8

When Models meet Data

In the first part of the book, we introduced the mathematics that form the foundations of many machine learning methods. The hope is that a reader would be able to learn the rudimentary forms of the language of mathematics, which we will now use to describe and discuss machine learning. The second part of the book introduces four pillars of machine learning:

- Regression (Chapter 9)
- Dimensionality reduction (Chapter 10)
- Density estimation (Chapter 11)
- Classification (Chapter 12)

Recall from Table 1.1 that these problems illustrate two supervised and two unsupervised learning methods — one discrete and another continuous. The main aim of this part of the book is to illustrate how the mathematical concepts introduced in the first part of the book can be used to design machine learning algorithms that can be used to solve tasks within the remit of the four pillars. We do not intend to introduce advanced machine learning concepts, but instead to provide a set of practical methods that allow the reader to apply the knowledge they had gained from the first part of the book. It also provides a gateway to the wider machine learning literature for readers already familiar with the mathematics.

It is worth at this point to pause and consider the problem that a machine learning algorithm is designed to solve. As discussed in Chapter 1, there are three major components of a machine learning system: data, models and learning. The main question of machine learning is "what do we mean by good models?". That is we are interested to find models that perform well on future data. The word *model* has many subtleties and we will revisit it multiple times in this chapter. It is also not entirely obvious how to objectively define the word "good", and one of the guiding principles of machine learning is that good models should perform well on unseen data. This requires us to define some performance metrics, such as accuracy or distance from ground truth, as well as figuring out ways to do well (under these performance metrics).

model

This chapter covers a few necessary bits and pieces of mathematical and statistical language that are commonly used to talk about machine

Table 8.1 Example data from a fictitious human resource database that is not in a numerical format.

Name	Gender	Degree	Postcode	Age	Annual Salary
Aditya	M	MSc	W21BG	36	89563
Bob	M	PhD	EC1A1BA	47	123543
Chloé	F	BEcon	SW1A1BH	26	23989
Daisuke	M	BSc	SE207AT	68	138769
Elisabeth	F	MBA	SE10AA	33	113888

Table 8.2 Example data from a fictitious human resource database (see Table 8.1), converted to a numerical format.

Gender ID	Degree	Latitude (in degrees)	Longitude (in degrees)	Age	Annual Salary (in thousands)
-1	2	51.5073	0.1290	36	89.563
-1	3	51.5074	0.1275	47	123.543
+1	1	51.5071	0.1278	26	23.989
-1	1	51.5075	0.1281	68	138.769
+1	2	51.5074	0.1278	33	113.888

learning models. By doing so, we briefly outline the current best practices for training a model such that we do well on data that we have not yet seen. We will introduce the framework for non-probabilistic models in Section 8.1, the principle of maximum likelihood in Section 8.2, and the idea of probabilistic models in Section 8.3. We briefly outline a graphical language for specifying probabilistic models in Section 8.4 and finally discuss model selection in Section 8.5. The rest of this section expands upon the three main components of machine learning: data, models and learning.

Data as Vectors

We assume that our data can be read by a computer, and represented adequately in a numerical format. Furthermore, data is assumed to be tabular, where we think of each row of the table to represent a particular instance or example, and each column to be a particular feature/representation of the instance. We do not discuss the important and challenging aspects of identifying good representations (features). Many of these aspects depend on domain expertise and require careful engineering, which in recent years have been put under the umbrella of data science (Stray, 2016; Adhikari and DeNero, 2018). For example, in Table 8.1, the gender column (a categorical variable) may be converted into numbers 0 representing "Male" and 1 representing "Female". Alternatively, the gender could be represented by numbers $-1, +1$, respectively (as shown in Table 8.2). Furthermore, it is often important to use domain knowledge when constructing the representation, such as knowing that university degrees progress from Bachelor's to Master's to PhD or realizing that the postcode provided is not just a string of characters but actually encodes an area in London. In Table 8.2, we converted the data from Table 8.1 to a numerical format, and each postcode is represented as two numbers, a latitude and longitude. Even numerical data that could potentially be directly read into a machine learning algorithm should be carefully con-

Data is assumed to be in a tidy format (Wickham, 2014; Codd, 1990).

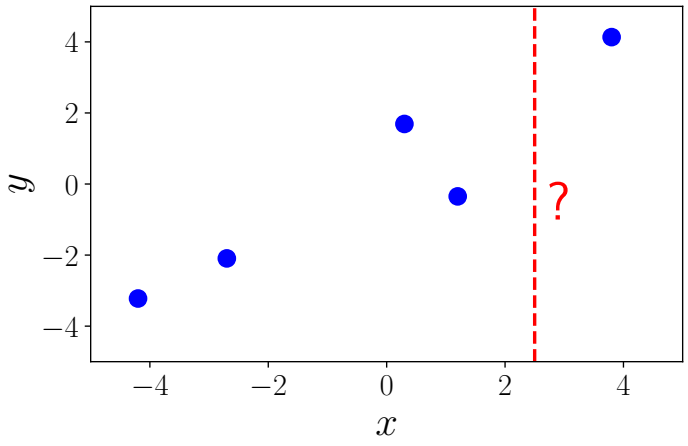


Figure 8.1 Toy data for linear regression. Training data in (x_n, y_n) pairs: $\{(-4.200, -3.222), (-2.700, -2.093), (+0.300, +1.690), (+1.200, -0.348), (+3.800, +4.134)\}$. We are interested in the value of the function at $x = 2.5$, which is not part of the training data.

sidered for units, scaling, and constraints. For the purposes of this book we assume that a domain expert already converted data appropriately, i.e., each input $\boldsymbol{x}_n$ is a D-dimensional vector of numbers, which are called *features*, *attributes* or *covariates*. In general, however, $\boldsymbol{x}_n$ could be a complex structured object (e.g., an image, a sentence, an email message, a time series, a molecular shape, a graph, etc).

Without additional information, one should shift and scale all columns of the dataset such that they mean 0 and variance 1.

features
attributes
covariates

In this part of the book, we will use N to denote the number of examples in a dataset and index the examples with lowercase $n = 1, \ldots, N$. We assume that we are given a set of numerical data, represented as an array of vectors, e.g., as illustrated in Figure 8.2. Each row is a particular individual $\boldsymbol{x}_n$ often referred to as an *example* or *data point* in machine learning. The subscript n refers to the fact that this is the n^{th} example out of a total of N examples in the dataset. Each column represents a particular *feature* of interest about the example, and we index the features as $d = 1, \ldots, D$. Recall that data is represented as vectors, which means that each example (each data point) is a D dimensional vector.

example
data point

feature

For supervised learning problems we have a label y_n associated with each example $\boldsymbol{x}_n$. A dataset is written as a set of example-label pairs $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$. The table of examples $\{\boldsymbol{x}_1, \ldots \boldsymbol{x}_N\}$ is often concatenated, and written as $\boldsymbol{X} \in \mathbb{R}^{N \times D}$. Figure 8.1 illustrates an example of a one dimensional input x and corresponding labels y.

The orientation of the table originates from the database community, although it would actually be more convenient in machine learning for vectors representing examples to be columns.

Representing data as vectors $\boldsymbol{x}_n$ allows us to use concepts from linear algebra (introduced in Chapter 2). In many machine learning algorithms, we need to additionally be able to compare two vectors. As we will see in Chapters 9 and 12, computing the similarity or distance between two examples allows us to formalize the intuition that examples with similar features should have similar labels. The comparison of two vectors requires that we construct a geometry (explained in Chapter 3), and allows us to optimize the resulting learning problem using techniques in Chapter 7.

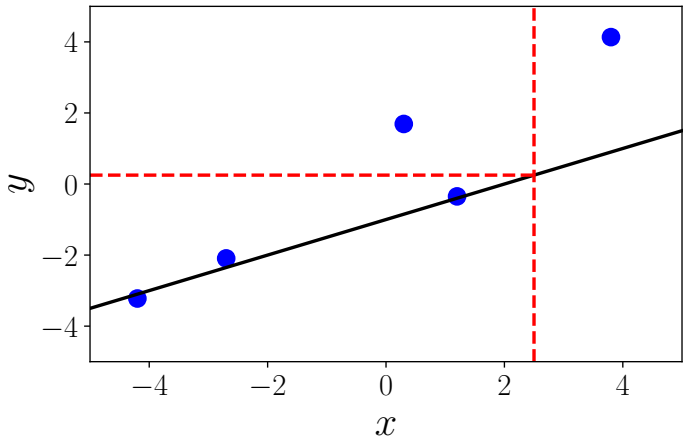


Figure 8.2 Example function (black solid diagonal line) and its prediction at $x = 2.5$. That is $f(2.5) = 0.25$.

Since we have vector representations of data, we can manipulate data to find potentially better representations of it. We will discuss finding good representations in two ways: finding lower-dimensional approximations of the original feature vector, and using nonlinear higher-dimensional combinations of the original feature vector. In Chapter 10 we will see an example of finding a low-dimensional approximation of the original data space by finding the principal components. Finding principal components is closely related to concepts of eigenvalue and singular value decomposition as introduced in Chapter 4. For the high-dimensional representation, we will see an explicit *feature map* $\phi(\cdot)$ that allows us to represent inputs $\boldsymbol{x}_n$ using a higher dimensional representation $\phi(\boldsymbol{x}_n)$. The main motivation for higher dimensional representations is that we can construct new features as non-linear combinations of the original features, which in turn may make the learning problem easier. We will discuss the feature map in Section 9.2 and show how this feature map leads to a *kernel* in Section 12.3.3. In recent years, deep learning methods (Goodfellow et al., 2016) have shown promise in using the data itself to learn the features, and has been very successful in areas such as computer vision, speech recognition and natural language processing. We will not cover neural networks in this part of the book, but the reader is referred to Section 5.6 for the mathematical description of backpropagation, a key concept for training neural networks.

feature map

kernel

Models are Functions

Once we have data in an appropriate vector representation, we can get to the business of constructing a predictive function (known as a *predictor*). In Chapter 1 we did not yet have the language to be precise about models. Using the concepts from the first part of the book, we can now introduce what ”model” means. We present two major approaches in this book: a

predictor

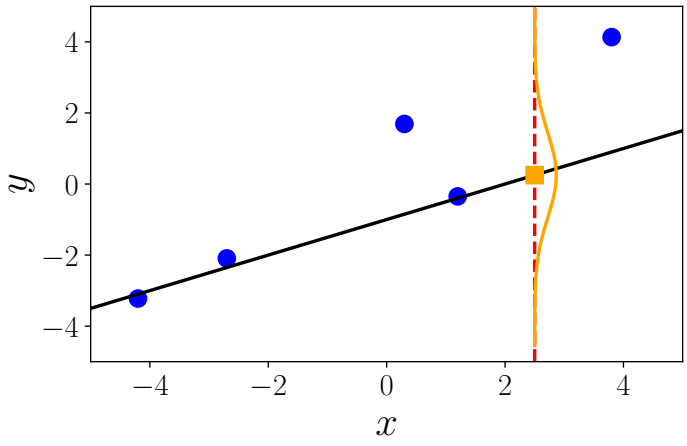


Figure 8.3 Example function (black solid diagonal line) and its predictive uncertainty at $x = 2.5$ (drawn as a Gaussian).

predictor as a function, and a predictor as a probabilistic model. We describe the former here and the latter in the next subsection.

A predictor is a function that, when given a particular input example (in our case a vector of features), produces an output. For now consider the output to be a single number, i.e., a real-valued scalar output. This can be written as

$$f : \mathbb{R}^D \to \mathbb{R}\,, \tag{8.1}$$

where the input vector $\boldsymbol{x}$ is D-dimensional (has D features), and the function f then applied to it (written as $f(\boldsymbol{x})$) returns a real number. Figure 8.2 illustrates a possible function that can be used to compute the value of the prediction for input values x.

In this book, we do not consider the general case of all functions, which would involve the need for functional analysis. Instead we consider the special case of linear functions

$$f(\boldsymbol{x}) = \boldsymbol{\theta}^\top \boldsymbol{x} + \theta_0\,. \tag{8.2}$$

This restriction means that the contents of Chapter 2 and 3 suffice for precisely stating the notion of a predictor for the non-probabilistic (in contrast to the probabilistic view described next) view of machine learning. Linear functions strike a good balance between the generality of the problems that can be solved and the amount of background mathematics that is needed.

Models are Probability Distributions

We often consider data to be noisy observations of some true underlying effect, and hope that by applying machine learning we can identify the signal from the noise. This requires us to have a language for quantifying the effect of noise. We often would also like to have predictors that express some sort of uncertainty, e.g., to quantify the confidence we have

about the value of the prediction for a particular test data point. As we have seen in Chapter 6 probability theory provides a language for quantifying uncertainty. Figure 8.3 illustrates the predictive uncertainty of the function as a Gaussian distribution.

Instead of considering a predictor as a single function, we could consider predictors to be probabilistic models, i.e., models describing the distribution of possible functions. We limit ourselves in this book to the special case of distributions with finite dimensional parameters, which allows us to describe probabilistic models without needing stochastic processes and random measures. For this special case we can think about probabilistic models as multivariate probability distributions, which already allow for a rich class of models.

We will introduce how to use concepts from probability (Chapter 6) to define machine learning models in Section 8.3, and introduce a graphical language for describing probabilistic models in a compact way in Section 8.4.

Learning is Finding Parameters

The goal of learning is to find a model and its corresponding parameters such that the resulting predictor will perform well on unseen data. There are conceptually three distinct algorithmic phases when discussing machine learning algorithms:

1. prediction or inference
2. training or parameter estimation
3. hyperparameter tuning or model selection

The prediction phase is when we use a trained predictor on previously unseen test data. In other words, the parameters and model choice is already fixed and the predictor is applied to new vectors representing new input data points. As outlined in Chapter 1 and the previous subsection, we will consider two schools of machine learning in this book, corresponding to whether the predictor is a function or a probabilistic model. When we have a probabilistic model (discussed further in Section 8.3) the prediction phase is called inference.

The training or parameter estimation phase is when we adjust our predictive model based on training data. We would like to find good predictors given training data, and there are two main strategies for doing so: finding the best predictor based on some measure of quality (sometimes called finding a point estimate), or using Bayesian inference. Finding a point estimate can be applied to both types of predictors, but Bayesian inference requires probabilistic models. For the non-probabilistic model, we follow the principle of *empirical risk minimization*, which we describe in Section 8.1. Empirical risk minimization directly provides an optimization problem for finding good parameters. With a statistical model the principle of *maximum likelihood* is used to find a good set of parameters (Sec-

empirical risk minimization

maximum likelihood

tion 8.2). We can additionally model the uncertainty of parameters using a probabilisitic model, which we will look at in more detail in Section 8.3.

We use numerical methods to find good parameters that "fit" the data, and most training methods can be thought of as hill climbing approaches to find the maximum of an objective, for example the maximum of a likelihood. To apply hill-climbing approaches we use the gradients described Chapter 5 and implement numerical optimization approaches from Chapter 7.

The convention in optimization is to minimize objectives. Hence, there is often an extra minus sign in machine learning objectives.

As mentioned in Chapter 1, we are interested in learning a model based on data such that it performs well on future data. It is not enough for the model to only fit the training data well, the predictor needs to perform well on unseen data. We simulate the behaviour of our predictor on future unseen data using cross validation (Section 8.1.4). As we will see in this chapter, to achieve the goal of performing well on unseen data, we will need to balance between fitting well on training data and finding "simple" explanations of the phenomenon. This trade off is achieved using regularization (Section 8.1.3) or by adding a prior (Section 8.2.2). In philosophy, this is considered to be neither induction or deduction, and is called *abduction*. According to the Stanford Encyclopedia of Philosophy, abduction is the process of inference to the best explanation (Douven, 2017).

abduction

A good movie title is "AI abduction".

We often need to make high level modeling decisions about the structure of the predictor, such as the number of components to use or the class of probability distributions to consider. The choice of the number of components is an example of a *hyperparameter*, and this choice can affect the performance of the model significantly. The problem of choosing between different models is called *model selection*, which we describe in Section 8.5. For non-probabilistic models, model selection is often done using *cross validation*, which is described in Section 8.1.4. We also use model selection to choose hyperparameters of our model.

hyperparameter

model selection

cross validation

Remark. The distinction between parameters and hyperparameters is somewhat arbitrary, and is mostly driven by the distinction between what can be numerically optimized versus what needs to utilize search techniques. Another way to consider the distinction is to consider parameters as the explicit parameters of a probabilistic model, and to consider hyperparameters (higher level parameters) as parameters that control the distribution of these explicit parameters. ♢

8.1 Empirical Risk Minimization

After having all the mathematics under our belt, we are now in a position to introduce what it means to learn. The "learning" part of machine learning boils down to estimating parameters based on training data.

In this section we consider the case of a predictor that is a function,

and consider the case of probabilistic models in Section 8.2. We describe the idea of empirical risk minimization, which was originally popularized by the proposal of the support vector machine (described in Chapter 12). However, its general principles are widely applicable and allows us to ask the question of what is learning without explicitly constructing probabilistic models. There are four main design choices, which we will cover in detail in the following subsections:

Section 8.1.1 What is the set of functions we allow the predictor to take?

Section 8.1.2 How do we measure how well the predictor performs on the training data?

Section 8.1.3 How do we construct predictors from only training data that performs well on unseen test data?

Section 8.1.4 What is the procedure for searching over the space of models?

8.1.1 Hypothesis Class of Functions

Assume we are given N examples $\boldsymbol{x}_n \in \mathbb{R}^D$ and corresponding scalar labels $y_n \in \mathbb{R}$. We consider the supervised learning setting, where we obtain pairs $(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)$. Given this data, we would like to estimate a predictor $f(\cdot, \boldsymbol{\theta}) : \mathbb{R}^D \to \mathbb{R}$, parameterized by $\boldsymbol{\theta}$. We hope to be able to find a good parameter $\boldsymbol{\theta}^*$ such that we fit the data well

$$f(\boldsymbol{x}_n, \boldsymbol{\theta}^*) \approx y_n \quad \text{for all} \quad n = 1, \dots, N\,. \tag{8.3}$$

In this section, we use the notation $\hat{y}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta}^*)$ to represent the output of the predictor.

Example 8.1
We introduce the problem of least squares regression to illustrate empirical risk minimization. A more comprehensive account of regression is given in Chapter 9. When the label y_n is real valued, a popular choice of function class for predictors is the set of linear functions,

$$f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}_n + \theta_0\,. \tag{8.4}$$

Observe that the predictor takes the vector of features representing a single example $\boldsymbol{x}_n$ as input and produces a real valued output. That is $f : \mathbb{R}^D \to \mathbb{R}$. The previous figures in this chapter had a straight line as a predictor, which means that we have assumed a linear function. For notational convenience we often concatenate an additional unit feature to $\boldsymbol{x}_n$, that is $\tilde{\boldsymbol{x}}_n = \begin{bmatrix} \boldsymbol{x}_n \\ 1 \end{bmatrix}$. This is so that we can correspondingly concatenate the

parameter vector $\tilde{\boldsymbol{\theta}} = \begin{bmatrix} \boldsymbol{\theta} \\ \theta_0 \end{bmatrix}$, and write the linear predictor as

$$f(\tilde{\boldsymbol{x}}_n, \tilde{\boldsymbol{\theta}}) = \tilde{\boldsymbol{\theta}}^\top \tilde{\boldsymbol{x}}_n \,. \tag{8.5}$$

We will often overload the notation in this book to have tidier presentation: $\boldsymbol{x}_n$ is used to mean the new concatenated vector.

Instead of a linear function, we may wish to consider non-linear functions as predictors. Recent advances in neural network frameworks allowed for efficient computation of more complex non-linear function classes.

Remark. For ease of presentation we will describe empirical risk minimization in terms of supervised learning. This simplifies the definition of the hypothesis class and the loss function. ♢

Given the class of functions we want to search for a good predictor, we now move on to the second ingredient of empirical risk minimization: how to measure how well the predictor fits the training data.

8.1.2 Loss Function for Training

Consider the label y_n for particular example; and the corresponding prediction $\hat{y}_n$ that we make based on $\boldsymbol{x}_n$. To define what it means to fit the data well, we need to specify a *loss function* $\ell(y_n, \hat{y}_n)$ that takes two values as input and produces a non-negative number (referred to as the loss) representing how much error we have made on this particular prediction. Our goal for finding a good parameter vector $\boldsymbol{\theta}^*$ is to minimize the average loss on the set of N training examples.

loss function

The word error is often used to mean loss.

One assumption that is commonly made in machine learning is that the set of examples $(x_1, y_1), \ldots, (x_N, y_N)$ are *independent and identically distributed*. The word independent (Section 6.4.3) means that two data points (x_i, y_i) and (x_j, y_j) do not statistically depend on each other, meaning that the empirical mean is a good estimate of the population mean (Section 6.4.1). This implies that we can use the empirical mean of the loss on the training data. For a given *training set* $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\}$ which we collect into an example matrix $\boldsymbol{X}$ and label vector $\boldsymbol{y}$, the average loss is given by

independent and identically distributed

training set

$$\mathbf{R}_{\text{emp}}(f, \boldsymbol{X}, \boldsymbol{y}) = \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \hat{y}_n) \tag{8.6}$$

where $\hat{y}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta}^*)$. Equation (8.6) is called the *empirical risk*. Note that the empirical risk depends on three arguments, the predictor f and the data $\boldsymbol{X}, \boldsymbol{y}$. This general strategy for learning is called *empirical risk minimization*.

empirical risk

empirical risk minimization

Example 8.2
Continuing the example of least squares regression, we specify that we measure cost of making an error during training using the squared loss $\ell(y_n, \hat{y}_n) = (y_n - \hat{y}_n)^2$. We wish to minimize the empirical risk, which is the average of the losses over the data

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^{N} (y_n - f(\boldsymbol{x}_n, \boldsymbol{\theta}))^2, \tag{8.7}$$

where we have substituted the predictor $\hat{y}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta})$. By using our choice of a linear predictor $f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}_n$ we obtain the optimization problem

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \sum_{n=1}^{N} (y_n - \boldsymbol{\theta}^\top \boldsymbol{x}_n)^2 \,. \tag{8.8}$$

This equation can be equivalently expressed in matrix form by collecting the labels into a vector $\boldsymbol{y} := [y_1, \ldots, y_N]^\top \in \mathbb{R}^N$ and collecting the dataset into a matrix $\boldsymbol{X} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]^\top \in \mathbb{R}^{N \times D}$.

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2 \,. \tag{8.9}$$

This is known as the least squares problem. There is a closed-form analytic solution for this, by solving the normal equations, which we will discuss in Section 9.2.

Note that we are not interested in a predictor that only performs well on the training data. We are actually interested in a predictor that performs well (has low risk) on unseen test data. More formally we are interested in finding a predictor f (with parameters fixed) that minimizes *expected risk*

expected risk

$$\mathbf{R}_{\text{true}}(f) = \mathbb{E}_{\boldsymbol{x},y} \ell(y, f(\boldsymbol{x})) \tag{8.10}$$

where y is the ground truth label, and $f(\boldsymbol{x})$ is the prediction based on the data $\boldsymbol{x}$. The notation $\mathbf{R}_{\text{true}}(f)$ indicates that this is the true risk if we had access to an infinite amount of data. The expectation is over the (infinite) set of all possible data and labels. There are two practical questions that arise from our desire to minimize expected risk which we address in the following two subsections:

Another phrase commonly used for expected risk is the population risk.

- How should we change our training procedure to generalize well?
- How do we estimate expected risk from (finite) data?

Remark. Many machine learning tasks are specified with an associated performance measure, e.g., accuracy of prediction or root mean squared error. The performance measure could be more complex, be cost sensitive

and capture details about the particular application. In principle, the design of the loss function for empirical risk minimization should correspond directly to the performance measure specified by the machine learning task. In practice there is a often mismatch between the design of the loss function and the performance measure. This could be due to issues such as ease of implementation or efficiency of optimization. ♢

8.1.3 Regularization to Reduce Overfitting

This section describes an addition to empirical risk minimization that allows it to generalize well (minimizing expected risk). Recall that the aim of training a machine learning predictor is so that we can perform well on unseen data, that is the predictor generalizes well. This unseen data is referred to as the *test set*. Given a sufficiently rich class of functions for the predictor f, we can essentially memorize the training data to obtain zero empirical risk. While this is great to minimize the loss (and therefore the risk) on the training data, we would not expect the predictor to generalize well to unseen data. In practice we have only a finite set of data, and hence we split our data into a training and a test set. The training set is used to fit the model, and the test set (not seen by the machine learning algorithm during training) is used to evaluate generalization performance. We use the subscript $_{\text{train}}$ and $_{\text{test}}$ to denote the training and test set respectively. We will revisit this idea of using a finite dataset to evaluate expected risk in Section 8.1.4.

test set

It turns out that empirical risk minimization can lead to *overfitting*, that is the predictor fits too closely to the training data and does not generalize well to new data (Mitchell, 1997). This general phenomenon of having very small training loss but large test loss tends to occur when we have little data and a complex hypothesis class. For a particular predictor f (with parameters fixed), the phenomenon of overfitting occurs when the risk estimate from the training data $\mathbf{R}_{\text{emp}}(f, \boldsymbol{X}_{\text{train}}, \boldsymbol{y}_{\text{train}})$ underestimates the expected risk $\mathbf{R}_{\text{true}}(f)$. Since we estimate the expected risk $\mathbf{R}_{\text{true}}(f)$ by using the empirical risk on the test set $\mathbf{R}_{\text{emp}}(f, \boldsymbol{X}_{\text{test}}, \boldsymbol{y}_{\text{test}})$ if the test risk is much larger than the training risk, this is an indication of overfitting.

overfitting

Therefore, we need to somehow bias the search for the minimizer of empirical risk by introducing a penalty term, which makes it harder for the optimizer to return an overly flexible predictor. In machine learning, the penalty term is referred to as *regularization*. Regularization is a way to compromise between accurate solution of empirical risk and the size or complexity of the solution.

regularization

Example 8.3
Regularization is used to improve the conditioning of ill-conditioned least squares problems. The simplest regularization strategy is to replace the

least squares problem in the previous example

$$\min_{\boldsymbol{\theta}} \frac{1}{N} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2 \ . \tag{8.11}$$

with the "regularized" problem by adding a penalty term involving only $\boldsymbol{\theta}$

$$\min_{\boldsymbol{\theta}} \frac{1}{N} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|^2 \ . \tag{8.12}$$

The additional term $\|\boldsymbol{\theta}\|^2$ is known as a regularizer, and the parameter λ is known as the regularization parameter. The regularization parameter trades off minimizing the loss on the training set and the size of the parameters $\boldsymbol{\theta}$.

The constant $\frac{1}{2}$ in front of the regularizer is so that when we take the derivative, the square and the half cancels.

The regularization term is sometimes called the penalty term, what biases the vector $\boldsymbol{\theta}$ to be closer to the origin. The idea of regularization also appears in probabilisitic models as the prior probability of the parameters. Recall from Section 6.7 that for the posterior distribution to be of the same form as the prior, the prior distribution and the likelihood need to be conjugate distributions. We will revisit this idea in Section 8.2.2. We will see in Chapter 12 that the idea of the regularizer is equivalent to the idea of a large margin.

8.1.4 Cross Validation to Assess the Generalization Performance

We mentioned in the previous section that we measure generalization error by estimating it by applying the predictor on test data. This data is also sometimes referred to as the *validation set*. The validation set is a subset of the available training data that we keep aside. A practical issue with this approach is that the amount of data is limited, and ideally we would use as much of the data available to train the model. This would require to keep our validation set $\mathcal{V}$ small, which then would lead to a noisy estimate (with high variance) of the predictive performance. One solution to these contradictory objectives (large training set, large validation set) is to use *cross validation*. K-fold cross validation effectively partitions the data into K chunks, $K-1$ of which form the training set $\tilde{\mathcal{D}}$, and the last chunk serves as the validation set $\mathcal{V}$ (similar to the idea outlined above). Cross-validation iterates through (ideally) all combinations of assignments of chunks to $\tilde{\mathcal{D}}$ and $\mathcal{V}$, see Figure 8.4. This procedure is repeated for all K choices for the validation set, and the performance of the model from the K runs is averaged.

validation set

cross validation

We partition our training set into two sets $\mathcal{D} = \tilde{\mathcal{D}} \cup \mathcal{V}$, such that they do not overlap $\tilde{\mathcal{D}} \cap \mathcal{V} = \emptyset$, where $\mathcal{V}$ is the validation set, and train our model on $\tilde{\mathcal{D}}$. After training, we assess the performance of the predictor f on the validation set $\mathcal{V}$ (e.g., by computing root mean square error (RMSE)

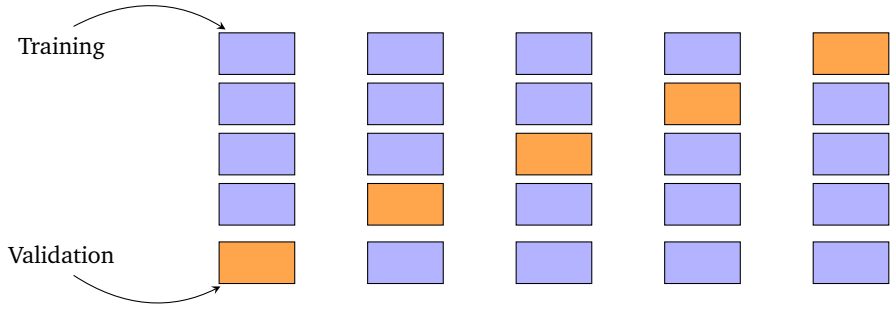


Figure 8.4 K-fold cross validation. The data set is divided into $K = 5$ chunks, $K - 1$ of which serve as the training set (blue) and one as the validation set (orange).

of the trained model on the validation set). We cycle through all possible partitionings of validation and training sets and compute the average generalization error of the predictor. Cross-validation effectively computes the expected generalization error

$$\mathbb{E}_{\mathcal{V}}[\mathbf{R}(f, \mathcal{V})] \approx \frac{1}{K} \sum_{k=1}^{K} \mathbf{R}(f, \mathcal{V}^{(k)}) \,, \tag{8.13}$$

where $\mathbf{R}(f, \mathcal{V})$ is the risk (e.g., RMSE) on the validation set $\mathcal{V}$ for predictor f.

A potential disadvantage of K-fold cross validation is the computational cost of training the model K times, which can be burdensome if the training cost is computationally expensive. In practice, it is often not sufficient to look at the direct parameters alone. For example, we need to explore multiple complexity parameters (e.g., multiple regularization parameters), which may not be direct parameters of the model. Evaluating the quality of the model, depending on these hyper-parameters may result in a number of training runs that is exponential in the number of model parameters.

However, cross validation is an *embarrassingly parallel* problem, i.e., little effort is needed to separate the problem into a number of parallel tasks. Given sufficient computing resources (e.g., cloud computing, server farms), cross validation does not require longer than a single performance assessment.

embarrassingly parallel

Further Reading

Due to the fact that the original development of empirical risk minimization (Vapnik, 1998) was couched in heavily theoretical language, many of the subsequent developments have been theoretical. The area of study is called *statistical learning theory* (von Luxburg and Schölkopf, 2011; Vapnik, 1999; Evgeniou et al., 2000). A recent machine learning textbook that builds on the theoretical foundations and develops efficient learning algorithms is Shalev-Shwartz and Ben-David (2014).

statistical learning theory

The idea of regularization has its roots in the solution of ill-posed in-

verse problems (Neumaier, 1998). It has deep relationships to the bias variance tradeoff and feature selection (Bühlmann and Geer, 2011).

An alternative to cross validation is bootstrap and jackknife (Efron and Tibshirani, 1993; Davidson and Hinkley, 1997; Hall, 1992).

8.2 Parameter Estimation

In Section 8.1 we did not explicitly model our problem using probability distributions. In this section, we will see how to use probability distributions to model our uncertainty due to the observation process and our uncertainty in the parameters of our predictors.

8.2.1 Maximum Likelihood Estimation

maximum likelihood estimation

likelihood

The idea behind *maximum likelihood estimation* (MLE) is to define a function of the parameters that enables us to find a model that fits the data well. The estimation problem is focused on the *likelihood* function, or more precisely its negative logarithm. For data represented by random variable $\boldsymbol{x}$ and for a family of probability densities $p(\boldsymbol{x} \mid \boldsymbol{\theta})$ parameterized by $\boldsymbol{\theta}$, the *negative log likelihood* is given by

negative log likelihood

$$\mathcal{L}_{\boldsymbol{x}}(\boldsymbol{\theta}) = -\log p(\boldsymbol{x} \mid \boldsymbol{\theta}). \tag{8.14}$$

The notation $\mathcal{L}_{\boldsymbol{x}}(\boldsymbol{\theta})$ emphasizes the fact that the parameter $\boldsymbol{\theta}$ is varying and the data $\boldsymbol{x}$ is fixed. We very often drop the reference to $\boldsymbol{x}$ when writing the negative log likelihood, as it is really a function of $\boldsymbol{\theta}$, and write it as $\mathcal{L}(\boldsymbol{\theta})$ when the random variable representing the uncertainty in the data is clear from the context.

Let us intepret what the probability density $p(\boldsymbol{x} \mid \boldsymbol{\theta})$ is modelling for a fixed value of $\boldsymbol{\theta}$. It is a distribution that models the uncertainty of the data. In other words, once we have chosen the type of function we want as a predictor, the likelihood provides the probability of observing data $\boldsymbol{x}$.

In a complementary view, if we consider the data to be fixed (because it has been observed), and we vary the parameters $\boldsymbol{\theta}$, what does $\mathcal{L}(\boldsymbol{\theta})$ tell us? It tells us the (negative log) likelihood of that parameter setting. Based on this second view, the maximum likelihood estimator is the parameter setting that maximizes the function.

We consider the supervised learning setting, where we obtain pairs $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$ with $\boldsymbol{x}_n \in \mathbb{R}^D$ and labels $y_n \in \mathbb{R}$. We are interested in constructing a predictor that takes a feature vector $\boldsymbol{x}_n$ as input and produces a prediction y_n (or something close to it). That is given a vector $\boldsymbol{x}_n$ we want the probability distribution of the label y_n. In other words we specify the conditional probability distribution of the labels given the examples for the particular parameter setting $\boldsymbol{\theta}$.

Example 8.4
The first example that is often used is to specify that the conditional probability of the labels given the examples is a Gaussian distribution. In other words we assume that we can explain our observation uncertainty by independent Gaussian noise (refer to Section 6.6) with zero mean, $\varepsilon_n \sim \mathcal{N}(0, \sigma^2)$. We further assume that the linear model $\boldsymbol{x}_n^\top \boldsymbol{\theta}$ is used for prediction. This means we specify a Gaussian likelihood for each example label pair $\boldsymbol{x}_n, y_n$,

$$p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) = \mathcal{N}\left(y_n \mid \boldsymbol{x}_n^\top \boldsymbol{\theta}, \sigma^2\right). \tag{8.15}$$

An illustration of a Gaussian likelihood for a given parameter $\boldsymbol{\theta}$ is shown in Figure 8.3. We will see in Section 9.2 how to explicitly expand the expression above out in terms of the Gaussian distribution.

We assume that the set of examples $(x_1, y_1), \ldots, (x_N, y_N)$ are *independent and identically distributed*. The word independent (Section 6.4.3) implies that the likelihood of the whole dataset ($\boldsymbol{y} = [y_1, \ldots, y_N]^\top$ and $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]^\top \in \mathbb{R}^{N \times D}$) factorizes into a product of the likelihoods of each individual example

independent and identically distributed

$$p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta}) = \prod_{n=1}^{N} p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}), \tag{8.16}$$

where $p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta})$ is a particular distribution (which was Gaussian in the example above (8.15)). The word identically distributed means that each term in the product above is the same and all of them share the same parameters. It is often easier from an optimization viewpoint to compute functions that can be decomposed into sums of simpler functions, and hence in machine learning we often consider the negative log-likelihood

Recall $\log(ab) = \log(a) + \log(b)$

$$\mathcal{L}(\boldsymbol{\theta}) = -\log p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}). \tag{8.17}$$

While it is temping to interpret the fact that $\boldsymbol{\theta}$ is on the right of the conditioning in $p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta})$ (8.15), and hence should be intepreted as observed and fixed, this interpretation is incorrect. The negative log likelihood $\mathcal{L}(\boldsymbol{\theta})$ is a function of $\boldsymbol{\theta}$.

Therefore, to find a good parameter vector $\boldsymbol{\theta}$ that explains the data $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$ well, we look for a $\boldsymbol{\theta}$ that minimizes the negative log likelihood

$$\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}). \tag{8.18}$$

Remark. The negative sign in (8.17) is a historical artefact that is due to the convention that we want to maximize likelihood, but numerical optimization literature tends to study minimization of functions. ♢

Example 8.5
Continuing on our example of Gaussian likelihoods (8.15), the negative log likelihood can be rewritten as

$$\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n, \boldsymbol{\theta}) \tag{8.19}$$

$$= -\sum_{n=1}^{N} \log \mathcal{N}\left(y_n \mid \boldsymbol{x}_n^\top \boldsymbol{\theta},\, \sigma^2\right) \tag{8.20}$$

$$= -\sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_n - \boldsymbol{x}_n^\top \boldsymbol{\theta})^2}{2\sigma^2}\right) \tag{8.21}$$

$$= -\sum_{n=1}^{N} \log \exp\left(-\frac{(y_n - \boldsymbol{x}_n^\top \boldsymbol{\theta})^2}{2\sigma^2}\right) - \sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}} \tag{8.22}$$

$$= \sum_{n=1}^{N} \frac{(y_n - \boldsymbol{x}_n^\top \boldsymbol{\theta})^2}{2\sigma^2} - \sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}}. \tag{8.23}$$

$$\tag{8.24}$$

Observe that the first term in the last equation above is the least squares problem.

It turns out that for Gaussian likelihoods the resulting optimization problem corresponding to maximum likelihood estimation has a closed-form solution. We will see more details on this in Chapter 9. For other likelihood functions, i.e., if we model our noise with non-Gaussian distributions, maximum likelihood estimation may not have a closed-form analytic solution. In this case, we resort to numerical optimization methods discussed in Chapter 7.

8.2.2 Maximum A Posteriori Estimation

If we have prior knowledge about the distribution of the parameters $\boldsymbol{\theta}$ of our distribution we can multiply an additional term to the likelihood. This additional term is a prior probability distribution on parameters $p(\boldsymbol{\theta})$. For a given prior, after observing some data $\boldsymbol{x}$, how should we update the distribution of $\boldsymbol{\theta}$? In other words, how should we represent the fact that we have more specific knowledge after observing data $\boldsymbol{x}$? Bayes' theorem, as discussed in Section 6.3, gives us a principled tool to update our probability distributions of random variables. It allows us to compute a *posterior* distribution $p(\boldsymbol{\theta} \mid \boldsymbol{x})$ (the more specific knowledge) on the paramters $\boldsymbol{\theta}$ from general *prior* statements (prior distribution) $p(\boldsymbol{\theta})$ and the function $p(\boldsymbol{x} \mid \boldsymbol{\theta})$ that links the parameters $\boldsymbol{\theta}$ and the observed data $\boldsymbol{x}$ (called the *likelihood*):

posterior

prior

likelihood

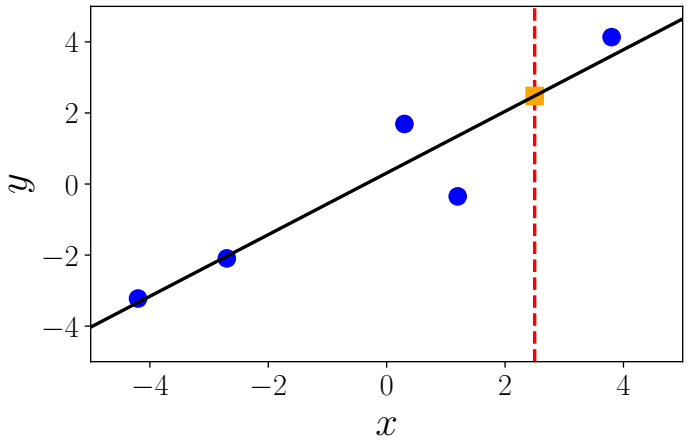


Figure 8.5 For the given data, the maximum likelihood estimate of the parameters results in the black diagonal line. The orange square shows the value of the maximum likelihood prediction at $x = 2.5$.

$$p(\boldsymbol{\theta} \mid \boldsymbol{x}) = \frac{p(\boldsymbol{x} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{x})} . \tag{8.25}$$

Recall that we are interested in finding the parameter $\boldsymbol{\theta}$ that maximizes likelihood, and the distribution $p(\boldsymbol{x})$ affects the value of the likelihood, but does not affect the value of the parameter that achieves the maximum likelihood. Therefore we can ignore the value of the denominator,

$$p(\boldsymbol{\theta} \mid \boldsymbol{x}) \propto p(\boldsymbol{x} \mid \boldsymbol{\theta})p(\boldsymbol{\theta}) . \tag{8.26}$$

The proportion relation above hides the density of the data $p(\boldsymbol{x})$ which may be difficult to estimate. Instead of estimating the minimum of the negative log likelihood, we now estimate the minimum of the negative log posterior, which is referred to as *maximum a posteriori estimation* (MAP).

maximum a posteriori estimation

Example 8.6
In addition to the assumption of Gaussian likelihood in the previous example, we assume that the parameter vector is distributed as a multivariate Gaussian with zero mean, that is $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$ where $\boldsymbol{\Sigma}$ is the covariance matrix (Section 6.6). Note that the conjugate prior of a Gaussian is also a Gaussian (Section 6.7.1) and therefore we expect the posterior distribution to also be a Gaussian. We will see the details of maximum a posteriori estimation in Chapter 9.

The idea of including prior knowledge about where good parameters lie is widespread in machine learning. An alternative view which we saw in Section 8.1 is the idea of regularization, which introduces an additional term that biases the resulting parameters to be close to the origin.

Remark. The maximum likelihood estimate $\boldsymbol{\theta}_{\text{ML}}$ possesses the following properties (Lehmann and Casella, 1998; Efron and Hastie, 2016):

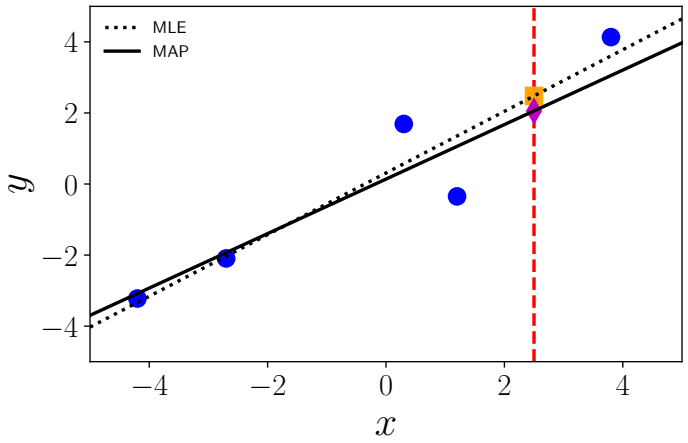


Figure 8.6 Comparing the Maximum Likelihood estimate and the Maximum A Posteriori estimate and their predictions at $x = 2.5$. The prior biases the slope to be less steep and the intercept to be closer to zero.

- Asymptotic consistency: The MLE converges to the true value in the limit of infinitely many observations, plus a random error that is approximately normal.
- The size of the samples necessary to achieve these properties can be quite large.
- The error's variance decays in $1/N$ where N is the number of data points.
- Especially, in the "small" data regime, maximum likelihood estimation can lead to *overfitting*.

♢

Further Reading

When considering probabilistic models the principle of maximum likelihood estimation generalizes the idea of least-squares regression for linear models (which we will discuss in detail in Chapter 9). When restricting the predictor to have linear form with an additional nonlinear function φ applied to the output,

$$p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta}) = \varphi(\boldsymbol{\theta}^\top \boldsymbol{x}_n) \tag{8.27}$$

we can consider other models for other prediction tasks, such as binary classification or modelling count data (McCullagh and Nelder, 1989). An alternative view of this is to consider likelihoods that are from the exponential family (Section 6.7). The class of models, which have linear dependence between parameters and data, and have potentially nonlinear transformation φ (called a link function) is referred to as generalized linear models (Agresti, 2002, Chapter 4).

Maximum likelihood estimation has a rich history, and was originally proposed by Sir Ronald Fisher in the 1930s. We will expand upon the idea of a probabilistic model in Section 8.3. One debate among researchers

who use probabilistic models, is the discussion between Bayesian and frequentist statistics. As mentioned in Section 6.1.1 it boils down to the definition of probability. Recall that one can consider probability to be a generalization of logical reasoning to allow for uncertainty (Cheeseman, 1985; Jaynes, 2003). The method of maximum likelihood estimation is frequentist in nature, and the interested reader is pointed to Efron and Hastie (2016) for a balanced view of both Bayesian and frequentist statistics.

There are some probabilisitic models where maximum likelihood estimation may not be possible. The reader is referred to more advanced statistical textbooks, e.g., Casella and Berger (2002), for approaches such as method of moments, M-estimation and estimating equations.

8.3 Probabilistic Modeling

In machine learning, we are frequently concerned with the interpretation and analysis of data, e.g., for prediction of future events and decision making. To make this task more tractable, we often build models that describe the process that generates the data. For example, when we want to describe the outcome of a coin-flip experiment, we can describe this process using a Bernoulli distribution as described in Chapter 6. In this example, we can say that an outcome $x \in \{\text{head, tail}\}$ can be described as the conditional distribution $p(x \mid \mu)$ where x is the outcome of the experiment and μ is the probability of "heads".

In this section, we will focus on probabilisitic models. The benefit of using probabilistic models is that we have the set of tools from probability (Chapter 6) available to us for modeling, inference, parameter estimation and model selection.

Remark. Thinking about empirical risk minimization (Section 8.1) as "probability free" is incorrect. There is an underlying unknown probability distribution $p(\boldsymbol{x}, y)$ that governs the data generation, but the approach of empirical risk minimization is agnostic to that choice of distribution. This is in contrast to standard statistical approaches that require the knowledge of $p(\boldsymbol{x}, y)$. Furthermore, since the distribution is a joint distribution on both examples $\boldsymbol{x}$ and labels y, the labels can be non-deterministic. In contrast to standard statistics we do not need to specify the noise distribution for the labels y. ♢

8.3.1 MLE, MAP, and Bayesian Inference

Let us revisit the discussion about modeling with probability distributions we had at the beginning of this chapter. There are three levels where we can use a probability distribution. At the first level, we can use a probability distribution to model our uncertainty about the observation. For example, in (8.15) we make the assumption that there is Gaussian noise

(with mean 0 and variance σ^2) that corrupts the observation of a linear function. A way to express this is to write

$$y_n = \boldsymbol{x}_n^\top \boldsymbol{\theta} + \varepsilon \quad \text{where} \quad \varepsilon \sim \mathcal{N}\left(0, \sigma^2\right). \tag{8.28}$$

By making this assumption, we obtain the likelihood described in Section 8.2.1 where we can then maximize.

At the second level, we can use a probability distribution to describe our uncertainty about the parameters $\boldsymbol{\theta}$. This is detailed in Section 8.2.2, where we place a probability distribution to model the parameter vector $\boldsymbol{\theta}$ that encodes our beliefs about the unknown parameters. The probability distribution over parameters is known as the prior distribution, and by using Bayes' Theorem we obtain the posterior distribution over the parameters $\boldsymbol{\theta}$, which describes an "updated" prior belief, i.e., the belief about the unknown parameters *after* having seen some data. Instead of maximizing the likelihood, we can maximize the posterior with respect to the model parameters $\boldsymbol{\theta}$. This approach is called *maximum a posteriori estimation* (*MAP estimation*), and it will generally yield a different result than maximum likelihood estimation. Note that in both maximum likelihood and maximum a posteriori cases in the previous paragraphs, the estimated best solution is a single value of the parameter $\boldsymbol{\theta}$.

maximum a posteriori estimation

MAP estimation

With maximum likelihood or MAP estimates, we obtain a single best parameter setting $\boldsymbol{\theta}^*$, which we can use when making predictions. More specifically, when predicting an outcome $\boldsymbol{x}_*$ we can do this by using $\boldsymbol{\theta}^*$ directly in the likelihood function that connects parameters and data to obtain a prediction $p(\boldsymbol{x}_* \mid \boldsymbol{\theta}^*)$. At the third level, we can use a probability distribution when making predictions, instead of focusing on a single parameter setting $\boldsymbol{\theta}^*$. To do so, we maintain a full probability distribution on the parameters (MLE and MAP estimation pick a single parameter value) and make predictions by accounting for all plausible parameter settings $\boldsymbol{\theta}$ under this distribution. This is done by (weighted) averaging, i.e., integration so that the predictive distribution

$$p(\boldsymbol{x}_*) = \mathbb{E}_{\boldsymbol{\theta}}[p(\boldsymbol{x}_* \mid \boldsymbol{\theta})] = \int p(\boldsymbol{x}_* \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta} \tag{8.29}$$

no longer depends on the parameters $\boldsymbol{\theta}$ – they have been marginalized/ integrated out. This is referred to as *Bayesian inference*.

Bayesian inference

8.3.2 Latent Variables

Taking a probabilistic view of machine learning implies that we also want to treat predictors (models) as random variables. While data $x_1, \ldots, x_N$ can be observed, these models themselves possess quantities/parameters that are not directly observed. In the coin-flip experiment described in the introduction to this section, the probability μ of "heads" is typically not

known and depends on the coin we use. We describe these kind of unknown quantities with a random variable. Given that these random variables cannot be observed but only inferred we call them *hidden variables* or *latent variables*. While we can make general statements about plausible values of these latent variables prior to observing any data (e.g., by using a prior distribution), a key challenge in machine learning is to infer more about these unobserved variables given a dataset.

hidden variables

latent variables

Remark. We tend to use the notation $\boldsymbol{\theta}$ to represent the vector of unobserved random variables. We also refer to $\boldsymbol{\theta}$ as the *parameters* of the model. ♢

parameters

Recall from Section 8.2.2 that Bayes' Theorem gives us a principled tool to update our probability distribution over $\boldsymbol{\theta}$ given observed data. Here we go from a prior distribution on the latent variables to a posterior distribution after taking the likelihood into account. Since we can write the numerator of (8.25) as the joint distribution $p(\boldsymbol{\theta}, \boldsymbol{x}) = p(\boldsymbol{x} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})$ of the latent variables and the data, this joint distribution is of central importance and sufficient to compute the quantities of interest, either by conditioning or marginalization (Section 6.2.1). For example, we obtain the posterior distribution by conditioning so that we can make informed statements about the latent variables, and we obtain the marginal likelihood (evidence) $p(\boldsymbol{x})$ via marginalization where we integrate out the latent variables. The marginal likelihood is very useful for model selection as we will discuss in Section 8.5. Hence, we can define a probabilistic model in machine learning as the joint distribution $p(\boldsymbol{\theta}, \boldsymbol{x})$ of all latent and observed variables.

A probabilistic model in machine learning describes the joint distribution of all latent and observed variables.

As mentioned above, in machine learning, it is important to get some information about the latent variables given a dataset. The posterior distribution $p(\boldsymbol{\theta} \mid \boldsymbol{x})$ gives us complete information about the parameters after observing the data. We can then use the full posterior distribution to make statements about future outcomes by averaging over all plausible settings of the latent variables, that is we can predict/generate/fantasize/hallucinate new data via

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}\,. \tag{8.30}$$

Unfortunately, in most cases (in particular, when we choose non-conjugate priors), we cannot compute the posterior distribution using Bayes' theorem because the computations quickly become intractable. A solution to this problem is to estimate a single parameter vector $\boldsymbol{\theta}^*$ that explains the available data "best", e.g., by maximum likelihood estimation as discussed in Section 8.2. Then, we can make a prediction of new data directly via the likelihood $p(\boldsymbol{x} \mid \boldsymbol{\theta}^*)$ – without needing integration.

Remark. In the machine learning literature, there can be a somewhat arbitrary separation between "variables" and "parameters". While parame-

ters are estimated (e.g., via maximum likelihood) variables are usually marginalized out as in (8.30). In this book, we are not so strict with this separation because, in principle, we can place a prior on any parameter and integrate it out, which would then turn the parameter into a variable according to the separation above. ♢

There are modelling situations in machine learning where we may wish to introduce new random variables $\boldsymbol{z}$ into the problem. In these scenarios, the direct model of the problem (involving only $\boldsymbol{x}, \boldsymbol{\theta}$) may be computationally difficult to solve, but introducing a set of latent variables $\boldsymbol{z}$ allows us to design an efficient algorithm. We will see an example of this in Chapter 11, where we introduce the Gaussian mixture model and use it for density estimation.

Further Reading

Probabilistic models in machine learning Bishop (2006); Barber (2012); Murphy (2012) provide a way for users to capture uncertainty about data and predictive models in a principled fashion. Ghahramani (2015) presents a short review of probabilistic models in machine learning. Given a probabilistic model, we may be lucky enough to be able to compute parameters of interest analytically. However, in general, analytic solutions are rare and computational methods such as sampling (Brooks et al., 2011) and variational inference (Blei et al., 2017) are used.

In recent years, there have been several proposed programming languages that aim to treat the variables defined in software as random variables corresponding to probability distributions. The long-term dream is to be able to write complex functions of probability distributions, while under the hood the compiler automatically takes care of the rules of Bayesian inference. This is a rapidly changing field, but several examples of promising languages at the present are:

Stan `http://mc-stan.org/`
Edward `http://edwardlib.org/`
PyMC `https://docs.pymc.io/`
Pyro `http://pyro.ai/`
Tensorflow Probability `https://github.com/tensorflow/probability`
Infer.NET `http://infernet.azurewebsites.net/`

8.4 Directed Graphical Models

In this section we introduce a graphical language for specifying a probabilistic models, called the *directed graphical model*. They provides a compact and succinct way to specify probabilistic models, and allows the reader to visually parse dependencies between random variables. A graphical model visually captures the way in which the joint distribution over

directed graphical model

Directed graphical models are also known as Bayesian networks.

all random variables can be decomposed into a product of factors depending only on a subset of these variables. In Section 8.3, we identified the joint distribution of a probabilistic model as the key quantity of interest because it comprises information about the prior, the likelihood and the posterior. However, the joint distribution by itself can be quite complicated, and it does not tell us anything about structural properties of the probabilistic model. For example, the joint distribution $p(a, b, c)$ does not tell us anything about independence relations. This is the point where graphical models come into play. This section relies on the concepts of independence and conditional independence, as described in Section 6.4.3.

In a *graphical model*, nodes are random variables; in Figure 8.7(a), the nodes of the random variables a, b, c represent their respective (marginal) probabilities $p(a)$, $p(b)$ and $p(c)$. Edges represent probabilistic relations between variables, e.g., conditional probabilities.

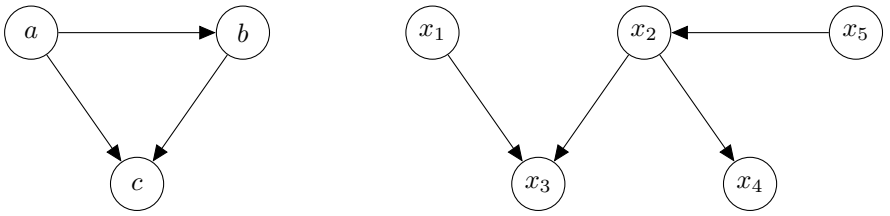
graphical model

Remark. Not every distribution can be represented in a particular choice of graphical model. A discussion of this can be found in Bishop (2006). ♢

Probabilistic graphical models have some convenient properties:

- They are a simple way to visualize the structure of a probabilistic model
- They can be used to design or motivate new kind of statistical models
- Inspection of the graph alone gives us insight into properties, e.g., conditional independence
- Complex computations for inference and learning in statistical models can be expressed in terms of graphical manipulations.

8.4.1 Graph Semantics



(a) Fully connected. (b) Not fully connected.

Figure 8.7 Examples of directed graphical models.

Directed graphical models/Bayesian networks are a method for representing conditional dependencies in a probabilistic model. They provide a visual description of the conditional probabilities, hence, providing a simple language for describing complex interdependence. The modular description also entails computational simplification. Directed links (arrows) between two nodes (random variables) are conditional probabilities. For example, the arrow between a and b in Figure 8.7(a) gives the conditional probability $p(b \mid a)$ of b given a.

Directed graphical models
Bayesian networks

With additional assumptions, the arrows can be used to indicate causal relationships (Pearl, 2009), but we do not make these assumptions here.

Directed graphical models can be derived from joint distributions if we know something about their factorization.

Example 8.7
Consider the joint distribution

$$p(a, b, c) = p(c \mid a, b)p(b \mid a)p(a) \tag{8.31}$$

of three random variables a, b, c. The factorization of the joint distribution in (8.31) tells us something about the relationship between the random variables:

- c depends directly on a and b
- b depends directly on a
- a depends neither on b nor on c

For the factorization in (8.31), we obtain the directed graphical model in Figure 8.7(a).

In general, we can construct the corresponding directed graphical model from a factorized joint distribution as follows:

1. Create a node for all random variables
2. For each conditional distribution, we add a directed link (arrow) to the graph from the nodes corresponding to the variables on which the distribution is conditioned on

The graph layout depends on the factorization of the joint distribution.

The graph layout depends on the choice of factorization of the joint distribution.

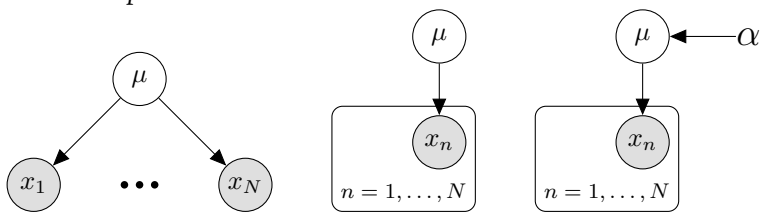
We discussed how to get from a known factorization of the joint distribution to the corresponding directed graphical model. Now, we will go exactly the opposite and describe how to extract the joint distribution of a set of random variables from a given graphical model.

Example 8.8
Let us look at the graphical model in Figure 8.7(b) and exploit two observations:

- The joint distribution $p(x_1, \ldots, x_5)$ we seek is the product of a set of conditionals, one for each node in the graph. In this particular example, we will need five conditionals.
- Each conditional depends only on the parents of the corresponding node in the graph. For example, x_4 will be conditioned on x_2.

With these two properties we arrive at the desired factorization of the joint distribution

$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_5)p(x_2 \mid x_5)p(x_3 \mid x_1, x_2)p(x_4 \mid x_2)\,. \tag{8.32}$$



(a) Version with x_n explicit. (b) Version with plate notation. (c) Hyperparameter α on the latent μ.

Figure 8.8 Graphical models for a repeated Bernoulli experiment.

In general, the joint distribution $p(\boldsymbol{x}) = p(x_1, \ldots, x_K)$ is given as

$$p(\boldsymbol{x}) = \prod_{k=1}^{K} p(x_k \,|\, \text{Pa}_k) \tag{8.33}$$

where Pa_k means "the parent nodes of x_k".

We conclude this subsection with a concrete example of the coin flip experiment. Consider a Bernoulli experiment where the probability that the outcome x of this experiment is "heads" is

$$p(x \,|\, \mu) = \text{Ber}(\mu)\,. \tag{8.34}$$

We now repeat this experiment N times and observe outcomes $x_1, \ldots, x_N$ so that we obtain the joint distribution

$$p(x_1, \ldots, x_N|\mu) = \prod_{n=1}^{N} p(x_n|\mu)\,. \tag{8.35}$$

The expression on the right hand side is a product of Bernoulli distributions on each individual outcome because the experiments are independent. Recall from Section 6.4.3 that statistical independence means that the distribution factorizes. To write the graphical model down for this setting, we make the distinction between unobserved/latent variables and observed variables. Graphically, observed variables are denoted by shaded nodes so that we obtain the graphical model in Figure 8.8(a). We see that the single parameter μ is the same for all x_n, $n = 1, \ldots, N$. A more compact, but equivalent, graphical model for this setting is given in Figure 8.8(b), where we use the *plate* notation. The plate (box) repeats everything inside (in this case the observations x_n) N times. Therefore, both graphical models are equivalent, but the plate notation is more compact. Graphical models immediately allow us to place a hyper-prior on μ. Figure 8.8(c) places a Beta(α) prior on the latent variable μ. If we treat α as a constant (deterministic parameter), i.e., not a random variable, we omit the circle around it.

plate

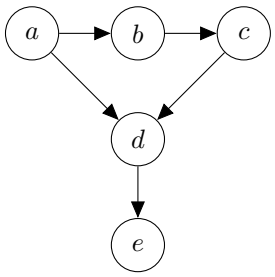


Figure 8.9 D-separation example.

8.4.2 Conditional Independence and D-Separation

Directed graphical models allow us to find conditional independence (Section 6.4.3) relationship properties of the joint distribution only by looking at the graph. A concept called *d-separation* (Pearl, 1988) is key to this.

d-separation

Consider a general directed graph in which $\mathcal{A}, \mathcal{B}, \mathcal{C}$ are arbitrary non-intersecting sets of nodes (whose union may be smaller than the complete set of nodes in the graph). We wish to ascertain whether a particular conditional independence statement, $\mathcal{A}$ is conditionally independent of $\mathcal{B}$ given $\mathcal{C}$, denoted by

$$\mathcal{A} \perp\!\!\!\perp \mathcal{B} \,|\, \mathcal{C}\,, \tag{8.36}$$

is implied by a given directed acyclic graph. To do so, we consider all possible paths from any node in $\mathcal{A}$ to any nodes in $\mathcal{B}$. Any such path is said to be blocked if it includes any node such that either

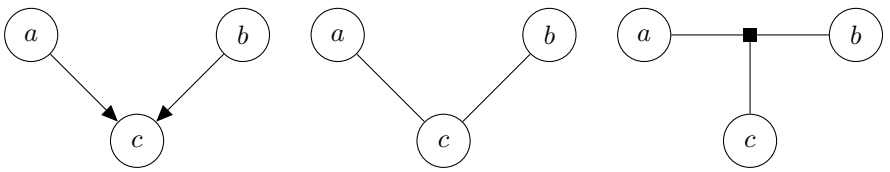
- the arrows on the path meet either head to tail or tail to tail at the node, and the node is in the set $\mathcal{C}$, or
- the arrows meet head to head at the node and neither the node nor any of its descendants is in the set $\mathcal{C}$.

If all paths are blocked, then $\mathcal{A}$ is said to be *d-separated* from $\mathcal{B}$ by $\mathcal{C}$, and the joint distribution over all of the variables in the graph will satisfy $\mathcal{A} \perp\!\!\!\perp \mathcal{B} \,|\, \mathcal{C}$.

Example 8.9 (Conditional Independence)
Consider the graphical model in Figure 8.9. By visual inspection we see that

$$b \perp\!\!\!\perp d \,|\, a, c\,, \tag{8.37a}$$
$$a \perp\!\!\!\perp c \,|\, b\,, \tag{8.37b}$$
$$b \not\perp\!\!\!\perp d \,|\, c\,, \tag{8.37c}$$
$$a \not\perp\!\!\!\perp c \,|\, b, e\,. \tag{8.37d}$$

Directed graphical models allow a compact representation of probabilisitic models, and we will see examples of directed graphical models in



(a) Directed graphical model (b) Undirected graphical model (c) Factor graph

Figure 8.10 Three types of graphical models: (a) Directed graphical models (Bayesian network); (b) Undirected graphical models (Markov random field); (c) Factor graphs.

Chapter 9, 10 and 11. The representation along with the concept of conditional independence, allows us to factorize the respective probabilisitic models into expressions that are easier to optimize.

Further Reading

An introduction to probabilistic graphical models can be found in Bishop (2006, Chapter 8), and an extensive description of the different applications and corresponding algorithmic implications can be found in Koller and Friedman (2009).

There are three main types of probabilistic graphical models:

Directed graphical models

Undirected graphical models

Factor graphs

- *Directed graphical models* (Bayesian networks), see Figure 8.11(a)
- *Undirected graphical models* (Markov random fields), see Figure 8.11(b)
- *Factor graphs*, see Figure 8.11(c)

Graphical models allow for graph-based algorithms for inference and learning, e.g., via local message passing. Applications range from ranking in online games (Herbrich et al., 2007) and computer vision (e.g., image segmentation, semantic labeling, image de-noising, image restoration (Sucar and Gillies, 1994; Shotton et al., 2006; Szeliski et al., 2008; Kittler and Föglein, 1984)) to coding theory (McEliece et al., 1998), solving linear equation systems (Shental et al., 2008) and iterative Bayesian state estimation in signal processing (Bickson et al., 2007; Deisenroth and Mohamed, 2012).

One topic which is particularly important in real applications that we do not discuss in this book is the idea of structured prediction (Bakir et al., 2007; Nowozin et al., 2014) which allow machine learning models to tackle predictions that are structured, for example sequences, trees and graphs. The popularity of neural network models has allowed more flexible probabilistic models to be used, resulting in many useful applications of structured models (Goodfellow et al., 2016, Chapter 16). In recent years, there has been a renewed interest in graphical models due to its applications to causal inference (Rosenbaum, 2017; Pearl, 2009; Imbens and Rubin, 2015; Peters et al., 2017).

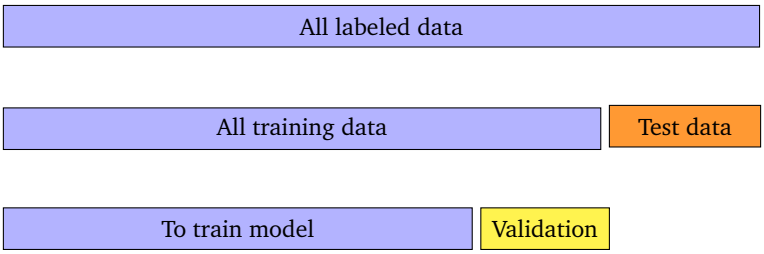


Figure 8.11 Nested cross validation. We perform two levels of K fold cross validation. The inner level is used to estimate the performance of a particular choice of model or hyperparameter on a internal validation set. The outer level is used to estimate generalization performance for *the best choice of model* chosen by the inner loop.

8.5 Model Selection

In machine learning, we often need to make high level modeling decisions that critically influence the performance of the model. The choices we make (e.g., the degree of the polynomial in a regression setting) influence the number and type of free parameters in the model and thereby also the flexibility and expressivity of the model. More complex models are more flexible in the sense that they can be used to describe more data sets. For instance, a polynomial of degree 1 (a line $y = a_0 + a_1 x$) can only be used to describe linear relations between inputs x and observations y. A polynomial of degree 2 can additionally describe quadratic relationships between inputs and observations.

Note that a polynomial $y = a_0 + a_1 x + a_2 x^2$ can also describe linear functions by setting $a_2 = 0$, i.e., it is strictly more expressive than a first-order polynomial.

One would now think that very flexible models are generally preferable to simple models because they are more expressive. A general problem is that at training time we can only use the training set to evaluate the performance of the model and learn its parameters. However, the performance on the training set is not really what we are interested in. In Section 8.2, we have seen that maximum likelihood estimation can lead to overfitting, especially when the training data set is small. Ideally, our model (also) works well on the test set (which is not available at training time). Therefore, we need some mechanisms for assessing how a model *generalizes* to unseen test data. *Model selection* is concerned with exactly this problem.

8.5.1 Nested Cross Validation

We have already seen an approach (cross validation in Section 8.1.4) that can be used for model selection. Recall that cross validation provides an estimate of the generalization error by repeatedly splitting the dataset into training and validation sets. We can apply this idea one more time, that is for each split, we can perform another round of cross validation. This is sometimes referred to as *nested cross validation*. We can test different model and hyperparameter choices in the inner loop. To distinguish the two levels, the set used to estimate the generalization performance is often

nested cross validation

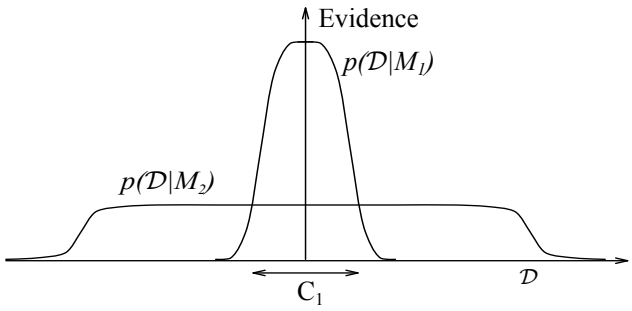


Figure 8.12 Bayesian inference embodies Occam's razor (MacKay, 2003), see text for description.

called the *test set* and the set used for choosing the best model is called the *validation set*.

test set
validation set

$$\mathbb{E}_{\mathcal{V}}[G(\mathcal{V}) \mid M] \approx \frac{1}{K} \sum_{k=1}^{K} G(\mathcal{V}^{(k)} \mid M)\,, \tag{8.38}$$

where $G(\mathcal{V})$ is the generalization error (e.g., RMSE) on the validation set $\mathcal{V}$ for model M. We repeat this procedure for all models and choose the model that performs best. Note that cross-validation not only gives us the expected generalization error, but we can also obtain high-order statistics, e.g., the standard error, an estimate of how uncertain the mean estimate is.

The standard error is defined as $\frac{\sigma}{\sqrt{K}}$, where K is the number of experiments and σ the standard deviation.

Once the model is chosen we can evaluate the final performance on the test set.

8.5.2 Bayesian Model Selection

There are many approaches to model selection, some of which are covered in this section. Generally, they all attempt to trade off model complexity and data fit: The objective is to find the simplest model that explains the data reasonably well. This concept is also known as *Occam's Razor*.

We assume that simpler models are less prone to overfitting than complex models.

Occam's Razor
We are looking for the simplest model that explains the data.

Remark. If we treat model selection as a hypothesis testing problem, we are looking for the simplest hypothesis that is consistent with the data (Murphy, 2012). ♢

One may consider placing a prior on models that favors simpler models. However, it is not necessary to do this: An "automatic Occam's Razor" is quantitatively embodied in the application of Bayesian probability (Spiegelhalter and Smith, 1980; MacKay, 1992; Jefferys and Berger, 1992). Figure 8.12 from MacKay (2003) gives us the basic intuition why complex and very expressive models may turn out to be a less probably choice for modeling a given dataset $\mathcal{D}$. Let us think of the horizontal axis representing the space of all possible datasets $\mathcal{D}$. If we are interested in the posterior probability $p(M_i \mid \mathcal{D})$ of model M_i given the data $\mathcal{D}$, we can

employ Bayes' theorem. Assuming a uniform prior $p(M)$ over all models, Bayes' theorem rewards models in proportion to how much they predicted the data that occurred. This probability of the data given model M_i, $p(\mathcal{D} \mid M_i)$, is called the *evidence* for M_i. A simple model M_1 can only predict a small number of datasets, which is shown by $p(\mathcal{D} \mid M_1)$; a more powerful model M_2 that has, e.g., more free parameters than M_1, is able to predict a greater variety of datasets. This means, however, that M_2 does not predict the datasets in region C_1 as strongly as M_1. Suppose that equal prior probabilities have been assigned to the two models. Then, if the data set falls in region C_1, the less powerful model M_1 is the more probable model.

Note that these predictions are quantified by a normalized probability distribution on $\mathcal{D}$, i.e., it needs to integrate/sum to 1.

evidence

Above, we argued that models need to be able to explain the data, i.e., there should be a way to generate data from a given model. Furthermore if the model has been appropriately learned from the data, then we expect that the generated data should be similar to the empirical data. For this, it is helpful to phrase model selection as a hierarchical inference problem, which allows us to compute the *posterior distribution over models*.

posterior distribution over models

Let us consider a finite number of models $M = \{M_1, \ldots, M_K\}$, where each model M_k possesses parameters $\boldsymbol{\theta}_k$. In *Bayesian model selection*, we place a prior $p(M)$ on the set of models. The corresponding *generative process* that allows us to generate data from this model is

$$M_k \sim p(M) \tag{8.39}$$

$$\boldsymbol{\theta}_k \mid M_k \sim p(\boldsymbol{\theta}_k) \tag{8.40}$$

$$\mathcal{D} \mid \boldsymbol{\theta}_k \sim p(\mathcal{D} \mid \boldsymbol{\theta}_k) \tag{8.41}$$

and illustrated in Figure 8.13.

Figure 8.13 Illustration of the hierarchical generative process in Bayesian model selection. We place a prior $p(M)$ on the set of models. For each model, there is a prior $p(\boldsymbol{\theta}_k \mid M_k)$ on the corresponding model parameters, which are then used to generate the data $\mathcal{D}$.

Bayesian model selection generative process

Given a training set $\mathcal{D}$, we apply Bayes' theorem and compute the posterior distribution over models as

$$p(M_k \mid \mathcal{D}) \propto p(M_k) p(\mathcal{D} \mid M_k) \,. \tag{8.42}$$

Note that this posterior no longer depends on the model parameters $\boldsymbol{\theta}_k$ because they have been integrated out in the Bayesian setting since

$$p(\mathcal{D} \mid M_k) = \int p(\mathcal{D} \mid \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k \mid M_k) d\boldsymbol{\theta}_k \,. \tag{8.43}$$

From the posterior in (8.42), we determine the MAP estimate as

$$M^* = \arg\max_{M_k} p(M_k \mid \mathcal{D}) \,. \tag{8.44}$$

With a uniform prior $p(M_k) = \frac{1}{K}$, which gives every model equal (prior) probability, determining the MAP estimate over models amounts to picking the model that maximizes the *model evidence/marginal likelihood*

model evidence marginal likelihood

$$p(\mathcal{D} \mid M_k) = \int p(\mathcal{D} \mid \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k \mid M_k) d\boldsymbol{\theta}_k \,, \tag{8.45}$$

where $p(\boldsymbol{\theta}_k \mid M_k)$ is the prior distribution of the model parameters $\boldsymbol{\theta}_k$ of model M_k.

Remark (Likelihood and Marginal Likelihood). There are some important differences between a likelihood and a marginal likelihood (evidence): While the likelihood is prone to overfitting, the marginal likelihood is typically not as the model parameters have been marginalized out (i.e., we no longer have to fit the parameters). Furthermore, the marginal likelihood automatically embodies a trade-off between model complexity and data fit (Occam's razor). ♢

8.5.3 Bayes Factors for Model Comparison

Consider the problem of comparing two probabilistic models M_1, M_2, given a data set $\mathcal{D}$. If we compute the posteriors $p(M_1 \mid \mathcal{D})$ and $p(M_2 \mid \mathcal{D})$, we can compute the ratio of the posteriors (*posterior odds*) posterior odds

$$\underbrace{\frac{p(M_1 \mid \mathcal{D})}{p(M_2 \mid \mathcal{D})}}_{\text{posterior odds}} = \frac{\frac{p(\mathcal{D} \mid M_1)p(M_1)}{p(\mathcal{D})}}{\frac{p(\mathcal{D} \mid M_2)p(M_2)}{p(\mathcal{D})}} = \underbrace{\frac{p(M_1)}{p(M_2)}}_{\text{prior odds}} \underbrace{\frac{p(\mathcal{D} \mid M_1)}{p(\mathcal{D} \mid M_2)}}_{\text{Bayes factor}} \tag{8.46}$$

The first fraction on the right-hand-side (prior odds) measures how much our prior (initial) beliefs favor M_1 over M_2. The ratio of the marginal likelihoods (second fraction on the right-hand-side) is called the *Bayes factor* and measures how well the data $\mathcal{D}$ is predicted by M_1 compared to M_2. Bayes factor

Remark. The *Jeffreys-Lindley paradox* states that the "Bayes factor always favors the simpler model since the probability of the data under a complex model with a diffuse prior will be very small" (Murphy, 2012). Here, a diffuse prior refers to a prior that does not favor specific models, i.e., many models are a priori plausible under this prior. ♢ Jeffreys-Lindley paradox

If we choose a uniform prior over models, the prior odds term in (8.46) is 1, i.e., the posterior odds is the ratio of the marginal likelihoods (Bayes factor)

$$\frac{p(\mathcal{D} \mid M_1)}{p(\mathcal{D} \mid M_2)}\,. \tag{8.47}$$

If the Bayes factor is greater than 1, we choose model M_1, otherwise model M_2.

Remark (Computing the Marginal Likelihood). The marginal likelihood plays an important role in model selection: We need to compute Bayes factors (8.46) and posterior distributions over models (8.42).

Unfortunately, computing the marginal likelihood requires us to solve an integral (8.45). This integration is generally analytically intractable, and we will have to resort to approximation techniques, e.g., numerical

integration (Stoer and Burlirsch, 2002), stochastic approximations using Monte Carlo (Murphy, 2012) or Bayesian Monte Carlo techniques (O'Hagan, 1991; Rasmussen and Ghahramani, 2003).

However, there are special cases in which we can solve it. In Section 6.7.1, we discussed conjugate models. If we choose a conjugate parameter prior $p(\boldsymbol{\theta})$, we can compute the marginal likelihood in closed form. In Chapter 9, we will do exactly this in the context of linear regression. ♢

Further Reading

We mentioned at the start of the section that there are high level modeling choices that influence the performance of the model. Examples include:

- The degree of a polynomial in a regression setting
- The number of components in a mixture model
- The network architecture of a (deep) neural network
- The type of kernel in a support vector machine
- The dimensionality of the latent space in PCA
- The learning rate (schedule) in an optimization algorithm

Rasmussen and Ghahramani (2001) showed that the automatic Occam's razor does not necessarily penalize the number of parameters in a model but it is active in terms of the complexity of functions. They also showed that the automatic Occam's razor also holds for Bayesian nonparametric models with many parameters, e.g., Gaussian processes.

In parametric models, the number of parameters is often related to the complexity of the model class.

If we focus on the maximum likelihood estimate, there exist a number of heuristics for model selection that discourage overfitting. These are called information criteria, and we choose the model with the largest value. The *Akaike Information Criterion (AIC)* (Akaike, 1974)

$$\log p(\boldsymbol{x} \mid \boldsymbol{\theta}) - M \tag{8.48}$$

corrects for the bias of the maximum likelihood estimator by addition of a penalty term to compensate for the overfitting of more complex models (with lots of parameters). Here, M is the number of model parameters.

The *Bayesian Information Criterion (BIC)* (Schwarz, 1978)

$$\ln p(\boldsymbol{x}) = \log \int p(\boldsymbol{x} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} \approx \log p(\boldsymbol{x} \mid \boldsymbol{\theta}) - \frac{1}{2} M \ln N \tag{8.49}$$

can be used for exponential family distributions. Here, N is the number of data points and M is the number of parameters. BIC penalizes model complexity more heavily than AIC.