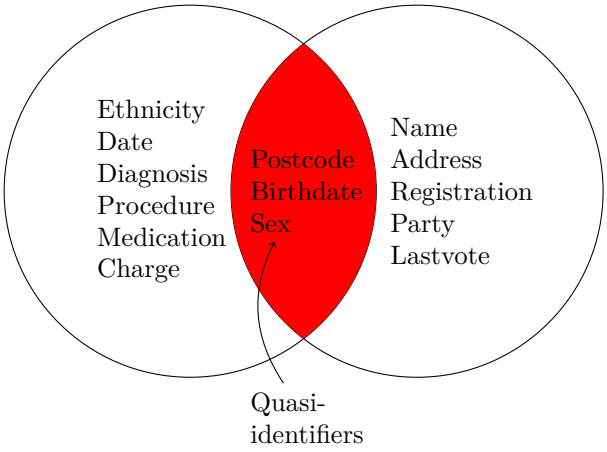


Figure 3.2: An example of two datasets, one containing sensitive and the other public information. The two datasets can be linked and individuals identified through the use of quasi-identifiers.

ID	Name	Salary	Deposits	Age	Postcode	Profession
1959060783	Li Pu	150,000	1e6	60	1001	Politician
1946061408	Sara Lee	300,000	-1e9	72	1001	Rentier
2100010101	A. B. Student	10,000	100,000	40	6732	Time Traveller

Example 13 (Typical relational database in a tax office).

Birthday	Name	Height	Weight	Age	Postcode	Profession
06/07		190	80	60-70	1001	Politician
06/14		185	110	70+	1001	Rentier
01/01		170	70	40-60	6732	Time Traveller

EXAMPLE 14 (Typical relational database in Tinder).

3.3 k-anonymity

k-anonymity

(a) Samarati (b) Sweeney

The concept of k-anonymity was introduced by Samarati and Sweeney [4] and provides good guarantees when accessing a single database

Definition 3.3.1 (k-anonymity)**.** A database provides k-anonymity if for every person in the database is indistinguishable from $k-1$ persons with respect to *quasi-identifiers*.

It's the analyst's job to define quasi-identifiers

Birthday	Name	Height	Weight	Age	Postcode	Profession
06/07	Li Pu	190	80	60+	1001	Politician
06/14	Sara Lee	185	110	60+	1001	Rentier
06/12	Nikos Papadopoulos	170	82	60+	1243	Politician
01/01	A. B. Student	170	70	40-60	6732	Time Traveller
05/08	Li Yang	175	72	30-40	6910	Time Traveller

Table 3.1: 1-anonymity.

Birthday	Name	Height	Weight	Age	Postcode	Profession
		180-190	80+	60+	1*	
		180-190	80+	60+	1*	
		170-180	60-80	69+	1*	
		170-180	60-80	20-60	6*	
		170-180	60-80	20-60	6*	

Table 3.2: 2-anonymity: the database can be partitioned in sets of at least 2 records

However, with enough information, somebody may still be able to infer something about the individuals

3.4 Differential privacy

While k-anonymity can protect against specific re-identification attacks when used with care, it says little about what to do when the adversary has a lot of power. For example, if the adversary knows the data of everybody that has participated in the database, it is trivial for them to infer what our own data is. Differential privacy offers protection against adversaries with unlimited side-information or computational power. Informally, an algorithmic computation is differentially-private if an adversary cannot distinguish two similar database based on the result of the computation. While the notion of similarity is for the analyst to define, it is common to say that two databases are similar when they are identical apart from the data of one person.

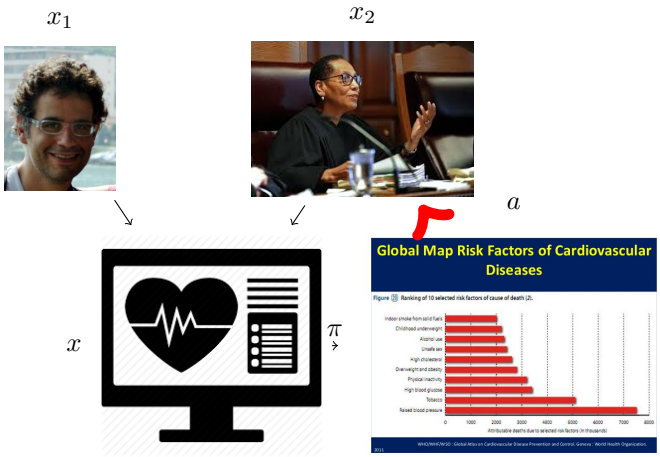


Figure 3.3: If two people contribute their data $x = (x_1, x_2)$ to a medical database, and an algorithm π computes some public output a from x, then it should be hard infer anything about the data from the public output.

Privacy desiderata

Consider a scenario where n persons give their data $x_1, \ldots, x_n$ to an analyst. This analyst then performs some calculation $f(x)$ on the data and published the result. The following properties are desirable from a general standpoint.

Anonymity. Individual participation in the study remains a secret. From the release of the calculations results, nobody can significantly increase their probability of identifying an individual in the database.

Secrecy. The data of individuals is not revealed. The release does not significantly increase the probability of inferring individual's information x_i.

Side-information. Even if an adversary has arbitrary side-information, he cannot use that to amplify the amount of knowledge he would have obtained from the release.

Utility. The released result has, with high probability, only a small error relative to a calculation that does not attempt to safeguard privacy.

Example: The prevalence of drug use in sport

Let's say you need to perform a statistical analysis of the drug-use habits of athletes. Obviously, even if you promise the athlete not to reveal their information, you still might not convince them. Yet, you'd like them to be truthful. The trick is to allow them to randomly change their answers, so that you can't be *sure* if they take drugs, no matter what they answer.

Algorithm for randomising responses about drug use

1. Flip a coin.
2. If it comes heads, respond truthfully.
3. Otherwise, flip another coin and respond `yes` if it comes heads and `no` otherwise.

Exercise 8. Assume that the observed rate of positive responses in a sample is p, that everybody follows the protocol, and the coin is fair. Then, what is the true rate q of drug use in the population?

Solution. Since the responses are random, we will deal with expectations first

$$\mathbb{E}\, p = \frac{1}{2} \times \frac{1}{2} + q \times \frac{1}{2} = \frac{1}{4} + \frac{q}{2}$$
$$q = 2\,\mathbb{E}\, p - \frac{1}{2}.$$

□

The problem with this approach, of course, is that we are effectively throwing away half of our data. In particular, if we repeated the experiment with a coin that came heads at a rate ϵ, then our error bounds would scale as $O(1/\sqrt{\epsilon n})$ for n data points.

The randomised response mechanism

The above idea can be generalised. Consider we have data $x_1, \ldots, x_n$ from n users and we transform it randomly to $y_1, \ldots, y_n$ using the following mapping.

Definition 3.4.1 (Randomised response)**.** The i-th user, whose data is $x_i \in \{0, 1\}$, responds with $a_i \in \{0, 1\}$ with probability

$$\pi(a_i = j \mid x_i = k) = p, \qquad \pi(a_i = k \mid x_i = k) = 1 - p,$$

where $j \neq k$.

Given the complete data x, the mechanism's output is $a = (a_1, \ldots, a_n)$. Since the algorithm independently calculates a new value for each data entry, the output is

$$\pi(a \mid x) = \prod_i \pi(a_i \mid x_i)$$

This mechanism satisfies so-called ϵ-differential privacy, which we will define later.

Exercise 9. Let the adversary have a prior $\xi(x = 0) = 1 - \xi(x = 1)$ over the values of the true response of an individual. we use the randomised response mechanism with p and the adversary observes the randomised data $a = 1$ for that individual, then what is $\xi(x = 1 \mid a = 1)$?

The local privacy model

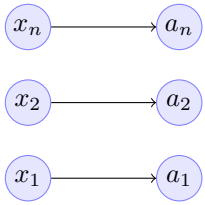
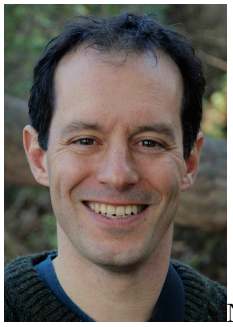


Figure 3.4: The local privacy model

In the local privacy model, the i-th individual's data x_i is used to generate a private response a_i. This means that no individual will provide their true data with certainty. This model allows us to publish a complete dataset of private responses.

Differential privacy.



Now let us take a look at a way to characterise the the inherent privacy properties of algorithms. This is called differential privacy, and it can be seen as a bound on the information an adversary with arbitrary power or side-information could extract from the result of a computation π on the data. For reasons that will be made clear later, this computation has to be stochastic.

Definition 3.4.2 (ϵ-Differential Privacy)**.** A stochastic algorithm $\pi : \mathcal{X} \to \mathcal{A}$, where $\mathcal{X}$ is endowed with a neighbourhood relation N, is said to be ϵ-differentially private if

$$\left| \ln \frac{\pi(a \mid x)}{\pi(a \mid x')} \right| \leq \epsilon, \qquad \forall x N x'. \tag{3.4.1}$$

Typically, algorithms are applied to datasets $x = (x_1, \ldots, x_n)$ composed of the data of n individuals. Thus, all privacy guarantees relate to the data contributed by these individuals.

In this context, two datasets are usually called neighbouring if $x = (x_1, \ldots, x_{i-1}, x_i, x_{i+1} x_n)$ and $x' = (x_1, \ldots, x_{i-1}, x_{i+1} x_n)$, i.e. if one dataset is missing an element.

A slightly weaker definition of neighbourhood is to say that xNx' if $x' = (x_1, \ldots, x_{i-1}, x'_i, x_{i+1} x_n)$, i.e. if one dataset has an altered element. We will usually employ this latter definition, especially for the local privacy model.

The definition of differential privacy

- First rigorous mathematical definition of privacy.

- Relaxations and generalisations possible.
- Connection to learning theory and reproducibility.

Current uses

- Apple. DP is used internally in the company to "protect user privacy". It is not clear exactly what they are doing but their efforts seem to be going in the right direction.
- Google. The company has a DP API available based on randomised response, RAPPOR.
- Uber. Elastic sensitivity for SQL queries, which is available as open source. This is a good thing, because it is easy to get things wrong with privacy.
- US 2020 Census. It uses differential privacy to protect the condidentiality of responders' information while maintaining data that are suitable for their intended uses.

Open problems

- Complexity of differential privacy.
- Verification of implementations and queries.

Remark 3.4.1. Any differentially private algorithm must be stochastic.

To prove that this is necessary, consider the example of counting how many people take drugs in a competition. If the adversary only doesn't know whether you in particular take drugs, but knows whether everybody else takes drugs, it's trivial to discover your own drug habits by looking at the total. This is because in this case, $f(x) = \sum_i x_i$ and the adversary knows x_i for all $i \neq j$. Then, by observing $f(x)$, he can recover $x_j = f(x) - \sum_{i \neq j} x_i$. Consequently, it is not possible to protect against adversaries with arbitrary side information without stochasticity.

Remark 3.4.2. The randomised response mechanism with $p \leq 1/2$ is $(\ln \frac{1-p}{p})$-DP.

Proof. Consider $x = (x_1, \ldots, x_j, \ldots, x_n)$, $x' = (x_1, \ldots, x'_j, \ldots, x_n)$. Then

$$\begin{aligned}
\pi(a \mid x) &= \prod_i \pi(a_i \mid x_i) \\
&= \pi(a_j \mid x_j) \prod_{i \neq j} \pi(a_i \mid x_i) \\
&\leq \frac{p}{1-p} \pi(a_j \mid x'_j) \prod_{i \neq j} \pi(a_i \mid x_i) \\
&= \frac{1-p}{p} \pi(a \mid x')
\end{aligned}$$

$\pi(a_j = k \mid x_j = k) = 1 - p$ so the ratio is $\max\{(1-p)/p, p/(1-p)\} \leq (1-p)/p$ for $p \leq 1/2$. □

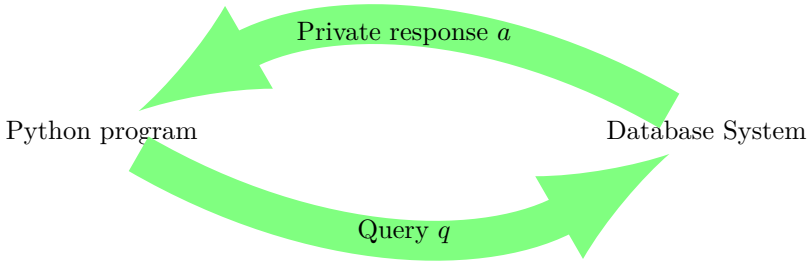


Figure 3.5: Private database access model

Response policy
The policy defines a distribution over responses a given the data x and the query q.

$$\pi(a \mid x, q)$$

Differentially private queries
There is no actual `DP-SELECT` statement, but we can imagine it.

The `DP-SELECT` statement

- `DP-SELECT` ϵ `column1, column2 FROM table;` This selects only some columns from the table
- `DP-SELECT` ϵ `* FROM table;` This selects all the columns from the table

Selecting rows

```
DP-SELECT ϵ * FROM table WHERE column = value;
```

Arithmetic queries
Here are some example SQL statements

- `DP-SELECT` ϵ `COUNT(column) FROM table WHERE condition;` This allows you to count the number of rows matching `condition`
- `DP-SELECT` ϵ `AVG(column) FROM table WHERE condition;` This lets you to count the number of rows matching `condition`

- `DP-SELECT` ϵ `SUM(column) FROM table WHERE condition;` This is used to sum up the values in a column.

Depending on the DP scheme, each query answered may leak privacy. In particular, if we always respond with an ϵ-DP mechanism, after T queries our privacy guarantee is $T\epsilon$. There exist mechanisms that do not respond to each query independently, which can bound the total privacy loss.

Definition 3.4.3 (T-fold adaptive composition)**.** In this privacy model, an adversary is allowed to compose T queries. The composition is *adaptive*, in the sense that the next query is allowed to depend on the previous queries and their results.

Theorem 3.4.1. *For any $\epsilon > 0$, the class of ϵ-differentially private mechanism satisfy $T\epsilon$-differential privacy under T-fold adaptive composition.*

Exercise 10. Adversary knowledge Assume that the adversary knows that the data is either $\mathbf{x}$ or $\mathbf{x}'$. For concreteness, assume the data is either

$$\mathbf{x} = (x_1, \dots, x_j = 0, \dots, x_n)$$

where x_i indicates whether or not the i-th person takes drugs, or

$$\mathbf{x}' = (x_1, \dots, x_j = 1, \dots, x_n).$$

In other words, the adversary knows the data of all people apart from one, the j-th person. We can assume that the adversary has some prior belief

$$\xi(\mathbf{x}) = 1 - \xi(\mathbf{x}')$$

for the two cases. Assume the adversary knows the output a of a mechanism π What can we say about the posterior distribution of the adversary $\xi(\mathbf{x} \mid a, \pi)$ after having seen the output, if π is ϵ-DP?

Solution

We can write the adversary posterior as follows.

$$\begin{aligned}
\xi(\mathbf{x} \mid a, \pi) &= \frac{\pi(a \mid \mathbf{x})\xi(\mathbf{x})}{\pi(a \mid \mathbf{x})\xi(\mathbf{x}) + \pi(a \mid \mathbf{x}')\xi(\mathbf{x}')} && (3.4.2)\\
&\geq \frac{\pi(a \mid \mathbf{x})\xi(\mathbf{x})}{\pi(a \mid \mathbf{x})\xi(\mathbf{x}) + \pi(a \mid \mathbf{x})e^{\epsilon}\xi(\mathbf{x}')} && \text{(from DP definition)}\\
&= \frac{\xi(\mathbf{x})}{\xi(\mathbf{x}) + e^{\epsilon}\xi(\mathbf{x}')} && (3.4.3)
\end{aligned}$$

But this is not very informative. We can also write

$$\frac{\xi(\mathbf{x} \mid a, \pi)}{\xi(\mathbf{x}' \mid a, \pi)} = \frac{\pi(a \mid \mathbf{x})\xi(\mathbf{x})}{\pi(a \mid \mathbf{x}')\xi(\mathbf{x}')} \geq \frac{\pi(a \mid \mathbf{x})\xi(\mathbf{x})}{\pi(a \mid \mathbf{x})e^{-\epsilon}\xi(\mathbf{x}')} = \frac{\xi(\mathbf{x})}{\xi(\mathbf{x}')}e^{\epsilon} \quad (3.4.4)$$

Dealing with multiple attributes.

Up to now we have been discussing the case where each individual only has one attribute. However, in general each individual t contributes multiple data $x_{t.i}$, which can be considered as a row $\mathbf{x}_t$ in a database. Then the mechanism can release each $a_{t,i}$ independently.

Independent release of multiple attributes.
For n users and k attributes, if the release of each attribute i is ϵ-DP then the data release is $k\epsilon$-DP. Thus to get ϵ-DP overall, we need ϵ/k-DP per attribute.

The result follows immediately from the composition theorem. We can see each attribute release as the result of an individual query.

3.4.1 Other differentially private mechanisms

The Laplace mechanism.

A simple method to obtain a differentially private algorithm from a deterministic function $f : \mathcal{X} \to \mathbb{R}$, is to use additive noise, so that the output of the algorithm is simply

$$a = f(x) + \omega, \qquad \omega \sim \mathit{Laplace}\,.$$

The amount of noise added, together with the smoothness of the function f, determine the amount of privacy we have.

Definition 3.4.4 (The Laplace mechanism)**.** For any function $f : \mathcal{X} \to \mathbb{R}$,

$$\pi(a \mid x) = \mathit{Laplace}(f(x), \lambda), \tag{3.4.5}$$

where the Laplace density is defined as

$$p(\omega \mid \mu, \lambda) = \frac{1}{2\lambda} \exp\left(-\frac{|\omega - \mu|}{\lambda}\right).$$

and has mean μ and variance $2\lambda^2$.

Here, $\mathit{Laplace}(\mu, \lambda)$ is the density $f(x) = \frac{\lambda}{2}\exp(-\lambda|x - \mu|)$.

Example 15 (Calculating the average salary).

- The i-th person receives salary x_i
- We wish to calculate the average salary in a private manner.

Local privacy model

- Obtain $y_i = x_i + \omega$, where $\omega \sim \mathit{Laplace}(\lambda)$.
- Return $a = n^{-1}\sum_{i=1}^{n} y_i$.

Centralised privacy model
Return $a = n^{-1}\sum_{i=1}^{n} x_i + \omega$, where $\omega \sim \mathit{Laplace}(\lambda')$.

How should we add noise in order to guarantee privacy?

The centralised privacy model

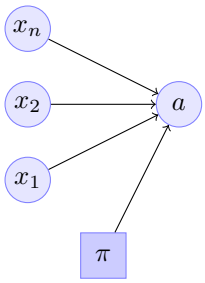


Figure 3.6: The centralised privacy model

Assumption 3.4.1. *The data x is collected and the result a is published by a trusted curator*

DP properties of the Laplace mechanism

Definition 3.4.5 (Sensitivity)**.** The sensitivity of a function f is

$$\mathbb{L}(f) \triangleq \sup_{xNx'} |f(x) - f(x')|$$

If we define a metric d, so that $d(x, x') = 1$ for xNx', then:

$$|f(x) - f(x')| \leq \mathbb{L}(f)\, d(x, x'),$$

i.e. f is $\mathbb{L}(f)$-Lipschitz with respect to d.

Example 16. If $f : \mathcal{X} \to [0, B]$, e.g. $\mathcal{X} = \mathbb{R}$ and $f(x) = \min\{B, \max\{0, x\}\}$, then $\mathbb{L}(f) = B$.

Example 17. If $f : [0, B]^n \to [0, B]$ is $f = \frac{1}{n}\sum_{t=1}^{n} x_t$, then $\mathbb{L}(f) = B/n$.

Proof. Consider two neighbouring datasets x, x' differing in example j. Then

$$f(x) - f(x') = \frac{1}{n}\left[f(x_j) - f(x'_j)\right] \leq \frac{1}{n}\left[B - 0\right]$$

□

Theorem 3.4.2. *The Laplace mechanism on a function f with sensitivity $\mathbb{L}(f)$, ran with $\mathcal{L}aplace(\lambda)$ is $\mathbb{L}(f)/\lambda$-DP.*

Proof.

$$\frac{\pi(a \mid x)}{\pi(a \mid x')} = \frac{e^{|a - f(x')|/\lambda}}{e^{|a - f(x)|/\lambda}} \leq \frac{e^{|a - f(x)|/\lambda + \mathbb{L}(f)/\lambda}}{e^{|a - f(x)|/\lambda}} = e^{\mathbb{L}(f)/\lambda}$$

□

So we need to use $\lambda = \mathbb{L}(f)/\epsilon$ for ϵ-DP. What is the effect of applying the Laplace mechanism in the local versus centralised model? Here let us assume $x_i \in [0, B]$ for all i and consider the problem of calculating the average.

Laplace in the local privacy model
The sensitivity of the individual data is B, so to obtain ϵ-DP we need to use $\lambda = B/\epsilon$. The variance of each component is $2(M/\epsilon)^2$, so the total variance is $2M^2/\epsilon^2 n$.

Laplace in the centralised privacy model
The sensitivity of f is M/n, so we only need to use $\lambda = \frac{M}{n\epsilon}$. The variance of a is $2(M/\epsilon n)^2$.

Thus the two models have a significant difference in the variance of the estimates obtained, for the same amount of privacy. While the central mechanism has variance $O(n^{-2})$, the local one is $O(n^{-1})$ and so our estimates will need much more data to be accurate under this mechanism. In particular, we need square the amount of data in the local model as we need in the central model. Nevertheless, the local model may be the only possible route if we have no specific use for the data.

3.4.2 Utility of queries

Rather than saying that we wish to calculate a private version of some specific function f, sometimes it is more useful to consider the problem from the perspective of the utility of different answers to queries. More precisely, imagine the interaction between a database system and a user:

Interactive queries

- System has data x.
- User asks query q.
- System responds with a.
- There is a common utility function $U : \mathcal{X}, \mathcal{A}, \mathcal{Q} \to \mathbb{R}$.

We wish to maximisation U with our answers, but are constrained by the fact that we also want to preserve privacy.

The utility $U(x, a, q)$ describes how appropriate each response a given by the system for a query r is given the data x. It can be seen as how useful the response is [1] It allows us to quantify exactly how much we would gain by replying correctly. The exponential mechanism, described below is a simple differentially private mechanism for responding to queries while trying to maximise utility for *any possible* utility function.

The Exponential Mechanism.

Here we assume that we can answer queries q, whereby each possible answer a to the query has a different utility to the DM: $U(q, a, x)$. Let $\mathbb{L}(U(q)) \triangleq \sup_{xNx'} |U(q, a, x) - U(q, a, x)|$ denote the sensitivity of a query. Then the following mechanism is ϵ-differentially private.

[1] This is essentially the utility to the user that asks the query, but it could be the utility to the person that answers. In either case, the motivation does not matter the action should maximise it, but is constrained by privacy.

Definition 3.4.6 (The Exponential mechanism)**.** For any utility function $U : \mathcal{Q} \times \mathcal{A} \times \mathcal{X} \to \mathbb{R}$, define the policy

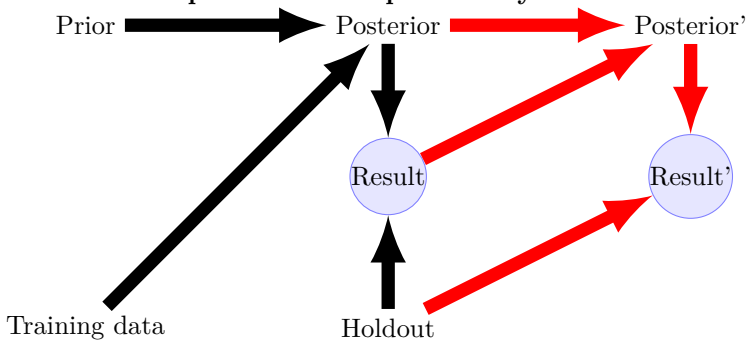
$$\pi(a \mid x) \triangleq \frac{e^{\epsilon U(q,a,x)/\mathbb{L}(U(q))}}{\sum_{a'} e^{\epsilon U(q,a',x)/\mathbb{L}(U(q))}} \tag{3.4.6}$$

Clearly, when $\epsilon \to 0$, this mechanism is uniformly random. When $\epsilon \to \infty$ the action maximising $U(q, a, x)$ is always chosen.

Although the exponential mechanism can be used to describe most known DP mechanisms, its best use is in settings where there is a natural utility function.

3.4.3 Privacy and reproducibility

The unfortunate practice of adaptive analysis



In the ideal data analysis, we start from some prior hypothesis, then obtain some data, which we split into training and holdout. We then examine the training data and obtain a posterior that corresponds to our conclusions. We can then measure the quality of these conclusions in the independent holdout set.

However, this is not what happens in general. Analysts typically use the same holdout repeatedly, in order to improve the performance of their algorithms. This can be seen as indirectly using the holdout data to obtain a new posterior, and so it is possible that you can overfit on the holdout data, even if you never directly see it. It turns out we can solve this problem if we use differential privacy, so that the analyst only sees a differentially private version of queries.

The reusable holdout[22]

One idea to solve this problem is to only allow the analyst to see a private version of the result. In particular, the analyst will only see whether or not the holdout result is τ-close to the training result.

Algorithm parameters

- Performance measure f.
- Threshold τ. How close do we want f to be on the training versus holdout set?
- Noise σ. How much noise should we add?
- Budget B. How much are we allowed to learn about the holdout set?

[2] Also see `https://ai.googleblog.com/2015/08/the-reusable-holdout-preserving.html`

Algorithm idea

Run algorithm λ on data D_T and get e.g. classifier parameters θ.
Run a DP version of the function $f(\theta, D_H) = \mathbb{I}\{U(\theta, D_T) \geq \tau U(\theta, D_H)\}$.

So instead of reporting the holdout performance at all, you just see if you are much worse than the training performance, i.e. if you're overfitting. The fact that the mechanism is DP also makes it difficult to learn the holdout set. See the thresholdout link for more details.

Available privacy toolboxes

k-anonymity

- `https://github.com/qiyuangong/Mondrian` Mondrian k-anonymity

Differential privacy

- `https://github.com/bmcmenamin/thresholdOut-explorations`Threshold out
- `https://github.com/steven7woo/Accuracy-First-Differential-Privacy`Accuracy-constrained DP
- `https://github.com/menisadi/pydp`Various DP algorithms
- `https://github.com/haiphanNJIT/PrivateDeepLearning` Deep learning and DP

Learning outcomes

Understanding

- Linkage attacks and k-anonymity.
- Inferring data from summary statistics.
- The local versus global differential privacy model.
- False discovery rates.

Skills

- Make a dataset satisfy k-anonymity with respect to identifying attributes.
- Apply the randomised response and Laplace mechanism to data.
- Apply the exponential mechanism to simple decision problems.
- Use differential privacy to improve reproducibility.

Reflection

- How can potentially identifying attributes be chosen to achieve k-anonymity?
- How should the parameters of the two ideas, ϵ-DP and k-anonymity be chosen?
- Does having more data available make it easier to achieve privacy?

Chapter 4

Fairness

When machine learning algorithms are applied at scale, it can be difficult to imagine

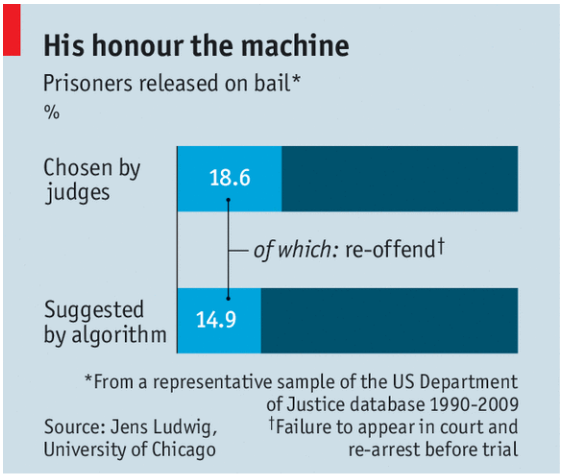


Figure 4.1: In some cases, it appears as though automating this procedure might lead to better outcomes. But is that generally true?

4.1 Fairness in machine learning

The problem of fairness in machine learning and artificial intelligence has only recently been widely recognised. When any algorithm is implemented at scale, no matter the original objective and whether it is satisfied, it has significant societal effects. In particular, even when considering the narrow objective of the algorithm, even if it improves it overall, it may increase inequality.

In this course we will look at two aspects of fairness. The first has to do with disadvantaged populations that form distinct social classes due to a shared income stratum, race or gender. The second has to do with meritocratic notions of fairness.

Bail decisions

For our example regarding disadvantaged populations, consider the example of bail decisions in the US court system. When a defendant is charged, the judge has the option to either place them in jail pending trial, or set them free, under the condition that the defendant pays some amount of bail. The amount of bail (if any) is set to an amount that would be expected to deter flight or a relapse.

Whites get lower scores than blacks[1]

In a different study, it was shown that a commonly used software tool for determining 'risk scores' in the US was biased towards white defendants, who seemed to be always getting lower scores than blacks.

[1] Pro-publica, 2016

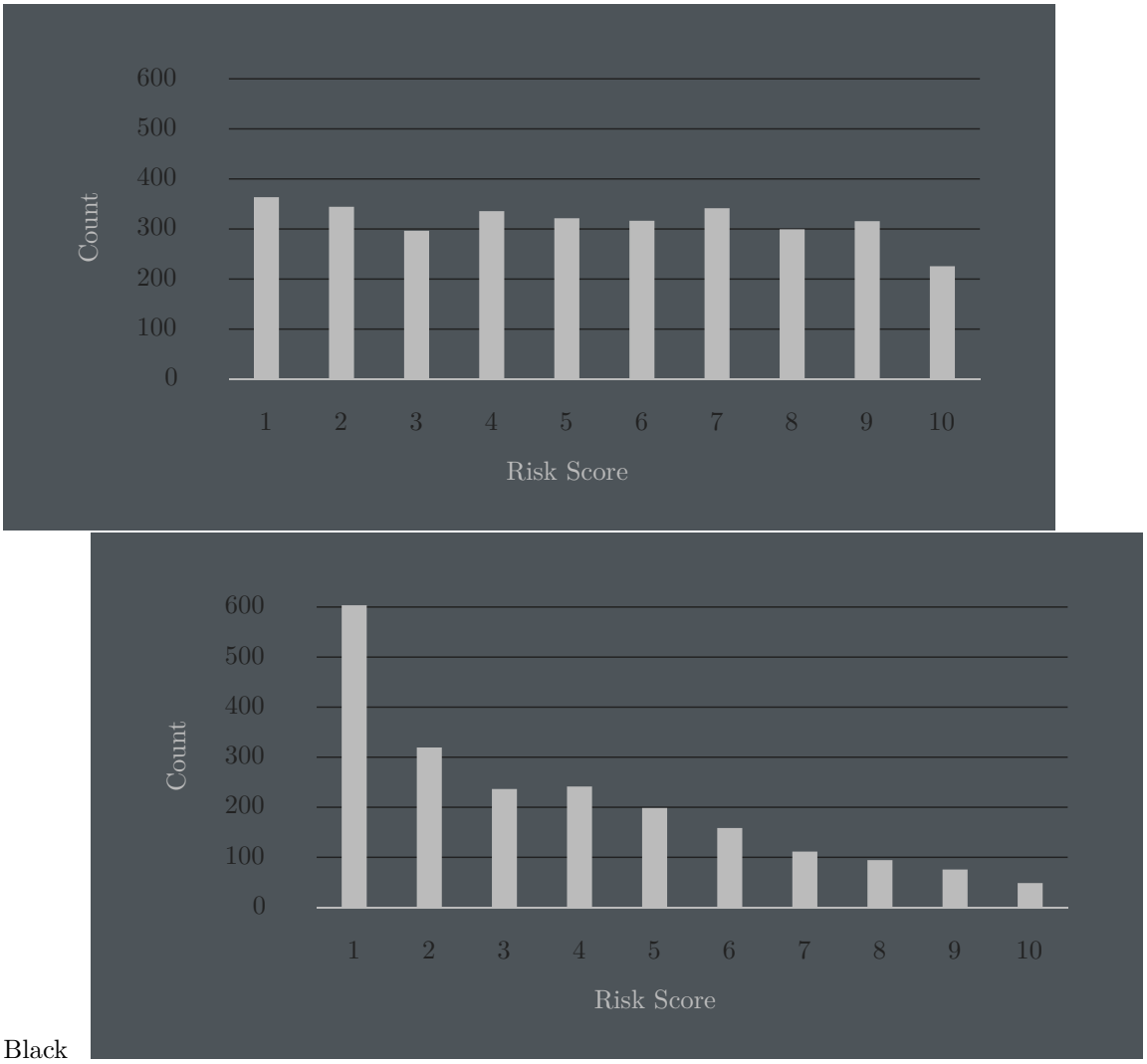


Figure 4.2: Apparent bias in risk scores towards black versus white defendants.

But scores equally accurately predict recidivsm[2]

On the other hand, the scores generated by the software seemed to be very predictive on whether or not defendants would re-offend, independently of their race.

[2]Washington Post, 2016

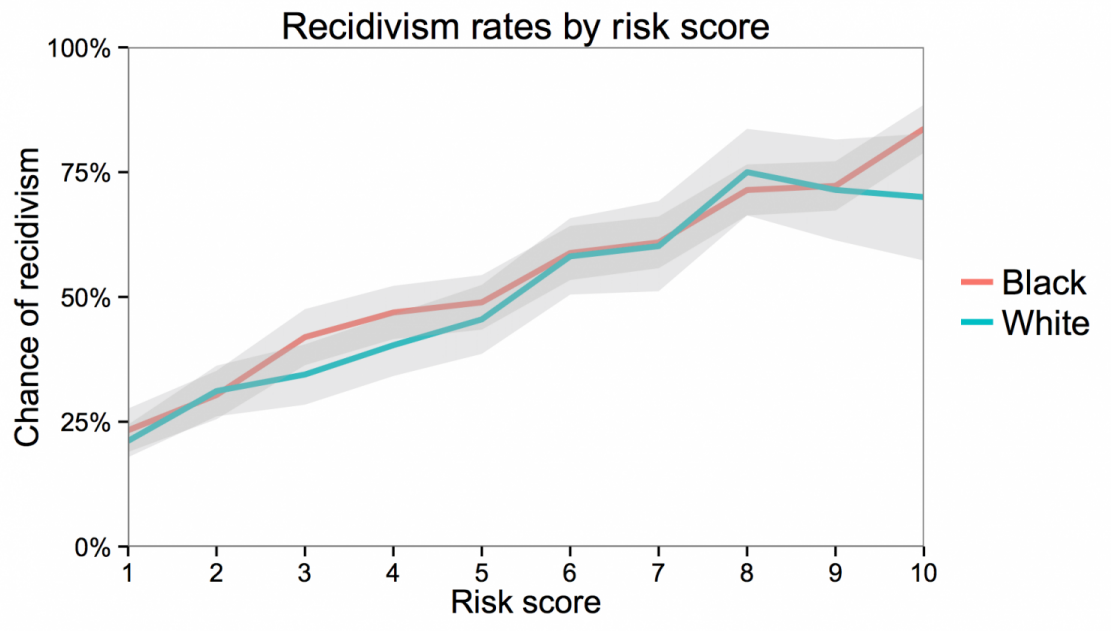


Figure 4.3: Recidivism rates by risk score.

But non-offending blacks get higher scores

On the third hand, we see that the system seemed to give higher risk scores to non-offending blacks. So, is there a way to fix that or not?

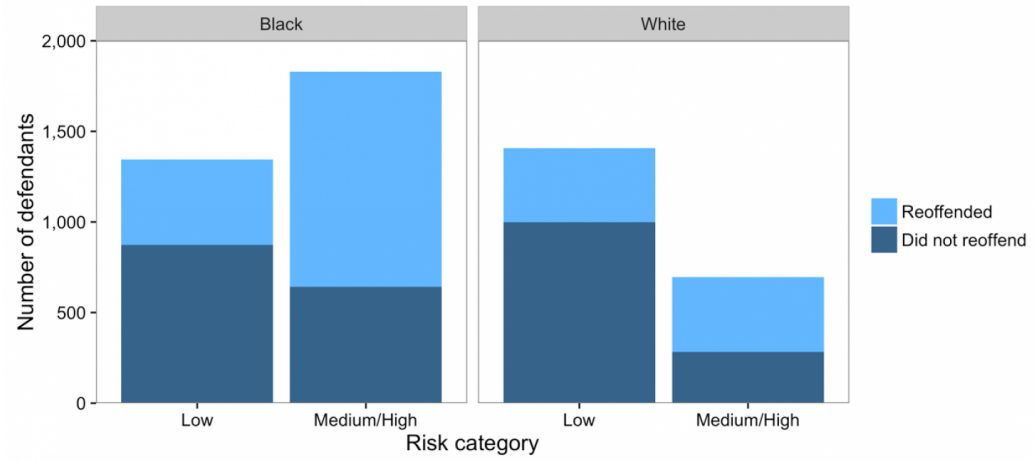


Figure 4.4: Score breakdown based on recidivism rates.

How can we explain this discrepancy? We can show that in fact, each one of these different measures of bias in our decision rules can be seen as a notion of conditional independence.

4.2 Graphical models

Graphical models are a very useful tool for modelling the relationship between multiple variables. The simplest such models, probabilistic graphical models (otherwise known as Bayesian networks) involve directed acyclic graphs between random variables.

Graphical models

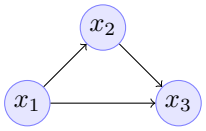


Figure 4.5: Graphical model for three variables.

Consider for example the model in Figure 117. It involves three variables, x_1, x_2, x_3 and there are three arrows, which show how one variable depends on another. Simply put, if you think of each x_k as a stochastic function, then x_k's value only depends on the values of its parents, i.e. the nodes that are point to it. In this example, x_1 does not depend on any other variable, but the value of x_2 depends on the value of x_1. Such models are useful when we want to describe the joint probability distribution of all the variables in the collection.

Joint probability
Let $\mathbf{x} = (x_1, \ldots, x_n)$. Then $\mathbf{x} : \Omega \to X$, $X = \prod_i X_i$ and:

$$\mathbb{P}(\mathbf{x} \in A) = P(\{\omega \in \Omega \mid \mathbf{x}(\omega) \in A\}).$$

When X_i are finite, we can typically write

$$\mathbb{P}(\mathbf{x} = \mathbf{a}) = P(\{\omega \in \Omega \mid \mathbf{x}(\omega) = \mathbf{a}\}),$$

for the probability that $x_i = a_i$ for all $i \in [n]$.

Factorisation
For any subsets $B \subset [n]$ and its complement C so that $\mathbf{x}_B = (x_i)_{i \in B}$, $\mathbf{x}_C = (x_i)_{i \notin B}$

$$\mathbb{P}(\mathbf{x}) = \mathbb{P}(\mathbf{x}_B \mid \mathbf{x}_C)\, \mathbb{P}(\mathbf{x}_C)$$

So we can write any joint distribution as

$$\mathbb{P}(x_1)\, \mathbb{P}(x_2 \mid x_1)\, \mathbb{P}(x_3 \mid x_1, x_2) \cdots \mathbb{P}(x_n \mid x_1, \ldots, x_{n-1}).$$

Although the above factorisation is always possible to do, sometimes our graphical model has a structure that makes the factors much simpler. In fact, the main reason for introducing graphical models is to represent dependencies between variables. For a given model, we can infer whether some variables are in fact dependent, independent, or conditionally independent.

Directed graphical models and conditional independence

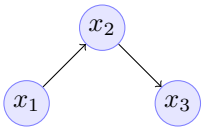


Figure 4.6: Graphical model for the factorisation $\mathbb{P}(x_1 \mid x_2)\,\mathbb{P}(x_2 \mid x_3)\,\mathbb{P}(x_3)$.

Conditional independence
We say x_i is conditionally independent of $\mathbf{x}_B$ given $\mathbf{x}_D$ and write $x_i \mid \mathbf{x}_D \perp\!\!\!\perp \mathbf{x}_B$ iff

$$\mathbb{P}(x_i, \mathbf{x}_B \mid \mathbf{x}_D) = \mathbb{P}(x_i \mid \mathbf{x}_D)\,\mathbb{P}(\mathbf{x}_D \mid \mathbf{x}_B).$$

Directed graphical models

A graphical model is a convenient way to represent conditional independence between variables. There are many variants of graphical models, whose name is context dependent. Other names used in the literature are probabilistic graphical models, Bayesian networks, causal graphs, or decision diagrams. In this set of notes we focus on directed graphical models that depict dependencies between ranom variables.

Definition 4.2.1 (Directed graphical model)**.** A collection of n random variables $x_i : \Omega \to X_i$, and let $X \triangleq \prod_i X_i$, with underlying probability measure P on Ω. Let $\mathbf{x} = (x_i)_{i=1}^n$ and for any subset $B \subset [n]$ let

$$\mathbf{x}_B \triangleq (x_i)_{i \in B} \tag{4.2.1}$$
$$\mathbf{x}_{-j} \triangleq (x_i)_{i \neq i} \tag{4.2.2}$$

In a Graphical model, conditional independence is represented through directed edges.

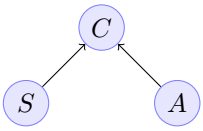


Figure 4.7: Smoking and lung cancer graphical model, where S: Smoking, C: cancer, A: asbestos exposure.

Example 18 (Smoking and lung cancer). It has been found by **?** that lung incidence not only increases with both asbestos exposure and smoking. This is in agreement with the graphical model shown. The study actually found that there is an amplification effect, whereby smoking and asbestos exposure increases cancer risk by 28 times compared to non-smokers. This implies that the risk is not simply additive. The graphical model only tells us that there is a dependency, and does not describe the nature of this dependency precisely.

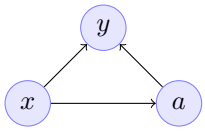


Figure 4.8: Kidney treatment model, where x: severity, y: result, a: treatment applied

Example 19 (Treatment effects).

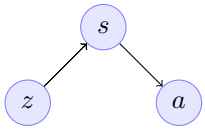


Figure 4.9: Simplified school admission graphical model, where z: gender, s: school applied to, a: whether you were admitted.

Example 20 (School admission).

Deciding conditional independence

There is an algorithm for deciding conditional independence of any two variables in a graphical model. However, this is beyond the scope of these notes. Here, we shall just use these models as a way to encode dependencies that we assume exist.

Measuring independence

The simplest way to measure independence is by looking at whether or not the distribution of the possibly dependent variable changes when we change the value of the other variables.

Theorem 4.2.1. *If* $x_i \mid \mathbf{x}_D \perp\!\!\!\perp \mathbf{x}_B$ *then*

$$\mathbb{P}(x_i \mid \mathbf{x}_B, \mathbf{x}_D) = \mathbb{P}(x_i \mid \mathbf{x}_D)$$

This implies

$$\mathbb{P}(x_i \mid \mathbf{x}_B, \mathbf{x}_D) = \mathbb{P}(x_i \mid \mathbf{x}'_B, \mathbf{x}_D)$$

so we can measure independence by seeing how the distribution of x_i changes when we vary $\mathbf{x}'_B$, keeping $\mathbf{x}_D$ fixed.

4.3 Concepts of fairness

Bail decisions, revisited

Let us think of this problem in terms of bail decisions made by a judge using some policy π with $\pi(a \mid x)$ being the probability that the judge decides a when she observes x. Let y be the outcome, which may or may not depend on a. In this particular case, a is either release or jail. And y is appears for trial or not. If we accept the tenets of decision theory, there is also a utility function $U(a, y)$ defined on which the judge bases her decision.

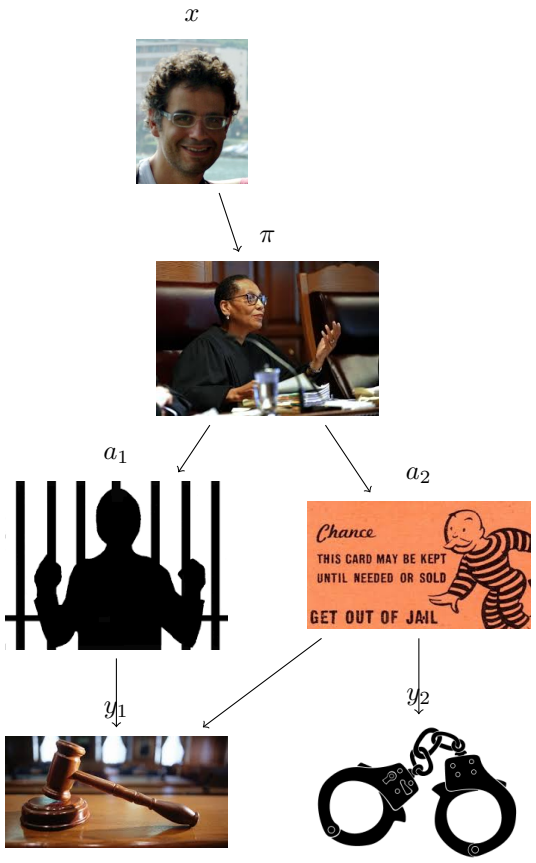


Figure 4.10: The bail decision process, simplified.

4.3.1 Fairness as independence

So how can we reframe the above fairness notions in a more precise way? Both of them involve conditional independence between y, a and a sensitive attribute z, such as race. The first notion says that the actions of the judge (or equivalently, the scores of the algorithm) are *calibrated* with respect to the outcomes. The second says that they are *balanced*, so that were the outcome known to the judge, she would be making a decision independently of the defendant's race. Both of these conditions were discussed in a more restricted setting by

Definition 4.3.1 (Calibration)**.** A policy π is calibrated for parameter θ with respect to z if

$$\mathbb{P}^{\pi}_{\theta}(y \mid a, z) = \mathbb{P}^{\pi}_{\theta}(y \mid a), \qquad \forall a, z. \tag{4.3.1}$$

You will observe that calibration here means that

$$y \perp\!\!\!\perp z \mid a, \theta, \pi$$

i.e. that y is independent of z given the judge's action a, so the distribution of outcomes is the same for every one of our actions no matter what the value of z is.

Definition 4.3.2 (Balance)**.** A policy π is balanced for parameter θ with respect to z if

$$\mathbb{P}^{\pi}_{\theta}(a \mid y, z) = \mathbb{P}^{\pi}_{\theta}(a \mid y), \qquad \forall y, z. \tag{4.3.2}$$

On the other hand, balance means that

$$a \perp\!\!\!\perp z \mid y,$$

i.e. that a is independent of z given the true outcome y.[3]

4.3.2 Fairness as meritocracy.

A different concept of fairness is meritocracy. For example, if one candidate for a job is better than another candidate, perhaps that candidate should be taken for the job.

Let us consider merit from the point of view of the decision maker, who can either hire ($a_t = 1$) or not hire ($a_t = 0$) the t-th applicant. If the applicant has characteristics x_t and merit y_t, the DM's decision has utility $U(a_t, y_t)$. In order to model meritocracy, we assign an inherent *quality* to y, expressed as an ordering, so that $U(1, y) \geq U(1, y')$ if $y \geq y'$. Assuming $P_\theta(x_t, y_t)$ is known to the DM then clearly she should make the decision by solving the following maximisation problem:

Meritocratic decision

$$a_t(\theta, x_t) \in \arg\max_a \mathbb{E}_\theta(U \mid a, x_t) = \int_{\mathcal{Y}} U(a_t, y)\, \mathbb{E}_\theta(U \mid a_t, x_t) \tag{4.3.3}$$

Here, the notion of meritocracy is defined through our utility function. Although it would be better to consider the candidate's utility instead, this is in practice difficult, because we'd have to somehow estimate each individual's utility function. Finally, we are taking the expectation here is because we may not know for certain what the quality attribute of a given person might be.

4.3.3 Fairness as similarity.

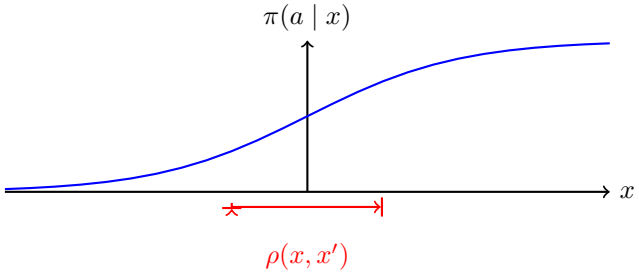
It makes sense to combine the idea of meritocracy with that of similarity. That is, similar people should be treated similarly. This means that we should find a policy π that maximises utility U and makes similar decisions for similar people.

Let $\mathcal{X}$ be equipped with a metric ρ, and let D be a divergence between distributions, such as the KL-divergence. We can then formalise the above intuition as follows:

$$D[\pi(a \mid x), \pi(a \mid x')] \leq \rho(x, x'). \tag{4.3.4}$$

[3]This definition only really makes sense when y does not depend on a at all. When this is not the case, it's easy to construct a random variable y' that does not depend on a so that y can be written as a function $y(y', a)$. Then we can achieve balance with respect to y'.

This is a so-called Lipschitz condition on the policy, and is illustrated in the figure below.



4.3.4 Bayesian fairness

In both cases, we defined conditional independence for a fixed probability distribution $P_\theta(x, y, z)$ on the various variables. However, this cannot be assumed to be known.

4.4 Project: Credit risk for mortgages

Consider a bank that must design a decision rule for giving loans to individuals. In this particular case, some of each individual's characteristics are partially known to the bank. We can assume that the insurer has a linear utility for money and wishes to maximise expected utility. Assume that the t-th individual is associated with relevant information x_t, sensitive information z_t and a potential outcome y_t, which is whether or not they will default on their mortgage. For each individual t, the decision rule chooses $a \in \mathcal{A}$ with probability $\pi(a_t = a \mid x_t)$.

As an example, take a look at the historical data in `data/credit/german.data-mumeric`, described in `data/credit/german.doc`. Here there are some attributes related to financial situation, as well as some attributes related to personal information such as gender and marital status.

A skeleton for the project is available at `https://github.com/olethrosdc/ml-society-science/tree/master/src/project-1`. Start with `random_banker.py` as a template, and create a new module `name_banker.py`. You can test your implementation with the `TestLending.py` program.

For ensuring progress, the project is split into two parts:

4.4.1 Deadline 1: September 14

The first part of the project focuses on a baseline implementation of a banker module.

1. Design a policy for giving or denying credit to individuals, given their probability for being credit-worthy. Assuming that if an individual is credit-worthy, you will obtain a return on investement of $r = 0.5\%$ per month. Take into account the length of the loan to calculate the utility through `NameBanker.expected_utility()`. Assume that the loan is either fully repaid at the end of the lending period n, or not at all to make things simple. If an individual is not credit-worthy you will lose your investment of m credits, otherwise you will gain $m[(1 + r)^n - 1]$. Ignore macroenomic aspects, such as inflation. In this section, simply assume you have a model for predicting creditworthiness as input to your policy, which you can access `NameBanker.get_proba()`.

2. Implement `NameBanker.fit()` to fit a model for calculating the probability of creditworthiness from the german data. Then implement `NameBanker.predict_proba()` to predict the probability of the loan being returned for new data. What are the implicit assumptions about the labelling process in the original data, i.e. what do the labels represent?

3. Combine the model with the first policy to obtain a policy for giving credit, given only the information about the individual and previous data seen. In other words, implement `Namebanker.get_best_action()`.

4. Finally, using `TestLending.py` as a baseline, create a jupyter notebook where you document your model development. Then compare your model against `RandomBanker`.

4.4.2 Deadline 2: September 28

The second part of the project focuses on issues of reproducibility, reliability, privacy and fairness. That is, how desirable would it be to use this model in practice? Here are some sample questions that you can explore, but you should be free to think about other questions.

1. Is it possible to ensure that your policy maximises revenue? How can you take into account the uncertainty due to the limited and/or biased data? What if you have to decide for credit for thousands of individuals and your model is wrong? How should you take that type of risk into account?[4]

2. Does the existence of this database raise any privacy concerns? If the database was secret (and only known by the bank), but the credit decisions were public, how would that affect privacy? (a) Explain how you would protect the data of the people in the training set. (b) Explain how would protect the data of the people that apply for new loans. (c) *Implement* a private decision making mechanism for (b),[5] and estimate the amount of loss in utility as you change the privacy guarantee.

3. Choose one concept of fairness, e.g. balance of decisions with respect to gender. How can you ensure that your policy is fair? How can you measure it? How does the original training data affect the fairness of your policy? [6]

Submit a final report about your project, either as a standalone PDF or as a jupyter notebook.

[4] You do not need to implement anything specific for this to pass the assignment, but you should outline an algorithm in a precise enough manner that it can be implemented. In either case you should explain how your solution mitigates this type of risk.

[5] If you have already implemented (a) as part of the tutorial, feel free to include the results in your report.

[6] You do not need to implement any type of fair policy a passing grade, but you should at least try to analyse the data or your decision function with simple statistics.

Chapter 5

Recommendation systems

Structured learning problems involve multiple latent variables with a complex structure. These range from clustering and spech recognition to DNA and biological and social network analysis. Since structured problems include relationships between many variables, they can be analysed using graphical models.

5.1 Recommendation systems

Figure 5.1: The recommendation problem

In many machine learning applications, we are dealing with the problem of proposing one or more alternatives to a human. The human can accept zero or more of these choices. As an example, when using an internet search engine, we typically see two things: (a) A list of webpages matching our search terms (b) A smaller list of advertisements that might be relevant to our search. At a high level,

The recommendation problem
At time t

1. A customer x_t appears. For the internet search problem, x_t would at least involve the search term used.
2. We present a choice a_t. For the matching website, the choice is ranked list of websites. For the advertisements, however, it is typical
3. The customer makes a choice y_t. This might include selecting one or more of items suggested in a_t.

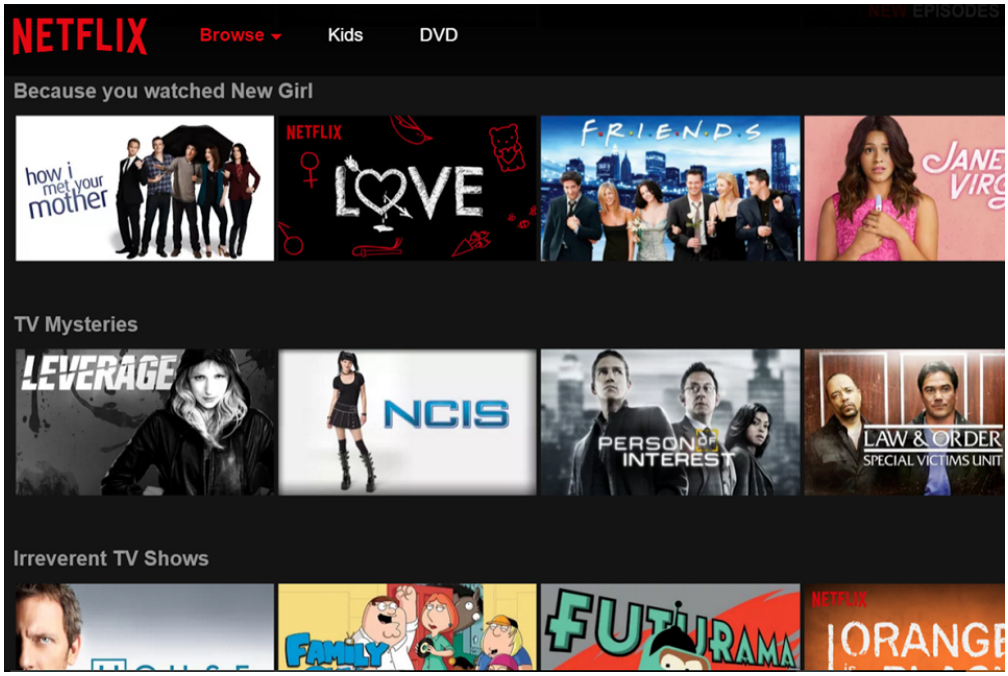


Figure 5.2: The Netflix recommendation problem

Example 21. In the case of Netflix and related services, we would like to suggest movies to users which they are more likely to watch, as shown in Figure 5.2. However, how can we tell which movies those can be? It is probably not useful to just recommend them to rewatch a previously watched movie. We need to somehow take into account information across our user database: if somebody watched mostly the same films as you, then maybe you'd be interested in watching those movies she has that you haven't seen.

In the Netflix catalogue, in particular, users also post reviews of the movies they have watched, as shown in Figure 5.3. This allows us to be able to guess the ratings of users from previous user's ratings.

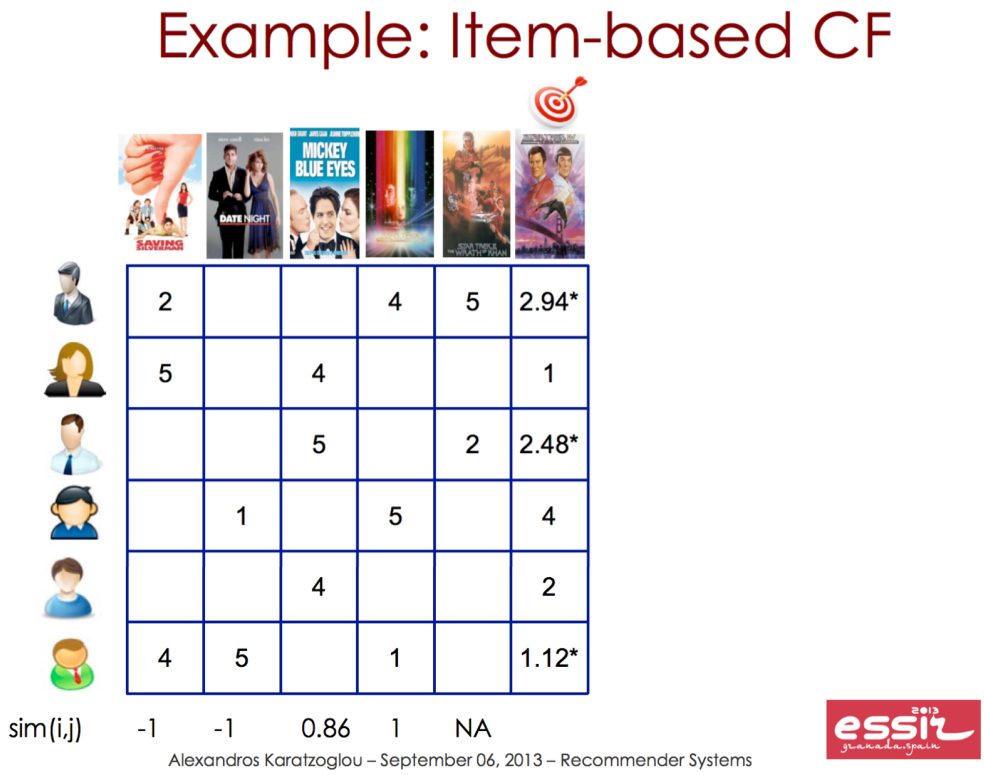


Figure 5.3: User ratings

Predictions based on similarity

Collaborative filtering

- *Similar users have similar tastes.* For example, consider two users t, u who have each watched a set of movies $\mathcal{M}_t$ and $\mathcal{M}_u$ respectively, and $\mathcal{M}_{t,u} = \mathcal{M}_t \cap \mathcal{M}_u$ is the set of common movies. If their ratings are the same for those movies, i.e. $x_{t.m} = x_{u,m} \forall m \in \mathcal{M}_{t,u}$, then it's a good guess that they might have the same ratings for movies they have not both watched.
- That means we can use similar user's *ratings* to predict the ratings for other users. The advantage is that ratings are readily available. The disadvantage is that new users have too few data to be matched to other users.

Content-based filtering.

- Users typically like similar items. For example, a horror movie fan typically rates horror movies highly.

- That means we can one user's ratings and *item information* to predict their ratings for other items. In this scenario

k-NN for similarity

EXERCISE 11.
- Define a distance $d : \mathcal{X}^M \times \mathcal{X}^M \to \mathbb{R}_+$ between user ratings.
- Apply a k-NN algorithm to prediction of user ratings from the dataset.

Preferences as clusters

As a simple model, we can assume that each person belongs to a *type*. Every type has the same preferences over films. In the simplest possible model, a user of type c_i that has watched a movie m will rate the film deterministically $x_{c,m}$. More generally, we can assume the following model.

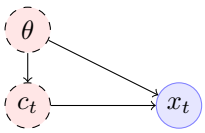


Figure 5.4: Preference model

Preference model

- User t.
- User type $c_t \in \mathcal{C}$. For simplicity, we can think of there being a finite number of types $\mathcal{C} = \{1, \dots, n\}$.
- User ratings $\mathbf{x}_t$ with $x_{t,m} \in \mathcal{X}$ rating for movie m. As an example, $\mathcal{X} = \{0, 1, 2, 3, 4, 5\}$, with 0 meaning no rating given. This is important, since
- Preference distribution $P_\theta(\mathbf{x}_t = \mathbf{x}|c_t = c)$.Typically, we can assume that ratings are independent given the type

$$P_\theta(\mathbf{x}_t = \mathbf{x}|c_t = c) = \prod_{m=1}^{M} P_\theta(x_{t,m} = x_m|c_t = c),$$

so that a single (vector) parameter $\theta_{c,m}$ will describe the distribution of ratings for a particular movie m and type c, i.e. $P_\theta(x_{t,m} = x_m|c_t = c) = P_\theta(x_{t,m} = x_m|c_t = c)$.

5.2 Clustering

Clustering is the problem of automatically seggregating data of different types into clusters. When the goal is *anomaly detection*, then there are typically two clusters. When the goal is *compression* or *auto-encoding* then there are typically as many clusters as needed for sufficienlty good accuracy.

Clusters as latent variables

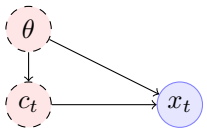


Figure 5.5: Graphical model for independent data from a cluster distribution.

The clustering distribution

The learning problem is to estimate the parameter θ describing the distribution of observations x_t and clusters c_t.

$$x_t \mid c_t = c, \theta \sim P_\theta(x|c), \qquad c_t \mid \theta \sim P_\theta(c)$$

Given a parameter θ, the clustering problem is to estimate the probability of each cluster for each new observation.

$$P_\theta(c_t \mid x_t) = \frac{P_\theta(x_t \mid c_t) P_\theta(c_t)}{\sum_{c'} P_\theta(x_t \mid c_t = c') P_\theta(c_t = c')}$$

Bayesian formulation of the clustering problem

- Prior ξ on parameter space Θ.
- Data $x^T = x_1, \ldots, x_T$. Cluster assignments c^T unknown.
- Posterior $\xi(\cdot \mid x^T)$.

Posterior distribution

The data we obtain do not include the cluster assignments, but we can still formulate the posterior distribution of parameters given the data.

$$\xi(\theta \mid x^T) = \frac{P_\theta(x^T)\xi(\theta)}{\int_\Theta P_{\theta'}(x^T)\,\mathrm{d}\xi(\theta')}, \qquad P_\theta(x^T) = \sum_{c^T \in \mathcal{C}^T} \overbrace{P_\theta(x^T \mid c^T)}^{\text{Cluster Density}} \underbrace{P_\theta(c^T)}_{\text{Cluster prior}} \tag{5.2.1}$$

We simply need to expand the data-dependent term to include all possible cluster assignments. This is of course not trivial, since the number of assignments is exponential in T. However, algorithms such as Markov Chain Monte Carlo can be used instead.

Marginal posterior prediction

$$P_\xi(c_t \mid x_t, x^T) = \int_\Theta P_\theta(c_t \mid x_t)\, \mathrm{d}\xi(\theta \mid x^T)$$

EXAMPLE 22 (Preference clustering). The learning problem is to estimate the parameter θ describing the distribution of observations x_t and clusters c_t. In this example, we can assume

$$\mathcal{C} = \{1, \dots, C\}, \qquad x_{t.m} \in \{0, 1\}.$$

This means that all movies are either watched or not, and we'd simply want to predict which movie somebody is likely to watch. This allows us to use the following simple priors, splitting the parameters in two parts $\theta = (\theta_1, \theta_2)$.

Model family

$$P_{\theta_1}(c_t = c) = \theta_{1,c}, \qquad c_t \sim \mathit{Multinomial}(\theta_1) \tag{5.2.2}$$

$$P_{\theta_2}(x_{t,m} = 1 \mid c_t = c) = \theta_{2,m,c} \qquad x_{t,m} \mid c_t = c \sim \mathit{Bernoulli}(\theta_{2,m,c}) \tag{5.2.3}$$

Since everything is discrete, it makes sense that we can use a Multinomial model for the cluster distribution and a Bernoulli model for whether or not a movie was watched. Now we only need to specify a useful prior for each one of those. The standard priors to use, are a Beta prior for the Bernoulli and the Dirichlet for the Multinomial, as they are conjuate.

Prior

$$\theta_1 \sim \mathit{Dirichlet}(\boldsymbol{\gamma}), \theta_2 \qquad \sim \mathit{Beta}(\alpha, \beta) \tag{5.2.4}$$

Typically $\boldsymbol{\gamma} = (1/2, \dots, 1/2)$ and $\alpha = \beta = 1/2$ to allow for the possibility of nearly deterministic behaviour.

5.3 Social networks

Social networks afford us another opportunity to take a look at data. We can use connections between users to infer their similarity: if two users are connected, then they are more likely to have similar preferences.

Network model

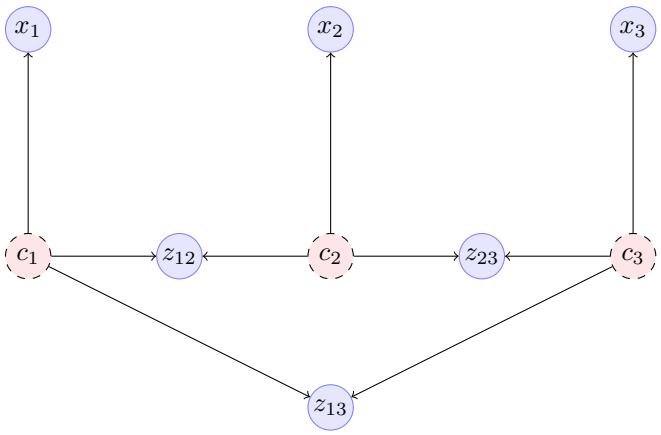


Figure 5.6: Graphical model for data from a social network.

In the model seen in Figure 5.6, each user t is characterised by their cluster membership c_t and emits data x_t. Users t, u are connected when $z_{t,u} = 1$.

5.4 Sequential structures

The simplest type of structure in data is sequences. Examples include speech, text and DNA sequences, as well as data acquired in any sequential decision making problem such as recommendation systems or robotics. Sequential data is always thought to arise from some Markovian processes, defined below.

Markov process

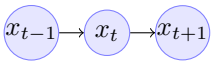


Figure 5.7: Graphical model for a Markov process.

Definition 5.4.1 (Markov process)**.** A Markov process is a sequence of variables $x_t : \Omega \to \mathcal{X}$ such that $x_{t+1} \mid x_t \perp\!\!\!\perp x_{t-k} \forall k \leq 1$.

DNA data

Hidden Markov model

Frequently the sequential dependency is not in the data itself, but in some hidden underlying markov process. In that case, the hidden variable x_t is the *state* of the process. The observed variable y_t is simply an observation.

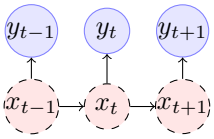


Figure 5.8: Graphical model for a hidden Markov model.

$$P_\theta(x_{t+1} \mid x_t) \qquad \text{(transition distribution)}$$
$$P_\theta(y_t \mid x_t) \qquad \text{(emission distribution)}$$

For any given parater value θ, it is easy to estimate the probability distribution over states given the observations $P_\theta(x^T \mid y^T)$. As an example, if y^T is raw speech data and x^T is a sequence of words, and θ are the parameters of our speech model, then we can obtain probabilities for every possible sequence of words that was uttered. Frequently, though, in speech recognition we are only interested in the most likely seuence of words. This makes the problem simple enough to be solved instantaneously by modern cellphones.

HMM modelling of DNA data

As a more detailed example, consider hidden Markov models for DNA data....

Chapter 6

Bandit problems

nothing

6.1 Introduction

This unit describes the very general formalism of Markov decision processes (MDPs) for formalising problems in sequential decision making. Thus a *Markov decision process* can be used to model stochastic path problems, stopping problems, reinforcement learning problems, experiment design problems, and control problems.

Markov decision proces

We being by taking a look at the problem of *experimental design*. One instance of this problem occurs when considering how to best allocate treatments with unknown efficacy to patients in an adaptive manner, so that the best treatment is found, or so as to maximise the number of patients that are treated successfully. The problem, originally considered by [? ?] , informally can be stated as follows.

experimental design

We have a number of treatments of unknown efficacy, i.e. some of them work better than the others. We observe patients one at a time. When a new patient arrives, we must choose which treatment to administer. Afterwards, we observe whether the patient improves or not. Given that the treatment effects are initially unknown, how can we maximise the number of cured patients? Alternatively, how can we discover the best treatment? The two different problems are formalised below.

Adaptive treatment allo

EXAMPLE 23. Consider k treatments to be administered to T volunteers. To each volunteer only a single treatment can be assigned. At the t-th trial, we treat one volunteer with some treatment $a_t \in \{1, \dots, k\}$. We then obtain obtain a reward $r_t = 1$ if the patient is treated and 0 otherwise. We wish to choose actions maximising the utility $U = \sum_t r_t$. This would correspond to maximising the number of patients that get treated over time.

tion

Adaptive hypothesis t

EXAMPLE 24. An alternative goal would be to do a *clinical trail*, in order to find the best possible treatment. For simplicity, consider the problem of trying to find out whether a particular treatment is better or not than a placebo. We are given a hypothesis set Ω, with each $\omega \in \Omega$ corresponding to different models for the effect of the treatment and the placebo. Since we don't know what is the right model, we place a prior ξ_0 on Ω. We can perform T experiments, after which we must make decide whether or not the treatment is significantly better than the placebo. To model this, we define a decision set $\mathcal{D} = \{d_0, d_1\}$ and a utility function $U : \mathcal{D} \times \Omega \to \mathbb{R}$, which models the effect of each decision d given different versions of reality ω. One hypothesis $\omega \in \Omega$ is true. To distinguish them, we can choose from a set of k possible experiments to be performed over T trials. At the t-th trial, we choose experiment $a_t \in \{1, \dots, k\}$ and observe outcome $x_t \in \mathcal{X}$, with $x_t \sim P_\omega$ drawn from the true hypothesis. Our posterior is

ing

$$\xi_t(\omega) \triangleq \xi_0(\omega \mid a_1, \dots, a_t, x_1, \dots, x_t).$$

The reward is $r_t = 0$ for $t < T$ and

$$r_T = \max_{d \in D} \mathbb{E}_{\xi_T}(U \mid d).$$

Our utility in this can again be expressed as a sum over individual rewards, $U = \sum_{t=1}^{T} r_t$.

Both formalizations correspond to so-called *bandit problems* which we take a closer look at in the following section.

6.2 Bandit problems

The simplest bandit problem is the stochastic n-armed bandit. We are faced with n different one-armed bandit machines, such as those found in casinos. In this problem, at time t, you have to choose one *action* (i.e. a machine) $a_t \in \mathcal{A} = \{1, \dots, n\}$. In this setting, each time t you play a machine, you receive a reward r_t, with fixed expected value $\omega_i = \mathbb{E}(r_t \mid a_t = i)$. Unfortunately,

you do not know ω_i, and consequently the best arm is also unknown. How do you then choose arms so as to maximise the total expected reward?

Definition 6.2.1 (The stochastic n-armed bandit problem.)**.** This is the problem of selecting a sequence of actions $a_t \in \mathcal{A}$, with $\mathcal{A} = \{1, \dots, n\}$, so as to maximise expected utility, where the utility is

$$U = \sum_{t=0}^{T-1} \gamma^t r_t,$$

count factor where $T \in (0, \infty]$ is the horizon and $\gamma \in (0, 1]$ is a *discount factor*. The reward r_t is stochastic, and only depends on the current action, with expectation $\mathbb{E}(r_t \mid a_t = i) = \omega_i$.

icy In order to select the actions, we must specify some *policy* or decision rule. This can only depend on the sequence of previously taken actions and observed rewards. Usually, the policy $\pi : \mathcal{A}^* \times \mathbb{R}^* \to \mathcal{A}$ is a deterministic mapping from the space of all sequences of actions and rewarsd to actions. That is, for every observation and action history $a_1, r_1, \dots, a_{t-1}, r_{t-1}$ it suggests a single action a_t. However, it could also be a stochastic policy, that specifies a mapping to action distributions. We use the following notation for stochastic history-dependent bandit policies,

$$\pi(a_t \mid a^{t-1}, r^{t-1}) \tag{6.2.1}$$

to mean the probability of actions a_t given the history until time t.

How can we solve bandit problems? One idea is to apply the Bayesian decision-theoretic framework we have developed earlier to maximise utility in expectation. More specifically, given the horizon $T \in (0, \infty]$ and the discount factor $\gamma \in (0, 1]$, we define our utility from time t to be:

$$U_t = \sum_{k=1}^{T-t} \gamma^k r_{t+k}. \tag{6.2.2}$$

To apply the decision theoretic framework, we need to define a suitable family of probability measures $\mathcal{F}$, indexed by parameter $\omega \in \Omega$ describing the reward distribution of each bandit, together with a prior distribution ξ on Ω. Since ω is unknown, we cannot maximise the expected utility with respect to it. However, we can always maximise expected utility with respect to our belief ξ. That is, we replace the ill-defined problem of maximising utility in an unknown model with that of maximising expected utility given a distribution over possible models. The problem can be written in a simple form:

$$\max_\pi \mathbb{E}_\xi^\pi U_t = \max_\pi \int_\Omega \mathbb{E}_\omega^\pi U_t \, \mathrm{d}\xi\omega. \tag{6.2.3}$$

The difficulty lies not in formalising the problem, but in the fact that the set of learning policies is quite large, rendering the optimisation infeasible. The following figure summarises the statement of the bandit problem in the Bayesian setting.

Decision-theoretic statement of the bandit problem

- Let $\mathcal{A}$ be the set of arms.
- Define a family of distributions $\mathcal{F} = \{P_{\omega,i} \mid \omega \in \Omega, i \in \mathcal{A}\}$ on $\mathbb{R}$.

- Assume the i.i.d model $r_t \mid \omega, a_t = i \sim P_{\omega,i}$.
- Define prior ξ on Ω.
- Select a policy $\pi : \mathcal{A}^* \times \mathbb{R}^* \to \mathcal{A}$ maximising

$$\mathbb{E}_\xi^\pi U = \mathbb{E}_\xi^\pi \sum_{t=0}^{T-1} \gamma^t r_t$$

There are two main difficulties with this approach. The first is specifying the family and the prior distribution: this is effectively part of the problem formulation and can severely influence the solution. The second is calculating the policy that maximises expected utility given a prior and family. The first problem can be resolved by either specifying a subjective prior distribution, or by selecting a prior distribution that has good worst-case guarantees. The second problem is hard to solve, because in general, such policies are history dependent and the set of all possible histories is exponential in the horizon T.

6.2.1 An example: Bernoulli bandits

As a simple illustration, consider the case when the reward for choosing one of the n actions is either 0 or 1, with some fixed, yet unknown probability depending on the chosen action. This can be modelled in the standard Bayesian framework using the Beta-Bernoulli conjugate prior. More specifically, we can formalise the problem as follows.

Consider n Bernoulli distributions with unknown parameters ω_i $(i = 1, \ldots, n)$ such that

$$r_t \mid a_t = i \sim \textit{Bernoulli}(\omega_i), \qquad \mathbb{E}(r_t \mid a_t = i) = \omega_i. \tag{6.2.4}$$

Each Bernoulli distribution thus corresponds to the distribution of rewards obtained from each bandit that we can play. In order to apply the statistical decision theoretic framework, we have to quantify our uncertainty about the parameters ω in terms of a probability distribution.

We model our belief for each bandit's parameter ω_i as a Beta distribution $\textit{Beta}(\alpha_i, \beta_i)$, with density $f(\omega \mid \alpha_i, \beta_i)$ so that

$$\xi(\omega_1, \ldots, \omega_n) = \prod_{i=1}^{n} f(\omega_i \mid \alpha_i, \beta_i).$$

Recall that the posterior of a Beta prior is also a Beta. Let

$$N_{t,i} \triangleq \sum_{k=1}^{t} \mathbb{I}\{a_k = i\}$$

be the number of times we played arm i and

$$\hat{r}_{t,i} \triangleq \frac{1}{N_{t,i}} \sum_{k=1}^{t} r_t \, \mathbb{I}\{a_k = i\}$$

be the *empirical reward* of arm i at time t. We can let this equal 0 when $N_{t,i} = 0$. Then, the posterior distribution for the parameter of arm i is

$$\xi_t = \textit{Beta}(\alpha_i + N_{t,i}\hat{r}_{t,i} \ , \ \beta_i + N_{t,i}(1 - \hat{r}_{t,i})).$$

Since $r_t \in \{0, 1\}$ the possible states of our belief given some prior are $\mathbb{N}^{2n}$.

In order for us to be able to evaluate a policy, we need to be able to predict the expected utility we obtain. This only depends on our current belief, and the state of our belief corresponds to the state of the bandit problem. This means that everything we know about the problem at time t can be summarised by ξ_t. For Bernoulli bandits, sufficient statistic for our belief is the number of times we played each bandit and the total reward from each bandit. Thus, our state at time t is entirely described by our priors α, β (the initial state) and the vectors

$$N_t = (N_{t,1}, \dots, N_{t,i}) \tag{6.2.5}$$

$$\hat{r}_t = (\hat{r}_{t,1}, \dots, \hat{r}_{t,i}). \tag{6.2.6}$$

At any time t, we can calculate the probability of observing $r_t = 1$ or $r_t = 0$ if we pull arm i as:

$$\xi_t(r_t = 1 \mid a_t = i) = \frac{\alpha_i + N_{t,i}\hat{r}_{t,i}}{\alpha_i + \beta_i + N_{t,i}}$$

So, not only we can predict the immediate reward based on our current belief, but we can also predict all next possible beliefs: the next state is well-defined and depends only on the current state. As we shall see later, this type of decision problem is more generally called a Markov decision process (Definition 7.1.1). For now, we shall more generally (and precisely) define the bandit process itself.

6.2.2 Decision-theoretic bandit process

The basic bandit process can be seen in Figure 6.2(a). We can now define the general decision-theoretic bandit process, not restricted to independent Bernoulli bandits.

Definition 6.2.2. Let $\mathcal{A}$ be a set of actions, not necessarily finite. Let Ω be a set of possible parameter values, indexing a family of probability measures $\mathcal{F} = \{P_{\omega,a} \mid \omega \in \Omega, a \in \mathcal{A}\}$. There is some $\omega \in \Omega$ such that, whenever we take action $a_t = a$, we observe reward $r_t \in \mathcal{R} \subset \mathbb{R}$ with probability measure:

$$P_{\omega,a}(R) \triangleq \mathbb{P}_\omega(r_t \in R \mid a_t = a), \qquad R \subseteq \mathbb{R}. \tag{6.2.7}$$

Let ξ_1 be a prior distribution on Ω and let the posterior distributions be defined as:

$$\xi_{t+1}(B) \propto \int_B P_{\omega,a_t}(r_t) \, \mathrm{d}\xi_t(\omega). \tag{6.2.8}$$

The next belief is random, since it depends on the random quantity r_t. In fact, the probability of the next reward lying in R if $a_t = a$ is given by the following marginal distribution:

$$P_{\xi_t,a}(R) \triangleq \int_\Omega P_{\omega,a}(R) \, \mathrm{d}\xi_t(\omega). \tag{6.2.9}$$

Finally, as ξ_{t+1} deterministically depends on ξ_t, a_t, r_t, the probability of obtaining a particular next belief is the same as the probability of obtaining the corresponding rewards leading to the next belief. In more detail, we can write:

$$\mathbb{P}(\xi_{t+1} = \xi \mid \xi_t, a_t) = \int_{\mathcal{R}} \mathbb{I}\left\{\xi_t(\cdot \mid a_t, r_t = r) = \xi\right\} \, \mathrm{d}P_{\xi_t,a}(r). \tag{6.2.10}$$

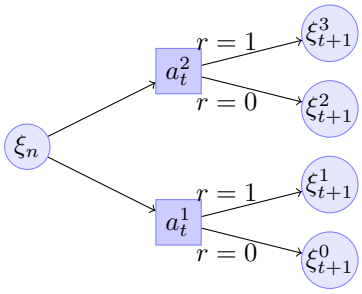


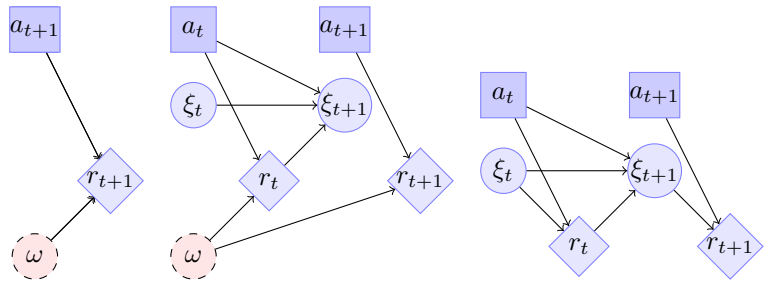
Figure 6.1: A partial view of the multi-stage process. Here, the probability that we obtain $r = 1$ if we take action $a_t = i$ is simply $P_{\xi_t,i}(\{1\})$.

In practice, although multiple reward sequences may lead to the same beliefs, we frequently ignore that possibility for simplicity. Then the process becomes a tree. A solution to the problem of what action to select is given by a backwards induction algorithm similar to that given in Section **??**.

$$U^*(\xi_t) = \max_{a_t} \mathbb{E}(r_t \mid \xi_t, a_t) + \sum_{\xi_{t+1}} \mathbb{P}(\xi_{t+1} \mid \xi_t, a_t) U^*(\xi_{t+1}). \tag{6.2.11}$$

The above equation is the *backwards induction* algorithm for bandits. If you look at this structure, you can see that next belief only depends on the current belief, action and reward, i.e. it satisfies the Markov property, as seen in Figure 6.1. Consequently, a decision-theoretic bandit process can be modelled more generally as a Markov decision process, explained in the following section. It turns out that backwards induction, as well as other efficient algorithms, can provide optimal solutions for Markov decision processes.

backwards induction



(a) The basic process (b) The full process (c) The lifted process

Figure 6.2: Three views of the bandit process. Figure 6.2(a) shows the basic bandit process, from the view of an external observer. The decision maker selects a_t, while the parameter ω of the process is hidden. It then obtains reward r_t. The process repeats for $t = 1, \ldots, T$. The decision-theoretic bandit process is shown in Figures 6.2(b) and 6.2(c). While ω is not known, at each time step t we maintain a belief ξ_t on Ω. The reward distribution is then defined through our belief. In Figure 6.2(b), we can see that complete process, where the dependency on ω is clear. In Figure 6.2(c), we marginalise out ω and obtain a model where the transitions only depend on the current belief and action.

In reality, the reward depends only on the action and the unknown ω, as can be seen in

Figure 6.2(b). This is the point of view of an external observer. However, from the point of view of the decision maker, the distribution of ω only depends on his current belief. Consequently, the distribution of rewards also only depends on the current belief, as we can marginalise over ω. This gives rise to the decision-theoretic bandit process shown in Figure 6.2(c). In the following section, we shall consider Markov decision processes more generally.

6.3 Experiment design

Chapter 7

Markov decision processes

7.1 Markov decision processes and reinforcement learning

Bandit problems are one of the simplest instances of reinforcement learning problems. Informally, speaking, these are problems of learning how to act in an unknown environment, only through interaction with the environment and limited reinforcement signals. The learning agent interacts with the environment through actions and observations, and simultaneously obtains rewards. For example, we can consider a rat running through a maze designed by an experimenter, which from time to time finds a piece of cheese, the reward. The goal of the agent is usually to maximise some measure of the total reward. In summary, we can state the problem as follows.

The reinforcement learning problem.
The reinforcement learning problem is the problem of *learning* how to act in an *unknown* environment, only by interaction and reinforcement.

Generally, we assume that the environment μ that we are acting in has an underlying state $s_t \in \mathcal{S}$, which changes with in discrete time steps t. At each step, the agent obtains an observation $x_t \in \mathcal{X}$ and chooses actions $a_t \in \mathcal{A}$. We usually assume that the environment is such that its next state s_{t+1} only depends on its current state s_t and the last action taken by the agent, a_t. In addition, the agent observes a reward signal r_t, and its goal is to maximise the total reward during its lifetime.

Doing so when the environment μ is unknown, is hard even in seemingly simple settings, like n-armed bandits, where the underlying state never changes. In many real-world applications, the problem is even harder, as the state is not directly observed. Instead, we may simply have some measurements x_t, which give only partial information about the true underlying state s_t.

Reinforcement learning problems typically fall into one of the following three groups: (1) Markov decision processes (MDPs), where the state s_t is observed directly, i.e. $x_t = s_t$; (2) Partially observable MDPs (POMDPs), where the state is hidden, i.e. x_t is only probabilistically dependent on the state; and (3) stochastic Markov games, where the next state also depends on the move of other agents. While all of these problem *descriptions* are different, in the Bayesian setting, they all can be reformulated as MDPs, by constructing an appropriate belief state, similarly to how we did it for the decision theoretic formulation of the bandit problem.

In this chapter, we shall restrict our attention to Markov decision processes. Hence, we shall not discuss the existence of other agents, or the case where we cannot observe the state directly.

nsition distribution

ard distribution

Definition 7.1.1 (Markov Decision Process)**.** A Markov decision process μ is a tuple $\mu = \langle \mathcal{S}, \mathcal{A}, \mathscr{P}, \mathscr{R} \rangle$, where $\mathcal{S}$ is the *state space* and $\mathcal{A}$ is the *action space*. The *transition distribution* being $\mathscr{P} = \{P(\cdot \mid s, a) \mid s \in \mathcal{S}, a \in \mathcal{A}\}$ is a collection of probability measures on $\mathcal{S}$, indexed in $\mathcal{S} \times \mathcal{A}$ and the *reward distribution* $\mathscr{R} = \{\rho(\cdot \mid s, a) \mid s \in \mathcal{S}, a \in \mathcal{A}\}$ is a collection of probability measures on $\mathbb{R}$, such that:

$$P(S \mid s, a) = \mathbb{P}_\mu(s_{t+1} \in S \mid s_t = s, a_t = a) \tag{7.1.1}$$

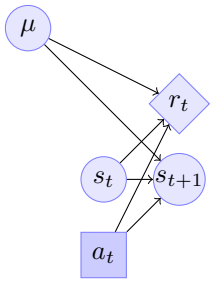
$$\rho(R \mid s, a) = \mathbb{P}_\mu(r_t \in R \mid s_t = s, a_t = a). \tag{7.1.2}$$

For simplicity, we shall also use

$$r_\mu(s, a) = \mathbb{E}_\mu(r_{t+1} \mid s_t = s, a_t = a), \tag{7.1.3}$$

for the expected reward.

Of course, the transition and reward distributions are different for different environments μ. For that reason, we shall usually subscript the relevant probabilities and expectations with μ, unless the MDP is clear from the context.



Markov property of the reward and state distribution

$$\mathbb{P}_\mu(s_{t+1} \in S \mid s_1, a_1, \ldots, s_t, a_t) = \mathbb{P}_\mu(s_{t+1} \in S \mid s_t, a_t) \tag{7.1.4}$$
$$\mathbb{P}_\mu(r_t \in R \mid s_1, a_1, \ldots, s_t, a_t) = \mathbb{P}_\mu(r_t \in R \mid s_t, a_t) \tag{7.1.5}$$

where $S \subset \mathcal{S}$ and $R \subset \mathcal{R}$ are reward and state subsets respectively.

Figure 7.1: The structure of a Markov decision process.

Dependencies of rewards. Sometimes it is more convenient to have rewards that depend on the next state as well, i.e.

$$r_\mu(s, a, s') = \mathbb{E}_\mu(r_{t+1} \mid s_t = s, a_t = a, s_{t+1} = s'), \tag{7.1.6}$$

though this is complicates the notation considerably since now the reward is obtained on the next time step. However, we can always replace this with the expected reward for a given state-action pair:

$$r_\mu(s, a) = \mathbb{E}_\mu(r_{t+1} \mid s_t = s, a_t = s) = \sum_{s' \in \mathcal{S}} P_\mu(s' \mid s, a) r_\mu(s, a, s') \tag{7.1.7}$$

In fact, it is notationally more convenient to have rewards that only depend on the current state:

$$r_\mu(s) = \mathbb{E}_\mu(r_t \mid s_t = s). \tag{7.1.8}$$

For simplicity, we shall mainly consider the latter case.

The agent. The environment does not exist in isolation. The actions are taken by an agent, who is interested in obtaining high rewards. Instead of defining an algorithm for choosing actions directly, we define an algorithm for computing policies, which define distributions on actions.

The agent's policy π

$$\mathbb{P}^\pi(a_t \mid s_t, \dots, s_1, a_{t-1}, \dots, a_1) \quad \text{(history-dependent policy)}$$
$$\mathbb{P}^\pi(a_t \mid s_t) \quad \text{(Markov policy)}$$

In some sense, the agent is defined by its *policy* π, which is a conditional distribution on actions given the history. The *policy* π is otherwise known as a *decision function*. In general, the policy can be history-dependent. In certain cases, however, there are optimal policies that are Markov. This is for example the case with additive utility functions. In paticular, the utility function maps from the sequence of all possible rewards to a real number $U : \mathcal{R}^* \to \mathbb{R}$, given below:

Definition 7.1.2 (Utility)**.** Given a horizon T and a discount factor $\gamma \in (0, 1]$, the utility function $U : \mathcal{R}^* \to \mathbb{R}$ is defined as

$$U(r_0, r_1, \dots, r_T) = \sum_{k=0}^{T} \gamma^k r_k. \tag{7.1.9}$$

It is convenient to give a special name to the utility starting from time t, i.e. the sum of rewards from that time on:

$$U_t \triangleq \sum_{k=0}^{T-t} \gamma^k r_{t+k}. \tag{7.1.10}$$

At any time t, the agent wants to to find a policy π *maximising* the *expected total future reward*

$$\mathbb{E}_\mu^\pi U_t = \mathbb{E}_\mu^\pi \sum_{k=0}^{T-t} \gamma^k r_{t+k}. \quad \text{(expected utility)}$$

This is so far identical to the expected utility framework we had seen so far, with the only difference that now the reward space is a sequence of numerical rewards and that we are acting within a dynamical system with state space $\mathcal{S}$. In fact, it is a good idea to think about the *value* of different states of the system under certain policies, in the same way that one things about how good different positions are in chess.

7.1.1 Value functions

A value function represents the expected utility of a given state, or state-and-action pair for a specific policy. They are really useful as shorthand notation and as the basis of algorithm development. The most basic of those is the state value function.

State value function

$$V_{\mu,t}^\pi(s) \triangleq \mathbb{E}_\mu^\pi(U_t \mid s_t = s) \tag{7.1.11}$$

The state value function for a particular policy π can be interpreted as how much utility you should expect if you follow the policy starting from state s at time t, for the particular MDP μ.

State-action value function

$$Q^{\pi}_{\mu,t}(s,a) \triangleq \mathbb{E}^{\pi}_{\mu}(U_t \mid s_t = s, a_t = a) \tag{7.1.12}$$

The state-action value function for a particular policy π can be interpreted as how much utility you should expect if you play action a, at state s at time t, and then follow the policy π, for the particular MDP μ.

It is also useful to define the optimal policy and optimal value functions for a given MDP. In the following, a star indicates optimal quantities. The *optimal policy* π^*

$$\pi^*(\mu) : V^{\pi^*(\mu)}_{t,\mu}(s) \geq V^{\pi}_{t,\mu}(s) \quad \forall \pi, t, s \tag{7.1.13}$$

dominates all other policies π everywhere in $\mathcal{S}$.

The *optimal value function* V^*

$$V^*_{t,\mu}(s) \triangleq V^{\pi^*(\mu)}_{t,\mu}(s), \quad Q^*_{t,\mu}(s) \triangleq Q^{\pi^*(\mu)}_{t,\mu}(s,a). \tag{7.1.14}$$

is the value function of the optimal policy π^*.

Finding the optimal policy when μ is known

When the MDP μ is known, the expected utility of any policy can be calculated. Therefore, one could find the optimal policy by brute force, i.e. by calculating the utility of every possible policy. This might be as reasonable strategy if the number of policies is small. However, there are many better appr. First, there are iterative/offline methods where an optimal policy is found for all states of the MDP. These either try to estimate the optimal value function directly, or try to iteratively improve a policy until it is optimal. The second type of methods tries to find an optimal policy online. That is, the optimal actions are estimated only for states which can be visited in the future starting from the current state. However, the same main ideas are used in all of these algorithms.

7.2 Finite horizon, undiscounted problems

The conceptually simplest type of problems are finite horizon problems where $T < \infty$ and $\gamma = 1$. The first thing we shall try to do is to evaluate a given policy for a given MDP. There are a number of algorithms that can achieve this.

7.2.1 Policy evaluation

Here we are interested in the problem of determining the value function of a policy π (for $\gamma = 1, T < \infty$). All the algorithms we shall consider can be recovered from the following

recursion. Noting that $U_{t+1} = \sum_{k=1}^{T-t} r_{t+k}$ we have:

$$V^\pi_{\mu,t}(s) \triangleq \mathbb{E}^\pi_\mu(U_t \mid s_t = s) \tag{7.2.1}$$

$$= \sum_{k=0}^{T-t} \mathbb{E}^\pi_\mu(r_{t+k} \mid s_t = s) \tag{7.2.2}$$

$$= \mathbb{E}^\pi_\mu(r_t \mid s_t = s) + \mathbb{E}^\pi_\mu(U_{t+1} \mid s_t = s) \tag{7.2.3}$$

$$= \mathbb{E}^\pi_\mu(r_t \mid s_t = s) + \sum_{i \in \mathcal{S}} V^\pi_{\mu,t+1}(i)\, \mathbb{P}^\pi_\mu(s_{t+1} = i | s_t = s). \tag{7.2.4}$$

Note that the last term can be calculated easily through marginalisation.

$$\mathbb{P}^\pi_\mu(s_{t+1} = i | s_t = s) = \sum_{a \in \mathcal{A}} \mathbb{P}_\mu(s_{t+1}{=}i | s_t{=}s, a_t{=}a)\, \mathbb{P}^\pi(a_t{=}a | s_t{=}s).$$

This derivation directly gives a number of *policy evaluation algorithms*.

Direct policy evaluation Direct policy evaluation is based on (7.2.2), which can be implemented by Algorithm 3. One needs to *marginalise out* all possible state sequences to obtain the expected reward given the state at time $t + k$ giving the following:

$$\mathbb{E}^\pi_\mu(r_{t+k} \mid s_t = s) = \sum_{s_{t+1}, \ldots, s_{t+k} \in \mathcal{S}^k} \mathbb{E}^\pi_\mu(r_{t+k} \mid s_{t+k})\, \mathbb{P}^\pi_\mu(s_{t+1}, \ldots, s_{t+1} \mid s_t).$$

By using the Markov property, we calculate the probability of reaching any state from any other state at different times, and then add up the expected reward we would get in that state under our policy. Then $\hat{V}_t(s) = V^\pi_{\mu,t}(s)$ by definition.

Unfortunately it is not a very good idea to use direct policy evaluation. The most efficient implementation involves calculating $P(s_t \mid s_0)$ recursively for every state. This would result in a total of $|\mathcal{S}|^3 T$ operations. Monte-Carlo evaluations should be considerably cheaper, especially when the transition structure is sparse.

Algorithm 3 Direct policy evaluation

1: **for** $s \in \mathcal{S}$ **do**
2: **for** $t = 0, \ldots, T$ **do**
3:

$$\hat{V}_t(s) = \sum_{k=t}^{T} \sum_{j \in \mathcal{S}} \mathbb{P}^\pi_\mu(s_k = j \mid s_t = s)\, \mathbb{E}^\pi_\mu(r_k \mid s_k = j).$$

4: **end for**
5: **end for**

7.2.2 Monte-Carlo policy evaluation

Another conceptually simple algorithm is Monte-Carlo policy evaluation shown as Algorithm 4. The idea is that instead of summing over all possible states to be visited, we just draw states from the Markov chain defined jointly by the policy and the Markov decision process. Unlike direct policy evaluation the algorithm needs a parameter K, the number of trajectories to generate. Nevertheless, this is a very useful method, employed within a number of more complex algorithms.

Algorithm 4 Monte-Carlo policy evaluation

for $s \in \mathcal{S}$ **do**
  for $k = 0, \dots, K$ **do**
    Choose initial state s_1.
    for $t = 1, \dots, T$ **do**
      $a_t \sim \pi(a_t \mid s_t)$ // Take action
      Observe reward r_t and next state s_{t+1}.
      Set $r_{t,k} = r_t$.
    end for
    Save total reward:

$$\hat{V}_k(s) = \sum_{t=1}^{T} r_{t,k}.$$

  end for
  Calculate estimate:

$$\hat{V}(s) = \frac{1}{K} \sum_{k=1}^{K} \hat{V}_k(s).$$

end for

Remark 7.2.1. The estimate $\hat{V}$ of the Monte Carlo evaluation algorithm satisfies

$$\|V - \hat{V}\|_\infty \leq \sqrt{\frac{\ln(2|\mathcal{S}|/\delta)}{2K}} \qquad \text{with probability } 1 - \delta$$

Proof. From Hoeffding's inequality (**??**) we have for any state s that

$$\mathbb{P}\left(|\hat{V}(s) - V(s)| \geq \sqrt{\frac{\ln(2|\mathcal{S}|/\delta)}{2K}} \right) \leq \delta/|\mathcal{S}|.$$

Consequently, using a union bound of the form $P(A_1 \cup A_2 \cup \ldots \cup A_n) \leq \sum_i P(A_i)$ gives the required result. □

The main advantage of Monte-Carlo policy evaluation is that it can be used in very general settings. It can be used not only in Markovian environments such as MDPs, but also in partially observable and multi-agent settings.

7.2.3 Backwards induction policy evaluation

Finally, the backwards induction algorithm shown as Algorithm 5 is similar to the backwards induction algorithm we saw for sequential sampling and bandit problems. However, here we are only evaluating a policy rather than finding the optimal one. This algorithm is slightly less generally applicable than the Monte-Carlo method because it makes Markovian assumptions. The Monte-Carlo algorithm, can be used for environments that with a non-Markovian variable s_t.

Algorithm 5 Backwards induction policy evaluation

For each state $s \in S$, for $t = 1, \dots, T-1$:

$$\hat{V}_t(s) = r^\pi_\mu(s) + \sum_{j \in S} \mathbb{P}^\pi_\mu(s_{t+1} = j \mid s_t = s)\hat{V}_{t+1}(j), \tag{7.2.5}$$

with $\hat{V}_T(s) = r^\pi_\mu(s)$.

Theorem 7.2.1. *The backwards induction algorithm gives estimates $\hat{V}_t(s)$ satisfying*

$$\hat{V}_t(s) = V^\pi_{\mu,t}(s) \tag{7.2.6}$$

Proof. For $t = T-1$, the result is obvious. We can prove the remainder by induction. Let (7.2.6) hold for all $t \geq n+1$. Now we prove that it holds for n. Note that from the recursion (7.2.5) we have:

$$\begin{aligned}
\hat{V}_t(s) &= r_\mu(s) + \sum_{j \in S} \mathbb{P}_{\mu,\pi}(s_{t+1} = j \mid s_t = s)\hat{V}_{t+1}(j) \\
&= r(s) + \sum_{j \in S} \mathbb{P}_{\mu,\pi}(s_{t+1} = j \mid s_t = s)V^\pi_{\mu,t+1}(j) \\
&= r(s) + \mathbb{E}_{\mu,\pi}(U_{t+1} \mid s_t = s) \\
&= \mathbb{E}_{\mu,\pi}(U_t \mid s_t = s) = V^\pi_{\mu,t}(s),
\end{aligned}$$

where the second equality is by the induction hypothesis, the third and fourth equalities are by the definition of the utility, and the last by definition of $V^\pi_{\mu,t}$. □

7.2.4 Backwards induction policy optimisation

Backwards induction as given in Alg 6 is the first non-naive algorithm for finding an optimal policy for the sequential problems with T stages. It is basically identical to the backwards induction algorithm we saw in Chapter **??**, which was for the very simple sequential sampling problem, as well as the backwards induction algorithm for the decision-theoretic bandit problem.

Algorithm 6 Finite-horizon backwards induction

Input μ, set $\mathcal{S}_T$ of states reachable within T steps.
Initialise $V_T(s) := \max_a r(s,a)$, for all $s \in \mathcal{S}_T$.
for $n = T-1, T-2, \dots, 1$ **do**
  for $s \in \mathcal{S}_n$ **do**
    $\pi_n(s) = \arg\max_a r(s,a) + \sum_{s' \in \mathcal{S}_{n+1}} P_\mu(s' \mid s, a)V_{n+1}(s')$
    $V_n(s) = r(s,a) + \sum_{s' \in \mathcal{S}_{n+1}} P_\mu(s' \mid s, \pi_n(s))V_{n+1}(s')$
  end for
end for
Return $\pi = (\pi_n)_{n=1}^T$.

Theorem 7.2.2. *For T-horizon problems, backwards induction is optimal, i.e.*

$$V_n(s) = V^*_{\mu,n}(s) \tag{7.2.7}$$

Proof. Note that the proof below also holds for $r(s,a) = r(s)$. First we show that $V_t \geq V_t^*$. For $n = T$ we evidently have $V_T(s) = \max_a r(s,a) = V_{\mu,T}^*(s)$. Now assume that for $n \geq t+1$, (7.2.7) holds. Then it also holds for $n = t$, since for any policy π'

$$\begin{aligned}
V_t(s) &= \max_a \left\{ r(s,a) + \sum_{j \in \mathcal{S}} P_\mu(j \mid s,a) V_{t+1}(j) \right\} \\
&\geq \max_a \left\{ r(s,a) + \sum_{j \in \mathcal{S}} P_\mu(j \mid s,a) V_{\mu,t+1}^*(j) \right\} \qquad \text{(by induction assumption)} \\
&\geq \max_a \left\{ r(s,a) + \sum_{j \in \mathcal{S}} P_\mu(j \mid s,a) V_{\mu,t+1}^{\pi'}(j) \right\} \\
&\geq V_t^{\pi'}(s).
\end{aligned}$$

This holds for any policy π', including $\pi' = \pi$, the policy returned by backwards induction. Then:

$$V_{\mu,t}^*(s) \geq V_{\mu,t}^{\pi}(s) = V_t(s) \geq V_{\mu,t}^*(s).$$

□

Remark 7.2.2. A similar theorem can be proven for arbitrary $\mathcal{S}$. This requires using sup instead of max and proving the existence of a π' that is arbitrary-close in value to V^*. For details, see[?] .

7.3 Infinite-horizon

When problems have no fixed horizon, they usually can be modelled as infinite horizon problems, sometimes with help of a *terminating state*, whose visit terminates the problem, or discounted rewards, which indicate that we care less about rewards further in the future. When reward discounting is exponential, these problems can be seen as undiscounted problems with random and geometrically distributed horizon. For problems with no discounting and no termination states there are some complications in the definition of optimal policy. However, we defer discussion of such problems to Chapter **??**.

7.3.1 Examples

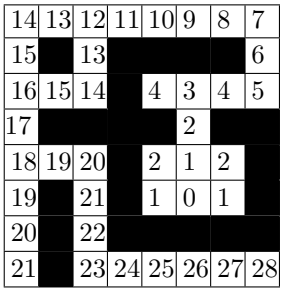
We begin with some examples, which will help elucidate the concept of terminating states and infinite horizon. The first is shortest path problems, where the aim is to find the shortest path to a particular goal. Although the process terminates when the goal is reached, not all policies may be able to reach the goal, and so the process may never terminate.

Shortest-path problems

We shall consider two types of shortest path problems, deterministic and stochastic. Although conceptually very different, both problems have essentially the same complexity.

Consider an agent moving in a maze, aiming to get to some terminating goal state X. That is, when reaching this state, the agent cannot move anymore, and receives a reward of 0. In general, the agent can move deterministically in the four cardinal directions, and receives a

negative reward at each time step. Consequently, the optimal policy is to move to X as quickly as possible.

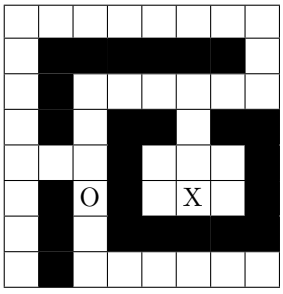


Properties

- $\gamma = 1$, $T \to \infty$.
- $r_t = -1$ unless $s_t = X$, in which case $r_t = 0$.
- $\mathbb{P}_\mu(s_{t+1} = X | s_t = X) = 1$.
- $\mathcal{A} = \{\text{North}, \text{South}, \text{East}, \text{West}\}$
- Transitions are deterministic and walls block.

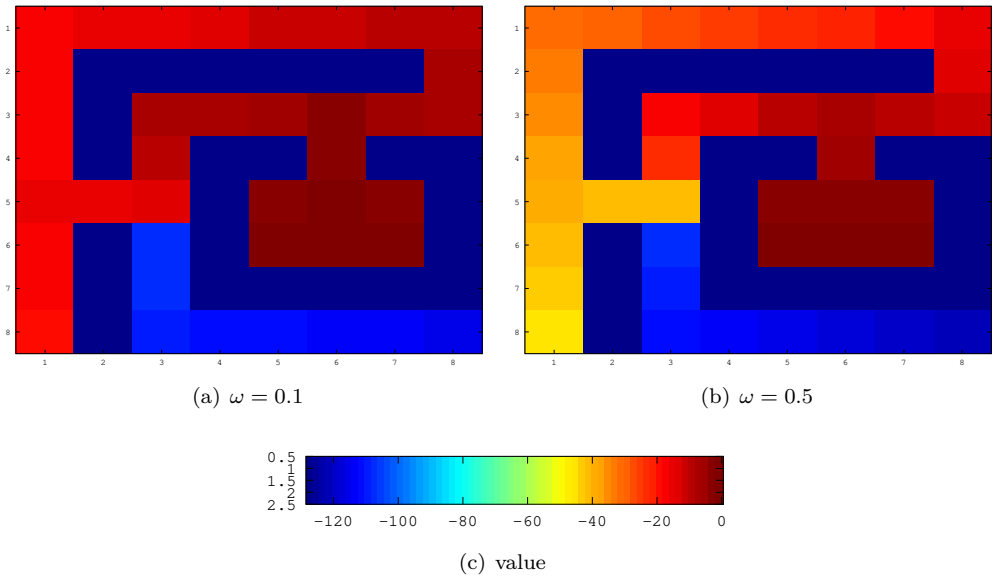
Solving the shortest path problem can be done simply by looking at the distance of any point to X. Then the reward obtained by the optimal policy starting from any point, is simply the negative distance. The optimal policy simply moves to the state with the smallest distance to X.

Stochastic shortest path problem with a pit Now assume the shortest path problem with stochastic dynamics. That is, at each time-step there is a small probability ω that move to a random direction. In addition, there is a pit O, that is a terminating state with a reward of -100.



Properties

- $\gamma = 1$, $T \to \infty$.
- $r_t = -1$, but $r_t = 0$ at X and -100 at O and episode ends.
- $\mathbb{P}_\mu(s_{t+1} = X | s_t = X) = 1$.
- $\mathcal{A} = \{\text{North}, \text{South}, \text{East}, \text{West}\}$
- Moves to a random direction with probability ω. Walls block.



(a) $\omega = 0.1$ (b) $\omega = 0.5$

(c) value

Figure 7.2: Pit maze solutions for two values of ω.

Randomness changes the solution significantly in this environment. When ω is relatively small, it is worthwhile (in expectation) for the agent to pass past the pit, even though there is a risk of falling in and getting a reward of -100. In the example given, even starting from the third row, the agent prefers taking the short-cut. For high enough ω, the optimal policy avoids approaching the pit. Still, the agent prefers jumping in the pit, than being trapped at the bottom of the maze forever.

Continuing problems

Finally, many problems have no natural terminating state, but are continuing *ad infinitum*. Frequently, we model those problems using a utility that discounts future rewards exponentially. This way, we can guarantee that the utility is bounded. In addition, exponential discounting also has some economical sense. This is partially because of the effects of inflation, and partially because money now may be more useful than money in the future. Both these effects diminish the value of money over time. As an example, consider the following inventory management problem.

Example 25 (Inventory management). There are K storage locations, and each location i can store n_i items. At each time-step there is a probability ϕ_i that a client tries to buy an item from location i, where $\sum_i \phi_i \leq 1$. If there is an item available, when this happens, you gain reward 1. There are two types of actions, one for ordering a certain number u units of stock, paying $c(u)$. Further one may move u units of stock from one location i to another location j, paying $\psi_{ij}(u)$.

An easy special case is when $K = 1$, and we assume that deliveries happen once every m timesteps, and each time-step a client arrives with probability ϕ. Then the state set $\mathcal{S} = \{0, 1, \ldots, n\}$ corresponds to the number of items we have, the action set $\mathcal{A} = \{0, 1, \ldots, n\}$ to the number of items we may order. The transition probabilities are given by $P(s'|s, a) = \binom{m}{d}\phi^d(1 - \phi)^{m-d}$, where $d = s + a - s'$, for $s + a \leq n$.

7.3.2 MDP Algorithms

Let us now look at three basic algorithms for solving a known Markov decision process. The first, *value iteration*, is a simple extension of the backwards induction algorithm to the infinite horizon case.

Value iteration

In this version of the algorithm, we assume that rewards are dependent only on the state. An algorithm for the case where reward only depends on the state can be obtained by replacing $r(s, a)$ with $r(s)$.

Algorithm 7 Value iteration

Input μ, $\mathcal{S}$.
Initialise $\boldsymbol{v}_0 \in \mathcal{V}$.
for $n = 1, 2, \ldots$ **do**
  for $s \in \mathcal{S}_n$ **do**
    $\pi_n(s) = \arg\max_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \sum_{s' \in \mathcal{S}} P_\mu(s' \mid s, a) \boldsymbol{v}_{n-1}(s') \right\}$
    $\boldsymbol{v}_n(s) = r(s, \pi_n(s)) + \gamma \sum_{s' \in \mathcal{S}} P_\mu(s' \mid s, \pi_n(s)) \boldsymbol{v}_{n-1}(s')$
  end for
  break if `termination-condition` is met
end for
Return π_n, V_n.

The value iteration algortihm is a direct extension of the backwards induction algorithm for an infinite horizon. However, since we know that stationary policies are optimal, we do not need to maintain the values and actions for all time steps. At each step, we can merely keep the previous value $\boldsymbol{v}_{n-1}$. However, since there is an infinite number of steps, we need to know whether the algorithm converges to the optimal value, and what is the error we make at a particular iteration.

Theorem 7.3.1. *The value iteration algorithm satisfies*

- $\lim_{n \to \infty} \|\boldsymbol{v}_n - \boldsymbol{v}^*\| = 0$.
- *For each* $\epsilon > 0$ *there exists* $N_\epsilon < \infty$ *such that for all* $n \geq N_\epsilon$

$$\|\boldsymbol{v}_{n+1} - \boldsymbol{v}_n\| \leq \epsilon(1 - \gamma)/2\gamma. \tag{7.3.1}$$

- *For* $n \geq N_\epsilon$ *the policy* π_ϵ *that takes action*

$$\arg\max_a r(s, a) + \gamma \sum_j p(j|s, a) \boldsymbol{v}_n(s')$$

  is ϵ*-optimal, i.e.* $V_\mu^{\pi_\epsilon}(s) \geq V_\mu^*(s) - \epsilon$ *for all states* s.

- $\|\boldsymbol{v}_{n+1} - \boldsymbol{v}^*\| < \epsilon/2$ *for* $n \geq N_\epsilon$.

Proof. The first two statements follow from the fixed-point Theorem **??**. Now note that

$$\|V_\mu^{\pi_\epsilon} - \boldsymbol{v}^*\| \leq \|V_\mu^{\pi_\epsilon} - \boldsymbol{v}_n\| + \|\boldsymbol{v}_n - \boldsymbol{v}^*\|$$

We can bound these two terms easily:

$$\begin{aligned}
\left\|V_\mu^{\pi_\epsilon} - \boldsymbol{v}_{n+1}\right\| &= \left\|\mathscr{L}_{\pi_\epsilon} V_\mu^{\pi_\epsilon} - \boldsymbol{v}_{n+1}\right\| && \text{(by definition of } \mathscr{L}_{\pi_\epsilon}) \\
&\le \left\|\mathscr{L}_{\pi_\epsilon} V_\mu^{\pi_\epsilon} - \mathscr{L}\boldsymbol{v}_{n+1}\right\| + \left\|\mathscr{L}\boldsymbol{v}_{n+1} - \boldsymbol{v}_{n+1}\right\| && \text{(triangle)} \\
&= \left\|\mathscr{L}_{\pi_\epsilon} V_\mu^{\pi_\epsilon} - \mathscr{L}_{\pi_\epsilon}\boldsymbol{v}_{n+1}\right\| + \left\|\mathscr{L}\boldsymbol{v}_{n+1} - \mathscr{L}\boldsymbol{v}_n\right\| && \text{(by definition)} \\
&\le \gamma \left\|V_\mu^{\pi_\epsilon} - \boldsymbol{v}_{n+1}\right\| + \gamma \left\|\boldsymbol{v}_{n+1} - \boldsymbol{v}_n\right\|. && \text{(by contraction)}
\end{aligned}$$

An analogous argument gives the same bound for the second term $\|\boldsymbol{v}_n - \boldsymbol{v}^*\|$. Then, rearranging we obtain

$$\|V^{\pi_\epsilon} - \boldsymbol{v}_{n+1}\| \le \frac{\gamma}{1-\gamma}\|\boldsymbol{v}_{n+1} - \boldsymbol{v}_n\|, \qquad \|\boldsymbol{v}_{n+1} - \boldsymbol{v}^*\| \le \frac{\gamma}{1-\gamma}\|\boldsymbol{v}_{n+1} - \boldsymbol{v}_n\|,$$

and the third and fourth statements follow from the second statement. □

The *termination condition* of value iteration has been left unspecified. However, the theorem above shows that if we terminate when (7.3.1) is true, then our error will be bounded by ϵ. However, better termination conditions can be obtained. *termination condition*

Now let us prove how fast value iteration converges.

Theorem 7.3.2 (Value iteration monotonicity)**.** *Let $\mathcal{V}$ be the set of value vectors with Bellman operator $\mathscr{L}$. Then:*

1. *Let $\boldsymbol{v}, \boldsymbol{v}' \in \mathcal{V}$ with $\boldsymbol{v}' \ge \boldsymbol{v}$. Then $\mathscr{L}\boldsymbol{v}' \ge \mathscr{L}\boldsymbol{v}$.*
2. *Let $\boldsymbol{v}_{n+1} = \mathscr{L}\boldsymbol{v}_n$. If there is an N s.t. $\mathscr{L}\boldsymbol{v}_N \le \boldsymbol{v}_N$, then $\mathscr{L}\boldsymbol{v}_{N+k} \le \boldsymbol{v}_{N+k}$ for all $k \ge 0$ and similarly for $\ge$.*

Proof. Let $\pi \in \arg\max_\pi \boldsymbol{r} + \gamma \boldsymbol{P}_{\mu,\pi}\boldsymbol{v}$. Then

$$\mathscr{L}\boldsymbol{v} = \boldsymbol{r} + \gamma \boldsymbol{P}_{\mu,\pi}\boldsymbol{v} \le \boldsymbol{r} + \gamma \boldsymbol{P}_{\mu,\pi}\boldsymbol{v}' \le \max_{\pi'} \boldsymbol{r} + \gamma \boldsymbol{P}_{\mu,\pi'}\boldsymbol{v}',$$

where the first inequality is due to the fact that $\boldsymbol{P}\boldsymbol{v} \ge \boldsymbol{P}\boldsymbol{v}'$ for any $\boldsymbol{P}$. For the second part,

$$\mathscr{L}\boldsymbol{v}_{N+k} = \boldsymbol{v}_{N+k+1} = \mathscr{L}^k \mathscr{L}\boldsymbol{v}_N \le \mathscr{L}^k \boldsymbol{v}_N = \boldsymbol{v}_{N+k}.$$

since $\mathscr{L}\boldsymbol{v}_N \le \boldsymbol{v}_N$ by assumption and consequently $\mathscr{L}^k\mathscr{L}\boldsymbol{v}_N \le \mathscr{L}^k\boldsymbol{v}_N$ by part one of the theorem. □

Thus, value iteration converges monotonically to V_μ^* if the initial value $\boldsymbol{v}_0 \le \boldsymbol{v}'$ for all $\boldsymbol{v}'$. If $r \ge 0$, it is sufficient to set $\boldsymbol{v}_0 = \boldsymbol{0}$. Then $\boldsymbol{v}_n$ is always a lower bound on the optimal value function.

Theorem 7.3.3. *Value iteration converges with error in $O(\gamma^n)$ More specifically, for $r \in [0,1]$ and $\boldsymbol{v}_0 = \boldsymbol{0}$,*

$$\|\boldsymbol{v}_n - V_\mu^*\| \le \frac{\gamma^n}{1-\gamma}, \qquad \|V_\mu^{\pi_n} - V_\mu^*\| \le \frac{2\gamma^n}{1-\gamma}.$$

Proof. The first part follows from the contraction property (Theorem **??**):

$$\|\boldsymbol{v}_{n+1} - \boldsymbol{v}^*\| = \|\mathscr{L}\boldsymbol{v}_n - \mathscr{L}\boldsymbol{v}^*\| \le \gamma\|\boldsymbol{v}_n - \boldsymbol{v}^*\|. \tag{7.3.2}$$

Now divide by γ^n to obtain the final result.

□

Although value iteration converges exponentially fast, the convergence is dominated by the discount factor γ. When γ is very close to one, convergence can be extremely slow. In fact, **?** showed that the number of iterations are on the order of $1/(1-\gamma)$, for bounded accuracy of the input data. The overall complexity is $\tilde{O}(|\mathcal{S}|^2|\mathcal{A}|L(1-\gamma)^{-1}$, omitting logarithmic factors, where L is the total number of bits used to represent the input.[1]

[1]Thus the result is *weakly* polynomial complexity, due to the dependence on the input size description.

Chapter 8

Safety

Nothing here

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