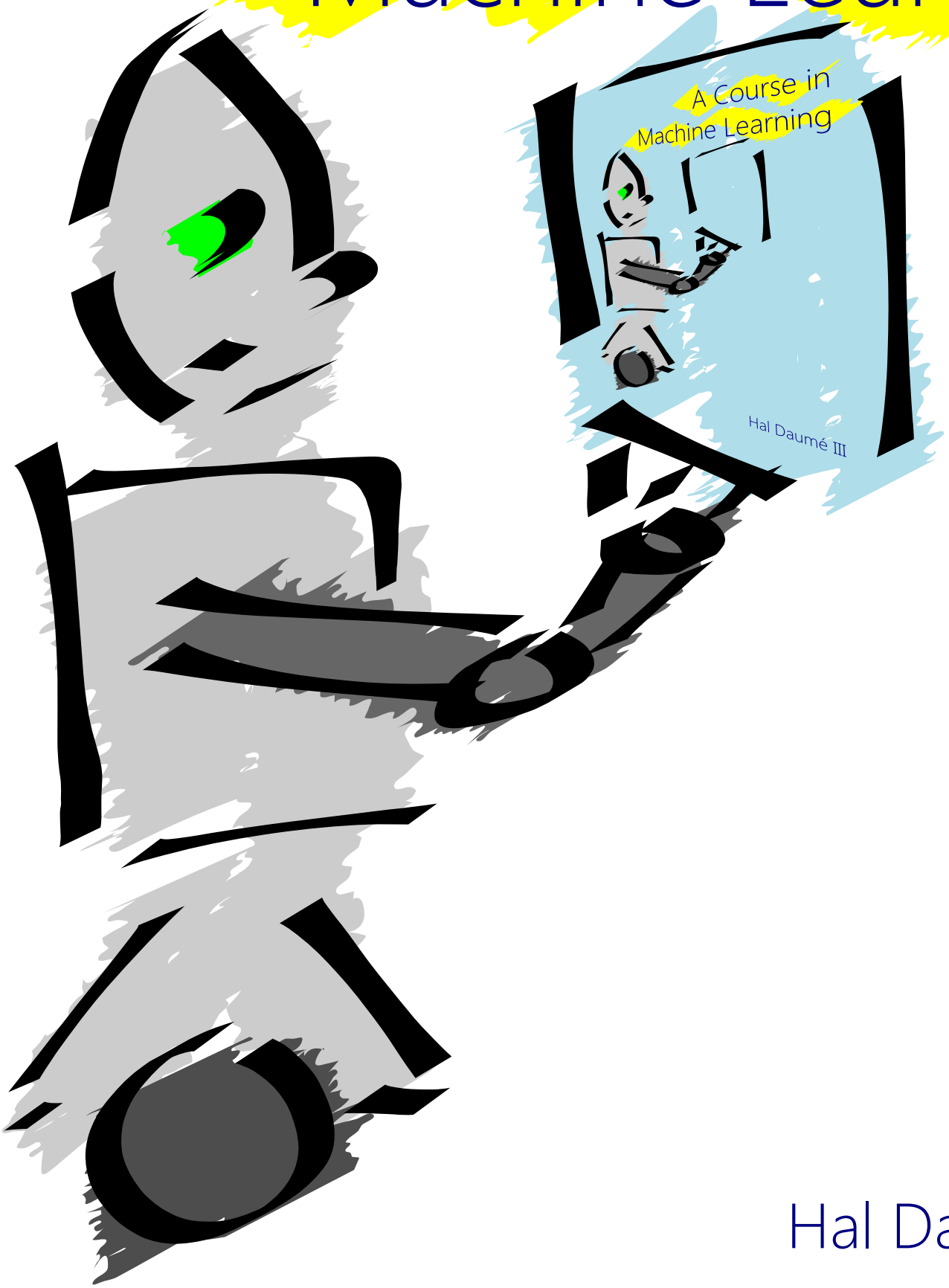
A Course in Machine Learning



Hal Daumé III

1 | Decision Trees

> The words printed here are concepts.
> You must go through the experiences. – Carl Frederick

Learning Objectives:

- Explain the difference between memorization and generalization.
- Define "inductive bias" and recognize the role of inductive bias in learning.
- Take a concrete task and cast it as a learning problem, with a formal notion of input space, features, output space, generating distribution and loss function.
- Illustrate how regularization trades off between underfitting and overfitting.
- Evaluate whether a use of test data is "cheating" or not.

Dependencies: None.

At a basic level, machine learning is about predicting the future based on the past. For instance, you might wish to predict how much a user Alice will like a movie that she hasn't seen, based on her ratings of movies that she has seen. This means making informed guesses about some unobserved property of some object, based on observed properties of that object.

The first question we'll ask is: what does it mean to learn? In order to develop learning machines, we must know what learning actually means, and how to determine success (or failure). You'll see this question answered in a very limited learning setting, which will be progressively loosened and adapted throughout the rest of this book. For concreteness, our focus will be on a very simple model of learning called a **decision tree**.

Vignette: Alice Decides which Classes to Take

todo

1.1 What Does it Mean to Learn?

Alice has just begun taking a course on machine learning. She knows that at the end of the course, she will be expected to have "learned" all about this topic. A common way of gauging whether or not she has learned is for her teacher, Bob, to give her a exam. She has done well at learning if she does well on the exam.

But what makes a reasonable exam? If Bob spends the entire semester talking about machine learning, and then gives Alice an exam on History of Pottery, then Alice's performance on this exam will *not* be representative of her learning. On the other hand, if the exam only asks questions that Bob has answered exactly during lectures, then this is also a bad test of Alice's learning, especially if it's an "open notes" exam. What is desired is that Alice observes *specific*

examples from the course, and then has to answer new, but related questions on the exam. This tests whether Alice has the ability to **generalize**. Generalization is perhaps the most central concept in machine learning.

As a running concrete example in this book, we will use that of a course recommendation system for undergraduate computer science students. We have a collection of students and a collection of courses. Each student has taken, and evaluated, a subset of the courses. The evaluation is simply a score from -2 (terrible) to $+2$ (awesome). The job of the recommender system is to **predict** how much a particular student (say, Alice) will like a particular course (say, Algorithms).

Given historical data from course ratings (i.e., the past) we are trying to predict unseen ratings (i.e., the future). Now, we could be unfair to this system as well. We could ask it whether Alice is likely to enjoy the History of Pottery course. This is unfair because the system has no idea what History of Pottery even is, and has no prior experience with this course. On the other hand, we could ask it how much Alice will like Artificial Intelligence, which she took last year and rated as $+2$ (awesome). We would expect the system to predict that she would really like it, but this isn't demonstrating that the system has learned: it's simply recalling its past experience. In the former case, we're expecting the system to generalize *beyond* its experience, which is unfair. In the latter case, we're not expecting it to generalize at all.

This general set up of predicting the future based on the past is at the core of most machine learning. The objects that our algorithm will make predictions about are **examples**. In the recommender system setting, an example would be some particular Student/Course pair (such as Alice/Algorithms). The desired prediction would be the rating that Alice would give to Algorithms.

To make this concrete, Figure 1.1 shows the general framework of **induction**. We are given **training data** on which our algorithm is expected to learn. This training data is the examples that Alice observes in her machine learning course, or the historical ratings data for the recommender system. Based on this training data, our learning algorithm induces a function f that will map a new example to a corresponding prediction. For example, our function might guess that $f(\text{Alice/Machine Learning})$ might be high because our training data said that Alice liked Artificial Intelligence. We want our algorithm to be able to make lots of predictions, so we refer to the collection of examples on which we will evaluate our algorithm as the **test set**. The test set is a closely guarded secret: it is the final exam on which our learning algorithm is being tested. If our algorithm gets to peek at it ahead of time, it's going to cheat and do better than it should.

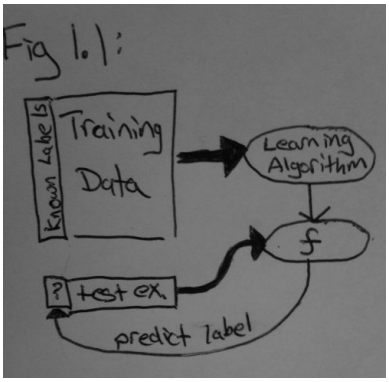


Figure 1.1: The general supervised approach to machine learning: a learning algorithm reads in training data and computes a learned function f. This function can then automatically label future text examples.

? Why is it bad if the learning algorithm gets to peek at the test data?

The goal of inductive machine learning is to take some training data and use it to induce a function f. This function f will be evaluated on the test data. The machine learning algorithm has succeeded if its performance on the test data is high.

1.2 Some Canonical Learning Problems

There are a large number of typical inductive learning problems. The primary difference between them is in what type of *thing* they're trying to predict. Here are some examples:

Regression: trying to predict a real value. For instance, predict the value of a stock tomorrow given its past performance. Or predict Alice's score on the machine learning final exam based on her homework scores.

Binary Classification: trying to predict a simple yes/no response. For instance, predict whether Alice will enjoy a course or not. Or predict whether a user review of the newest Apple product is positive or negative about the product.

Multiclass Classification: trying to put an example into one of a number of classes. For instance, predict whether a news story is about entertainment, sports, politics, religion, etc. Or predict whether a CS course is Systems, Theory, AI or Other.

Ranking: trying to put a set of objects in order of relevance. For instance, predicting what order to put web pages in, in response to a user query. Or predict Alice's ranked preferences over courses she hasn't taken.

? For each of these types of canonical machine learning problems, come up with one or two concrete examples.

The reason that it is convenient to break machine learning problems down by the type of object that they're trying to predict has to do with measuring error. Recall that our goal is to build a system that can make "good predictions." This begs the question: what does it mean for a prediction to be "good?" The different types of learning problems differ in how they define goodness. For instance, in regression, predicting a stock price that is off by \$0.05 is perhaps much better than being off by \$200.00. The same does not hold of multiclass classification. There, accidentally predicting "entertainment" instead of "sports" is no better or worse than predicting "politics."

1.3 The Decision Tree Model of Learning

The **decision tree** is a classic and natural model of learning. It is closely related to the fundamental computer science notion of "divide and conquer." Although decision trees can be applied to many

learning problems, we will begin with the simplest case: binary classification.

Suppose that your goal is to predict whether some unknown user will enjoy some unknown course. You must simply answer "yes" or "no." In order to make a guess, you're allowed to ask binary questions about the user/course under consideration. For example:

You: Is the course under consideration in Systems?
Me: Yes
You: Has this student taken any other Systems courses?
Me: Yes
You: Has this student liked most previous Systems courses?
Me: No
You: *I predict this student will not like this course.*

The goal in learning is to figure out what questions to ask, in what order to ask them, and what answer to predict once you have asked enough questions.

The decision tree is so-called because we can write our set of questions and guesses in a tree format, such as that in Figure 1.2. In this figure, the questions are written in the internal tree nodes (rectangles) and the guesses are written in the leaves (ovals). Each non-terminal node has two children: the left child specifies what to do if the answer to the question is "no" and the right child specifies what to do if it is "yes."

In order to learn, I will give you training data. This data consists of a set of user/course examples, paired with the correct answer for these examples (did the given user enjoy the given course?). From this, you must construct your questions. For concreteness, there is a small data set in Table **??** in the Appendix of this book. This training data consists of 20 course rating examples, with course ratings and answers to questions that you might ask about this pair. We will interpret ratings of 0, $+1$ and $+2$ as "liked" and ratings of -2 and -1 as "hated."

In what follows, we will refer to the questions that you can ask as **features** and the responses to these questions as **feature values**. The rating is called the **label**. An example is just a set of feature values. And our training data is a set of examples, paired with labels.

There are a lot of logically possible trees that you could build, even over just this small number of features (the number is in the millions). It is computationally infeasible to consider all of these to try to choose the "best" one. Instead, we will build our decision tree *greedily.* We will begin by asking:

If I could only ask one question, what question would I ask?

You want to find a feature that is *most useful* in helping you guess whether this student will enjoy this course.[1] A useful way to think

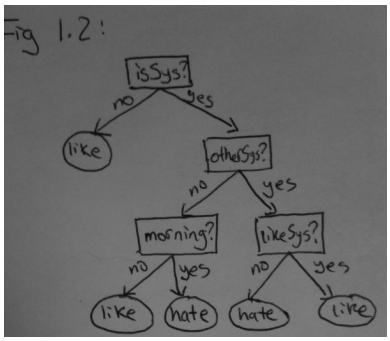


Figure 1.2: A decision tree for a course recommender system, from which the in-text "dialog" is drawn.

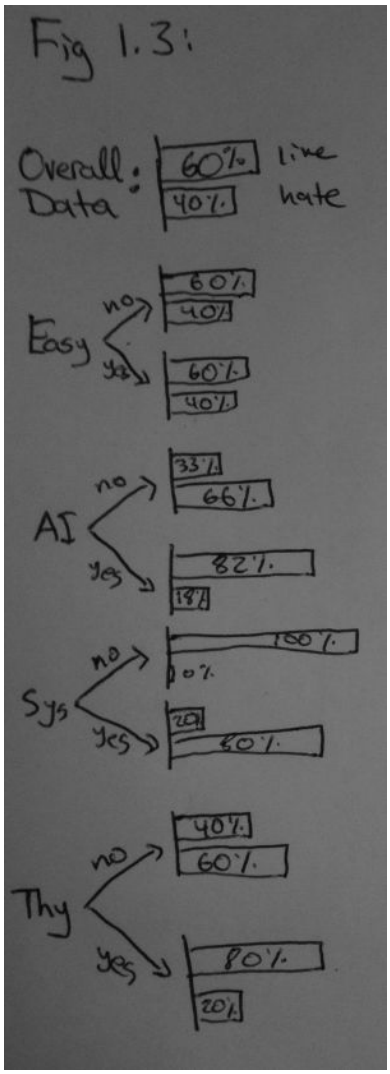


Figure 1.3: A histogram of labels for (a) the entire data set; (b-e) the examples in the data set for each value of the first four features.

[1] A colleague related the story of getting his 8-year old nephew to guess a number between 1 and 100. His nephew's first four questions were: Is it bigger than 20? (YES) Is it even? (YES) Does it have a 7 in it?

about this is to look at the **histogram** of labels for each feature. This is shown for the first four features in Figure 1.3. Each histogram shows the frequency of "like"/"hate" labels for each possible value of an associated feature. From this figure, you can see that asking the first feature is not useful: if the value is "no" then it's hard to guess the label; similarly if the answer is "yes." On the other hand, asking the second feature *is* useful: if the value is "no," you can be pretty confident that this student will hate this course; if the answer is "yes," you can be pretty confident that this student will like this course.

More formally, you will consider each feature in turn. You might consider the feature "Is this a System's course?" This feature has two possible value: no and yes. Some of the training examples have an answer of "no" – let's call that the "NO" set. Some of the training examples have an answer of "yes" – let's call that the "YES" set. For each set (NO and YES) we will build a histogram over the labels. This is the second histogram in Figure 1.3. Now, suppose you were to ask this question on a random example and observe a value of "no." Further suppose that you must *immediately* guess the label for this example. You will guess "like," because that's the more prevalent label in the NO set (actually, it's the *only* label in the NO set). Alternatively, if you recieve an answer of "yes," you will guess "hate" because that is more prevalent in the YES set.

So, for this single feature, you know what you *would* guess if you had to. Now you can ask yourself: if I made that guess on the *training data*, how well would I have done? In particular, how many examples would I classify *correctly?* In the NO set (where you guessed "like") you would classify all 10 of them correctly. In the YES set (where you guessed "hate") you would classify 8 (out of 10) of them correctly. So overall you would classify 18 (out of 20) correctly. Thus, we'll say that the *score* of the "Is this a System's course?" question is 18/20.

? How many training examples would you classify correctly for each of the other three features from Figure 1.3?

You will then repeat this computation for each of the available features to us, compute the scores for each of them. When you must choose which feature consider first, you will want to choose the one with the highest score.

But this only lets you choose the *first* feature to ask about. This is the feature that goes at the *root* of the decision tree. How do we choose subsequent features? This is where the notion of divide and conquer comes in. You've already decided on your first feature: "Is this a Systems course?" You can now *partition* the data into two parts: the NO part and the YES part. The NO part is the subset of the data on which value for this feature is "no"; the YES half is the rest. This is the *divide* step.

Algorithm 1 DECISIONTREETRAIN(*data*, *remaining features*)

```
guess ← most frequent answer in data                    // default answer for this data
if the labels in data are unambiguous then
    return LEAF(guess)                                  // base case: no need to split further
else if remaining features is empty then
    return LEAF(guess)                                  // base case: cannot split further
else                                                    // we need to query more features
    for all f ∈ remaining features do
        NO ← the subset of data on which f=no
        YES ← the subset of data on which f=yes
        score[f] ← # of majority vote answers in NO
                   + # of majority vote answers in YES
                                                        // the accuracy we would get if we only queried on f
    end for
    f ← the feature with maximal score(f)
    NO ← the subset of data on which f=no
    YES ← the subset of data on which f=yes
    left ← DECISIONTREETRAIN(NO, remaining features \ {f})
    right ← DECISIONTREETRAIN(YES, remaining features \ {f})
    return NODE(f, left, right)
end if
```

Algorithm 2 DECISIONTREETEST(*tree*, *test point*)

```
if tree is of the form LEAF(guess) then
    return guess
else if tree is of the form NODE(f, left, right) then
    if f = yes in test point then
        return DECISIONTREETEST(left, test point)
    else
        return DECISIONTREETEST(right, test point)
    end if
end if
```

The *conquer* step is to recurse, and run the *same* routine (choosing the feature with the highest score) on the NO set (to get the left half of the tree) and then separately on the YES set (to get the right half of the tree).

At some point it will become useless to query on additional features. For instance, once you know that this is a Systems course, you *know* that everyone will hate it. So you can immediately predict "hate" without asking any additional questions. Similarly, at some point you might have already queried every available feature and still not whittled down to a single answer. In both cases, you will need to create a leaf node and guess the most prevalent answer in the current piece of the training data that you are looking at.

Putting this all together, we arrive at the algorithm shown in Algorithm 1.3.[2] This function, DECISIONTREETRAIN takes two argu-

[2] There are more nuanced algorithms for building decision trees, some of which are discussed in later chapters of this book. They primarily differ in how they compute the *score* funciton.

ments: our data, and the set of as-yet unused features. It has two base cases: either the data is unambiguous, or there are no remaining features. In either case, it returns a LEAF node containing the most likely guess at this point. Otherwise, it loops over all remaining features to find the one with the highest score. It then partitions the data into a NO/YES split based on the best feature. It constructs its left and right subtrees by recursing on itself. In each recursive call, it uses one of the partitions of the data, and removes the just-selected feature from consideration.

The corresponding *prediction* algorithm is shown in Algorithm 1.3. This function recurses down the decision tree, following the edges specified by the feature values in some *test point*. When it reaches a leaf, it returns the guess associated with that leaf.

TODO: define outlier somewhere!

? Is Algorithm 1.3 guaranteed to terminate?

1.4 Formalizing the Learning Problem

As you've seen, there are several issues that we must take into account when formalizing the notion of learning.

- The performance of the learning algorithm should be measured on unseen "test" data.
- The way in which we measure performance should depend on the problem we are trying to solve.
- There should be a strong relationship between the data that our algorithm sees at training time and the data it sees at test time.

In order to accomplish this, let's assume that someone gives us a **loss function**, $\ell(\cdot, \cdot)$, of two arguments. The job of ℓ is to tell us how "bad" a system's prediction is in comparison to the truth. In particular, if y is the truth and $\hat{y}$ is the system's prediction, then $\ell(y, \hat{y})$ is a measure of error.

For three of the canonical tasks discussed above, we might use the following loss functions:

Regression: **squared loss** $\ell(y, \hat{y}) = (y - \hat{y})^2$
or **absolute loss** $\ell(y, \hat{y}) = |y - \hat{y}|$.

Binary Classification: **zero/one loss** $\ell(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ 1 & \text{otherwise} \end{cases}$

This notation means that the loss is zero if the prediction is correct and is one otherwise.

Multiclass Classification: also zero/one loss.

? Why might it be a bad idea to use zero/one loss to measure performance for a regression problem?

Note that the loss function is something that *you* must decide on based on the goals of learning.

Now that we have defined our loss function, we need to consider where the data (training *and* test) comes from. The model that we will use is the *probabilistic* model of learning. Namely, there is a probability distribution $\mathcal{D}$ over input/output pairs. This is often called the **data generating distribution**. If we write $\boldsymbol{x}$ for the input (the user/course pair) and y for the output (the rating), then $\mathcal{D}$ is a distribution over $(\boldsymbol{x}, y)$ pairs.

A useful way to think about $\mathcal{D}$ is that it gives *high probability* to reasonable $(\boldsymbol{x}, y)$ pairs, and *low probability* to unreasonable $(\boldsymbol{x}, y)$ pairs. A $(\boldsymbol{x}, y)$ pair can be unreasonable in two ways. First, $\boldsymbol{x}$ might be an unusual input. For example, a $\boldsymbol{x}$ related to an "Intro to Java" course might be highly probable; a $\boldsymbol{x}$ related to a "Geometric and Solid Modeling" course might be less probable. Second, y might be an unusual rating for the paired $\boldsymbol{x}$. For instance, if Alice were to take AI 100 times (without remembering that she took it before!), she would give the course a $+2$ almost every time. Perhaps some semesters she might give a slightly lower score, but it would be unlikely to see $\boldsymbol{x}$ =Alice/AI paired with $y = -2$.

It is important to remember that we are not making *any* assumptions about what the distribution $\mathcal{D}$ looks like. (For instance, we're not assuming it looks like a Gaussian or some other, common distribution.) We are also not assuming that we know what $\mathcal{D}$ is. In fact, if you know *a priori* what your data generating distribution is, your learning problem becomes significantly easier. Perhaps the hardest thing about machine learning is that we *don't* know what $\mathcal{D}$ is: all we get is a random sample from it. This random sample is our training data.

Our learning problem, then, is defined by two quantities:

1. The loss function ℓ, which captures our notion of what is *important* to learn.
2. The data generating distribution $\mathcal{D}$, which defines what sort of data we expect to see.

? Consider the following prediction task. Given a paragraph written about a course, we have to predict whether the paragraph is a *positive* or *negative* review of the course. (This is the sentiment analysis problem.) What is a reasonable loss function? How would you define the data generating distribution?

We are given access to **training data**, which is a random sample of input/output pairs drawn from $\mathcal{D}$. Based on this training data, we need to **induce** a function f that maps new inputs $\hat{\boldsymbol{x}}$ to corresponding prediction $\hat{y}$. The key property that f should obey is that it should do well (as measured by ℓ) on future examples that are *also* drawn from $\mathcal{D}$. Formally, it's **expected loss** ϵ over $\mathcal{D}$ with repsect to ℓ should be as small as possible:

$$\epsilon \triangleq \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}\big[\ell(y, f(\boldsymbol{x}))\big] = \sum_{(\boldsymbol{x},y)} \mathcal{D}(\boldsymbol{x}, y)\ell(y, f(\boldsymbol{x})) \tag{1.1}$$

The difficulty in minimizing our **expected loss** from Eq (1.1) is that we *don't know what $\mathcal{D}$ is!* All we have access to is some training data sampled from it! Suppose that we denote our training data set by D. The training data consists of N-many input/output pairs, $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_N, y_N)$. Given a learned function f, we can compute our **training error**, $\hat{\epsilon}$:

$$\hat{\epsilon} \triangleq \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(\boldsymbol{x}_n)) \tag{1.8}$$

That is, our training error is simply our *average error* over the training data.

Of course, we can drive $\hat{\epsilon}$ to zero by simply memorizing our training data. But as Alice might find in memorizing past exams, this might not generalize well to a new exam!

This is the fundamental difficulty in machine learning: the thing we have access to is our training error, $\hat{\epsilon}$. But the thing we care about minimizing is our expected error ϵ. In order to get the expected error down, our learned function needs to **generalize** beyond the training data to some future data that it might not have seen yet!

So, putting it all together, we get a formal definition of induction machine learning: **Given (i) a loss function ℓ and (ii) a sample D from some unknown distribution $\mathcal{D}$, you must compute a function f that has low expected error ϵ over $\mathcal{D}$ with respect to ℓ.**

? Verify by calculation that we can write our training error as $\mathbb{E}_{(\boldsymbol{x},y)\sim D}[\ell(y, f(\boldsymbol{x}))]$, by thinking of D as a distribution that places probability $1/N$ to each example in D and probabiliy 0 on everything else.

1.5 *Inductive Bias: What We Know Before the Data Arrives*

MATH REVIEW | EXPECTATED VALUES

In this book, we will often write things like $\mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(y, f(\boldsymbol{x}))]$ for the expected loss. Here, as always, expectation means "average." In words, this is saying "if you drew a bunch of (x, y) pairs independently at random from $\mathcal{D}$, what would your *average* loss be? (More formally, what would be the average of $\ell(y, f(\boldsymbol{x}))$ be over these random draws?)

More formally, if $\mathcal{D}$ is a discrete probability distribution, then this expectation can be expanded as:

$$\mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\ell(y, f(\boldsymbol{x}))] = \sum_{(\boldsymbol{x},y)\in\mathcal{D}} [\mathcal{D}(\boldsymbol{x}, y)\ell(y, f(\boldsymbol{x}))] \tag{1.2}$$

This is *exactly* the weighted average loss over the all $(\boldsymbol{x}, y)$ pairs in $\mathcal{D}$, weighted by their probability (namely, $\mathcal{D}(\boldsymbol{x}, y)$) under this distribution $\mathcal{D}$.

In particular, if D is a *finite discrete distribution*, for instance one defined by a finite data set $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\}$ that puts equal weight on each example (in this case, equal weight means probability $1/N$), then we get:

$$\mathbb{E}_{(\boldsymbol{x},y)\sim D}[\ell(y, f(\boldsymbol{x}))] = \sum_{(\boldsymbol{x},y)\in D} [D(\boldsymbol{x}, y)\ell(y, f(\boldsymbol{x}))] \qquad \text{definition of expectation} \tag{1.3}$$

$$= \sum_{n=1}^{N} [D(\boldsymbol{x}_n, y_n)\ell(y_n, f(\boldsymbol{x}_n))] \qquad D \text{ is discrete and finite} \tag{1.4}$$

$$= \sum_{n=1}^{N} [\frac{1}{N}\ell(y_n, f(\boldsymbol{x}_n))] \qquad \text{definition of } D \tag{1.5}$$

$$= \frac{1}{N}\sum_{n=1}^{N} [\ell(y_n, f(\boldsymbol{x}_n))] \qquad \text{rearranging terms} \tag{1.6}$$

Which is exactly the average loss on that dataset.

In the case that the distribution is continuous, we need to replace the discrete sum with a continuous integral over some space Ω:

$$\mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\ell(y, f(\boldsymbol{x}))] = \int_{\Omega} \mathcal{D}(\boldsymbol{x}, y)\ell(y, f(\boldsymbol{x}))\mathrm{d}\boldsymbol{x}\mathrm{d}y \tag{1.7}$$

This is exactly the same but in continuous space rather than discrete space.
The most important thing to remember is that there are two equivalent ways to think about expections:

1. The expectation of some function g is the *weighted average value of* g, where the weights are given by the underlying probability distribution.
2. The expectation of some function g is your *best guess of the value of* g if you were to draw a single item from the underlying probability distribution.

Figure 1.4:

In Figure 1.5 you'll find training data for a binary classification problem. The two labels are "A" and "B" and you can see five examples for each label. Below, in Figure 1.6, you will see some test data. These images are left unlabeled. Go through quickly and, based on the training data, label these images. (Really do it before you read further! I'll wait!)

Most likely you produced one of two labelings: either ABBAAB or ABBABA. Which of these solutions is right?

The answer is that you cannot tell based on the training data. If you give this same example to 100 people, $60-70$ of them come up with the ABBAAB prediction and $30-40$ come up with the ABBABA prediction. Why are they doing this? Presumably because the first group believes that the relevant distinction is between "bird" and "non-bird" while the second group believes that the relevant distinction is between "fly" and "no-fly."

This preference for one distinction (bird/non-bird) over another (fly/no-fly) is a bias that different human learners have. In the context of machine learning, it is called **inductive bias**: in the absense of data that narrow down the relevant concept, what type of solutions are we more likely to prefer? Two thirds of people seem to have an inductive bias in favor of bird/non-bird, and one third seem to have an inductive bias in favor of fly/no-fly.

Throughout this book you will learn about several approaches to machine learning. The decision tree model is the first such approach. These approaches differ primarily in the sort of inductive bias that they exhibit.

Consider a variant of the decision tree learning algorithm. In this variant, we will not allow the trees to grow beyond some pre-defined maximum depth, d. That is, once we have queried on d-many features, we cannot query on any more and must just make the best guess we can at that point. This variant is called a **shallow decision tree**.

The key question is: What is the inductive bias of shallow decision trees? Roughly, their bias is that decisions can be made by only looking at a small number of features. For instance, a shallow decision tree would be very good at learning a function like "students only like AI courses." It would be very bad at learning a function like "if this student has liked an odd number of his past courses, he will like the next one; otherwise he will not." This latter is the *parity* function, which requires you to inspect every feature to make a prediction. The inductive bias of a decision tree is that the sorts of things we want to learn to predict are more like the first example and less like the second example.

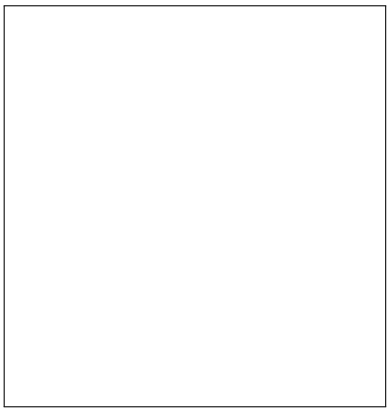


Figure 1.5: `dt:bird`: bird training images

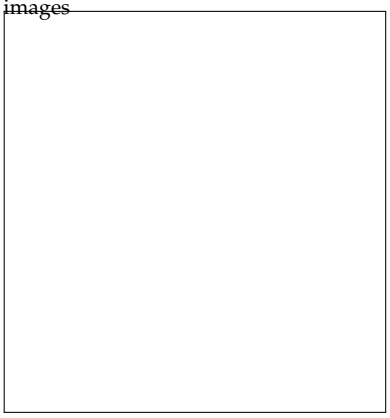


Figure 1.6: `dt:birdtest`: bird test images

? It is also possible that the correct classification on the test data is BABAAA. This corresponds to the bias "is the background in focus." Somehow no one seems to come up with this classification rule.

1.6 Not Everything is Learnable

Although machine learning works well—perhaps astonishingly well—in many cases, it is important to keep in mind that it is not magical. There are many reasons why a machine learning algorithm might fail on some learning task.

There could be **noise** in the training data. Noise can occur both at the feature level and at the label level. Some features might correspond to measurements taken by sensors. For instance, a robot might use a laser range finder to compute its distance to a wall. However, this sensor might fail and return an incorrect value. In a sentiment classification problem, someone might have a typo in their review of a course. These would lead to noise at the feature level. There might also be noise at the label level. A student might write a scathingly negative review of a course, but then accidentally click the wrong button for the course rating.

The features available for learning might simply be insufficient. For example, in a medical context, you might wish to diagnose whether a patient has cancer or not. You may be able to collect a large amount of data about this patient, such as gene expressions, X-rays, family histories, etc. But, even knowing all of this information exactly, it might still be impossible to judge for sure whether this patient has cancer or not. As a more contrived example, you might try to classify course reviews as positive or negative. But you may have erred when downloading the data and only gotten the first five characters of each review. If you had the rest of the features you might be able to do well. But with this limited feature set, there's not much you can do.

Some examples may not have a single correct answer. You might be building a system for "safe web search," which removes offensive web pages from search results. To build this system, you would collect a set of web pages and ask people to classify them as "offensive" or not. However, what one person considers offensive might be completely reasonable for another person. It is common to consider this as a form of label noise. Nevertheless, since you, as the designer of the learning system, have some control over this problem, it is sometimes helpful to isolate it as a source of difficulty.

Finally, learning might fail because the inductive bias of the learning algorithm is too far away from the concept that is being learned. In the bird/non-bird data, you might think that if you had gotten a few more training examples, you might have been able to tell whether this was intended to be a bird/non-bird classification or a fly/no-fly classification. However, no one I've talked to has ever come up with the "background is in focus" classification. Even with many

more training points, this is such an unusual distinction that it may be hard for anyone to figure out it. In this case, the inductive bias of the learner is simply too misaligned with the target classification to learn.

Note that the inductive bias source of error is fundamentally different than the other three sources of error. In the inductive bias case, it is the *particular* learning algorithm that you are using that cannot cope with the data. Maybe if you switched to a different learning algorithm, you would be able to learn well. For instance, Neptunians might have evolved to care greatly about whether backgrounds are in focus, and for them this would be an easy classification to learn. For the other three sources of error, it is not an issue to do with the particular learning algorithm. The error is a fundamental part of the learning problem.

1.7 Underfitting and Overfitting

As with many problems, it is useful to think about the *extreme cases* of learning algorithms. In particular, the extreme cases of decision trees. In one extreme, the tree is "empty" and we do not ask any questions at all. We simply immediately make a prediction. In the other extreme, the tree is "full." That is, every possible question is asked along every branch. In the full tree, there may be leaves with no associated training data. For these we must simply choose arbitrarily whether to say "yes" or "no."

Consider the course recommendation data from Table **??**. Suppose we were to build an "empty" decision tree on this data. Such a decision tree will make the same prediction regardless of its input, because it is not allowed to ask any questions about its input. Since there are more "likes" than "hates" in the training data (12 versus 8), our empty decision tree will simply always predict "likes." The training error, $\hat{\epsilon}$, is $8/20 = 40\%$.

On the other hand, we could build a "full" decision tree. Since each row in this data is unique, we can guarantee that any leaf in a full decision tree will have either 0 or 1 examples assigned to it (20 of the leaves will have one example; the rest will have none). For the leaves corresponding to training points, the full decision tree will always make the correct prediction. Given this, the training error, $\hat{\epsilon}$, is $0/20 = 0\%$.

Of course our goal is *not* to build a model that gets 0% error on the training data. This would be easy! Our goal is a model that will do well on *future, unseen* data. How well might we expect these two models to do on future data? The "empty" tree is likely to do not much better and not much worse on future data. We might expect

that it would continue to get around 40% error.

Life is more complicated for the "full" decision tree. Certainly if it is given a test example that is identical to one of the training examples, it will do the right thing (assuming no noise). But for everything else, it will only get about 50% error. This means that even if every other test point happens to be identical to one of the training points, it would only get about 25% error. In practice, this is probably optimistic, and maybe only one in every 10 examples would match a training example, yielding a 35% error.

So, in one case (empty tree) we've achieved about 40% error and in the other case (full tree) we've achieved 35% error. This is not very promising! One would hope to do better! In fact, you might notice that if you simply queried on a *single* feature for this data, you would be able to get very low training error, but wouldn't be forced to "guess" randomly.

? Convince yourself (either by proof or by simulation) that even in the case of imbalanced data – for instance data that is on average 80% positive and 20% negative – a predictor that guesses randomly (50/50 positive/negative) will get about 50% error.

This example illustrates the key concepts of **underfitting** and **overfitting**. Underfitting is when you had the opportunity to learn something but didn't. A student who hasn't studied much for an upcoming exam will be underfit to the exam, and consequently will not do well. This is also what the empty tree does. Overfitting is when you pay too much attention to idiosyncracies of the training data, and aren't able to generalize well. Often this means that your model is fitting noise, rather than whatever it is supposed to fit. A student who memorizes answers to past exam questions without understanding them has overfit the training data. Like the full tree, this student also will not do well on the exam. A model that is neither overfit nor underfit is the one that is expected to do best in the future.

? Which feature is it, and what is it's training error?

1.8 Separation of Training and Test Data

Suppose that, after graduating, you get a job working for a company that provides personalized recommendations for pottery. You go in and implement new algorithms based on what you learned in your machine learning class (you have learned the power of generalization!). All you need to do now is convince your boss that you have done a good job and deserve a raise!

How can you convince your boss that your fancy learning algorithms are really working?

Based on what we've talked about already with underfitting and overfitting, it is not enough to just tell your boss what your training error is. Noise notwithstanding, it is easy to get a training error of zero using a simple database query (or `grep`, if you prefer). Your boss will not fall for that.

The easiest approach is to *set aside* some of your available data as

"test data" and use this to evaluate the performance of your learning algorithm. For instance, the pottery recommendation service that you work for might have collected 1000 examples of pottery ratings. You will select 800 of these as **training data** and set aside the final 200 as **test data**. You will run your learning algorithms *only* on the 800 training points. Only once you're done will you apply your learned model to the 200 test points, and report your **test error** on those 200 points to your boss.

The hope in this process is that however well you do on the 200 test points will be indicative of how well you are likely to do in the future. This is analogous to estimating support for a presidential candidate by asking a small (random!) sample of people for their opinions. Statistics (specifically, concentration bounds of which the "Central limit theorem" is a famous example) tells us that if the sample is large enough, it will be a good representative. The 80/20 split is not magic: it's simply fairly well established. Occasionally people use a 90/10 split instead, especially if they have a *lot* of data.

? If you have more data at your disposal, why might a 90/10 split be preferable to an 80/20 split?

The cardinal rule of machine learning is: never touch your test data. Ever. If that's not clear enough:

Never *ever* touch your test data!

If there is only one thing you learn from this book, let it be that. Do not look at your test data. Even once. Even a tiny peek. Once you do that, it is not test data any more. Yes, perhaps your algorithm hasn't seen it. But you have. And you are likely a better learner than your learning algorithm. Consciously or otherwise, you might make decisions based on whatever you might have seen. Once you look at the test data, your model's performance on it is no longer indicative of it's performance on future unseen data. This is simply because future data is unseen, but your "test" data no longer is.

1.9 Models, Parameters and Hyperparameters

The general approach to machine learning, which captures many existing learning algorithms, is the **modeling** approach. The idea is that we come up with some formal model of our data. For instance, we might model the classification decision of a student/course pair as a decision tree. The choice of using a *tree* to represent this model is *our choice.* We also could have used an arithmetic circuit or a polynomial or some other function. The model tells us what sort of things we can learn, and also tells us what our inductive bias is.

For most models, there will be associated parameters. These are the things that we use the data to decide on. Parameters in a decision

tree include: the specific questions we asked, the order in which we asked them, and the classification decisions at the leaves. The job of our decision tree learning algorithm DECISIONTREETRAIN is to take data and figure out a good set of parameters.

Many learning algorithms will have additional knobs that you can adjust. In most cases, these knobs amount to tuning the inductive bias of the algorithm. In the case of the decision tree, an obvious knob that one can tune is the **maximum depth** of the decision tree. That is, we could modify the DECISIONTREETRAIN function so that it *stops* recursing once it reaches some pre-defined maximum depth. By playing with this depth knob, we can adjust between underfitting (the empty tree, depth$= 0$) and overfitting (the full tree, depth$= \infty$).

Such a knob is called a **hyperparameter**. It is so called because it is a parameter that controls other parameters of the model. The exact definition of hyperparameter is hard to pin down: it's one of those things that are easier to identify than define. However, one of the key identifiers for hyperparameters (and the main reason that they cause consternation) is that they cannot be naively adjusted using the training data.

? Go back to the DECISIONTREETRAIN algorithm and modify it so that it takes a maximum depth parameter. This should require adding two lines of code and modifying three others.

In DECISIONTREETRAIN, as in most machine learning, the learning algorithm is essentially trying to adjust the parameters of the model so as to minimize training error. This suggests an idea for choosing hyperparameters: choose them so that they minimize training error.

What is wrong with this suggestion? Suppose that you were to treat "maximum depth" as a hyperparameter and tried to tune it on your training data. To do this, maybe you simply build a collection of decision trees, tree_0, tree_1, tree_2, ..., tree_{100}, where tree_d is a tree of maximum depth d. We then computed the training error of each of these trees and chose the "ideal" maximum depth as that which minimizes training error? Which one would it pick?

The answer is that it would pick $d = 100$. Or, in general, it would pick d as large as possible. Why? Because choosing a bigger d will *never hurt* on the training data. By making d larger, you are simply encouraging overfitting. But by evaluating on the training data, overfitting actually looks like a good idea!

An alternative idea would be to tune the maximum depth on test data. This is promising because test data peformance is what we really want to optimize, so tuning this knob on the test data seems like a good idea. That is, it won't accidentally reward overfitting. Of course, it breaks our cardinal rule about test data: that you should never touch your test data. So that idea is immediately off the table.

However, our "test data" wasn't magic. We simply took our 1000 examples, called 800 of them "training" data and called the other 200

"test" data. So instead, let's do the following. Let's take our original 1000 data points, and select 700 of them as training data. From the remainder, take 100 as **development data**[3] and the remaining 200 as test data. The job of the development data is to allow us to tune hyperparameters. The general approach is as follows:

[3] Some people call this "**validation data**" or "**held-out data**."

1. Split your data into 70% training data, 10% development data and 20% test data.
2. For each possible setting of your hyperparameters:
   (a) Train a model using that setting of hyperparameters on the training data.
   (b) Compute this model's error rate on the development data.
3. From the above collection of models, choose the one that achieved the lowest error rate on development data.
4. Evaluate that model on the test data to estimate future test performance.

? In step 3, you could either choose the model (trained on the 70% training data) that did the best on the development data. Or you could choose the hyperparameter settings that did best and *retrain* the model on the 80% union of training and development data. Is either of these options obviously better or worse?

1.10 Chapter Summary and Outlook

At this point, you should be able to use decision trees to do machine learning. Someone will give you data. You'll split it into training, development and test portions. Using the training and development data, you'll find a good value for maximum depth that trades off between underfitting and overfitting. You'll then run the resulting decision tree model on the test data to get an estimate of how well you are likely to do in the future.

You might think: why should I read the rest of this book? Aside from the fact that machine learning is just an awesome fun field to learn about, there's a lot left to cover. In the next two chapters, you'll learn about two models that have very different inductive biases than decision trees. You'll also get to see a very useful way of thinking about learning: the geometric view of data. This will guide much of what follows. After that, you'll learn how to solve problems more complicated that simple binary classification. (Machine learning people like binary classification a lot because it's one of the simplest non-trivial problems that we can work on.) After that, things will diverge: you'll learn about ways to think about learning as a formal optimization problem, ways to speed up learning, ways to learn without labeled data (or with very little labeled data) and all sorts of other fun topics.

But throughout, we will focus on the view of machine learning that you've seen here. You select a model (and its associated inductive biases). You use data to find parameters of that model that work well on the training data. You use development data to avoid underfitting and overfitting. And you use test data (which you'll never look at or touch, right?) to estimate future model performance. Then you conquer the world.

1.11 *Exercises*

Exercise 1.1. TODO...