

combination of 20 decision stumps suffices to fit the 100 examples exactly. As more stumps are added to the ensemble, the error remains at zero. The graph also shows that the test set performance continues to increase long after the training set error has reached zero. At M=20, the test performance is 0.95 (or 0.05 error), and the performance increases to 0.98 as late as M=137, before gradually dropping to 0.95.

This finding, which is quite robust across data sets and hypothesis spaces, came as quite a surprise when it was first noticed. Ockham's razor tells us not to make hypotheses more complex than necessary, but the graph tells us that the predictions *improve* as the ensemble hypothesis gets more complex! Various explanations have been proposed for this. One view is that boosting approximates **Bayesian learning** (see Chapter 20), which can be shown to be an optimal learning algorithm, and the approximation improves as more hypotheses are added. Another possible explanation is that the addition of further hypotheses enables the ensemble to be *more definite* in its distinction between positive and negative examples, which helps it when it comes to classifying new examples.

## 18.5 WHY LEARNING WORKS: COMPUTATIONAL LEARNING THEORY

The main unanswered question posed in Section 18.2 was this: how can one be sure that one's learning algorithm has produced a theory that will correctly predict the future? In formal terms, how do we know that the hypothesis h is close to the target function f if we don't know what f is? These questions have been pondered for several centuries. Until we find answers, machine learning will, at best, be puzzled by its own success.

The approach taken in this section is based on **computational learning theory**, a field at the intersection of AI, statistics, and theoretical computer science. The underlying principle is the following: any hypothesis that is seriously wrong will almost certainly be "found out" with high probability after a small number of examples, because it will make an incorrect prediction. Thus, any hypothesis that is consistent with a sufficiently large set of training examples is unlikely to be seriously wrong: that is, it must be **probably approximately correct**. Any learning algorithm that returns hypotheses that are probably approximately correct is called a **PAC-learning** algorithm.

There are some subtleties in the preceding argument. The main question is the connection between the training and the test examples; after all, we want the hypothesis to be approximately correct on the test set, not just on the training set. The key assumption is that the training and test sets are drawn randomly and independently from the same population of examples with the *same probability distribution*. This is called the **stationarity** assumption. Without the stationarity assumption, the theory can make no claims at all about the future, because there would be no necessary connection between future and past. The stationarity assumption amounts to supposing that the process that selects examples is not malevolent. Obviously, if the training set consists only of weird examples—two-headed dogs, for instance—then the learning algorithm cannot help but make unsuccessful generalizations about how to recognize dogs.

COMPUTATIONAL

I FARNING THEORY



PROBABLY APPROXIMATEL CORRECT

PAC-LEARNING

STATIONARITY

## How many examples are needed?

In order to put these insights into practice, we will need some notation:

- Let X be the set of all possible examples.
- Let D be the distribution from which examples are drawn.
- Let **H** be the set of possible hypotheses.
- Let N be the number of examples in the training set.

Initially, we will assume that the true function f is a member of  $\mathbf{H}$ . Now we can define the **error** of a hypothesis h with respect to the true function f given a distribution D over the examples as the probability that h is different from f on an example:

$$\operatorname{error}(h) = P(h(x) \neq f(x) | x \operatorname{drawn from } D)$$
.

This is the same quantity being measured experimentally by the learning curves shown earlier.

A hypothesis h is called **approximately correct** if  $\operatorname{error}(h) \leq \epsilon$ , where  $\epsilon$  is a small constant. The plan of attack is to show that after seeing N examples, with high probability, all consistent hypotheses will be approximately correct. One can think of an approximately correct hypothesis as being "close" to the true function in hypothesis space: it lies inside what is called the  $\epsilon$ -ball around the true function f. Figure 18.12 shows the set of all hypotheses  $\mathbf{H}$ , divided into the  $\epsilon$ -ball around f and the remainder, which we call  $\mathbf{H}_{\text{bad}}$ .

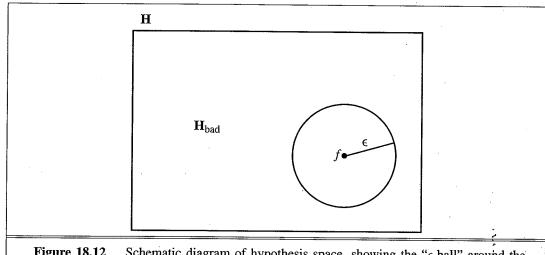


Figure 18.12 Schematic diagram of hypothesis space, showing the " $\epsilon$ -ball" around the true function f.

We can calculate the probability that a "seriously wrong" hypothesis  $h_b \in \mathbf{H}_{bad}$  is consistent with the first N examples as follows. We know that  $\operatorname{error}(h_b) > \epsilon$ . Thus, the probability that it agrees with a given example is at Jeast  $1 - \epsilon$ . The bound for N examples is

$$P(h_b \text{ agrees with } N \text{ examples}) \leq (1 - \epsilon)^N$$

The probability that  $\mathbf{H}_{bad}$  contains at least one consistent hypothesis is bounded by the sum of the individual probabilities:

$$P(\mathbf{H}_{\text{bad}} \text{ contains a consistent hypothesis}) \leq |\mathbf{H}_{\text{bad}}|(1-\epsilon)^N \leq |\mathbf{H}|(1-\epsilon)^N$$
,

ERROR

 $\epsilon$ -Ball

where we have used the fact that  $|\mathbf{H}_{bad}| \leq |\mathbf{H}|$ . We would like to reduce the probability of this event below some small number  $\delta$ :

$$|\mathbf{H}|(1-\epsilon)^N \leq \delta$$
.

Given that  $1 - \epsilon \le e^{-\epsilon}$ , we can achieve this if we allow the algorithm to see

$$N \ge \frac{1}{\epsilon} \left( \ln \frac{1}{\delta} + \ln |\mathbf{H}| \right) \tag{18.1}$$

examples. Thus, if a learning algorithm returns a hypothesis that is consistent with this many examples, then with probability at least  $1-\delta$ , it has error at most  $\epsilon$ . In other words, it is probably approximately correct. The number of required examples, as a function of  $\epsilon$  and  $\delta$ , is called the **sample complexity** of the hypothesis space.

It appears, then, that the key question is the size of the hypothesis space. As we saw earlier, if **H** is the set of all Boolean functions on n attributes, then  $|\mathbf{H}| = 2^{2^n}$ . Thus, the sample complexity of the space grows as  $2^n$ . Because the number of possible examples is also  $2^n$ , this says that any learning algorithm for the space of all Boolean functions will do no better than a lookup table if it merely returns a hypothesis that is consistent with all known examples. Another way to see this is to observe that for any unseen example, the hypothesis space will contain as many consistent hypotheses that predict a positive outcome as it does hypotheses that predict a negative outcome.

The dilemma we face, then, is that unless we restrict the space of functions the algorithm can consider, it will not be able to learn; but if we do restrict the space, we might eliminate the true function altogether. There are two ways to "escape" this dilemma. The first way is to insist that the algorithm return not just any consistent hypothesis, but preferably a simple one (as is done in decision tree learning). The theoretical analysis of such algorithms is beyond the scope of this book, but in cases where finding simple consistent hypotheses is tractable, the sample complexity results are generally better than for analyses based only on consistency. The second escape, which we pursue here, is to focus on learnable subsets of the entire set of Boolean functions. The idea is that in most cases we do not need the full expressive power of Boolean functions, and can get by with more restricted languages. We now examine one such restricted language in more detail.

### Learning decision lists

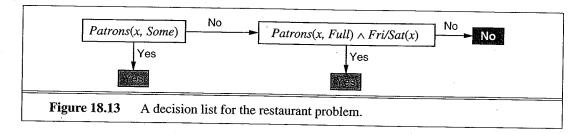
DECISION LIST

A **decision list** is a logical expression of a restricted form. It consists of a series of tests, each of which is a conjunction of literals. If a test succeeds when applied to an example description, the decision list specifies the value to be returned. If the test fails, processing continues with the next test in the list.<sup>6</sup> Decision lists resemble decision trees, but their overall structure is simpler. In contrast, the individual tests are more complex. Figure 18.13 shows a decision list that represents the following hypothesis:

$$\forall x \ WillWait(x) \Leftrightarrow Patrons(x, Some) \lor (Patrons(x, Full) \land Fri/Sat(x))$$
.

If we allow tests of arbitrary size, then decision lists can represent any Boolean function (Exercise 18.15). On the other hand, if we restrict the size of each test to at most k literals,

<sup>&</sup>lt;sup>6</sup> A decision list is therefore identical in structure to a COND statement in Lisp.



k-dl $\cdot$  k-dt

then it is possible for the learning algorithm to generalize successfully from a small number of examples. We call this language k-DL. The example in Figure 18.13 is in 2-DL. It is easy to show (Exercise 18.15) that k-DL includes as a subset the language k-DT, the set of all decision trees of depth at most k. It is important to remember that the particular language referred to by k-DL depends on the attributes used to describe the examples. We will use the notation k-DL(n) to denote a k-DL language using n Boolean attributes.

The first task is to show that k-DL is learnable—that is, that any function in k-DL can be approximated accurately after training on a reasonable number of examples. To do this, we need to calculate the number of hypotheses in the language. Let the language of tests—conjunctions of at most k literals using n attributes—be Conj(n,k). Because a decision list is constructed of tests, and because each test can be attached to either a Yes or a No outcome or can be absent from the decision list, there are at most  $3^{|Conj(n,k)|}$  distinct sets of component tests. Each of these sets of tests can be in any order, so

$$|k$$
-DL $(n)| \leq 3^{|Conj(n,k)|} |Conj(n,k)|!$ .

The number of conjunctions of k literals from n attributes is given by

$$|Conj(n,k)| = \sum_{i=0}^{k} {2n \choose i} = O(n^k)$$
.

Hence, after some work, we obtain

$$|k\text{-DL}(n)| = 2^{O(n^k \log_2(n^k))}$$

We can plug this into Equation (18.1) to show that the number of examples needed for PAC-learning a k-DL function is polynomial in n:

$$\stackrel{\cdot}{N} \ge \frac{1}{\epsilon} \left( \ln \frac{1}{\delta} + O(n^k \log_2(n^k)) \right) .$$

Therefore, any algorithm that returns a consistent decision list will PAC-learn a k-DL function in a reasonable number of examples, for small k.

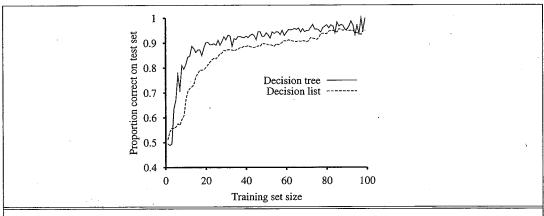
The next task is to find an efficient algorithm that returns a consistent decision list. We will use a greedy algorithm called DECISION-LIST-LEARNING that repeatedly finds a test that agrees exactly with some subset of the training set. Once it finds such a test, it adds it to the decision list under construction and removes the corresponding examples. It then constructs the remainder of the decision list, using just the remaining examples. This is repeated until there are no examples left. The algorithm is shown in Figure 18.14.

This algorithm does not specify the method for selecting the next test to add to the decision list. Although the formal results given earlier do not depend on the selection method,

function DECISION-LIST-LEARNING(examples) returns a decision list, or failure

if examples is empty then return the trivial decision list No  $t \leftarrow$  a test that matches a nonempty subset examples, of examples such that the members of  $examples_t$  are all positive or all negative if there is no such t then return failure if the examples in examples, are positive then  $o \leftarrow Yes$  else  $o \leftarrow No$ **return** a decision list with initial test t and outcome o and remaining tests given by DECISION-LIST-LEARNING (examples - examples<sub>t</sub>)

**Figure 18.14** An algorithm for learning decision lists.



Learning curve for DECISION-LIST-LEARNING algorithm on the restaurant **Figure 18.15** data. The curve for DECISION-TREE-LEARNING is shown for comparison.

it would seem reasonable to prefer small tests that match large sets of uniformly classified examples, so that the overall decision list will be as compact as possible. The simplest strategy is to find the smallest test t that matches any uniformly classified subset, regardless of the size of the subset. Even this approach works quite well, as Figure 18.15 suggests.

#### Discussion

IDENTIFICATION IN THE LIMIT

Computational learning theory has generated a new way of looking at the problem of learning. In the early 1960s, the theory of learning focused on the problem of identification in the limit. According to this notion, an identification algorithm must return a hypothesis that exactly matches the true function. One way to do that is as follows: First, order all the hypotheses in H according to some measure of simplicity. Then, choose the simplest hypothesis consistent with all the examples so far. As new examples arrive, the method will abandon a simpler hypothesis that is invalidated and adopt a more complex one instead. Once it reaches the true function, it will never abandon it. Unfortunately, in many hypothesis spaces, the number of examples and the computation time required to reach the true function are enormous. Thus, computational learning theory does not insist that the learning agent find the "one true law" governing its environment, but instead that it find a hypothesis with a certain degree of predictive accuracy. Computational learning theory also brings sharply into focus the tradeoff between the expressiveness of the hypothesis language and the complexity of learning, and has lead directly to an important class of learning algorithms called support vector machines.

The PAC-learning results we have shown are worst-case complexity results and do not necessarily reflect the average-case sample complexity as measured by the learning curves we have shown. An average-case analysis must also make assumptions about the distribution of examples and the distribution of true functions that the algorithm will have to learn. As these issues become better understood, computational learning theory continues to provide valuable guidance to machine learning researchers who are interested in predicting or modifying the learning ability of their algorithms. Besides decision lists, results have been obtained for almost all known subclasses of Boolean functions, for neural networks (see Chapter 20), and for sets of first-order logical sentences (see Chapter 19). The results show that the pure inductive learning problem, where the agent begins with no prior knowledge about the target function, is generally very hard. As we show in Chapter 19, the use of prior knowledge to guide inductive learning makes it possible to learn quite large sets of sentences from reasonable numbers of examples, even in a language as expressive as first-order logic.

## 18.6 SUMMARY

This chapter has concentrated on inductive learning of deterministic functions from examples. The main points were as follows:

- Learning takes many forms, depending on the nature of the performance element, the component to be improved, and the available feedback.
- If the available feedback, either from a teacher or from the environment, provides the correct value for the examples, the learning problem is called **supervised learning**. The task, also called **inductive learning**, is then to learn a function from examples of its inputs and outputs. Learning a discrete-valued function is called **classification**; learning a continuous function is called **regression**.
- Inductive learning involves finding a **consistent** hypothesis that agrees with the examples. **Ockham's razor** suggests choosing the simplest consistent hypothesis. The difficulty of this task depends on the chosen representation.
- Decision trees can represent all Boolean functions. The information gain heuristic provides an efficient method for finding a simple, consistent decision tree.
- The performance of a learning algorithm is measured by the learning curve, which shows the prediction accuracy on the test set as a function of the training set size.
- Ensemble methods such as **boosting** often perform better than individual methods.
- Computational learning theory analyzes the sample complexity and computational complexity of inductive learning. There is a tradeoff between the expressiveness of the hypothesis language and the ease of learning.

# BIBLIOGRAPHICAL AND HISTORICAL NOTES

Chapter 1 outlined the history of philosophical investigations into inductive learning. William of Ockham (1280–1349), the most influential philosopher of his century and a major contributer to medieval epistemology, logic, and metaphysics, is credited with a statement called "Ockham's Razor"—in Latin, *Entia non sunt multiplicanda praeter necessitatem*, and in English, "Entities are not to be multiplied beyond necessity." Unfortunately, this laudable piece of advice is nowhere to be found in his writings in precisely these words.

EPAM, the "Elementary Perceiver And Memorizer" (Feigenbaum, 1961), was one of the earliest systems to use decision trees (or **discrimination nets**). EPAM was intended as a cognitive-simulation model of human concept learning. CLS (Hunt *et al.*, 1966) used a heuristic look-ahead method to construct decision trees. ID3 (Quinlan, 1979) added the crucial idea of using information content to provide the heuristic function. Information theory itself was developed by Claude Shannon to aid in the study of communication (Shannon and Weaver, 1949). (Shannon also contributed one of the earliest examples of machine learning, a mechanical mouse named Theseus that learned to navigate through a maze by trial and error.) The  $\chi^2$  method of tree pruning was described by Quinlan (1986). C4.5, an industrial-strength decision tree package, can be found in Quinlan (1993). An independent tradition of decision tree learning exists in the statistical literature. *Classification and Regression Trees* (Breiman *et al.*, 1984), known as the "CART book," is the principal reference.

Many other algorithmic approaches to learning have been tried. The current-best-hypothesis approach maintains a single hypothesis, specializing it when it proves too broad and generalizing it when it proves too narrow. This is an old idea in philosophy (Mill, 1843). Early work in cognitive psychology also suggested that it is a natural form of concept learning in humans (Bruner et al., 1957). In AI, the approach is most closely associated with the work of Patrick Winston, whose Ph.D. thesis (Winston, 1970) addressed the problem of learning descriptions of complex objects. The version space method (Mitchell, 1977, 1982) takes a different approach, maintaining the set of all consistent hypotheses and eliminating those found to be inconsistent with new examples. The approach was used in the Meta-DENDRAL expert system for chemistry (Buchanan and Mitchell, 1978), and later in Mitchell's (1983) LEX system, which learns to solve calculus problems. A third influential thread was formed by the work of Michalski and colleagues on the AQ series of algorithms, which learned sets of logical rules (Michalski, 1969; Michalski et al., 1986b).

Ensemble learning is an increasingly popular technique for improving the performance of learning algorithms. **Bagging** (Breiman, 1996), the first effective method, combines hypotheses learned from multiple **bootstrap** data sets, each generated by subsampling the original data set. The **boosting** method described in the chapter originated with theoretical work by Schapire (1990). The ADABOOST algorithm was developed by Freund and Schapire (1996) and analyzed theoretically by Schapire (1999). Friedman *et al.* (2000) explain boosting from a statistician's viewpoint.

Theoretical analysis of learning algorithms began with the work of Gold (1967) on identification in the limit. This approach was motivated in part by models of scientific

BAGGING

discovery from the philosophy of science (Popper, 1962), but has been applied mainly to the problem of learning grammars from example sentences (Osherson et al., 1986).

KOLMOGOROV COMPLEXITY Whereas the identification-in-the-limit approach concentrates on eventual convergence, the study of Kolmogorov complexity or algorithmic complexity, developed independently by Solomonoff (1964) and Kolmogorov (1965), attempts to provide a formal definition for the notion of simplicity used in Ockham's razor. To escape the problem that simplicity depends on the way in which information is represented, it is proposed that simplicity be measured by the length of the shortest program for a universal Turing machine that correctly reproduces the observed data. Although there are many possible universal Turing machines, and hence many possible "shortest" programs, these programs differ in length by at most a constant that is independent of the amount of data. This beautiful insight, which essentially shows that *any* initial representation bias will eventually be overcome by the data itself, is marred only by the undecidability of computing the length of the shortest program. Approximate measures such as the **minimum description length**, or MDL (Rissanen, 1984) can be used instead and have produced excellent results in practice. The text by Li and Vitanyi (1993) is the best source for Kolmogorov complexity.

Computational learning theory—that is, the theory of PAC-learning—was inaugurated by Leslie Valiant (1984). Valiant's work stressed the importance of computational and sample complexity. With Michael Kearns (1990), Valiant showed that several concept classes cannot be PAC-learned tractably, even though sufficient information is available in the examples. Some positive results were obtained for classes such as decision lists (Rivest, 1987).

An independent tradition of sample complexity analysis has existed in statistics, beginning with the work on **uniform convergence theory** (Vapnik and Chervonenkis, 1971). The so-called **VC dimension** provides a measure roughly analogous to, but more general than, the ln |**H**| measure obtained from PAC analysis. The VC dimension can be applied to continuous function classes, to which standard PAC analysis does not apply. PAC-learning theory and VC theory were first connected by the "four Germans" (none of whom actually is German): Blumer, Ehrenfeucht, Haussler, and Warmuth (1989). Subsequent developments in VC theory led to the invention of the **support vector machine** or SVM (Boser *et al.*, 1992; Vapnik, 1998), which we describe in Chapter 20.

A large number of important papers on machine learning have been collected in *Readings in Machine Learning* (Shavlik and Dietterich, 1990). The two volumes *Machine Learning 1* (Michalski *et al.*, 1983) and *Machine Learning 2* (Michalski *et al.*, 1986a) also contain many important papers, as well as huge bibliographies. Weiss and Kulikowski (1991) provide a broad introduction to function-learning methods from machine learning, statistics, and neural networks. The STATLOG project (Michie *et al.*, 1994) is by far the most exhaustive investigation into the comparative performance of learning algorithms. Good current research in machine learning is published in the annual proceedings of the International Conference on Machine Learning and the conference on Neural Information Processing Systems, in *Machine Learning* and the *Journal of Machine Learning Research*, and in mainstream AI journals. Work in computational learning theory also appears in the annual ACM Workshop on Computational Learning Theory (COLT), and is described in the texts by Kearns and Vazirani (1994) and Anthony and Bartlett (1999).

MINIMUM DESCRIPTION LENGTH

UNIFORM CONVERGENCE THEORY VC DIMENSION