CHAPTER 5
Overfitting and Complexity Control

Fundamental concepts: *Generalization; Fitting and overfitting; Complexity control.*

Exemplary techniques: *Cross-validation; Attribute selection; Tree pruning; Regularization.*

One of the most important fundamental notions of data science is that of overfitting and generalization. If we allow ourselves enough flexibility in searching for patterns in a particular dataset, we will find patterns. Unfortunately, these "patterns" may be just chance occurrences in the data. As discussed previously, we are interested in patterns that generalize—that predict well for instances that we have not yet observed. Finding chance occurrences in data that look like interesting patterns, but which do not generalize, is called *overfitting* the data.

Generalization

Consider the following (extreme) scenario from our familiar churn problem. You're a manager at MegaTelCo, responsible for reducing customer churn. I run a data mining consulting group. You give my data science team a set of historical data on customers who have stayed with the company and customers who have departed within six months of contract expiration. My job is to build a model to distinguish customers who are likely to churn based on some features, as we've discussed previously. I mine the data and build a model. I give you back the code for the model, to implement in your company's churn-reduction system.

Of course you are interested in whether my model is any good, so you ask your technical team to check the performance of the model on the historical data. You understand that historical performance is no guarantee of future success, but your experience tells you that churn patterns remain relatively stable, except for major changes to the industry (such as the introduction of the iPhone), and you know of no such major changes since this data was collected. So, the tech team runs the historical dataset through the model. Your technical lead reports back that this data science team is amazing: the model is 100% accurate. It does not make a single mistake, identifying correctly all the churners as well as the nonchurners.

You're experienced enough not to be comfortable with that answer. You've had experts looking at churn behavior for a long time, and if there really were 100% accurate indicators, you figure you would be doing better than you currently are. Maybe this is just a lucky fluke?

It was not a lucky fluke. Our data science team can do that every time. Here is how we built the model. We stored the feature vector for each customer who has churned in a database table. Let's call that T_c. Then, in use, when the model is presented with a customer to determine the likelihood of churning, it takes the customer's feature vector, looks her up in T_c, and reports "100% likelihood of churning" if she is in T_c and "0% likelihood of churning" if she is not in T_c. So, when the tech team applies our model to the historical dataset, the model predicts perfectly.[1]

Call this simple approach a *table model*. It memorizes the training data and performs no generalization. What is the problem with this? Consider how we'll use the model in practice. When a *previously unseen* customer's contract is about to expire, we'll want to apply the model. Of course, this customer was not part of the historical dataset, so the lookup will fail since there will be no exact match, and the model will predict "0% likelihood of churning" for this customer. In fact, the model will predict this for every customer (not in the training data). A model that looked perfect would be completely useless in practice!

This may seem like an absurd scenario. In reality, no one would throw raw customer data into a table and claim it was a "predictive model" of anything. But it is important to think about why this is a bad idea, because it fails for the same reason other, more realistic data mining efforts may fail. It is an extreme example of two related fundamental concepts of data science: *generalization* and *overfitting*. Generalization is the property of a model or modeling process, whereby the model applies to data that were not used to build the model. In this example, the model does not generalize at all beyond the data that were used to build it. It is tailored, or "fit," perfectly to the training data. In fact, it is "overfit."

This is the important point. Every dataset is a finite sample of a population—in this case, the population of phone customers. We want models to apply not just to the exact training set but to the general population from which the training data came. We may worry that the training data were not representative of the true population,

1 Technically, this is not necessarily true: there may be two customers with the same feature vector description, one of whom churns and the other does not. We can ignore that possibility for the sake of this example. For example, we can assume that the unique customer ID is one of the features.

but that is not the problem here. The data were representative, but the data mining did not create a model that generalized beyond the training data.

Overfitting

Overfitting is the tendency of data mining procedures to tailor models to the training data, at the expense of generalization to previously unseen data points. The example from the previous section was contrived; the data mining built a model using pure memorization, the most extreme overfitting procedure possible. However, all data mining procedures have the tendency to overfit to some extent—some more than others. The idea is that if we look hard enough we will find patterns in a dataset. As the Nobel Laureate Ronald Coase said, "If you torture the data long enough, it will confess."

Unfortunately, the problem is insidious. The answer is not to use a data mining procedure that doesn't overfit because all of them do. Nor is the answer to simply use models that produce less overfitting, because there is a fundamental trade-off between the ability to represent complex relationships and the possibility of overfitting. Sometimes we may simply want more complex models, because they will better capture the real complexities of the application and thereby be more accurate. There is no single choice or procedure that will eliminate overfitting. The best strategy is to recognize overfitting and to manage complexity in a principled way.

The rest of this chapter discusses overfitting in more detail, methods for assessing the degree of overfitting at modeling time, as well as methods for avoiding overfitting as much as possible.

Overfitting Examined

Before discussing what to do about overfitting, we need to know how to recognize it.

Holdout Data and Fitting Graphs

Let's now introduce a simple analytic tool: the *fitting graph*. A fitting graph shows the accuracy of a model as a function of complexity. To examine *over*fitting, we need to introduce a concept that is fundamental to evaluation in data science: *holdout* data.

The problem in the prior section was that the model was evaluated on exactly the same data that was used to build it, and that provides no assessment of how well the model generalizes to unseen cases. What we need to do is to "hold out" some data for which we know the value of the target variable, but which will not be used to build the model. These are not the actual *use* data, for which we ultimately would like to predict the value of the target variable. Instead, creating holdout data is like creating a "lab test" of generalization performance. We will simulate the use scenario on these holdout data: we will hide from the model (and possibly from the modelers) the actual values for the target on the holdout data. The model will predict the values. Then we estimate the *generalization performance* by comparing the predicted values with the hidden true values. There is likely to be a difference between the model's accuracy on the training set (sometimes called the "in-sample" accuracy) and the model's generalization accuracy, as estimated on the holdout data. Thus, when the holdout data are used in this manner, they often are called the "test set."

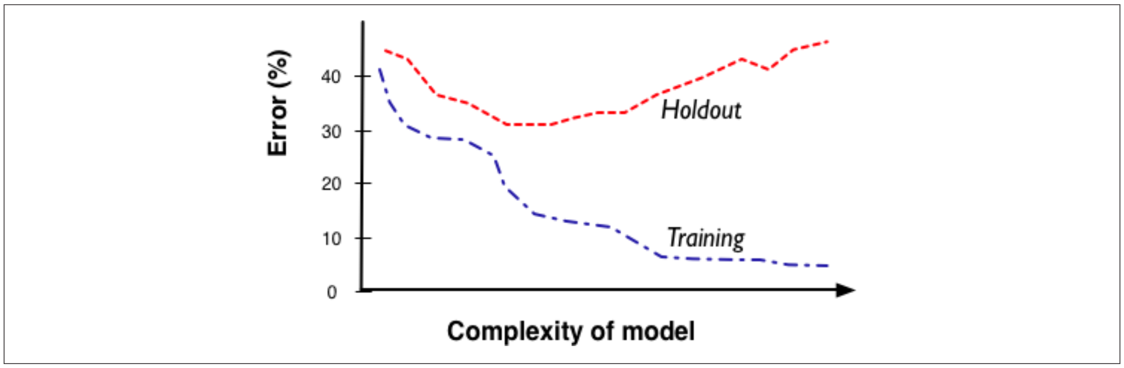


Figure 5-1. A typical fitting graph. Each point on a curve represents an error estimate of a model with a specified complexity (x axis). Accuracy estimates on training data and testing data vary differently based on how complex we allow a model to be. When the model is not allowed to be complex enough, it is not very accurate. As the models get too complex, they look very accurate on the training data, but in fact are overfitting—the training accuracy diverges from the holdout (generalization) accuracy.

The accuracy of a model depends on how complex we allow it to be. A model can be complex in different ways, as we will discuss in this chapter. First let us use this distinction between training and holdout data to define the fitting graph more precisely. The fitting graph (see Figure 5-1) shows the difference between a modeling procedure's accuracy on the training data and the accuracy on holdout data as model complexity changes. Generally, there will be more overfitting as one allows the model to be more complex. (Technically, the chance of overfitting increases as one allows the modeling procedure more flexibility in the models it can produce; we will ignore that distinction in this book).

Figure 5-2 shows a fitting graph for the customer churn "table model" described earlier. Since this was an extreme example the fitting graph will be peculiar. Again, the *x* axis measures the complexity of the model; in this case, the number of rows allowed in the table. The *y* axis measures the error. As we allow the table to increase in size, we can memorize more and more of the training set, and with each new row the training set error decreases. Eventually the table is large enough to contain the entire training set (marked N on the *x* axis) and the error goes to zero and remains there. However, the testing (holdout) set error starts at some value (let's call it *b*) and never decreases, because there is never an overlap between the training and holdout sets. The large gap between the two is a strong indication of memorization.

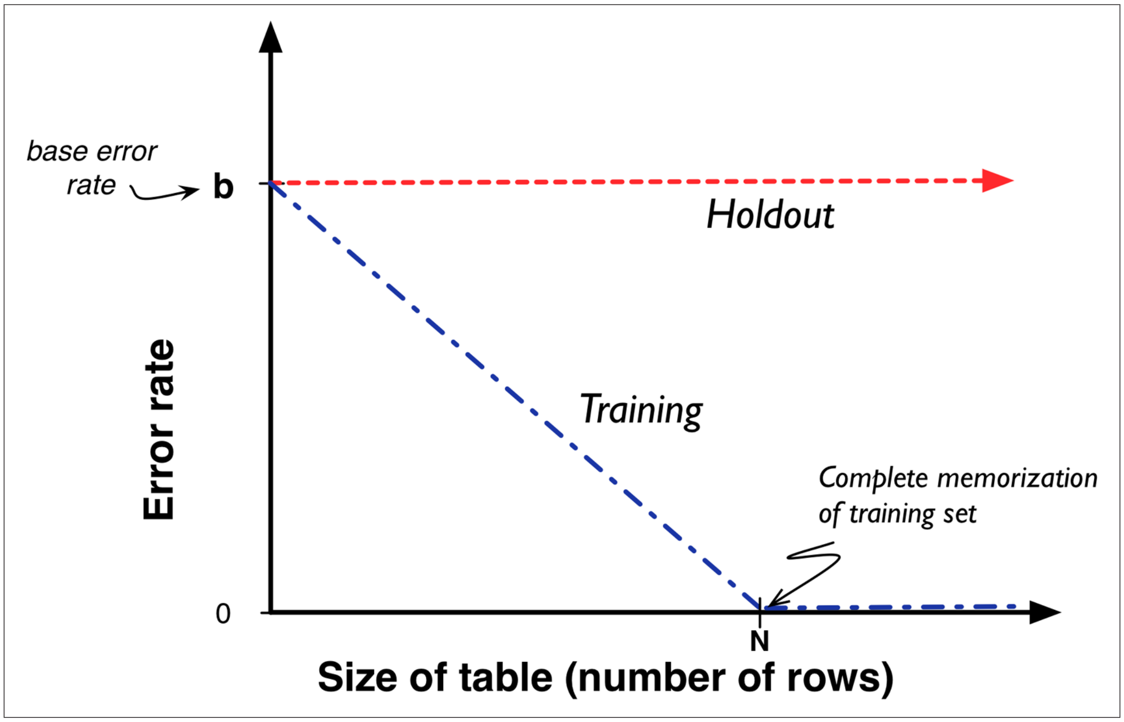
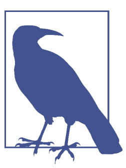


Figure 5-2. A fitting graph for the customer churn (table) model.



Note: Base rate

What would *b* be? Since the table model always predicts `no churn` for every new case, it will get every `no churn` case right and every `churn` case wrong. Thus the error rate will be the percentage of `churn` cases in the population. This is known as the *base rate*, and a classifier that always selects the majority class is called a base rate classifier.

A corresponding baseline for a regression model is a simple model that always predicts the mean or median value of the target variable.

You will occasionally hear reference to "base rate performance," especially as an important baseline against which to compare, and this is what it refers to. We will revisit the base rate in the next chapter.

We've discussed in the previous chapters two very different sorts of modeling procedures: recursive partitioning of the data as done for tree induction, and fitting a numeric model by finding an optimal set of parameters, for example the weights in a linear model. We can now examine overfitting for each of these procedures.

Overfitting in Tree Induction

Recall how we built tree-structured models for classification. We applied a fundamental ability to find important, predictive individual attributes repeatedly (recursively) to smaller and smaller data subsets. Let's assume for illustration that the dataset does not have two instances with exactly the same feature vector but different target values. If we continue to split the data, eventually the subsets will be pure—all instances in any chosen subset will have the same value for the target variable. These will be the leaves of our tree. There might be multiple instances at a leaf, all with the same value for the target variable. If we have to, we can keep splitting on attributes, and subdividing our data until we're left with a single instance at each leaf node, which is pure by definition.

What have we just done? We've essentially built a version of the lookup table discussed in the prior section as an extreme example of overfitting! Any training instance given to the tree for classification will make its way down, eventually landing at the appropriate leaf—the leaf corresponding to the subset of the data that includes this particular training instance. What will be the accuracy of this tree on the training set? It will be perfectly accurate, predicting correctly the class for every training instance.

Will it generalize? Possibly. This tree should be slightly better than the lookup table because every previously unseen instance will arrive at *some* classification, rather than just failing to match; the tree will give a nontrivial classification even for instances it has not seen before. Therefore, it is useful to examine empirically how well the accuracy on the training data tends to correspond to the accuracy on test data.

A procedure that grows trees until the leaves are pure tends to overfit. Tree-structured models are very flexible in what they can represent. Indeed, they can represent any function of the features, and if allowed to grow without bound they can fit it to arbitrary precision. But the trees may need to be huge in order to do so. The complexity of the tree lies in the number of nodes.

Figure 5-3 shows a typical fitting graph for tree induction. Here we artificially limit the maximum size of each tree, as measured by the number of nodes it's allowed to have, indicated on the x axis (which is log scale for convenience). For each tree size we create a new tree from scratch, using the training data. We measure two values: its accuracy on the training set and its accuracy on the holdout (test) set. If the data subsets at the leaves are not pure, we will predict the target variable based on some average over the target values in the subset, as we discussed in Chapter 3.

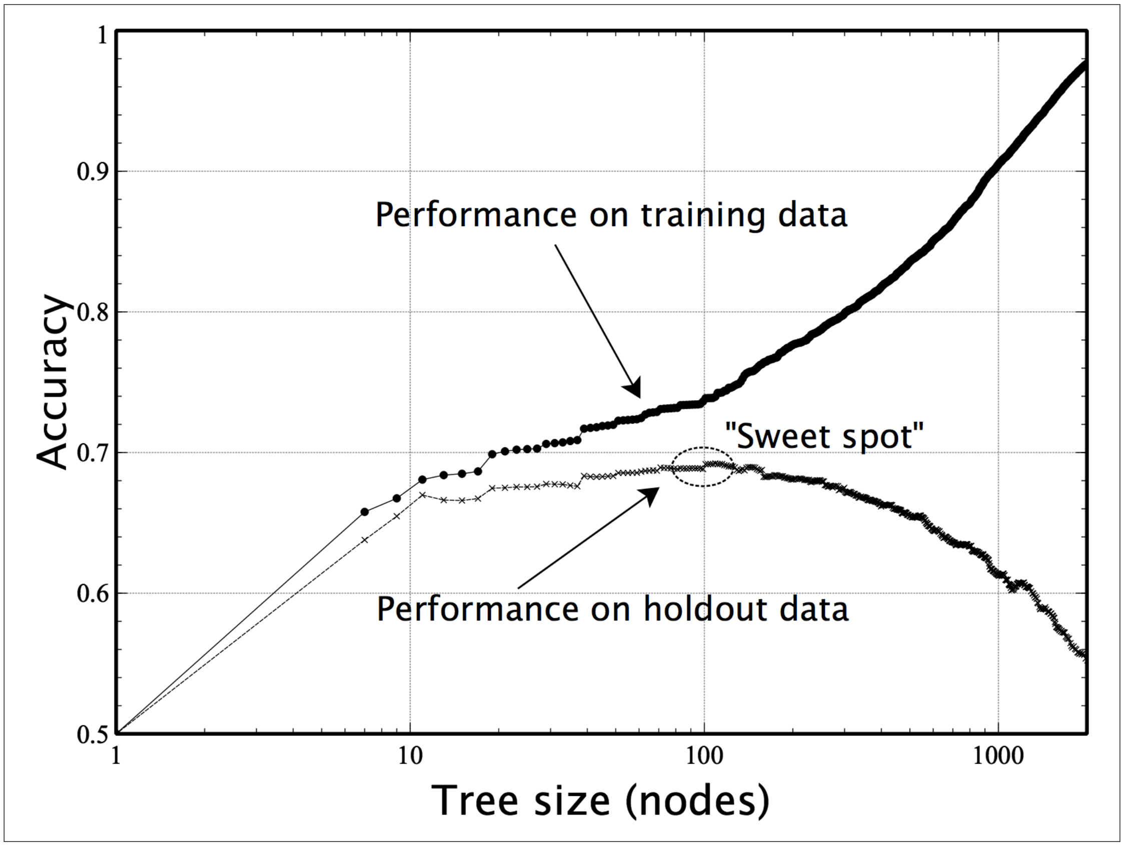


Figure 5-3. A typical fitting graph for tree induction.

Beginning at the left, the tree is very small and has poor performance. As it is allowed more nodes it improves rapidly, and both training-set accuracy and holdout-set accuracy improve. Also we see that training-set accuracy always is at least a little better than holdout-set accuracy, since we did get to look at the training data when building the model. But at some point the tree starts to overfit: it acquires details of the training set that are not characteristic of the population in general, as represented by the holdout set. In this example overfitting starts to dominate at around $x = 100$ nodes, denoted the "sweet spot" in the graph. As the trees are allowed to get larger, the training-set accuracy continues to increase—in fact, it is capable of memorizing the entire training set if we let it, leading to an accuracy of 1.0 (not shown). But the holdout accuracy declines as the tree grows past its "sweet spot"; the data subsets at the leaves get smaller and smaller, and the model generalizes from fewer and fewer data. Such inferences will be increasingly error-prone and the performance on the holdout data suffers.

In summary, from this fitting graph we may infer that overfitting on this dataset starts to dominate at around 100 nodes, so we should restrict tree size to this value.[2] This represents the best trade-off between the extremes of (i) not splitting the data at all and simply using the average target value in the entire dataset, and (ii) building a complete tree until the leaves are pure.

Unfortunately, no one has come up with a way to determine this sweet spot theoretically so we have to rely on empirical techniques. Before discussing those, let's examine overfitting in our second sort of modeling procedure.

Overfitting in Mathematical Functions

There are different ways to allow more or less complexity in mathematical functions. There are entire books on the topic. This section discusses one very important way, and "* Avoiding Overfitting for Parameter Optimization" on page 146 discusses a second one. We urge you to at least skim that advanced (starred) section because it introduces concepts and vocabulary in common use by data scientists these days, that can make a non-data scientist's head swim. Here we will summarize and give you enough to understand such discussions at a conceptual level.[3] But first, let's discuss a much more straightforward way in which functions can become too complex.

One way mathematical functions can become more complex is by adding more variables (more attributes). For example, say that we have a linear model as described in Equation 4-2:

$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3$$

As we add more x_i's, the function becomes more complicated, because each x_i has a corresponding w_i, which is a parameter of the model that must be learned.

Modelers sometimes even change the function from being truly linear in the original attributes by adding new attributes that are nonlinear versions of original attributes. For example, I might add a fourth attribute $x_4 = x_1^2$. Also, we might expect that the ratio of x_2 and x_3 is important, so we add a new attribute $x_5 = x_2/x_3$. Now we're trying to find the parameters (weights) of:

$$f(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4 + w_5 x_5$$

2 Note that 100 nodes is not some special universal value; it is specific to this particular dataset. If we changed the data significantly, or even just used a different tree-building algorithm, we'd want to create another fitting graph to be sure the sweet spot hadn't moved.

3 We also will have enough of a conceptual toolkit by that point to understand support vector machines a little better—as being almost equivalent to logistic regression with complexity (overfitting) control.

Either way, a dataset may end up with a very large number of attributes, and using all of them gives the modeling procedure much leeway to fit the training set. You might recall from geometry that in two dimensions you can fit a line to any two points and in three dimensions you can fit a plane to any three points. This concept generalizes: as you increase the dimensionality, you can perfectly fit larger and larger sets of arbitrary points. And even if you cannot fit the dataset perfectly, you can fit it better and better with more dimensions—that is, with more attributes.

Often, modelers carefully prune the attributes in order to avoid overfitting. Modelers will use a sort of holdout technique introduced above to assess the information in the individual attributes. Careful manual attribute selection is a wise practice in cases where considerable human effort can be spent on modeling, and where there are reasonably few attributes. In many modern applications, where large numbers of models are built automatically or where there are large numbers of attributes, manual selection may not be feasible. For example, companies that do data science-driven targeting of online display advertisements can build thousands of models each day, sometimes with millions of possible features. In such cases there is no choice but to employ automatic feature selection (or to ignore feature selection all together).

Example: Overfitting Linear Functions

In "An Example of Mining a Linear Discriminant from Data" on page 95, we introduced a simple dataset called Iris, comprising data of two species of Iris flowers. Now let's revisit that to see the effects of overfitting in action.

Figure 5-4 shows the original Iris dataset graphed with its two attributes, Petal width and Sepal width. Recall that each instance is one flower and corresponds to one dot on the graph. The filled dots are of the species *Iris Setosa* and the circles are instances of the species *Iris Versicolor*. Note several things here: first, the two classes of iris are very distinct and separable. In fact, there is a wide gap between the two groups of instances. Both logistic regression (LR) and the support vector machine (SVM) place separating boundaries (lines) in the middle.

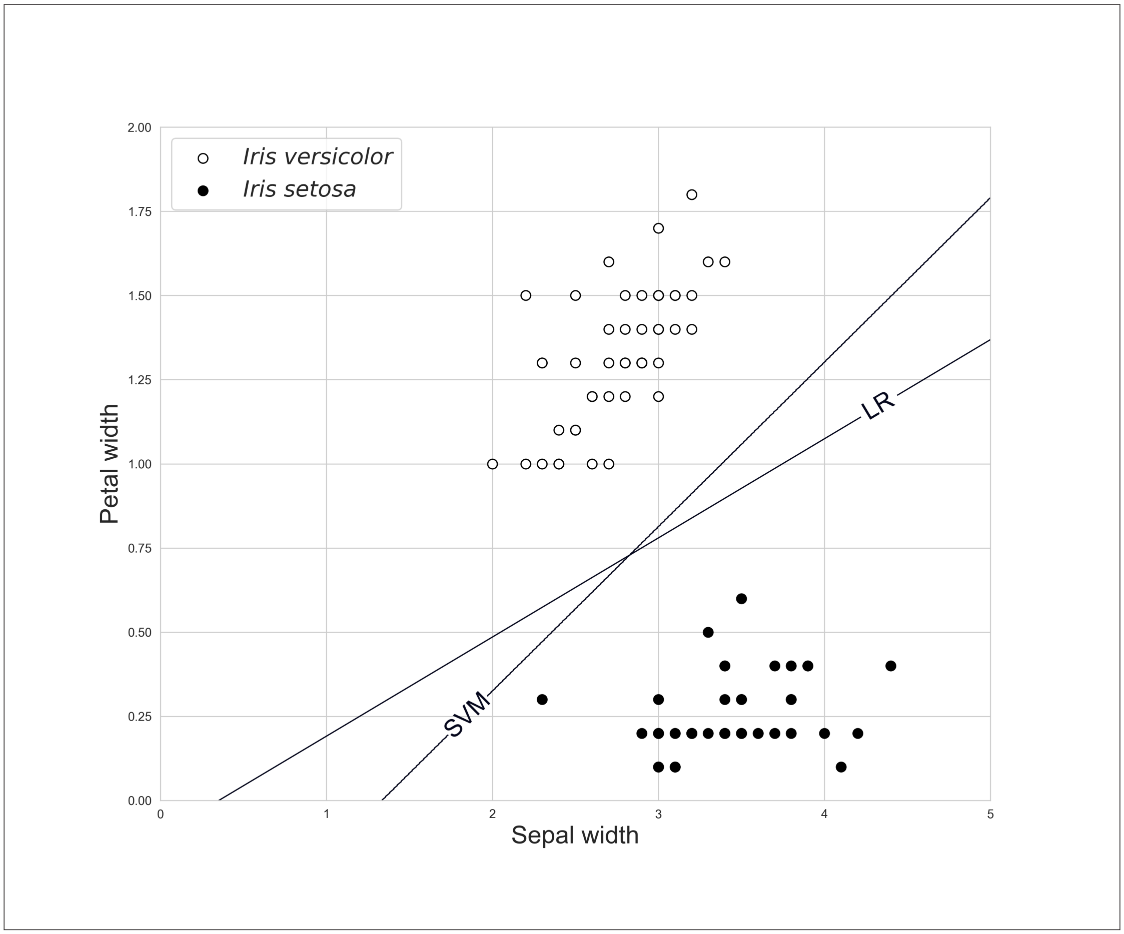


Figure 5-4. The original Iris dataset and the models (boundary lines) learned by two linear methods, logistic regression (LR) and a support vector machine (SVM).

In Figure 5-5, we've added a single new example: an *Iris Setosa* point at (3,1). Realistically, we might consider this example to be an outlier or an error since it's much closer to the *Versicolor* examples than the *Setosas*. Notice how the LR line moves in response: it separates the two groups perfectly, while the SVM line barely moves at all.

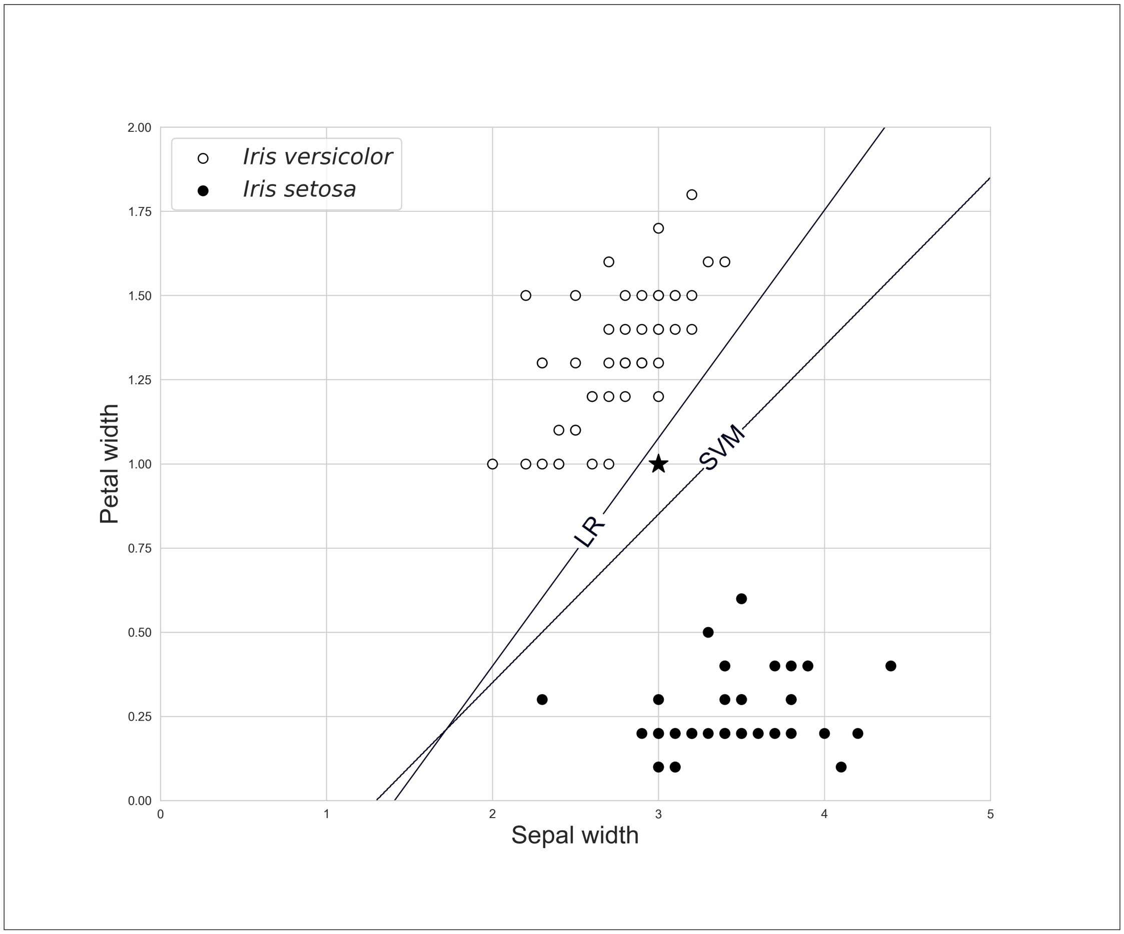


Figure 5-5. The Iris dataset from Figure 5-4 with a single new Iris Setosa example added (shown by the black star). Note how the boundary created by logistic regression (LR) has changed considerably, whereas the support vector machine's has not.

In Figure 5-6 we've added a different outlier at (4,0.7), this time a *Versicolor* example down in the *Setosa* region. Again, the support vector machine line moves very little in response, but the logistic regression line moves considerably.

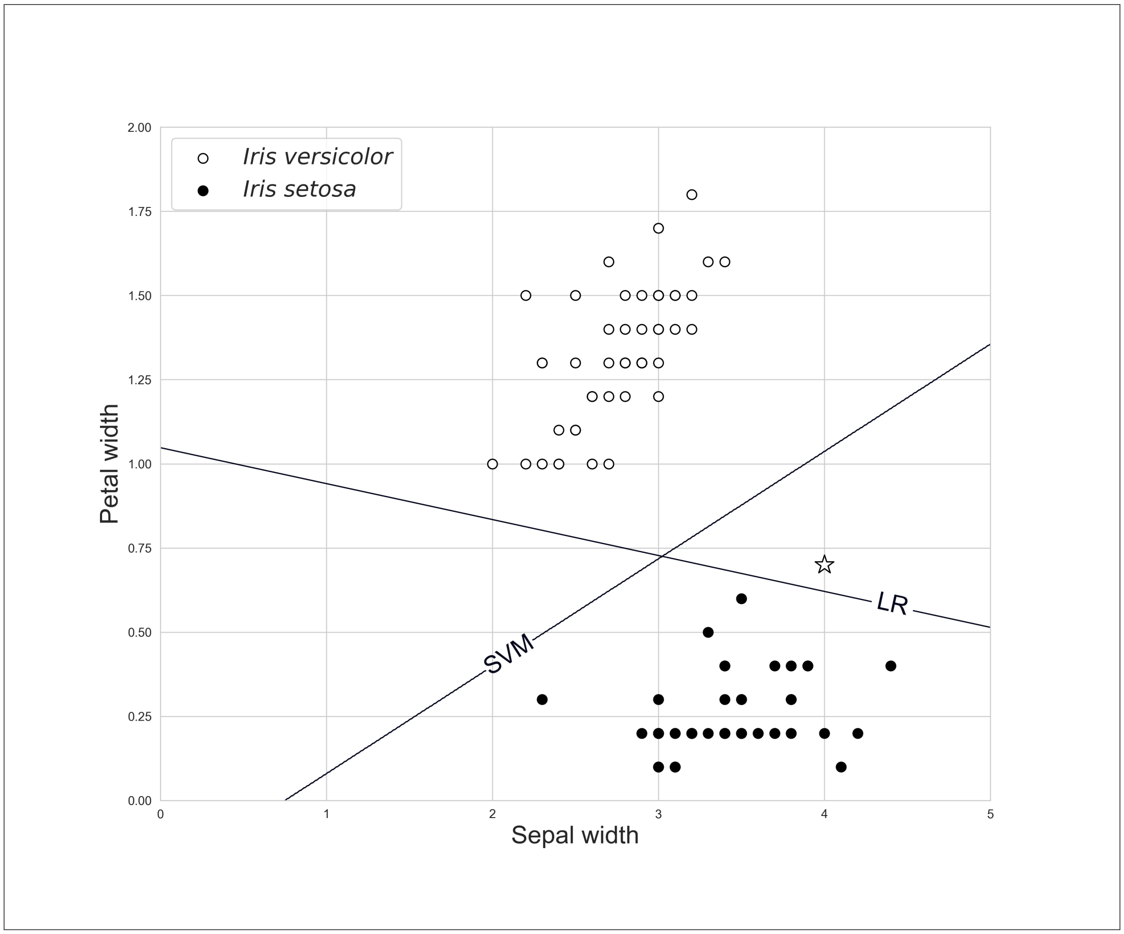


Figure 5-6. The Iris dataset from Figure 5-4 with a single new Iris Versicolor example added (shown by the white star). Note how logistic regression again changes its model considerably.

In Figure 5-5 and Figure 5-6, Logistic regression appears to be overfitting. Arguably, the single examples introduced in each figure are outliers that should not have much influence on the model since each contributes little to the overall "mass" of examples. Yet logistic regression is strongly influenced. If a linear boundary exists, logistic regression will find it,[4] even if this means moving the boundary to accommodate outliers. The SVM tends to be less sensitive to individual examples. The SVM training procedure incorporates complexity control, which we will describe technically later.

4 Technically, only *some* logistic regression algorithms are guaranteed to find it. Some do not have this guarantee. However, this fact is not germane to the overfitting point we're making here.

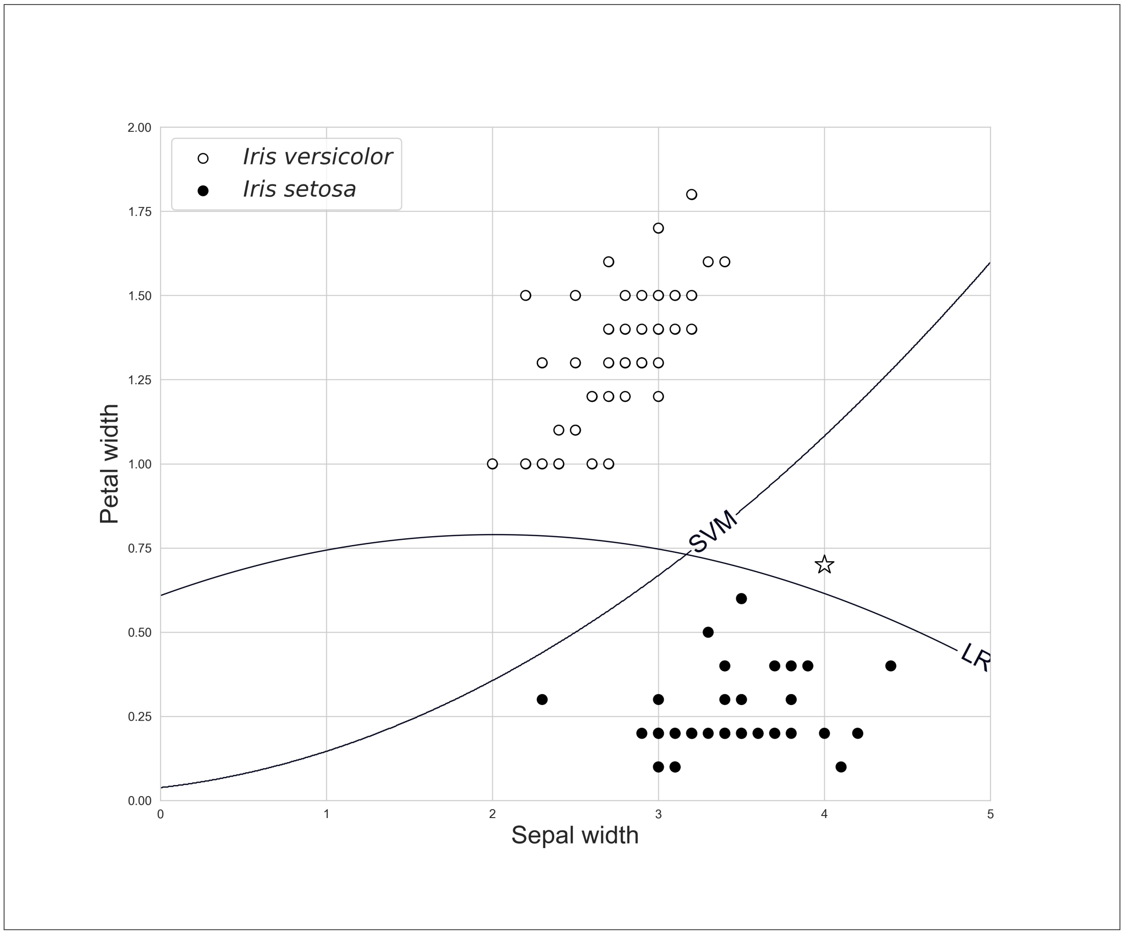


Figure 5-7. The Iris dataset from Figure 5-6 with both logistic regression and the support vector machine given an additional feature, ***Sepal width***^{2}*. This feature allows both methods the freedom to create more complex, nonlinear models (boundaries).*

As we said earlier, another way mathematical functions can become more complex is by adding more variables. In Figure 5-7, we have done just this: we used the same dataset as in Figure 5-6 but we added a single extra attribute: the square of the Sepal width. This attribute provides the methods with more flexibility in fitting the data because they may assign a weight to it. Geometrically, this means the separating boundary can be not just a line but a *parabola*, and this new freedom allows both methods to create curved surfaces that fit the regions more closely. In some cases curved surfaces may be necessary, but allowing them gives the methods far more opportunity to overfit. Note that, although the SVM's boundary is now curved, the boundary is used to keep the margin larger rather than to achieve perfect separation of the classes, as logistic regression has done.

* Example: Why Is Overfitting Bad?

Technical Details Ahead

At the beginning of the chapter, we said that a model that only memorizes is useless because it is incapable of generalizing. But technically this only demonstrates that overfitting only hinders model improvement; it does not explain why overfitting often causes models to become *worse*, as Figure 5-3 shows. This section goes into a detailed example showing how this may happen and why. It may be skipped without loss of continuity.

Why does performance sometimes degrade? The short answer is that as a model is allowed to become more complex it may pick up spurious correlations in the data. Some complexity is just extra unnecessary structure, but some may be harmful. These correlations are idiosyncrasies of the specific training set used and do not represent general characteristics of the population. The harm occurs when these spurious correlations produce *incorrect* generalizations in the model, causing performance to degrade when overfitting occurs. In this section we go through an example in detail to show how this can happen.

Consider a simple two-class problem with classes c_1 and c_2 and attributes x and y. Assume we have a population of examples, evenly balanced between the classes. Attribute x has two values, p and q, and y has two values, r and s. In the general population, $x = p$ occurs 75% of the time in class c_1 examples and in 25% of the c_2 examples, so x provides some prediction of the class. By design, y has no predictive power at all, and indeed we see that in the data sample both of y's values occur in both classes equally. In short, the instances in this domain are difficult to separate, with only x providing some predictive power. The best we can achieve is 75% accuracy by looking at x.

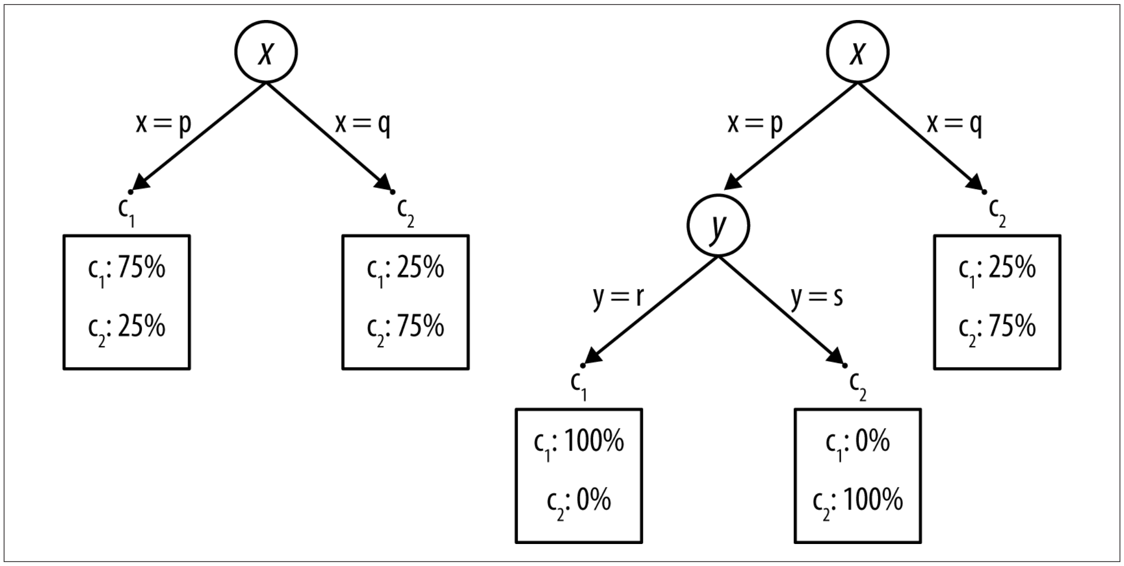


Figure 5-8. Classification trees for the overfitting example. (a) The optimal tree. (b) An overfit tree learned from the data in Table 5-1.

What would a classification tree learner ideally do samples of data from this population? Attribute *x* provides some leverage so a tree learner would split on it and create the tree shown on the left side of Figure 5-8. Since *x* provides the only leverage, this should be the optimal tree. Its error rate is 25%—equal to the theoretical minimum error rate.

Table 5-1. A small set of training examples

Instance	x	y	Class
1	p	r	c_1
2	p	r	c_1
3	p	r	c_1
4	q	s	c_1
5	p	s	c_2
6	q	r	c_2
7	q	s	c_2
8	q	r	c_2

Table 5-1 shows a very small training set of examples from this domain. *In this particular* dataset *y*'s values of *r* and *s* are not evenly split between the classes, so *y* seems to provide some predictiveness. Specifically, once we choose *x*=p (instances 1-4), we see that *y*=r predicts c_1 perfectly (instances 1-3). Hence, from this dataset, tree induction would achieve information gain by splitting on y's values and create two new leaf nodes, shown on the right side of Figure 5-8.

Based on our training set, this second, larger tree performs better than the optimal one. It classifies seven of the eight training examples correctly, whereas the optimal tree classifies only six out of eight correctly. But this is due to the fact that y=r purely by chance correlates with class c_1 in this data sample; in the general population there is no such correlation. The extra branch in the larger tree is not simply extraneous, it is harmful. Recall that we defined the general population to have x=p occurring in 75% of the class c_1 examples and 25% of the c_2 examples. But the spurious y=s branch predicts c_2, which is wrong in the general population. In fact, we expect this spurious branch to contribute one in eight errors made by the tree. Overall, the overfit tree will have an expected accuracy of 62.5%, while the optimal tree will have an accuracy of 75%.

In summary,

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Accuracy	Optimal tree	Overfit tree
Training set	75%	87.5%
True population	75%	62.5%

Several points should be emphasized here. First, this phenomenon is not particular to trees. Trees are merely convenient for this example because it is easy to point to a portion of a tree and declare it to be spurious, but all model types are susceptible to overfitting. Second, this phenomenon is not due to the training data in Table 5-1 being atypical or biased. Every dataset is a finite sample of a larger population, and samples will have variations even when there is no bias in the sampling. Third, the answer is not simply to increase the training set size, hoping that overfitting will go away. As we've seen, many models will expand to (over)fit the increasing amounts of training data. Finally, as we have said before, there is no general analytic way to determine in advance whether a model has overfit. In this example we defined the true population so we could declare that a given model had overfit. In practice, you will not have such knowledge and it will be necessary to use a holdout set to detect overfitting.

From Holdout Evaluation to Cross-Validation

Later we will present a general technique to help avoid overfitting, but first we need to discuss holdout evaluation in more detail. Before we can work to avoid overfitting, we need to be able to avoid being fooled by overfitting. At the beginning of this chapter we introduced the idea that in order to have a fair evaluation of the generalization performance of a model, we should estimate its accuracy on holdout data—data not used in building the model, but for which we do know the actual value of the target variable. Holdout testing is similar to other sorts of evaluation in a "laboratory" setting.

While a holdout set will indeed give us an estimate of generalization performance, it is just a single estimate. Should we have any confidence in a single estimate of model accuracy? It might have just been a single particularly lucky (or unlucky) choice of training and test data. We will not go into the details of computing confidence intervals on such quantities, but it is important to discuss a general testing procedure that will end up helping in several ways.

Cross-validation is a more sophisticated holdout training and testing procedure. We would like not only a simple estimate of the generalization performance, but also some statistics on it, such as the mean and variance, so that we can understand how performance varies across datasets. This variance is critical for assessing confidence in the performance estimate, as you might have learned in a statistics class.

Cross-validation also makes better use of a limited dataset. Unlike splitting the data into one training and one holdout set, cross-validation computes its estimates over *all* the data by performing multiple splits and systematically swapping out samples for testing.

Sidebar: Obtaining additional data

Because additional labeled data usually improves performance, you probably want to save the data processed by your system and add it to the training data you already have. There are subtleties with this that can cause problems: a deployed system may alter the population it sees, which can introduce selection bias. For example, a system that decides credit worthiness for loans will only see the results of loans that are approved—not the ones that are denied. We discuss this issue further in "A Brief Digression on Selection Bias" on page 303.

Cross-validation begins by splitting a labeled dataset into k partitions called *folds*. Typically, k will be five or ten. The top pane of Figure 5-9 shows a labeled dataset (the original dataset) split into five folds. Cross-validation then iterates training and testing k times, in a particular way. As depicted in the bottom pane of Figure 5-9, in each iteration of the cross-validation, a different fold is chosen as the test data. In this iteration, the other k–1 folds are combined to form the training data. So, in each iteration we have (k–1)/k of the data used for training and 1/k used for testing.

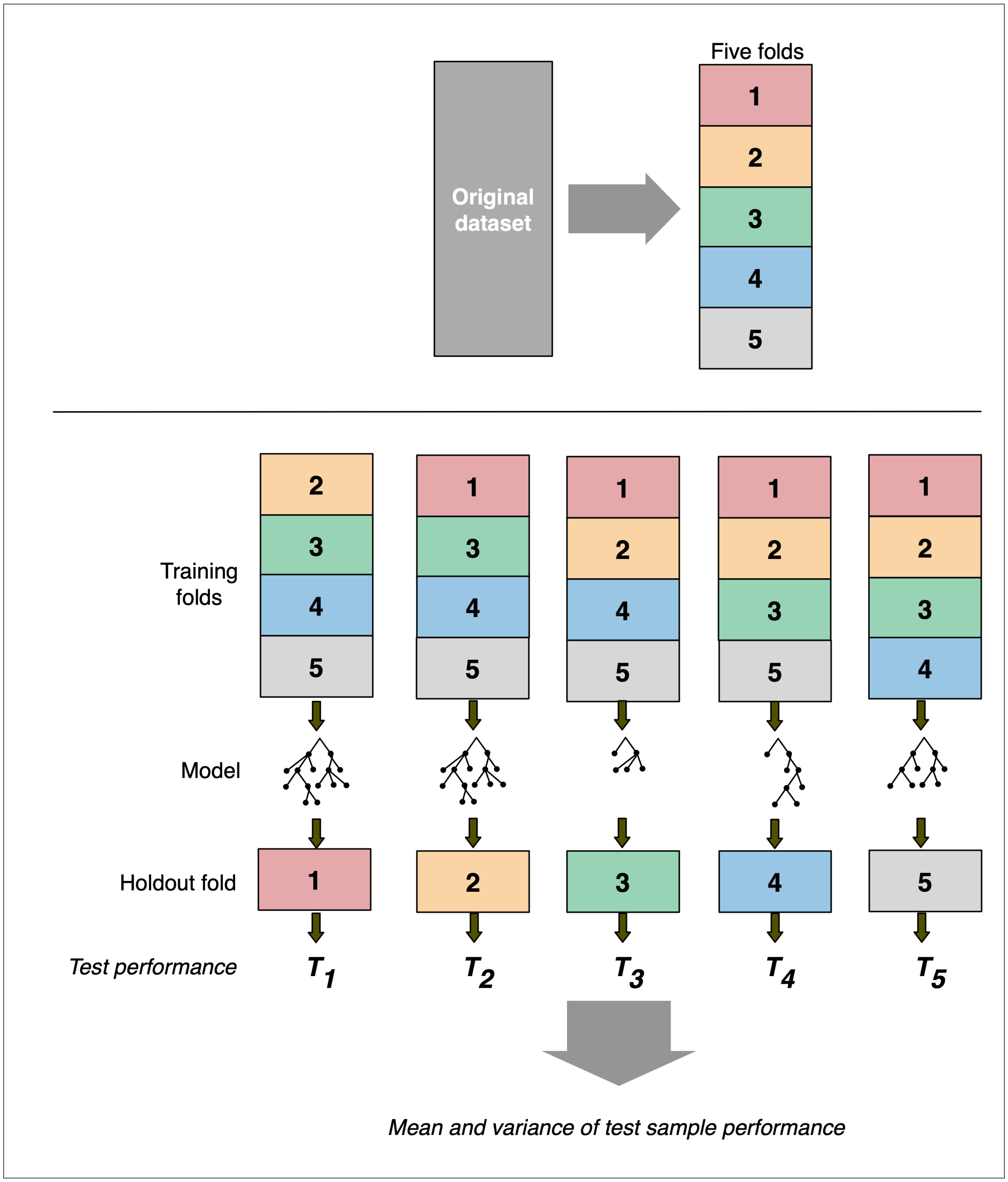

Figure 5-9. An illustration of cross-validation. The purpose of cross-validation is to use labeled data efficiently to estimate the performance of a modeling procedure. Here we show five-fold cross-validation: the original dataset is split randomly into five equal-sized pieces. Then, each piece is used in turn as the test set, with the other four used to train a model. The result is five accuracy estimates, which then can be used to compute the mean and its variance.

Each iteration produces one model, and thereby one estimate of generalization performance. When cross-validation is finished, every example will have been used only once for testing but *k*–1 times for training. At this point we have performance estimates from all the *k* folds and we can compute the average and standard deviation.

The Churn Dataset Revisited

Consider again the churn dataset introduced in "Example: Addressing the Churn Problem with Tree Induction" on page 80. In that section we used the entire dataset both for training and testing, and we reported an accuracy of 73%. We ended the section by asking, *Do you trust this number?* By this point you should know enough to mistrust any performance measurement taken from the training set, because overfitting is a very real possibility. Now that we have introduced cross-validation we can redo the evaluation more carefully.

Figure 5-10 shows the results of ten-fold cross-validation. In fact, two model types are shown. The top graph shows results with logistic regression, and the bottom graph shows results with classification trees. To be precise: the dataset was first shuffled, then divided into ten partitions. Each partition in turn served as a single holdout set while the other nine were collectively used for training. The horizontal line in each graph is the average of accuracies of the ten models of that type.

There are several things to observe here. First, the average accuracy of the folds with classification trees is 68.6%—significantly lower than our previous measurement of 73%. This means there was some overfitting occurring with the classification trees, and this new (lower) number is a more realistic measure of what we can expect. Second, there is variation in the performance on the different folds (the standard deviation of the fold accuracies is 1.1), and thus it is a good idea to average them to get a notion of the performance as well as the variation we can expect from inducing classification trees on this dataset.

Finally, compare the fold accuracies between logistic regression and classification trees. There are certain commonalities in both graphs—for example, neither model type did very well on Fold Three and both performed well on Fold Ten. But there are definite differences between the two. An important thing to notice is that logistic regression models show slightly lower average accuracy (64.1%) and higher variation (standard deviation of 1.3) than the classification trees do. On this particular dataset, trees may be preferable to logistic regression because of their greater stability and performance. But this is not absolute; other datasets will produce different results, as we shall see.

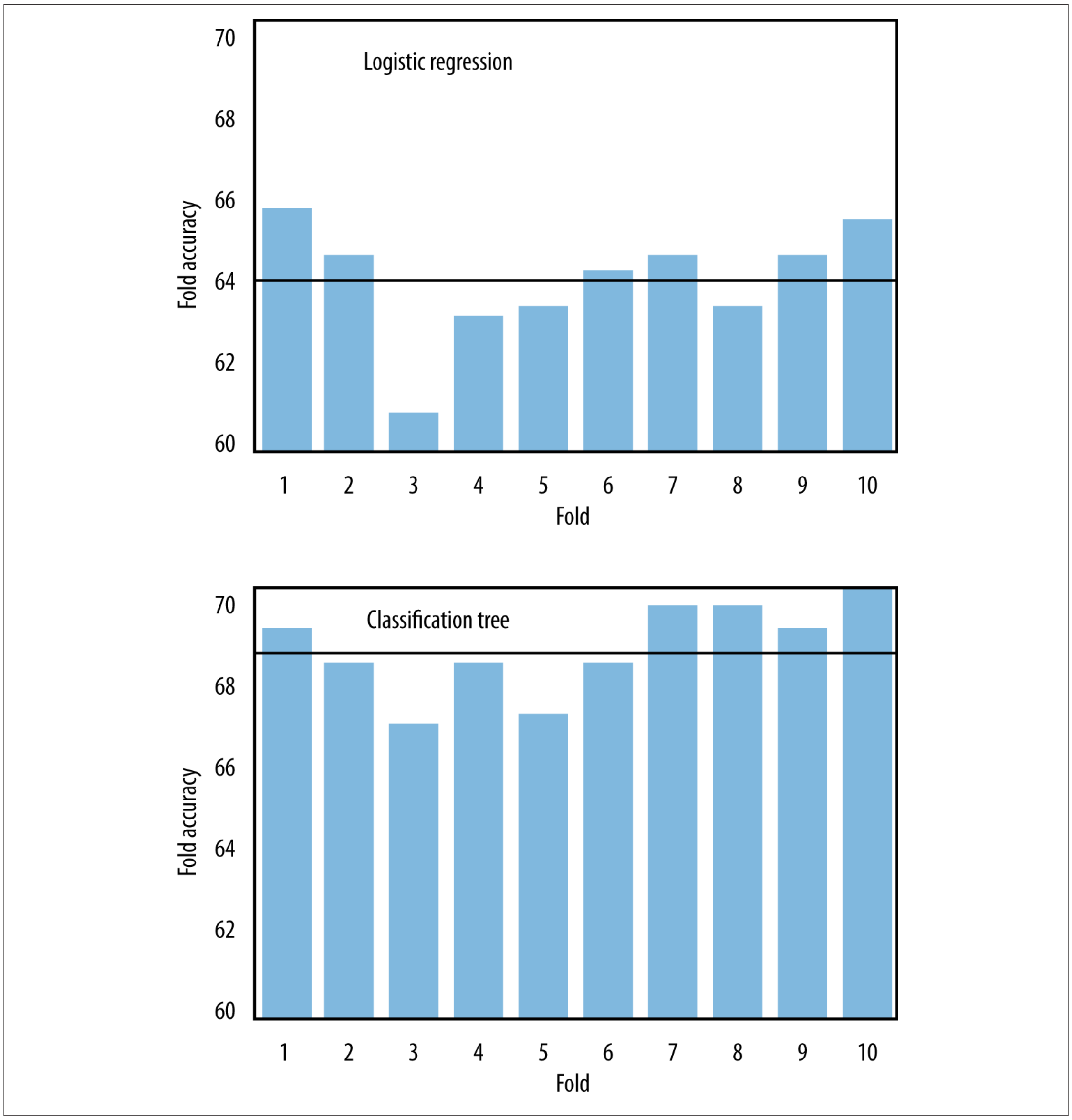

Figure 5-10. Fold accuracies for cross-validation on the churn problem. At the top are accuracies of logistic regression models trained on a dataset of 20,000 instances divided into ten folds. At the bottom are accuracies of classification trees on the same folds. In each graph the horizontal line shows the average accuracy of the folds. (Note the selection of the range of the y axis, which emphasizes the differences in accuracy.)

Learning Curves

If the training set size changes, you should expect generalization performance to change as well. All else being equal, model performance usually improves with more training data, up to a point. A plot of the generalization performance against the amount of training data is called a *learning curve*. The learning curve is another important analytical tool.

Learning curves for tree induction and logistic regression are shown in Figure 5-11 for the telecommunications churn problem.[5] Learning curves usually have a characteristic shape. They are steep initially as the modeling procedure finds the most apparent regularities in the dataset. Then as the modeling procedure is allowed to train on larger and larger datasets, it finds more accurate models. However, the marginal advantage of having more data decreases, so the learning curve becomes less steep. In some cases, the curve flattens out completely because the procedure can no longer improve accuracy even with more training data.

It is important to understand the difference between learning curves and fitting graphs (or fitting curves). A learning curve shows the generalization performance—the performance only on testing data, plotted against the *amount of training data* used. A fitting graph shows the generalization performance as well as the performance on the training data, but plotted against model *complexity*. Fitting graphs generally are shown for a fixed amount of training data.

Even on the same data, different modeling procedures can produce very different learning curves. In Figure 5-11, observe that for smaller training-set sizes, logistic regression yields better generalization accuracy than tree induction. However, as the training sets get larger, the learning curve for logistic regression levels off faster, the curves cross, and tree induction soon is more accurate. This performance relates back to the fact that with more flexibility comes more overfitting. Given the same set of features, classification trees are a more flexible model representation than linear logistic regression. This means two things: for smaller data, tree induction will tend to overfit more. Often, as we observe in Figure 5-11, this leads logistic regression to perform better on smaller datasets. On the other hand, the figure also shows that the flexibility of tree induction can be an advantage with larger training sets: the tree can represent nonlinear relationships between the features and the target. Whether the tree induction can actually *capture* those relationships is another question, and it needs to be evaluated empirically using an analytical tool such as learning curves.

5 Perlich et al. (2003) analyze learning curves for tree induction and logistic regression for dozens of classification problems.

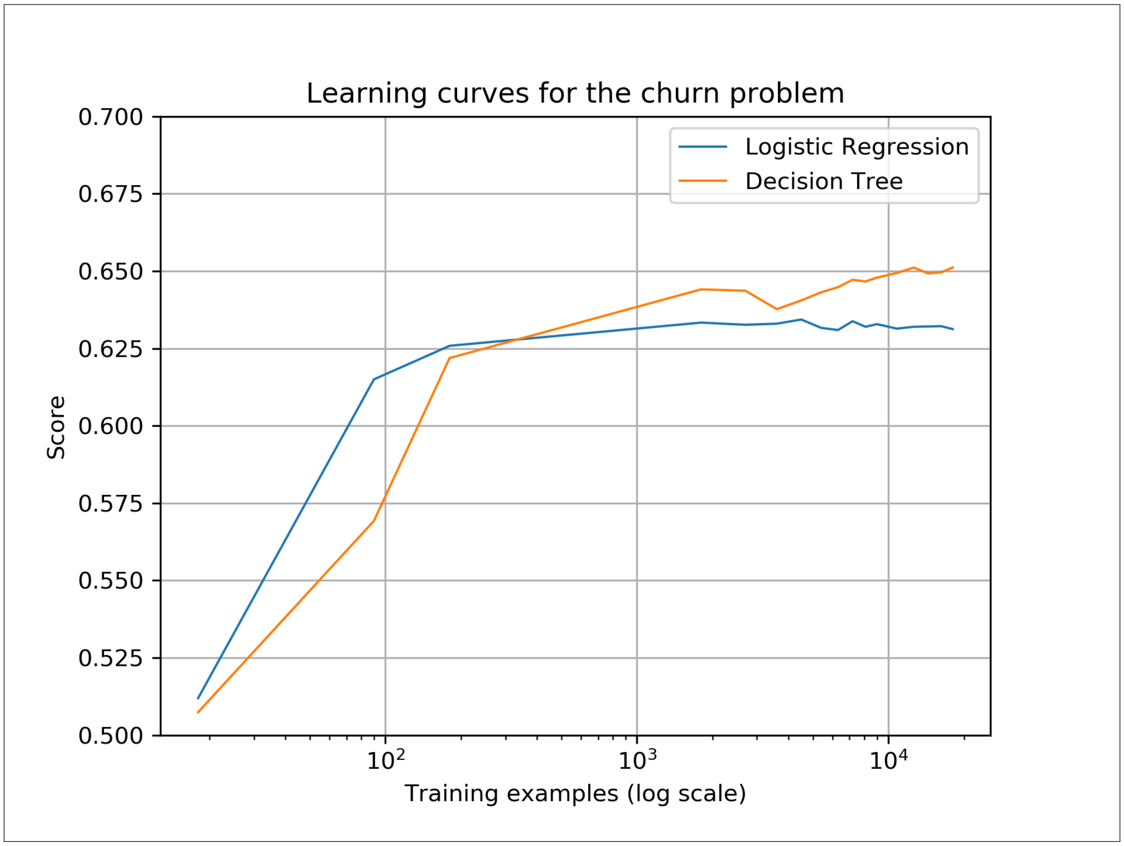

Figure 5-11. Learning curves for tree induction and logistic regression for the churn problem. As the training size grows (x axis), generalization performance (y axis) improves. Importantly, the improvement rates are different for the two induction techniques and change differently with the amount of training data. Logistic regression has less flexibility, allowing it to overfit less with small data, but in the long run keeping it from modeling the full complexity of the data. Tree induction is much more flexible, leading it to overfit more with small data, but to model more complex regularities with larger training sets.

The learning curve has additional analytical uses. For example, we've made the point that data can be an asset. The learning curve may show that generalization performance has leveled off so investing in more training data is probably not worthwhile; instead, one should accept the current performance or look for another way to improve the model, such as by devising better features. Alternatively, the learning curve might show generalization accuracy continuing to improve, so obtaining more training data could be a good investment.

Overfitting Avoidance and Complexity Control

To avoid overfitting, we control the complexity of the models induced from the data. Let's start by examining complexity control in tree induction, since tree induction has much flexibility and therefore will tend to overfit a good deal without some mechanism to avoid it. This discussion in the context of trees will lead us to a very general mechanism that will be applicable to other models.

Avoiding Overfitting with Tree Induction

The main problem with tree induction is that it will keep growing the tree to fit the training data until it creates pure leaf nodes. This will likely result in large, overly complex trees that overfit the data. We have seen how this can be detrimental. Tree induction commonly uses two techniques to avoid overfitting. These strategies are (i) to stop growing the tree before it gets too complex, and (ii) to grow the tree until it is too large, then "prune" it back, reducing its size (and thereby its complexity).

There are various methods for accomplishing each. The simplest method for limiting tree size is to specify a minimum number of instances that must be present in a leaf. The idea behind this minimum-instance stopping criterion is that for predictive modeling, we essentially are using the data at the leaf to make a statistical estimate of the value of the target variable for future cases that would fall to that leaf. If predictions are made based on very few instances, the predictions may be inaccurate—especially since tree construction is specifically designed to get pure leaves. A nice property of controlling complexity in this way is that tree induction will automatically grow the tree branches that have a lot of data and cut short branches that have fewer data—thereby automatically adapting the model based on the data distribution.

A key question becomes what threshold we should use. How few instances are we willing to tolerate at a leaf? Five instances? Thirty? One hundred? There is no fixed number, though practitioners tend to have their own preferences based on experience. However, researchers have developed techniques to decide the stopping point statistically. Statistics provides the notion of a "hypothesis test," which you might recall from a basic statistics class. Roughly, a hypothesis test tries to assess whether a difference in some statistic is not due simply to chance. In most cases, the hypothesis test is based on a "p-value," which imposes a limit on the probability that the difference in statistic is due to chance. If this value is below a threshold (often 5%), then the hypothesis test concludes that the difference is likely not due to chance. So, for stopping tree growth, an alternative to setting an instance minimum for the leaves is to conduct a hypothesis test at every leaf to determine whether the observed difference in (say) information gain could have been due to chance. If the test concludes that it was likely not due to chance, then the split is accepted and the tree growing continues. (See "Sidebar: Beware of "multiple comparisons"" on page 149.)

The second strategy for reducing overfitting is to "prune" an overly large tree after it has been built. In computer science, pruning means to cut off branches, replacing them with leaves. There are many ways to do this, and the interested reader can look into the data mining literature for details. One general idea is to estimate whether replacing a set of leaves or a branch with a leaf would reduce accuracy. If not, then go ahead and prune. The process can be iterated on progressive subtrees until any removal or replacement would reduce accuracy.

We conclude our example of avoiding overfitting in tree induction with the method that will generalize to many different data modeling techniques. Consider the following idea: what if we built trees with all sorts of different complexities? For example, say we stop building the tree after only one node. Then build a tree with two nodes. Then three nodes, etc. We have a set of trees of different complexities. Now, if only there were a way to estimate their generalization performance, we could pick the one that is (estimated to be) the best!

A General Method for Avoiding Overfitting

More generally, if we have a collection of models with different complexities, we could choose the best simply by estimating the generalization performance of each. But how could we estimate their generalization performance? On the (labeled) test data? There's one big problem with that: test data should be strictly *independent* of model building so that we can get an independent estimate of model accuracy. For example, we might want to estimate the ultimate business performance or to compare the best model we can build from one family (say, classification trees) against the best model from another family (say, logistic regression). If we don't care about comparing models or getting an independent estimate of the model accuracy and/or variance, then we could pick the best model based on the testing data.

However, even if we do want these things, we still can proceed. The key is to realize that there was nothing special about the first training/test split we made. Let's say we are saving the test set for a final assessment. We can take the training set and split it again into a training subset and a testing subset. Then we can build models on this training subset and pick the best model based on this testing subset. Let's call the former the *sub-training set* and the latter the *validation set* for clarity. The validation set is separate from the final test set, on which we are never going to make any modeling decisions. This procedure is often called *nested* holdout testing.

Returning to our classification tree example, we can induce trees of many complexities from the subtraining set, then we can estimate the generalization performance for each from the validation set. This would correspond to choosing the top of the inverted-U-shaped holdout curve in Figure 5-3. Say the best model by this assessment has a complexity of 122 nodes (the "sweet spot"). Then we could use this model as our best choice, possibly estimating the actual generalization performance on the final holdout test set. We also could add one more twist. This model was built on a subset of our training data, since we had to hold out the validation set in order to choose the complexity. But once we've chosen the complexity, why not induce a *new* tree with 122 nodes from the whole, original training set? Then we might get the best of both worlds: using the subtraining/validation split to pick the best complexity without tainting the test set, *and* building a model of this best complexity on the entire training set (subtraining plus validation).

This approach is used in many sorts of modeling algorithms to control complexity. The general method is to choose the value for some complexity parameter by using some sort of nested holdout procedure. Again, it is nested because a second holdout procedure is performed on the training set selected by the first holdout procedure.

Often, *nested cross-validation* is used. Nested cross-validation is more complicated, but it works as you might expect. Say we would like to do cross-validation to assess the generalization accuracy of a new modeling technique, which has an adjustable complexity parameter *C*, but we do not know how to set it. So, we run cross-validation as described above. However, before building the model for each fold, we take the training set (refer to Figure 5-9) and first run an experiment: we run another entire cross-validation on just that training set to find the value of *C* estimated to give the best accuracy. The result of that experiment is used only to set the value of *C* to build the actual model for that fold of the cross-validation. Then we build another model using the entire training fold, using that value for *C*, and test on the corresponding test fold. The only difference from regular cross-validation is that for each fold we first run this experiment to find *C*, using another, smaller, cross-validation.

If you understood all that, you would realize that the number of models built depends on how many values of *C* we want to try in the "inner loop." Let's say that we want to try 10 possible values for *C* and we always use 5-fold cross-validation. Then we actually have built 255 total models in the process! This sort of experimental complexity-controlled modeling has only become practical in the last decade or so because its obvious computational expense.

This idea of using the data to choose the complexity experimentally, as well as to build the resulting model, applies across different induction algorithms and different sorts of complexity. For example, we mentioned that complexity increases with the size of the feature set, so it is usually desirable to cull the feature set. A common method for doing this is to run with many different feature sets, using this sort of nested holdout procedure to pick the best.

For example, *sequential forward selection* (SFS) of features uses a nested holdout procedure to first pick the best individual feature, by looking at all models built using just one feature. After choosing a first feature, SFS tests all models that add a second feature to this first chosen feature. The best pair is then selected. Next the same procedure is done for three, then four, and so on. When adding a feature does not improve estimated generalization performance on the validation data, the SFS process stops. (There is a similar procedure called *sequential backward elimination* of features. As you might guess, it works by starting with all features and discarding features one at a time. It continues to discard features as long as there is no estimated performance loss.)

This is a common approach. In modern environments with plentiful data and computational power, the data scientist routinely sets modeling parameters by experimenting using some tactical, nested holdout testing (often nested cross-validation).

The next section shows a different way that this method applies to controlling overfitting when learning numerical functions (as described in Chapter 4). We urge you to at least skim the following section because it introduces concepts and vocabulary in common use by data scientists these days.

* Avoiding Overfitting for Parameter Optimization

As just described, avoiding overfitting involves complexity control: finding the "right" balance between the fit to the data and the complexity of the model. In trees we saw various ways for trying to keep the tree from getting too large (too complex) when fitting the data. For equations, such as logistic regression, that unlike trees do not automatically select what attributes to include, complexity can be controlled by choosing a "right" set of attributes.

Chapter 4 introduced the popular family of methods that builds models by explicitly optimizing the fit to the data via a set of numerical parameters. We discussed various linear members of this family, including linear discriminant learners, linear regression, and logistic regression. Many nonlinear models are fit to the data in exactly the same way.

As might be expected given our discussion so far in this chapter and the figures in "Example: Overfitting Linear Functions" on page 129, these procedures also can overfit the data. However, their explicit optimization framework provides an elegant, if technical, method for complexity control. The general strategy is that instead of just optimizing the fit to the data, we optimize some combination of fit and simplicity. Models will be better if they fit the data better, but they also will be better if they are simpler. This general methodology is called *regularization*, a term that is heard often in data science discussions.

Technical Details Ahead

The rest of this section discusses briefly (and slightly technically) how regularization is done. Don't worry if you don't really understand the technical details. Do remember that regularization is trying to optimize not just the fit to the data, but a combination of model fit and model simplicity.

Recall from Chapter 4 that to fit a model involving numeric parameters w to the data we find the set of parameters that maximizes some "objective function" indicating how well it fits the data:

$$\arg\max_{\mathbf{w}} \text{fit}(\mathbf{x}, \mathbf{w})$$

(The $\arg_{\mathbf{w}}\max$ just means that you want to maximize the fit over all possible arguments **w**, and are interested in the particular argument **w** that gives the maximum. These would be the parameters of the final model.)

Complexity control via regularization works by adding to this objective function a penalty for complexity:

$$\arg\max_{\mathbf{w}} \left[\text{fit}(\mathbf{x}, \mathbf{w}) - \lambda \cdot \text{penalty}(\mathbf{w})\right]$$

The λ term is simply a weight that determines how much importance the optimization procedure should place on the penalty, compared to the data fit. At this point, the modeler has to choose λ and the penalty function.

So, as a concrete example, recall from "* Logistic Regression: Some Technical Details" on page 108 that to learn a standard logistic regression model, from data, we find the numeric parameters **w** that yield the linear model most likely to have generated the observed data—the "maximum likelihood" model. Let's represent that as:

$$\arg\max_{\mathbf{w}} g_{\text{likelihood}}(\mathbf{x}, \mathbf{w})$$

To learn a "regularized" logistic regression model we would instead compute:

$$\arg\max_{\mathbf{w}} \left[g_{\text{likelihood}}(\mathbf{x}, \mathbf{w}) - \lambda \cdot \text{penalty}(\mathbf{w})\right]$$

There are different penalties that can be applied, with different properties.[6] The most commonly used penalty is the sum of the squares of the weights, sometimes called the "L2-norm" of w. The reason is technical, but basically functions can fit data better if they are allowed to have very large positive and negative weights. The sum of the squares of the weights gives a large penalty when weights have large absolute values.

6 The book *The Elements of Statistical Learning* (Hastie, Tibshirani, & Friedman, 2009) contains an excellent technical discussion of these.

If we incorporate the L2-norm penalty into standard least-squares linear regression, we get the statistical procedure called *ridge regression*. If instead we use the sum of the absolute values (rather than the squares), known as the L1-norm, we get a procedure known as the *lasso* (Hastie et al., 2009). More generally, this is called L1-regularization. For reasons that are quite technical, L1-regularization ends up zeroing out many coefficients. Since these coefficients are the multiplicative weights on the features, L1-regularization effectively performs an automatic form of feature selection.

Now we have the machinery to describe in more detail the linear support vector machine, introduced in "Support Vector Machines, Briefly" on page 98. There we waved our hands and told you that the support vector machine "maximizes the margin" between the classes by fitting the "fattest bar" between the classes. Separately we discussed that it uses hinge loss (see "Sidebar: Loss functions" on page 103) to penalize errors. We now can connect these together, and directly to logistic regression. Specifically, linear support vector machine learning is almost equivalent to the L2-regularized logistic regression just discussed; the only difference is that a support vector machine uses hinge loss instead of likelihood in its optimization. The support vector machine optimizes this equation:

$$\arg\max_{\mathbf{w}} \left[-g_{\text{hinge}}(\mathbf{x}, \mathbf{w}) - \lambda \cdot \text{penalty}(\mathbf{w}) \right]$$

where g_{hinge}, the hinge loss term, is negated because lower hinge loss is better.

Finally, you may be saying to yourself: all this is well and good, but a lot of magic seems to be hidden in this λ parameter, which the modeler has to choose. How in the world would the modeler choose that for some real domain like churn prediction, or online ad targeting, or fraud detection?

It turns out that we already have a straightforward way to choose λ. We've discussed how a good tree size and a good feature set can be chosen via nested cross-validation on the training data. We can choose λ the same way. This cross-validation would essentially conduct automated experiments on subsets of the training data and find a good λ value. Then this λ would be used to learn a regularized model on all the training data. This has become the standard procedure for building numerical models that give a good balance between data fit and model complexity. This approach to optimizing the parameter values of a data mining procedure is known as "grid search," as with two parameters it searches systematically through a grid of parameter values.

Sidebar: Beware of "multiple comparisons"

Consider the following scenario. You run an investment firm. Five years ago, you wanted to have some marketable small-cap mutual fund products to sell, but your analysts had been awful at picking small-cap stocks. So you undertook the following procedure. You started 1,000 different mutual funds, each including a small set of stocks randomly chosen from those that make up the Russell 2000 index (the main index for small-cap stocks). Your firm invested in all 1,000 of these funds, but told no one about them. Now, five years later, you look at their performance. Since they have different stocks in them, they will have had different returns. Some will be about the same as the index, some will be worse, and some will be better. The best one might be a lot better. Now, you liquidate all the funds but the best few, and you present these to the public. You can "honestly" claim that their 5-year return is substantially better than the return of the Russell 2000 index.

So, what's the problem? The problem is that you randomly chose the stocks! You have no idea whether the stocks in these "best" funds performed better because they indeed are fundamentally better, or because you cherry-picked the best from a large set that simply varied in performance. If you flip 1,000 fair coins many times each, one of them will have come up heads much more than 50% of the time. However, choosing that coin as the "best" of the coins for later flipping obviously is silly. These are instances of "the problem of multiple comparisons," a very important statistical phenomenon that business analysts and data scientists should always keep in mind. Beware whenever someone does many tests and then picks the results that look good. Statistics books warn against the practice of running multiple hypothesis tests and then looking only at the ones that give "significant" results. These usually violate the assumptions behind the tests, and the significance of the results is dubious.

The underlying reasons for overfitting when building models from data are essentially problems of multiple comparisons (Jensen & Cohen, 2000). Note that even the procedures for avoiding overfitting themselves undertake multiple comparisons (e.g., choosing the best complexity for a model by comparing many complexities). There is no silver bullet or magic formula to truly get "the optimal" model to fit the data. Nonetheless, care can be taken to reduce overfitting as much as possible, by using the holdout procedures described in this chapter and if possible by looking carefully at the results before declaring victory. For example, if the fitting graph truly has an inverted-U-shape, one can be much more confident that the top represents a "good" complexity than if the curve jumps around randomly.

Summary

We have devoted an entire chapter to overfitting because it is so important. Generalization is central to data science, and finding the right generalization is a balancing act between underfitting data and overfitting it.[7] A complex model may be necessary if the phenomenon producing the data is itself complex, but complex models run the risk of overfitting training data (i.e., modeling details of the data that are not found in the general population). An overfit model will not generalize to other data well, even if they are from the same population.

All model types can be overfit. There is no single choice or technique to eliminate overfitting. The best strategy is to recognize overfitting by testing with a holdout set. Several types of curves can help detect and measure overfitting. A *fitting graph* has two curves showing the model performance on the training and testing data as a function of model complexity. A fitting curve on testing data usually has an approximate U or inverted-U-shape (depending on whether error or accuracy is plotted). The accuracy starts off low when the model is simple, increases as complexity increases, flattens out, then starts to decrease again as overfitting sets in. A *learning curve* shows model performance on testing data plotted against the *amount of training data* used. Usually model performance increases with the amount of data, but the rate of increase and the final asymptotic performance can be quite different between models.

A common experimental methodology called *cross-validation* specifies a systematic way of splitting up a single dataset such that it generates multiple performance measures. These values tell the data scientist what average behavior the model yields as well as the variation to expect.

The general method for reining in model complexity to avoid overfitting is called model *regularization*. Techniques include restricting or reducing tree size, feature selection, and employing explicit complexity penalties into the objective function used for fitting models to data.

7 Put this way, you may be wondering: why not devote a chapter to *underfitting*? The answer is that underfitting is straightforward: you increase the complexity of the model and performance genuinely improves. Overfitting is pernicious because the same thing appears to happen *but the improvement is illusory*.