

# 1 Introduction

Machine learning is a rapidly growing field of study whose primary concern is the design and analysis of algorithms which enable computers to learn. While still a young discipline, with much more awaiting to be discovered than is currently known, today machine learning can be used to teach computers to perform a wide array of useful tasks. This includes tasks like the automatic detection of objects in images (a crucial component of driver-assisted and self-driving cars), speech recognition (which powers voice command technology), knowledge discovery in the medical sciences (used to improve our understanding of complex diseases), and predictive analytics (leveraged for sales and economic forecasting). In this chapter we give a high level introduction to the field of machine learning and the contents of this textbook. To get a big picture sense of how machine learning works we begin by discussing a simple toy machine learning problem: teaching a computer how to distinguish between pictures of cats from those with dogs. This will allow us to informally describe the procedures used to solve machine learning problems in general.

# 1.1 Teaching a computer to distinguish cats from dogs

To teach a child the difference between "cat" versus "dog", parents (almost!) never give their children some kind of formal scientific definition to distinguish the two; i.e., that a dog is a member of Canis Familiaris species from the broader class of Mammalia, and that a cat while being from the same class belongs to another species known as Felis Catus. No, instead the child is naturally presented with many images of what they are told are either "dogs" or "cats" until they fully grasp the two concepts. How do we know when a child can successfully distinguish between cats and dogs? Intuitively, when they encounter new (images of) cats and dogs, and can correctly identify each new example. Like human beings, computers can be taught how to perform this sort of task in a similar manner. This kind of task, where we aim to teach a computer to distinguish between different types of things, is referred to as a *classification* problem in machine learning.

**1. Collecting data** Like human beings, a computer must be trained to recognize the difference between these two types of animal by learning from a batch of examples, typically referred to as a *training set* of data. Figure 1.1 shows such a training set consisting



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Fig. 1.1 A training set of six cats (left panel) and six dogs (right panel). This set is used to train a machine learning model that can distinguish between future images of cats and dogs. The images in this figure were taken from [31].

of a few images of different cats and dogs. Intuitively, the larger and more diverse the training set the better a computer (or human) can perform a learning task, since exposure to a wider breadth of examples gives the learner more experience.

**2. Designing features** Think for a moment about how you yourself tell the difference between images containing cats from those containing dogs. What do you look for in order to tell the two apart? You likely use color, size, the shape of the ears or nose, and/or some combination of these *features* in order to distinguish between the two. In other words, you do not just look at an image as simply a collection of many small square pixels. You pick out details, or features, from images like these in order to identify what it is you are looking at. This is true for computers as well. In order to successfully train a computer to perform this task (and any machine learning task more generally) we need to provide it with properly designed features or, ideally, have it find such features itself.

This is typically not a trivial task, as designing quality features can be very application dependent. For instance, a feature like "number of legs" would be unhelpful in discriminating between cats and dogs (since they both have four!), but quite helpful in telling cats and snakes apart. Moreover, extracting the features from a training dataset can also be challenging. For example, if some of our training images were blurry or taken from a perspective where we could not see the animal's head, the features we designed might not be properly extracted.

However, for the sake of simplicity with our toy problem here, suppose we can easily extract the following two features from each image in the training set:

- 1. size of nose, relative to the size of the head (ranging from small to big);
- 2. shape of ears (ranging from round to pointy).

Examining the training images shown in Fig. 1.1, we can see that cats all have *small* noses and *pointy* ears, while dogs all have *big* noses and *round* ears. Notice that with the current choice of features each image can now be represented by just two numbers:



### 1.1 Teaching a computer to distinguish cats from dogs

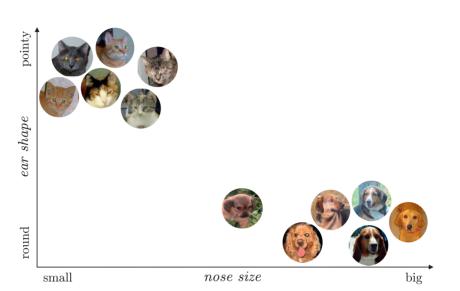


Fig. 1.2 Feature space representation of the training set where the horizontal and vertical axes represent the features "nose size" and "ear shape" respectively. The fact that the cats and dogs from our training set lie in distinct regions of the feature space reflects a good choice of features.

a number expressing the relative nose size, and another number capturing the pointyness or round-ness of ears. Therefore we now represent each image in our training set in a 2-dimensional *feature space* where the features "nose size" and "ear shape" are the horizontal and vertical coordinate axes respectively, as illustrated in Fig. 1.2. Because our designed features distinguish cats from dogs in our training set so well the feature representations of the cat images are all clumped together in one part of the space, while those of the dog images are clumped together in a different part of the space.

**3. Training a model** Now that we have a good feature representation of our training data the final act of teaching a computer how to distinguish between cats and dogs is a simple geometric problem: have the computer find a line or *linear model* that clearly separates the cats from the dogs in our carefully designed feature space. Since a line (in a 2-dimensional space) has two parameters, a slope and an intercept, this means finding the right values for both. Because the parameters of this line must be determined based on the (feature representation) of the training data the process of determining proper parameters, which relies on a set of tools known as *numerical optimization*, is referred to as the training of a model.

Figure 1.3 shows a trained linear model (in black) which divides the feature space into cat and dog regions. Once this line has been determined, any future image whose feature representation lies above it (in the blue region) will be considered a cat by the computer, and likewise any representation that falls below the line (in the red region) will be considered a dog.

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While generally speaking we could instead find a curve or *nonlinear model* that separates the data, we will see that linear models are by far the most common choice in practice when features are designed properly.



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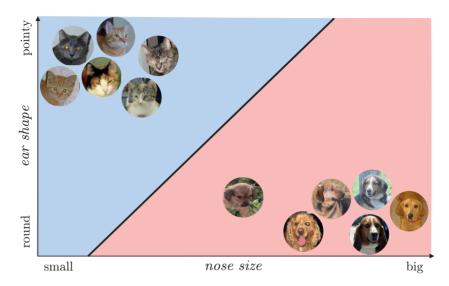


Fig. 1.3 A trained linear model (shown in black) perfectly separates the two classes of animal present in the training set. Any new image received in the future will be classified as a cat if its feature representation lies above this line (in the blue region), and a dog if the feature representation lies below this line (in the red region).



Fig. 1.4 A testing set of cat and dog images also taken from [31]. Note that one of the dogs, the Boston terrier on the top right, has both a short nose and pointy ears. Due to our chosen feature representation the computer will think this is a cat!

**4. Testing the model** To test the efficacy of our learner we now show the computer a batch of previously unseen images of cats and dogs (referred to generally as a *testing set* of data) and see how well it can identify the animal in each image. In Fig. 1.4 we show a sample testing set for the problem at hand, consisting of three new cat and dog images. To do this we take each new image, extract our designed features (nose size and ear shape), and simply check which side of our line the feature representation falls on. In this instance, as can be seen in Fig. 1.5 all of the new cats and all but one dog from the testing set have been identified correctly.



### 1.1 Teaching a computer to distinguish cats from dogs

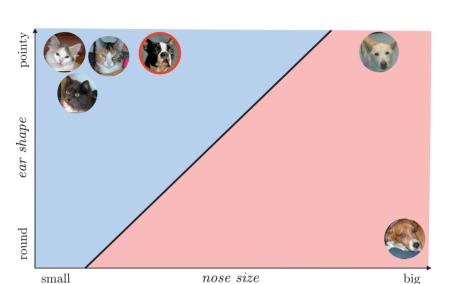


Fig. 1.5 Identification of (the feature representation of) our test images using our trained linear model. Notice that the Boston terrier is misclassified as a cat since it has pointy ears and a short nose, just like the cats in our training set.

The misidentification of the single dog (a Boston terrier) is due completely to our choice of features, which we designed based on the training set in Fig. 1.1. This dog has been misidentified simply because its features, a small nose and pointy ears, match those of the cats from our training set. So while it first appeared that a combination of nose size and ear shape could indeed distinguish cats from dogs, we now see that our training set was too small and not diverse enough for this choice of features to be completely effective.

To improve our learner we must begin again. First we should collect more data, forming a larger and more diverse training set. Then we will need to consider designing more discriminating features (perhaps eye color, tail shape, etc.) that further help distinguish cats from dogs. Finally we must train a new model using the designed features, and test it in the same manner to see if our new trained model is an improvement over the old one.

# 1.1.1 The pipeline of a typical machine learning problem

Let us now briefly review the previously described process, by which a trained model was created for the toy task of differentiating cats from dogs. The same process is used to perform essentially all machine learning tasks, and therefore it is worthwhile to pause for a moment and review the steps taken in solving typical machine learning problems. We enumerate these steps below to highlight their importance, which we refer to all together as the general pipeline for solving machine learning problems, and provide a picture that compactly summarizes the entire pipeline in Fig. 1.6.

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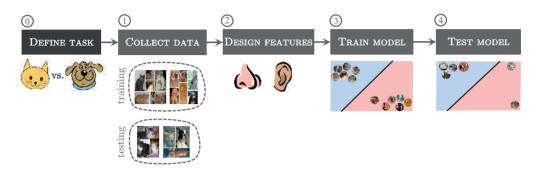


Fig. 1.6 The learning pipeline of the cat versus dog classification problem. The same general pipeline is used for essentially all machine learning problems.

- $\bigcirc$  **Define the problem.** What is the task we want to teach a computer to do?
- 1) Collect data. Gather data for training and testing sets. The larger and more diverse the data the better.
- 2 Design features. What kind of features best describe the data?
- 3 **Train the model.** Tune the parameters of an appropriate model on the training data using numerical optimization.
- 4 **Test the model.** Evaluate the performance of the trained model on the testing data. If the results of this evaluation are poor, re-think the particular features used and gather more data if possible.

# 1.2 Predictive learning problems

Predictive learning problems constitute the majority of tasks machine learning can be used to solve today. Applicable to a wide array of situations and data types, in this section we introduce the two major predictive learning problems: *regression* and *classification*.

# 1.2.1 Regression

Suppose we wanted to predict the share price of a company that is about to go public (that is, when a company first starts offering its shares of stock to the public). Following the pipeline discussed in Section 1.1.1, we first gather a training set of data consisting of a number of corporations (preferably active in the same domain) with known share prices. Next, we need to design feature(s) that are thought to be relevant to the task at



### 1.2 Predictive learning problems



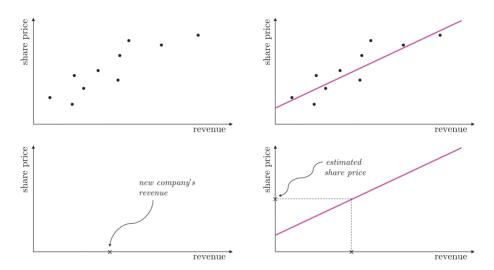


Fig. 1.7 (top left panel) A toy training dataset of ten corporations with their associated share price and revenue values. (top right panel) A linear model is fit to the data. This trend line models the overall trajectory of the points and can be used for prediction in the future as shown in the bottom left and bottom right panels.

hand. The company's revenue is one such potential feature, as we can expect that the higher the revenue the more expensive a share of stock should be.<sup>2</sup> Now in order to connect the share price to the revenue we train a linear model or *regression line* using our training data.

The top panels of Fig. 1.7 show a toy dataset comprising share price versus revenue information for ten companies, as well as a linear model fit to this data. Once the model is trained, the share price of a new company can be predicted based on its revenue, as depicted in the bottom panels of this figure. Finally, comparing the predicted price to the actual price for a testing set of data we can test the performance of our regression model and apply changes as needed (e.g., choosing a different feature). This sort of task, fitting a model to a set of training data so that predictions about a continuous-valued variable (e.g., share price) can be made, is referred to as *regression*. We now discuss some further examples of regression.

### **Example 1.1** The rise of student loan debt in the United States

Figure 1.8 shows the total student loan debt, that is money borrowed by students to pay for college tuition, room and board, etc., held by citizens of the United States from 2006 to 2014, measured quarterly. Over the eight year period reflected in this plot total student debt has tripled, totaling over one trillion dollars by the end of 2014. The regression line (in magenta) fit to this dataset represents the data quite well and, with its sharp positive slope, emphasizes the point that student debt is rising dangerously fast. Moreover, if

 $<sup>^{2} \ \</sup> Other \ potential \ features \ could \ include \ total \ assets, \ total \ equity, \ number \ of \ employees, \ years \ active, \ etc.$ 



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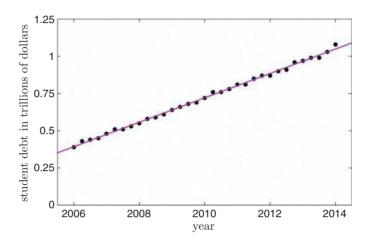


Fig. 1.8 Total student loan debt in the United States measured quarterly from 2006 to 2014. The rapid increase of the debt, measured by the slope of the trend line fit to the data, confirms the concerning claim that student debt is growing (dangerously) fast. The debt data shown in this figure was taken from [46].

this trend continues, we can use the regression line to predict that total student debt will reach a total of two trillion dollars by the year 2026.

#### Example 1.2 Revenue forecasting

In 1983, Academy Award winning screenwriter William Goldman coined the phrase "nobody knows anything" in his book *Adventures in the Screen Trade*, referring to his belief that at the time it was impossible to predict the success or failure of Hollywood movies. However, in the post-internet era of today, accurate estimation of box office revenue to be earned by upcoming movies is becoming possible. In particular, the quantity of internet searches for trailers, as well as the amount of discussion about a movie on social networks like Facebook and Twitter, have been shown to reliably predict a movie's opening weekend box office takings up to a month in advance (see e.g., [14, 62]). Sales forecasting for a range of products/services, including box office sales, is often performed using regression. Here the input feature can be for instance the volume of web searches for a movie trailer on a certain date, with the output being revenue made during the corresponding time period. Predicted revenue of a new movie can then be estimated using a regression model learned on such a dataset.

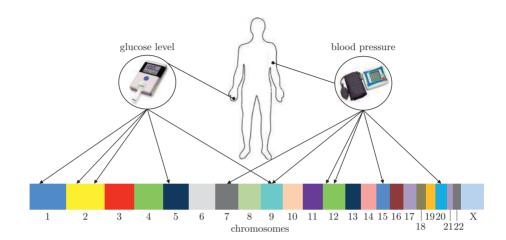
### **Example 1.3** Associating genes with quantitative traits

Genome-wide association (GWA) studies (Fig. 1.9) aim at understanding the connections between tens of thousands of genetic markers, taken from across the human genome of numerous subjects, with diseases like high blood pressure/cholesterol, heart



1.2 Predictive learning problems

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**Fig. 1.9** Conceptual illustration of a GWA study employing regression, wherein a quantitative trait is to be associated with specific genomic locations.

disease, diabetes, various forms of cancer, and many others [26, 76, 80]. These studies are undertaken with the hope of one day producing gene-targeted therapies, like those used to treat diseases caused by a single gene (e.g., cystic fibrosis), that can help individuals with these multifactorial diseases. Regression as a commonly employed tool in GWA studies, is used to understand complex relationships between genetic markers (features) and quantitative traits like level of cholesterol or glucose (a continuous output variable).

### 1.2.2 Classification

The machine learning task of *classification* is similar in principle to that of regression. The key difference between the two is that instead of predicting a continuous-valued output (e.g., share price, blood pressure, etc.), with classification what we aim at predicting takes on discrete values or *classes*. Classification problems arise in a host of forms. For example *object recognition*, where different objects from a set of images are distinguished from one another (e.g., handwritten digits for the automatic sorting of mail or street signs for semi-autonomous and self-driving cars), is a very popular classification problem. The toy problem of distinguishing cats from dogs discussed in Section 1.1 was such a problem. Other common classification problems include speech recognition (recognizing different spoken words for voice recognition systems), determining the general sentiment of a social network like Twitter towards a particular product or service, as well as determining what kind of hand gesture someone is making from a finite set of possibilities (for use in e.g., controlling a computer without a mouse).

Geometrically speaking, a common way of viewing the task of classification is one of finding a separating line (or hyperplane in higher dimensions) that separates the two<sup>3</sup>

<sup>&</sup>lt;sup>3</sup> Some classification problems (e.g., handwritten digit recognition) have naturally more than two classes for which we need a better model than a single line to separate the classes. We discuss in detail how multiclass classification is done later in Sections 4.4 and 6.3.



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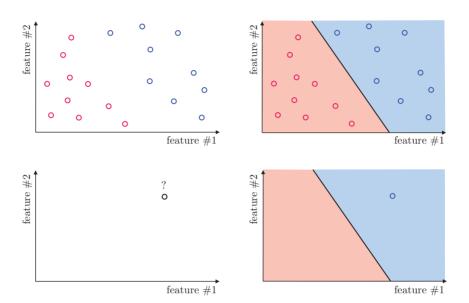


Fig. 1.10 (top left panel) A toy 2-dimensional training set consisting of two distinct classes, red and blue. (top right panel) A linear model is trained to separate the two classes. (bottom left panel) A test point whose class is unknown. (bottom right panel) The test point is classified as blue since it lies on the blue side of the trained linear classifier.

classes of data from a training set as best as possible. This is precisely the perspective on classification we took in describing the toy example in Section 1.1, where we used a line to separate (features extracted from) images of cats and dogs. New data from a testing set is then automatically classified by simply determining which side of the line/hyperplane the data lies on. Figure 1.10 illustrates the concept of a linear model or *classifier* used for performing classification on a 2-dimensional toy dataset.

### **Example 1.4 Object detection**

Object detection, a common classification problem, is the task of automatically identifying a specific object in a set of images or videos. Popular object detection applications include the detection of faces in images for organizational purposes and camera focusing, pedestrians for autonomous driving vehicles,<sup>4</sup> and faulty components for automated quality control in electronics production. The same kind of machine learning framework, which we highlight here for the case of face detection, can be utilized for solving many such detection problems.

After training a linear classifier on a set of training data consisting of facial and non-facial images, faces are sought after in a new test image by sliding a (typically) square

While the problem of detecting pedestrians is a particularly well-studied classification problem [29, 32, 53], a standard semi-autonomous or self-driving car will employ a number of detectors that scan the vehicle's surroundings for other important objects as well, like road markings, signs, and other cars on the road.