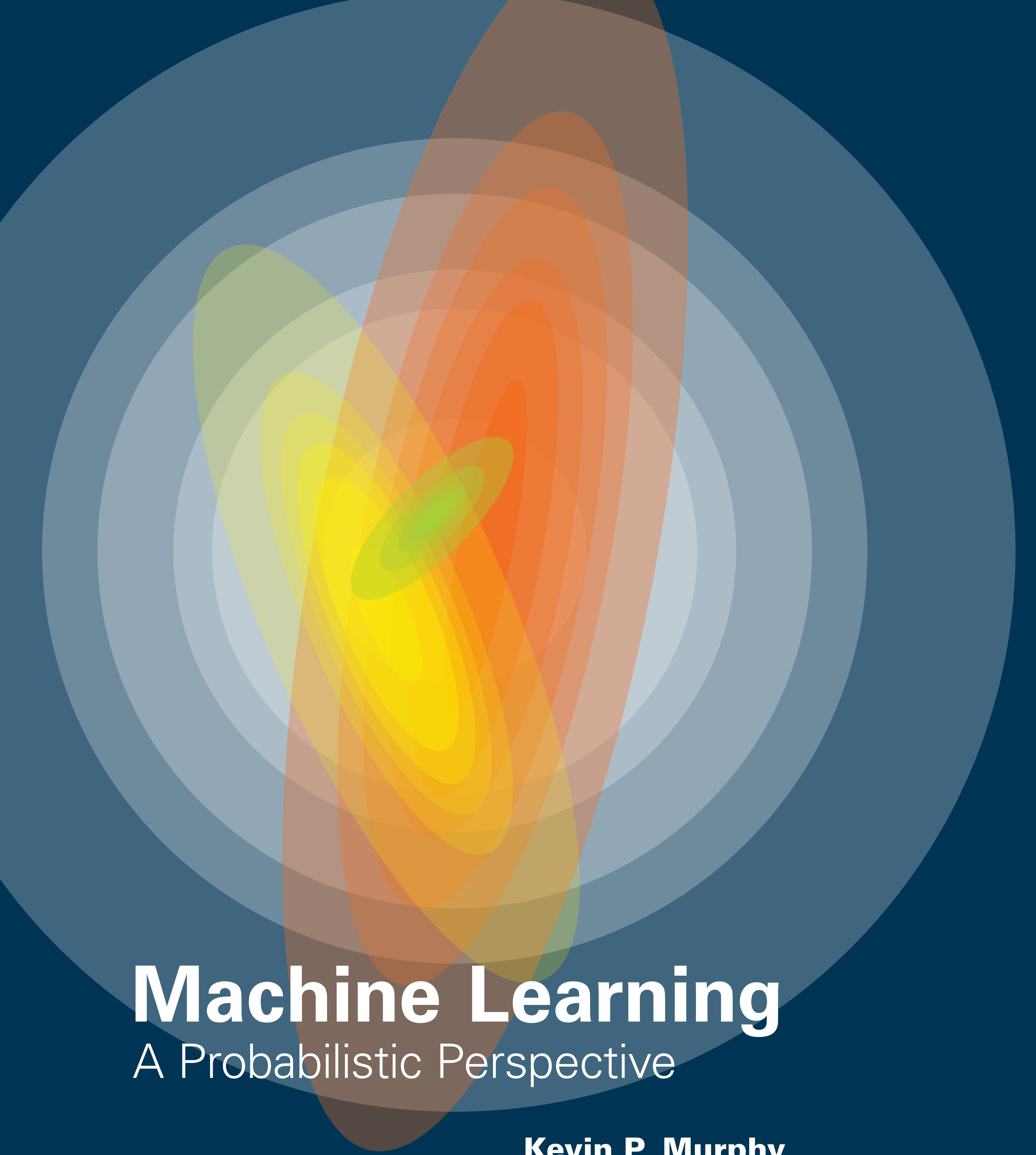

Machine Learning

A Probabilistic Perspective

Kevin P. Murphy

Machine Learning: A Probabilistic Perspective

Machine Learning
A Probabilistic Perspective

Kevin P. Murphy

The MIT Press
Cambridge, Massachusetts
London, England

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This book was set in the LaTeX programming language by the author. Printed and bound in the United States of America.

Library of Congress Cataloging-in-Publication Information

Murphy, Kevin P.
Machine learning : a probabilistic perspective / Kevin P. Murphy.
p. cm. — (Adaptive computation and machine learning series)
Includes bibliographical references and index.
ISBN 978-0-262-01802-9 (hardcover : alk. paper)
1. Machine learning. 2. Probabilities. I. Title.
Q325.5.M87 2012
006.3'1—dc23
2012004558

10 9 8 7 6 5 4 3 2 1

This book is dedicated to Alessandro, Michael and Stefano,
and to the memory of Gerard Joseph Murphy.

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Preface

Introduction

With the ever increasing amounts of data in electronic form, the need for automated methods for data analysis continues to grow. The goal of machine learning is to develop methods that can automatically detect patterns in data, and then to use the uncovered patterns to predict future data or other outcomes of interest. Machine learning is thus closely related to the fields of statistics and data mining, but differs slightly in terms of its emphasis and terminology. This book provides a detailed introduction to the field, and includes worked examples drawn from application domains such as molecular biology, text processing, computer vision, and robotics.

Target audience

This book is suitable for upper-level undergraduate students and beginning graduate students in computer science, statistics, electrical engineering, econometrics, or any one else who has the appropriate mathematical background. Specifically, the reader is assumed to already be familiar with basic multivariate calculus, probability, linear algebra, and computer programming. Prior exposure to statistics is helpful but not necessary.

A probabilistic approach

This books adopts the view that the best way to make machines that can learn from data is to use the tools of probability theory, which has been the mainstay of statistics and engineering for centuries. Probability theory can be applied to any problem involving uncertainty. In machine learning, uncertainty comes in many forms: what is the best prediction (or decision) given some data? what is the best model given some data? what measurement should I perform next? etc.

The systematic application of probabilistic reasoning to all inferential problems, including inferring parameters of statistical models, is sometimes called a Bayesian approach. However, this term tends to elicit very strong reactions (either positive or negative, depending on who you ask), so we prefer the more neutral term “probabilistic approach”. Besides, we will often use techniques such as maximum likelihood estimation, which are not Bayesian methods, but certainly fall within the probabilistic paradigm.

Rather than describing a cookbook of different heuristic methods, this book stresses a principled model-based approach to machine learning. For any given model, a variety of algorithms can often be applied. Conversely, any given algorithm can often be applied to a variety of models. This kind of modularity, where we distinguish model from algorithm, is good pedagogy and good engineering.

We will often use the language of graphical models to specify our models in a concise and intuitive way. In addition to aiding comprehension, the graph structure aids in developing efficient algorithms, as we will see. However, this book is not primarily about graphical models; it is about probabilistic modeling in general.

A practical approach

Nearly all of the methods described in this book have been implemented in a MATLAB software package called **PMTK**, which stands for probabilistic modeling toolkit. This is freely available from `pmtk3.googlecode.com` (the digit 3 refers to the third edition of the toolkit, which is the one used in this version of the book). There are also a variety of supporting files, written by other people, available at `pmtksupport.googlecode.com`. These will be downloaded automatically, if you follow the setup instructions described on the PMTK website.

MATLAB is a high-level, interactive scripting language ideally suited to numerical computation and data visualization, and can be purchased from `www.mathworks.com`. Some of the code requires the Statistics toolbox, which needs to be purchased separately. There is also a free version of Matlab called **Octave**, available at `http://www.gnu.org/software/octave/`, which supports most of the functionality of MATLAB. Some (but not all) of the code in this book also works in Octave. See the PMTK website for details.

PMTK was used to generate many of the figures in this book; the source code for these figures is included on the PMTK website, allowing the reader to easily see the effects of changing the data or algorithm or parameter settings. The book refers to files by name, e.g., `naiveBayesFit`. In order to find the corresponding file, you can use two methods: within Matlab you can type `which naiveBayesFit` and it will return the full path to the file; or, if you do not have Matlab but want to read the source code anyway, you can use your favorite search engine, which should return the corresponding file from the `pmtk3.googlecode.com` website.

Details on *how to use* PMTK can be found on the website, which will be udpated over time. Details on the *underlying theory* behind these methods can be found in this book.

Acknowledgments

A book this large is obviously a team effort. I would especially like to thank the following people: my wife Margaret, for keeping the home fires burning as I toiled away in my office for the last six years; Matt Dunham, who created many of the figures in this book, and who wrote much of the code in PMTK; Baback Moghaddam, who gave extremely detailed feedback on every page of an earlier draft of the book; Chris Williams, who also gave very detailed feedback; Cody Severinski and Wei-Lwun Lu, who assisted with figures; generations of UBC students, who gave helpful comments on earlier drafts; Daphne Koller, Nir Friedman, and Chris Manning, for letting me use their latex style files; Stanford University, Google Research and Skyline College for hosting me during part of my sabbatical; and various Canadian funding agencies (NSERC, CRC and CIFAR) who have supported me financially over the years.

In addition, I would like to thank the following people for giving me helpful feedback on

parts of the book, and/or for sharing figures, code, exercises or even (in some cases) text: David Blei, Hannes Bretschneider, Greg Corrado, Arnaud Doucet, Mario Figueiredo, Nando de Freitas, Mark Girolami, Gabriel Goh, Tom Griffiths, Katherine Heller, Geoff Hinton, Aapo Hyvarinen, Tommi Jaakkola, Mike Jordan, Charles Kemp, Emtiyaz Khan, Bonnie Kirkpatrick, Daphne Koller, Zico Kolter, Honglak Lee, Julien Mairal, Andrew McPherson, Tom Minka, Ian Nabney, Arthur Pope, Carl Rassmussen, Ryan Rifkin, Ruslan Salakhutdinov, Mark Schmidt, Daniel Selsam, David Sontag, Erik Sudderth, Josh Tenenbaum, Kai Yu, Martin Wainwright, Yair Weiss.

Kevin Patrick Murphy
Palo Alto, California
June 2012

1 *Introduction*

1.1 Machine learning: what and why?

We are drowning in information and starving for knowledge. — John Naisbitt.

We are entering the era of **big data**. For example, there are about 1 trillion web pages[1]; one hour of video is uploaded to YouTube every second, amounting to 10 years of content every day[2]; the genomes of 1000s of people, each of which has a length of 3.8×10^9 base pairs, have been sequenced by various labs; Walmart handles more than 1M transactions per hour and has databases containing more than 2.5 petabytes (2.5×10^{15}) of information (Cukier 2010); and so on.

This deluge of data calls for automated methods of data analysis, which is what **machine learning** provides. In particular, we define machine learning as a set of methods that can automatically detect patterns in data, and then use the uncovered patterns to predict future data, or to perform other kinds of decision making under uncertainty (such as planning how to collect more data!).

This books adopts the view that the best way to solve such problems is to use the tools of probability theory. Probability theory can be applied to any problem involving uncertainty. In machine learning, uncertainty comes in many forms: what is the best prediction about the future given some past data? what is the best model to explain some data? what measurement should I perform next? etc. The probabilistic approach to machine learning is closely related to the field of statistics, but differs slightly in terms of its emphasis and terminology[3].

We will describe a wide variety of probabilistic models, suitable for a wide variety of data and tasks. We will also describe a wide variety of algorithms for learning and using such models. The goal is not to develop a cook book of ad hoc techiques, but instead to present a unified view of the field through the lens of probabilistic modeling and inference. Although we will pay attention to computational efficiency, details on how to scale these methods to truly massive datasets are better described in other books, such as (Rajaraman and Ullman 2011; Bekkerman et al. 2011).

1. `http://googleblog.blogspot.com/2008/07/we-knew-web-was-big.html`
2. Source: `http://www.youtube.com/t/press_statistics`.
3. Rob Tibshirani, a statistician at Stanford university, has created an amusing comparison between machine learning and statistics, available at `http://www-stat.stanford.edu/~tibs/stat315a/glossary.pdf`.

It should be noted, however, that even when one has an apparently massive data set, the effective number of data points for certain cases of interest might be quite small. In fact, data across a variety of domains exhibits a property known as the **long tail**, which means that a few things (e.g., words) are very common, but most things are quite rare (see Section 2.4.6 for details). For example, 20% of Google searches each day have never been seen before[4]. This means that the core statistical issues that we discuss in this book, concerning generalizing from relatively small samples sizes, are still very relevant even in the big data era.

1.1.1 Types of machine learning

Machine learning is usually divided into two main types. In the **predictive** or **supervised learning** approach, the goal is to learn a mapping from inputs $\mathbf{x}$ to outputs y, given a labeled set of input-output pairs $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$. Here $\mathcal{D}$ is called the **training set**, and N is the number of training examples.

In the simplest setting, each training input $\mathbf{x}_i$ is a D-dimensional vector of numbers, representing, say, the height and weight of a person. These are called **features**, **attributes** or **covariates**. In general, however, $\mathbf{x}_i$ could be a complex structured object, such as an image, a sentence, an email message, a time series, a molecular shape, a graph, etc.

Similarly the form of the output or **response variable** can in principle be anything, but most methods assume that y_i is a **categorical** or **nominal** variable from some finite set, $y_i \in \{1, \ldots, C\}$ (such as male or female), or that y_i is a real-valued scalar (such as income level). When y_i is categorical, the problem is known as **classification** or **pattern recognition**, and when y_i is real-valued, the problem is known as **regression**. Another variant, known as **ordinal regression**, occurs where label space $\mathcal{Y}$ has some natural ordering, such as grades A–F.

The second main type of machine learning is the **descriptive** or **unsupervised learning** approach. Here we are only given inputs, $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^N$, and the goal is to find "interesting patterns" in the data. This is sometimes called **knowledge discovery**. This is a much less well-defined problem, since we are not told what kinds of patterns to look for, and there is no obvious error metric to use (unlike supervised learning, where we can compare our prediction of y for a given $\mathbf{x}$ to the observed value).

There is a third type of machine learning, known as **reinforcement learning**, which is somewhat less commonly used. This is useful for learning how to act or behave when given occasional reward or punishment signals. (For example, consider how a baby learns to walk.) Unfortunately, RL is beyond the scope of this book, although we do discuss decision theory in Section 5.7, which is the basis of RL. See e.g., (Kaelbling et al. 1996; Sutton and Barto 1998; Russell and Norvig 2010; Szepesvari 2010; Wiering and van Otterlo 2012) for more information on RL.

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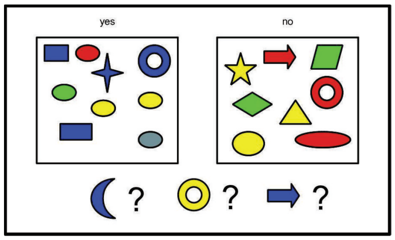
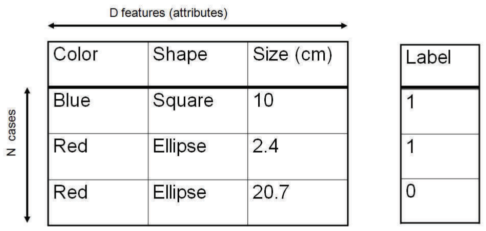
4. `http://certifiedknowledge.org/blog/are-search-queries-becoming-even-more-unique-statistics-from-google`.



(a)


D features (attributes)
N cases

Color	Shape	Size (cm)	Label
Blue	Square	10	1
Red	Ellipse	2.4	1
Red	Ellipse	20.7	0

(b)

Figure 1.1 Left: Some labeled training examples of colored shapes, along with 3 unlabeled test cases. Right: Representing the training data as an $N \times D$ design matrix. Row i represents the feature vector $\mathbf{x}_i$. The last column is the label, $y_i \in \{0, 1\}$. Based on a figure by Leslie Kaelbling.

1.2 Supervised learning

We begin our investigation of machine learning by discussing supervised learning, which is the form of ML most widely used in practice.

1.2.1 Classification

In this section, we discuss classification. Here the goal is to learn a mapping from inputs $\mathbf{x}$ to outputs y, where $y \in \{1, \ldots, C\}$, with C being the number of classes. If $C = 2$, this is called **binary classification** (in which case we often assume $y \in \{0, 1\}$); if $C > 2$, this is called **multiclass classification**. If the class labels are not mutually exclusive (e.g., somebody may be classified as tall and strong), we call it **multi-label classification**, but this is best viewed as predicting multiple related binary class labels (a so-called **multiple output model**). When we use the term “classification”, we will mean multiclass classification with a single output, unless we state otherwise.

One way to formalize the problem is as **function approximation**. We assume $y = f(\mathbf{x})$ for some unknown function f, and the goal of learning is to estimate the function f given a labeled training set, and then to make predictions using $\hat{y} = \hat{f}(\mathbf{x})$. (We use the hat symbol to denote an estimate.) Our main goal is to make predictions on novel inputs, meaning ones that we have not seen before (this is called **generalization**), since predicting the response on the training set is easy (we can just look up the answer).

1.2.1.1 Example

As a simple toy example of classification, consider the problem illustrated in Figure 1.1(a). We have two classes of object which correspond to labels 0 and 1. The inputs are colored shapes. These have been described by a set of D features or attributes, which are stored in an $N \times D$ design matrix $\mathbf{X}$, shown in Figure 1.1(b). The input features $\mathbf{x}$ can be discrete, continuous or a combination of the two. In addition to the inputs, we have a vector of training labels $\mathbf{y}$.

In Figure 1.1, the test cases are a blue crescent, a yellow circle and a blue arrow. None of these have been seen before. Thus we are required to **generalize** beyond the training set. A reasonable guess is that blue crescent should be $y = 1$, since all blue shapes are labeled 1 in the training set. The yellow circle is harder to classify, since some yellow things are labeled $y = 1$ and some are labeled $y = 0$, and some circles are labeled $y = 1$ and some $y = 0$. Consequently it is not clear what the right label should be in the case of the yellow circle. Similarly, the correct label for the blue arrow is unclear.

1.2.1.2 The need for probabilistic predictions

To handle ambiguous cases, such as the yellow circle above, it is desirable to return a probability. The reader is assumed to already have some familiarity with basic concepts in probability. If not, please consult Chapter 2 for a refresher, if necessary.

We will denote the probability distribution over possible labels, given the input vector $\mathbf{x}$ and training set $\mathcal{D}$ by $p(y|\mathbf{x}, \mathcal{D})$. In general, this represents a vector of length C. (If there are just two classes, it is sufficient to return the single number $p(y = 1|\mathbf{x}, \mathcal{D})$, since $p(y = 1|\mathbf{x}, \mathcal{D}) + p(y = 0|\mathbf{x}, \mathcal{D}) = 1$.) In our notation, we make explicit that the probability is conditional on the test input $\mathbf{x}$, as well as the training set $\mathcal{D}$, by putting these terms on the right hand side of the conditioning bar $|$. We are also implicitly conditioning on the form of model that we use to make predictions. When choosing between different models, we will make this assumption explicit by writing $p(y|\mathbf{x}, \mathcal{D}, M)$, where M denotes the model. However, if the model is clear from context, we will drop M from our notation for brevity.

Given a probabilistic output, we can always compute our "best guess" as to the "true label" using

$$\hat{y} = \hat{f}(\mathbf{x}) = \operatorname*{argmax}_{c=1}^{C} p(y = c|\mathbf{x}, \mathcal{D}) \tag{1.1}$$

This corresponds to the most probable class label, and is called the **mode** of the distribution $p(y|\mathbf{x}, \mathcal{D})$; it is also known as a **MAP estimate** (MAP stands for **maximum a posteriori**). Using the most probable label makes intuitive sense, but we will give a more formal justification for this procedure in Section 5.7.

Now consider a case such as the yellow circle, where $p(\hat{y}|\mathbf{x}, \mathcal{D})$ is far from 1.0. In such a case we are not very confident of our answer, so it might be better to say "I don't know" instead of returning an answer that we don't really trust. This is particularly important in domains such as medicine and finance where we may be risk averse, as we explain in Section 5.7. Another application where it is important to assess risk is when playing TV game shows, such as Jeopardy. In this game, contestants have to solve various word puzzles and answer a variety of trivia questions, but if they answer incorrectly, they lose money. In 2011, IBM unveiled a computer system called Watson which beat the top human Jeopardy champion. Watson uses a variety of interesting techniques (Ferrucci et al. 2010), but the most pertinent one for our present purposes is that it contains a module that estimates how confident it is of its answer. The system only chooses to "buzz in" its answer if sufficiently confident it is correct. Similarly, Google has a system known as SmartASS (ad selection system) that predicts the probability you will click on an ad based on your search history and other user and ad-specific features (Metz 2010). This probability is known as the **click-through rate** or **CTR**, and can be used to maximize expected profit. We will discuss some of the basic principles behind systems such as SmartASS later in this book.

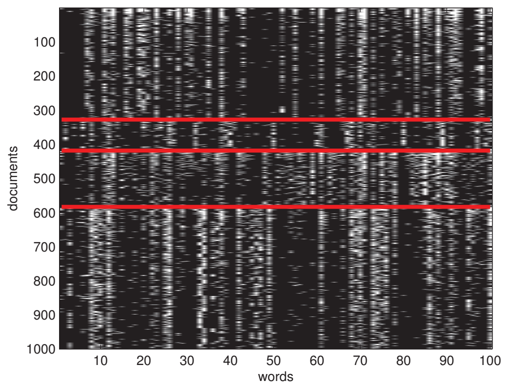


Figure 1.2 Subset of size 16242 x 100 of the 20-newsgroups data. We only show 1000 rows, for clarity. Each row is a document (represented as a bag-of-words bit vector), each column is a word. The red lines separate the 4 classes, which are (in descending order) comp, rec, sci, talk (these are the titles of USENET groups). We can see that there are subsets of words whose presence or absence is indicative of the class. The data is available from `http://cs.nyu.edu/~roweis/data.html`. Figure generated by `newsgroupsVisualize`.

1.2.1.3 Real-world applications

Classification is probably the most widely used form of machine learning, and has been used to solve many interesting and often difficult real-world problems. We have already mentioned some important applciations. We give a few more examples below.

Document classification and email spam filtering

In **document classification**, the goal is to classify a document, such as a web page or email message, into one of C classes, that is, to compute $p(y = c|\mathbf{x}, \mathcal{D})$, where $\mathbf{x}$ is some representation of the text. A special case of this is **email spam filtering**, where the classes are spam $y = 1$ or ham $y = 0$.

Most classifiers assume that the input vector $\mathbf{x}$ has a fixed size. A common way to represent variable-length documents in feature-vector format is to use a **bag of words** representation. This is explained in detail in Section 3.4.4.1, but the basic idea is to define $x_{ij} = 1$ iff word j occurs in document i. If we apply this transformation to every document in our data set, we get a binary document $\times$ word co-occurrence matrix: see Figure 1.2 for an example. Essentially the document classification problem has been reduced to one that looks for subtle changes in the pattern of bits. For example, we may notice that most spam messages have a high probability of containing the words “buy”, “cheap”, “viagra”, etc. In Exercise 8.1 and Exercise 8.2, you will get hands-on experience applying various classification techniques to the spam filtering problem.

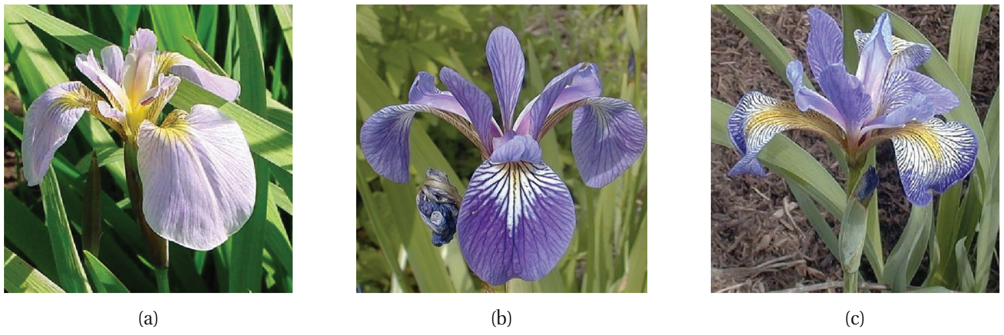


Figure 1.3 Three types of iris flowers: setosa, versicolor and virginica. Source: `http://www.statlab.uni-heidelberg.de/data/iris/` . Used with kind permission of Dennis Kramb and SIGNA.

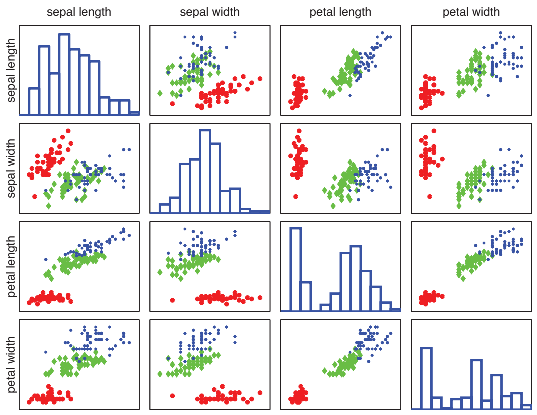


Figure 1.4 Visualization of the Iris data as a pairwise scatter plot. The diagonal plots the marginal histograms of the 4 features. The off diagonals contain scatterplots of all possible pairs of features. Red circle = setosa, green diamond = versicolor, blue star = virginica. Figure generated by `fisheririsDemo`.

Classifying flowers

Figure 1.3 gives another example of classification, due to the statistician Ronald Fisher. The goal is to learn to distinguish three different kinds of iris flower, called setosa, versicolor and virginica. Fortunately, rather than working directly with images, a botanist has already extracted 4 useful features or characteristics: sepal length and width, and petal length and width. (Such **feature extraction** is an important, but difficult, task. Most machine learning methods use features chosen by some human. Later we will discuss some methods that can learn good features from the data.) If we make a **scatter plot** of the iris data, as in Figure 1.4, we see that it is easy to distinguish setosas (red circles) from the other two classes by just checking if their petal length

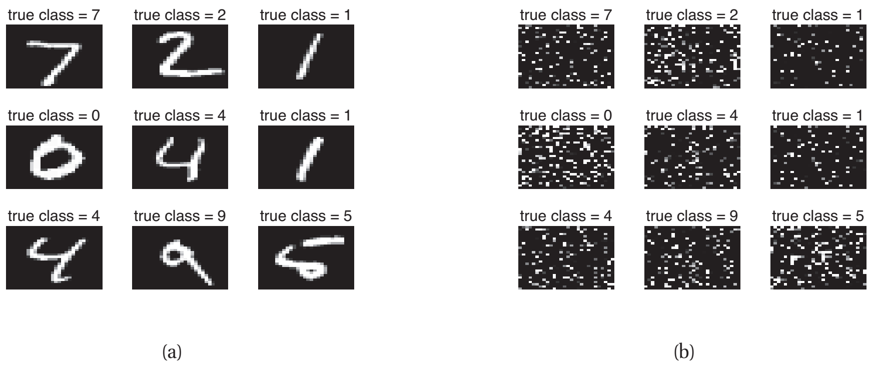


Figure 1.5 (a) First 9 test MNIST gray-scale images. (b) Same as (a), but with the features permuted randomly. Classification performance is identical on both versions of the data (assuming the training data is permuted in an identical way). Figure generated by `shuffledDigitsDemo`.

or width is below some threshold. However, distinguishing versicolor from virginica is slightly harder; any decision will need to be based on at least two features. (It is always a good idea to perform **exploratory data analysis**, such as plotting the data, before applying a machine learning method.)

Image classification and handwriting recognition

Now consider the harder problem of classifying images directly, where a human has not pre-processed the data. We might want to classify the image as a whole, e.g., is it an indoors or outdoors scene? is it a horizontal or vertical photo? does it contain a dog or not? This is called **image classification**.

In the special case that the images consist of isolated handwritten letters and digits, for example, in a postal or ZIP code on a letter, we can use classification to perform **handwriting recognition**. A standard dataset used in this area is known as **MNIST**, which stands for "Modified National Institute of Standards"[5]. (The term "modified" is used because the images have been preprocessed to ensure the digits are mostly in the center of the image.) This dataset contains 60,000 training images and 10,000 test images of the digits 0 to 9, as written by various people. The images are size 28×28 and have grayscale values in the range $0 : 255$. See Figure 1.5(a) for some example images.

Many generic classification methods ignore any structure in the input features, such as spatial layout. Consequently, they can also just as easily handle data that looks like Figure 1.5(b), which is the same data except we have randomly permuted the order of all the features. (You will verify this in Exercise 1.1.) This flexibility is both a blessing (since the methods are general purpose) and a curse (since the methods ignore an obviously useful source of information). We will discuss methods for exploiting structure in the input features later in the book.

5. Available from `http://yann.lecun.com/exdb/mnist/`.

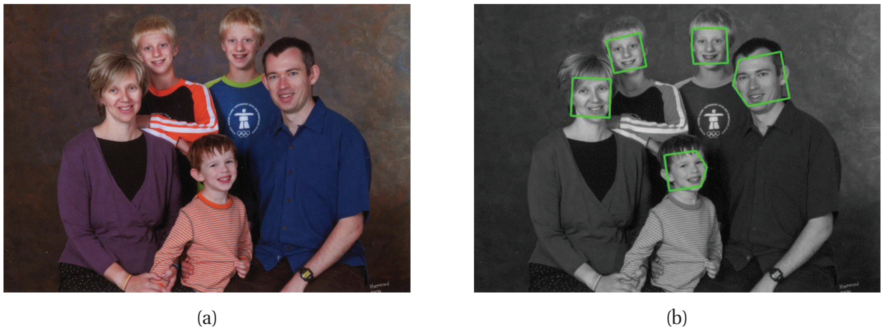


Figure 1.6 Example of face detection. (a) Input image (Murphy family, photo taken 5 August 2010). Used with kind permission of Bernard Diedrich of Sherwood Studios. (b) Output of classifier, which detected 5 faces at different poses. This was produced using the online demo at `http://demo.pittpatt.com/`. The classifier was trained on 1000s of manually labeled images of faces and non-faces, and then was applied to a dense set of overlapping patches in the test image. Only the patches whose probability of containing a face was sufficiently high were returned. Used with kind permission of Pittpatt.com

Face detection and recognition

A harder problem is to find objects within an image; this is called **object detection** or **object localization**. An important special case of this is **face detection**. One approach to this problem is to divide the image into many small overlapping patches at different locations, scales and orientations, and to classify each such patch based on whether it contains face-like texture or not. This is called a **sliding window detector**. The system then returns those locations where the probability of face is sufficiently high. See Figure 1.6 for an example. Such face detection systems are built-in to most modern digital cameras; the locations of the detected faces are used to determine the center of the auto-focus. Another application is automatically blurring out faces in Google's StreetView system.

Having found the faces, one can then proceed to perform **face recognition**, which means estimating the identity of the person (see Figure 1.10(a)). In this case, the number of class labels might be very large. Also, the features one should use are likely to be different than in the face detection problem: for recognition, subtle differences between faces such as hairstyle may be important for determining identity, but for detection, it is important to be **invariant** to such details, and to just focus on the differences between faces and non-faces. For more information about visual object detection, see e.g., (Szeliski 2010).

1.2.2 Regression

Regression is just like classification except the response variable is continuous. Figure 1.7 shows a simple example: we have a single real-valued input $x_i \in \mathbb{R}$, and a single real-valued response $y_i \in \mathbb{R}$. We consider fitting two models to the data: a straight line and a quadratic function. (We explain how to fit such models below.) Various extensions of this basic problem can arise, such as having high-dimensional inputs, outliers, non-smooth responses, etc. We will discuss ways to handle such problems later in the book.

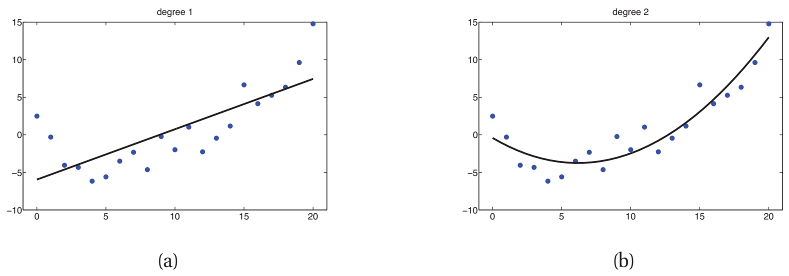


Figure 1.7 (a) Linear regression on some 1d data. (b) Same data with polynomial regression (degree 2). Figure generated by `linregPolyVsDegree`.

Here are some examples of real-world regression problems.

- Predict tomorrow's stock market price given current market conditions and other possible side information.
- Predict the age of a viewer watching a given video on YouTube.
- Predict the location in 3d space of a robot arm end effector, given control signals (torques) sent to its various motors.
- Predict the amount of prostate specific antigen (PSA) in the body as a function of a number of different clinical measurements.
- Predict the temperature at any location inside a building using weather data, time, door sensors, etc.

1.3 Unsupervised learning

We now consider **unsupervised learning**, where we are just given output data, without any inputs. The goal is to discover "interesting structure" in the data; this is sometimes called **knowledge discovery**. Unlike supervised learning, we are not told what the desired output is for each input. Instead, we will formalize our task as one of **density estimation**, that is, we want to build models of the form $p(\mathbf{x}_i|\boldsymbol{\theta})$. There are two differences from the supervised case. First, we have written $p(\mathbf{x}_i|\boldsymbol{\theta})$ instead of $p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$; that is, supervised learning is conditional density estimation, whereas unsupervised learning is unconditional density estimation. Second, $\mathbf{x}_i$ is a vector of features, so we need to create multivariate probability models. By contrast, in supervised learning, y_i is usually just a single variable that we are trying to predict. This means that for most supervised learning problems, we can use univariate probability models (with input-dependent parameters), which significantly simplifies the problem. (We will discuss multi-output classification in Chapter 19, where we will see that it also involves multivariate probability models.)

Unsupervised learning is arguably more typical of human and animal learning. It is also more widely applicable than supervised learning, since it does not require a human expert to