CHAPTER 7

DECISION TREE LEARNING

Decision tree learning is one of the most widely used and practical methods for inductive inference. It is a method for approximating discrete-valued functions that is robust to noisy data and capable of learning disjunctive expressions. This chapter describes a family of decision tree learning algorithms that includes widely used algorithms such as ID3, ASSISTANT, and C4.5. These decision tree learning methods search a completely expressive hypothesis space and thus avoid the difficulties of restricted hypothesis spaces. Their inductive bias is a preference for small trees over large trees.

3.1 INTRODUCTION

Decision tree learning is a method for approximating discrete-valued target functions, in which the learned function is represented by a decision tree. Learned trees can also be re-represented as sets of if-then rules to improve human readability. These learning methods are among the most popular of inductive inference algorithms and have been successfully applied to a broad range of tasks from learning to diagnose medical cases to learning to assess credit risk of loan applicants.

3.2 DECISION TREE REPRESENTATION

Decision trees classify instances by sorting them down the tree from the root to some leaf node, which provides the classification of the instance. Each node in the tree specifies a test of some *attribute* of the instance, and each branch descending

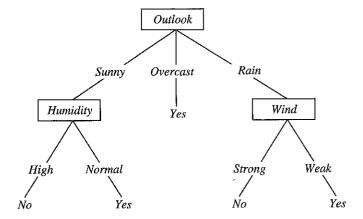


FIGURE 3.1

A decision tree for the concept *PlayTennis*. An example is classified by sorting it through the tree to the appropriate leaf node, then returning the classification associated with this leaf (in this case, *Yes* or *No*). This tree classifies Saturday mornings according to whether or not they are suitable for playing tennis.

from that node corresponds to one of the possible values for this attribute. An instance is classified by starting at the root node of the tree, testing the attribute specified by this node, then moving down the tree branch corresponding to the value of the attribute in the given example. This process is then repeated for the subtree rooted at the new node.

Figure 3.1 illustrates a typical learned decision tree. This decision tree classifies Saturday mornings according to whether they are suitable for playing tennis. For example, the instance

$$\langle Outlook = Sunny, Temperature = Hot, Humidity = High, Wind = Strong \rangle$$

would be sorted down the leftmost branch of this decision tree and would therefore be classified as a negative instance (i.e., the tree predicts that PlayTennis = no). This tree and the example used in Table 3.2 to illustrate the ID3 learning algorithm are adapted from (Quinlan 1986).

In general, decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances. Each path from the tree root to a leaf corresponds to a conjunction of attribute tests, and the tree itself to a disjunction of these conjunctions. For example, the decision tree shown in Figure 3.1 corresponds to the expression

$$(Outlook = Sunny \land Humidity = Normal)$$
 $\lor \qquad (Outlook = Overcast)$
 $\lor \qquad (Outlook = Rain \land Wind = Weak)$

3.3 APPROPRIATE PROBLEMS FOR DECISION TREE LEARNING

Although a variety of decision tree learning methods have been developed with somewhat differing capabilities and requirements, decision tree learning is generally best suited to problems with the following characteristics:

- Instances are represented by attribute-value pairs. Instances are described by a fixed set of attributes (e.g., Temperature) and their values (e.g., Hot). The easiest situation for decision tree learning is when each attribute takes on a small number of disjoint possible values (e.g., Hot, Mild, Cold). However, extensions to the basic algorithm (discussed in Section 3.7.2) allow handling real-valued attributes as well (e.g., representing Temperature numerically).
- The target function has discrete output values. The decision tree in Figure 3.1 assigns a boolean classification (e.g., yes or no) to each example. Decision tree methods easily extend to learning functions with more than two possible output values. A more substantial extension allows learning target functions with real-valued outputs, though the application of decision trees in this setting is less common.
- Disjunctive descriptions may be required. As noted above, decision trees naturally represent disjunctive expressions.
- The training data may contain errors. Decision tree learning methods are robust to errors, both errors in classifications of the training examples and errors in the attribute values that describe these examples.
- The training data may contain missing attribute values. Decision tree methods can be used even when some training examples have unknown values (e.g., if the *Humidity* of the day is known for only some of the training examples). This issue is discussed in Section 3.7.4.

Many practical problems have been found to fit these characteristics. Decision tree learning has therefore been applied to problems such as learning to classify medical patients by their disease, equipment malfunctions by their cause, and loan applicants by their likelihood of defaulting on payments. Such problems, in which the task is to classify examples into one of a discrete set of possible categories, are often referred to as classification problems.

The remainder of this chapter is organized as follows. Section 3.4 presents the basic ID3 algorithm for learning decision trees and illustrates its operation in detail. Section 3.5 examines the hypothesis space search performed by this learning algorithm, contrasting it with algorithms from Chapter 2. Section 3.6 characterizes the inductive bias of this decision tree learning algorithm and explores more generally an inductive bias called Occam's razor, which corresponds to a preference for the most simple hypothesis. Section 3.7 discusses the issue of overfitting the training data, as well as strategies such as rule post-pruning to deal with this problem. This section also discusses a number of more advanced topics such as extending the algorithm to accommodate real-valued attributes, training data with unobserved attributes, and attributes with differing costs.

MACHINE LEARNING

3.3 APPROPRIATE PROBLEMS FOR DECISION TREE LEARNING

Although a variety of decision tree learning methods have been developed with somewhat differing capabilities and requirements, decision tree learning is generally best suited to problems with the following characteristics:

- easiest situation for decision tree learning is when each attribute takes on a extensions to the basic algorithm (discussed in Section 3.7.2) allow handling a fixed set of attributes (e.g., Temperature) and their values (e.g., Hot). The small number of disjoint possible values (e.g., Hot, Mild, Cold). However, Instances are represented by attribute-value pairs. Instances are described by real-valued attributes as well (e.g., representing Temperature numerically).
- with real-valued outputs, though the application of decision trees in this tree methods easily extend to learning functions with more than two possible output values. A more substantial extension allows learning target functions assigns a boolean classification (e.g., yes or no) to each example. Decision The target function has discrete output values. The decision tree in Figure 3.1 setting is less common.
 - Disjunctive descriptions may be required. As noted above, decision trees naturally represent disjunctive expressions.
- The training data may contain errors. Decision tree learning methods are robust to errors, both errors in classifications of the training examples and errors in the attribute values that describe these examples.
 - (e.g., if the Humidity of the day is known for only some of the training ods can be used even when some training examples have unknown values The training data may contain missing attribute values. Decision tree methexamples). This issue is discussed in Section 3.7.4.

in which the task is to classify examples into one of a discrete set of possible cision tree learning has therefore been applied to problems such as learning to classify medical patients by their disease, equipment malfunctions by their cause, and loan applicants by their likelihood of defaulting on payments. Such problems, Many practical problems have been found to fit these characteristics. Decategories, are often referred to as classification problems.

with this problem. This section also discusses a number of more advanced topics to a preference for the most simple hypothesis. Section 3.7 discusses the issue of learning algorithm, contrasting it with algorithms from Chapter 2. Section 3.6 plores more generally an inductive bias called Occam's razor, which corresponds overfitting the training data, as well as strategies such as rule post-pruning to deal .1. to accommodate real-valued attributes, training in detail. Section 3.5 examines the hypothesis space search performed by this characterizes the inductive bias of this decision tree learning algorithm and ex-The remainder of this chapter is organized as follows. Section 3.4 presents the basic ID3 algorithm for learning decision trees and illustrates its operation

3.4 THE BASIC DECISION TREE LEARNING ALGORITHM

decision tree learning, corresponding approximately to the ID3 algorithm. In Section 3.7 we consider a number of extensions to this basic algorithm, including space of possible decision trees. This approach is exemplified by the ID3 algorithm ocus of our discussion here. In this section we present the basic algorithm for extensions incorporated into C4.5 and other more recent algorithms for decision ations on a core algorithm that employs a top-down, greedy search through the (Quinlan 1986) and its successor C4.5 (Quinlan 1993), which form the primary Most algorithms that have been developed for learning decision trees are vari-

rithm, specialized to learning boolean-valued functions (i.e., concept learning), is A descendant of the root node is then created for each possible value of this attribute, and the training examples are sorted to the appropriate descendant node The entire process is then repeated using the training examples associated with This forms a greedy search for an acceptable decision tree, in which the algorithm of the tree?" To answer this question, each instance attribute is evaluated using a statistical test to determine how well it alone classifies the training examples. The best attribute is selected and used as the test at the root node of the tree. each descendant node to select the best attribute to test at that point in the tree. never backtracks to reconsider earlier choices. A simplified version of the algodown, beginning with the question "which attribute should be tested at the root (i.e., down the branch corresponding to the example's value for this attribute). Our basic algorithm, ID3, learns decision trees by constructing them topdescribed in Table 3.1.

3.4.1 Which Attribute Is the Best Classifier?

for classifying examples. What is a good quantitative measure of the worth of measures how well a given attribute separates the training examples according to their target classification. ID3 uses this information gain measure to select among an attribute? We will define a statistical property, called information gain, that The central choice in the ID3 algorithm is selecting which attribute to test at each node in the tree. We would like to select the attribute that is most useful the candidate attributes at each step while growing the tree.

3.4.1.1 ENTROPY MEASURES HOMOGENEITY OF EXAMPLES

of an arbitrary collection of examples. Given a collection S, containing positive monly used in information theory, called entropy, that characterizes the (im)purity and negative examples of some target concept, the entropy of S relative to this In order to define information gain precisely, we begin by defining a measure comboolean classification is

Tutuni(C) = -n.log. n. - n.log. n.

ID3(Examples, Target_attribute, Attributes)

Examples are the training examples. Target_attribute is the attribute whose value is to be predicted by the tree. Attributes is a list of other attributes that may be tested by the learned decision tree. Returns a decision tree that correctly classifies the given Examples.

- · Create a Root node for the tree
- If all Examples are positive, Return the single-node tree Root, with label = +
- If all Examples are negative, Return the single-node tree Root, with label = -
- If Attributes is empty, Return the single-node tree Root, with label = most common value of Target_attribute in Examples
- · Otherwise Begin
 - $A \leftarrow$ the attribute from Attributes that best* classifies Examples
 - The decision attribute for Root ← A
 - For each possible value, v_i , of A,
 - ullet Add a new tree branch below Root, corresponding to the test $A=v_l$
 - Let $Examples_{v_i}$ be the subset of Examples that have value v_i for A
 - If Examples vi is empty
 - Then below this new branch add a leaf node with label = most common value of Target_attribute in Examples
 - Else below this new branch add the subtree
 ID3(Examples_{vi}, Target_attribute, Attributes {A}))
- End
- Return Root

TABLE 3.1

Summary of the ID3 algorithm specialized to learning boolean-valued functions. ID3 is a greedy algorithm that grows the tree top-down, at each node selecting the attribute that best classifies the local training examples. This process continues until the tree perfectly classifies the training examples, or until all attributes have been used.

where p_{\oplus} is the proportion of positive examples in S and p_{\ominus} is the proportion of negative examples in S. In all calculations involving entropy we define $0 \log 0$ to be 0.

To illustrate, suppose S is a collection of 14 examples of some boolean concept, including 9 positive and 5 negative examples (we adopt the notation [9+,5-] to summarize such a sample of data). Then the entropy of S relative to this boolean classification is

$$Entropy([9+, 5-]) = -(9/14) \log_2(9/14) - (5/14) \log_2(5/14)$$
$$= 0.940$$
(3.2)

Notice that the entropy is 0 if all members of S belong to the same class. For example, if all members are positive $(p_{\oplus} = 1)$, then p_{\ominus} is 0, and $Entropy(S) = -1 \cdot \log_2(1) - 0 \cdot \log_2 0 = -1 \cdot 0 - 0 \cdot \log_2 0 = 0$. Note the entropy is 1 when the collection contains an equal number of positive and negative examples. If the collection contains unequal numbers of positive and negative examples, the

^{*} The best attribute is the one with highest *information gain*, as defined in Equation (3.4).

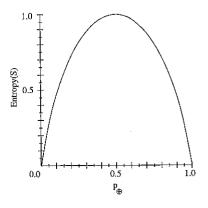


FIGURE 3.2 The entropy function relative to a boolean classification, as the proportion, p_{\oplus} , of positive examples varies between 0 and 1.

entropy is between 0 and 1. Figure 3.2 shows the form of the entropy function relative to a boolean classification, as p_{\oplus} varies between 0 and 1.

One interpretation of entropy from information theory is that it specifies the minimum number of bits of information needed to encode the classification of an arbitrary member of S (i.e., a member of S drawn at random with uniform probability). For example, if p_{\oplus} is 1, the receiver knows the drawn example will be positive, so no message need be sent, and the entropy is zero. On the other hand, if p_{\oplus} is 0.5, one bit is required to indicate whether the drawn example is positive or negative. If p_{\oplus} is 0.8, then a collection of messages can be encoded using on average less than 1 bit per message by assigning shorter codes to collections of positive examples and longer codes to less likely negative examples.

Thus far we have discussed entropy in the special case where the target classification is boolean. More generally, if the target attribute can take on c different values, then the entropy of S relative to this c-wise classification is defined as

$$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i$$
 (3.3)

where p_i is the proportion of S belonging to class i. Note the logarithm is still base 2 because entropy is a measure of the expected encoding length measured in bits. Note also that if the target attribute can take on c possible values, the entropy can be as large as $\log_2 c$.

3.4.1.2 INFORMATION GAIN MEASURES THE EXPECTED REDUCTION IN ENTROPY

Given entropy as a measure of the impurity in a collection of training examples, we can now define a measure of the effectiveness of an attribute in classifying the training data. The measure we will use, called *information gain*, is simply the expected reduction in entropy caused by partitioning the examples according to this attribute. More precisely, the information gain, Gain(S, A) of an attribute A,

relative to a collection of examples S, is defined as

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$
 (3.4)

where Values(A) is the set of all possible values for attribute A, and S_v is the subset of S for which attribute A has value v (i.e., $S_v = \{s \in S | A(s) = v\}$). Note the first term in Equation (3.4) is just the entropy of the original collection S, and the second term is the expected value of the entropy after S is partitioned using attribute A. The expected entropy described by this second term is simply the sum of the entropies of each subset S_v , weighted by the fraction of examples $\frac{|S_v|}{|S|}$ that belong to S_v . Gain(S, A) is therefore the expected reduction in entropy caused by knowing the value of attribute A. Put another way, Gain(S, A) is the information provided about the target function value, given the value of some other attribute A. The value of Gain(S, A) is the number of bits saved when encoding the target value of an arbitrary member of S, by knowing the value of attribute A.

For example, suppose S is a collection of training-example days described by attributes including Wind, which can have the values Weak or Strong. As before, assume S is a collection containing 14 examples, [9+, 5-]. Of these 14 examples, suppose 6 of the positive and 2 of the negative examples have Wind = Weak, and the remainder have Wind = Strong. The information gain due to sorting the original 14 examples by the attribute Wind may then be calculated as

$$Values(Wind) = Weak, Strong$$

$$S = [9+, 5-]$$

$$S_{Weak} \leftarrow [6+, 2-]$$

$$S_{Strong} \leftarrow [3+, 3-]$$

$$Gain(S, Wind) = Entropy(S) - \sum_{v \in \{Weak, Strong\}} \frac{|S_v|}{|S|} Entropy(S_v)$$

$$= Entropy(S) - (8/14) Entropy(S_{Weak})$$

$$- (6/14) Entropy(S_{Strong})$$

$$= 0.940 - (8/14)0.811 - (6/14)1.00$$

$$= 0.048$$

Information gain is precisely the measure used by ID3 to select the best attribute at each step in growing the tree. The use of information gain to evaluate the relevance of attributes is summarized in Figure 3.3. In this figure the information gain of two different attributes, Humidity and Wind, is computed in order to determine which is the better attribute for classifying the training examples shown in Table 3.2.

Gain (3)
= .9= .1

FIGUR Humid stands positiv [3+, 4partitic

3.4.2 To il

> traini have on of

Day

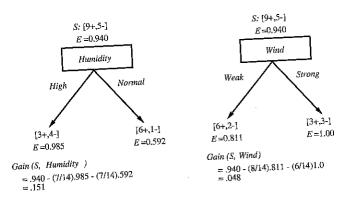
D1 D2 D3 D4 D5 D6 D7 D8 D9 D10 D11

TABI Train

D12 D13

D14

Which attribute is the best classifier?



Humidity provides greater information gain than Wind, relative to the target classification. Here, E stands for entropy and S for the original collection of examples. Given an initial collection S of 9positive and 5 negative examples, [9+, 5-], sorting these by their Humidity produces collections of [3+,4-] (Humidity = High) and [6+,1-] (Humidity = Normal). The information gained by this partitioning is .151, compared to a gain of only .048 for the attribute Wind.

An Illustrative Example 3.4.2

To illustrate the operation of ID3, consider the learning task represented by the training examples of Table 3.2. Here the target attribute PlayTennis, which can have values yes or no for different Saturday mornings, is to be predicted based on other attributes of the morning in question. Consider the first step through

	Outlook	Temperature	Humidity	Wind	PlayTennis
Day D1 D2 D3 D4 D5 D6 D7 D8 D9 D10 D11 D12 D13 D14	Sunny Sunny Overcast Rain Rain Overcast Sunny Sunny Rain Sunny Overcast Overcast Rain	Hot Hot Hot Mild Cool Cool Cool Mild Cool Mild Mild Mild Mild Hot Mild	High High High Normal Normal Normal High Normal Normal Normal Normal Normal Normal	Weak Strong Weak Weak Strong Strong Weak Weak Strong Strong Weak Strong Strong Strong	No No Yes Yes Yes No Yes No Yes Yes Yes Yes Yes Yos

Training examples for the target concept PlayTennis.

the algorithm, in which the topmost node of the decision tree is created. Which attribute should be tested first in the tree? ID3 determines the information gain for each candidate attribute (i.e., *Outlook, Temperature, Humidity*, and *Wind*), then selects the one with highest information gain. The computation of information gain for two of these attributes is shown in Figure 3.3. The information gain values for all four attributes are

Gain(S, Outlook) = 0.246 Gain(S, Humidity) = 0.151 Gain(S, Wind) = 0.048 Gain(S, Temperature) = 0.029

where S denotes the collection of training examples from Table 3.2.

According to the information gain measure, the Outlook attribute provides the best prediction of the target attribute, PlayTennis, over the training examples. Therefore, Outlook is selected as the decision attribute for the root node, and branches are created below the root for each of its possible values (i.e., Sunny, Overcast, and Rain). The resulting partial decision tree is shown in Figure 3.4, along with the training examples sorted to each new descendant node. Note that every example for which Outlook = Overcast is also a positive example of PlayTennis. Therefore, this node of the tree becomes a leaf node with the classification PlayTennis = Yes. In contrast, the descendants corresponding to Outlook = Sunny and Outlook = Rain still have nonzero entropy, and the decision tree will be further elaborated below these nodes.

The process of selecting a new attribute and partitioning the training examples is now repeated for each nonterminal descendant node, this time using only the training examples associated with that node. Attributes that have been incorporated higher in the tree are excluded, so that any given attribute can appear at most once along any path through the tree. This process continues for each new leaf node until either of two conditions is met: (1) every attribute has already been included along this path through the tree, or (2) the training examples associated with this leaf node all have the same target attribute value (i.e., their entropy is zero). Figure 3.4 illustrates the computations of information gain for the next step in growing the decision tree. The final decision tree learned by ID3 from the 14 training examples of Table 3.2 is shown in Figure 3.1.

3.5 HYPOTHESIS SPACE SEARCH IN DECISION TREE LEARNING

As with other inductive learning methods, ID3 can be characterized as searching a space of hypotheses for one that fits the training examples. The hypothesis space searched by ID3 is the set of possible decision trees. ID3 performs a simple-to-complex, hill-climbing search through this hypothesis space, beginning with the empty tree, then considering progressively more elaborate hypotheses in search of a decision tree that correctly classifies the training data. The evaluation function

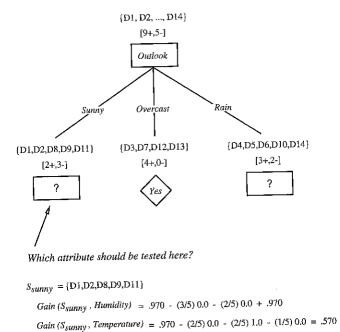
(D1,

 S_{SU}

FIGUE The parter and the expansion of th

that is de

some



Gain (S_{sunny} , Wind) = .970 - (2/5) 1.0 - (3/5) .918 = .019

FIGURE 3.4

The partially learned decision tree resulting from the first step of ID3. The training examples are sorted to the corresponding descendant nodes. The Overcast descendant has only positive examples and therefore becomes a leaf node with classification Yes. The other two nodes will be further expanded, by selecting the attribute with highest information gain relative to the new subsets of examples.

that guides this hill-climbing search is the information gain measure. This search is depicted in Figure 3.5.

By viewing ID3 in terms of its search space and search strategy, we can get some insight into its capabilities and limitations.

- ID3's hypothesis space of all decision trees is a complete space of finite discrete-valued functions, relative to the available attributes. Because every finite discrete-valued function can be represented by some decision tree, ID3 avoids one of the major risks of methods that search incomplete hypothesis spaces (such as methods that consider only conjunctive hypotheses): that the hypothesis space might not contain the target function.
- ID3 maintains only a single current hypothesis as it searches through the space of decision trees. This contrasts, for example, with the earlier version space Candidate-Elimination method, which maintains the set of all hypotheses consistent with the available training examples. By determining only a single hypothesis, ID3 loses the capabilities that follow from

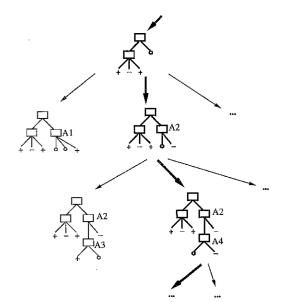


FIGURE 3.5
Hypothesis space search by ID3.
ID3 searches through the space of possible decision trees from simplest to increasingly complex, guided by the information gain heuristic.

explicitly representing all consistent hypotheses. For example, it does not have the ability to determine how many alternative decision trees are consistent with the available training data, or to pose new instance queries that optimally resolve among these competing hypotheses.

- ID3 in its pure form performs no backtracking in its search. Once it selects an attribute to test at a particular level in the tree, it never backtracks to reconsider this choice. Therefore, it is susceptible to the usual risks of hill-climbing search without backtracking: converging to locally optimal solutions that are not globally optimal. In the case of ID3, a locally optimal solution corresponds to the decision tree it selects along the single search path it explores. However, this locally optimal solution may be less desirable than trees that would have been encountered along a different branch of the search. Below we discuss an extension that adds a form of backtracking (post-pruning the decision tree).
- ID3 uses all training examples at each step in the search to make statistically based decisions regarding how to refine its current hypothesis. This contrasts with methods that make decisions incrementally, based on individual training examples (e.g., Find-S or Candidate-Elimination). One advantage of using statistical properties of all the examples (e.g., information gain) is that the resulting search is much less sensitive to errors in individual training examples. ID3 can be easily extended to handle noisy training data by modifying its termination criterion to accept hypotheses that imperfectly fit the training data.

3.6 II

What is to class from Cl the train future in

trees co fore con tent hyp It choos climbin ID3 sea (b) sele the root tic used to chara approxi comple

this inc searche all tree consiste search search precise viewed to atter search

it exhit find the with hi

3.6.1

There by ID3

3.6 INDUCTIVE BIAS IN DECISION TREE LEARNING

What is the policy by which ID3 generalizes from observed training examples to classify unseen instances? In other words, what is its inductive bias? Recall from Chapter 2 that inductive bias is the set of assumptions that, together with the training data, deductively justify the classifications assigned by the learner to future instances.

Given a collection of training examples, there are typically many decision trees consistent with these examples. Describing the inductive bias of ID3 therefore consists of describing the basis by which it chooses one of these consistent hypotheses over the others. Which of these decision trees does ID3 choose? It chooses the first acceptable tree it encounters in its simple-to-complex, hill-climbing search through the space of possible trees. Roughly speaking, then, the ID3 search strategy (a) selects in favor of shorter trees over longer ones, and (b) selects trees that place the attributes with highest information gain closest to the root. Because of the subtle interaction between the attribute selection heuristic used by ID3 and the particular training examples it encounters, it is difficult to characterize precisely the inductive bias exhibited by ID3. However, we can approximately characterize its bias as a preference for short decision trees over complex trees.

Approximate inductive bias of ID3: Shorter trees are preferred over larger trees.

In fact, one could imagine an algorithm similar to ID3 that exhibits precisely this inductive bias. Consider an algorithm that begins with the empty tree and searches breadth first through progressively more complex trees, first considering all trees of depth 1, then all trees of depth 2, etc. Once it finds a decision tree consistent with the training data, it returns the smallest consistent tree at that search depth (e.g., the tree with the fewest nodes). Let us call this breadth-first search algorithm BFS-ID3. BFS-ID3 finds a shortest decision tree and thus exhibits precisely the bias "shorter trees are preferred over longer trees." ID3 can be viewed as an efficient approximation to BFS-ID3, using a greedy heuristic search to attempt to find the shortest tree without conducting the entire breadth-first search through the hypothesis space.

Because ID3 uses the information gain heuristic and a hill climbing strategy, it exhibits a more complex bias than BFS-ID3. In particular, it does not always find the shortest consistent tree, and it is biased to favor trees that place attributes with high information gain closest to the root.

A closer approximation to the inductive bias of ID3: Shorter trees are preferred over longer trees. Trees that place high information gain attributes close to the root are preferred over those that do not.

3.6.1 Restriction Biases and Preference Biases

There is an interesting difference between the types of inductive bias exhibited by ID3 and by the Candidate-Elimination algorithm discussed in Chapter 2.

Consider the difference between the hypothesis space search in these two approaches:

- ID3 searches a *complete* hypothesis space (i.e., one capable of expressing any finite discrete-valued function). It searches *incompletely* through this space, from simple to complex hypotheses, until its termination condition is met (e.g., until it finds a hypothesis consistent with the data). Its inductive bias is solely a consequence of the ordering of hypotheses by its search strategy. Its hypothesis space introduces no additional bias.
- The version space Candidate-Elimination algorithm searches an *incomplete* hypothesis space (i.e., one that can express only a subset of the potentially teachable concepts). It searches this space *completely*, finding every hypothesis consistent with the training data. Its inductive bias is solely a consequence of the expressive power of its hypothesis representation. Its search strategy introduces no additional bias.

In brief, the inductive bias of ID3 follows from its *search strategy*, whereas the inductive bias of the Candidate-Elimination algorithm follows from the definition of its *search space*.

The inductive bias of ID3 is thus a *preference* for certain hypotheses over others (e.g., for shorter hypotheses), with no hard restriction on the hypotheses that can be eventually enumerated. This form of bias is typically called a *preference bias* (or, alternatively, a *search bias*). In contrast, the bias of the CANDIDATE-ELIMINATION algorithm is in the form of a categorical *restriction* on the set of hypotheses considered. This form of bias is typically called a *restriction bias* (or, alternatively, a *language bias*).

Given that some form of inductive bias is required in order to generalize beyond the training data (see Chapter 2), which type of inductive bias shall we prefer; a preference bias or restriction bias?

Typically, a preference bias is more desirable than a restriction bias, because it allows the learner to work within a complete hypothesis space that is assured to contain the unknown target function. In contrast, a restriction bias that strictly limits the set of potential hypotheses is generally less desirable, because it introduces the possibility of excluding the unknown target function altogether.

Whereas ID3 exhibits a purely preference bias and Candidate-Elimination a purely restriction bias, some learning systems combine both. Consider, for example, the program described in Chapter 1 for learning a numerical evaluation function for game playing. In this case, the learned evaluation function is represented by a linear combination of a fixed set of board features, and the learning algorithm adjusts the parameters of this linear combination to best fit the available training data. In this case, the decision to use a linear function to represent the evaluation function introduces a restriction bias (nonlinear evaluation functions cannot be represented in this form). At the same time, the choice of a particular parameter tuning method (the LMS algorithm in this case) introduces a preference bias stemming from the ordered search through the space of all possible parameter values.

3.6.2 Why

Is ID3's indiing beyond to for centuries was one of to often goes b

Occam

Of cour prefer simple inductive bia of the plane because ther combinatorial coincidental hypotheses subsequent a more 500-nd 20 training a sion trees co decision tree tree is less I the 500-node

Upon above argun prefer decisi use the deci numerical or same reason an arbitrary many small Why should trees with shother small s

A seco of a hypothe the learner. arrive at diffuccam's raz tree in Figur learner that

[†]Apparently wl

3.6.2 Why Prefer Short Hypotheses?

Is ID3's inductive bias favoring shorter decision trees a sound basis for generalizing beyond the training data? Philosophers and others have debated this question for centuries, and the debate remains unresolved to this day. William of Occam was one of the first to discuss† the question, around the year 1320, so this bias often goes by the name of Occam's razor.

Occam's razor: Prefer the simplest hypothesis that fits the data.

Of course giving an inductive bias a name does not justify it. Why should one prefer simpler hypotheses? Notice that scientists sometimes appear to follow this inductive bias. Physicists, for example, prefer simple explanations for the motions of the planets, over more complex explanations. Why? One argument is that because there are fewer short hypotheses than long ones (based on straightforward combinatorial arguments), it is less likely that one will find a short hypothesis that coincidentally fits the training data. In contrast there are often many very complex hypotheses that fit the current training data but fail to generalize correctly to subsequent data. Consider decision tree hypotheses, for example. There are many more 500-node decision trees than 5-node decision trees. Given a small set of 20 training examples, we might expect to be able to find many 500-node decision trees consistent with these, whereas we would be more surprised if a 5-node decision tree could perfectly fit this data. We might therefore believe the 5-node tree is less likely to be a statistical coincidence and prefer this hypothesis over the 500-node hypothesis.

Upon closer examination, it turns out there is a major difficulty with the above argument. By the same reasoning we could have argued that one should prefer decision trees containing exactly 17 leaf nodes with 11 nonleaf nodes, that use the decision attribute A_1 at the root, and test attributes A_2 through A_{11} , in numerical order. There are relatively few such trees, and we might argue (by the same reasoning as above) that our a priori chance of finding one consistent with an arbitrary set of data is therefore small. The difficulty here is that there are very many small sets of hypotheses that one can define—most of them rather arcane. Why should we believe that the small set of hypotheses consisting of decision trees with *short descriptions* should be any more relevant than the multitude of other small sets of hypotheses that we might define?

A second problem with the above argument for Occam's razor is that the size of a hypothesis is determined by the particular representation used *internally* by the learner. Two learners using different internal representations could therefore arrive at different hypotheses, both justifying their contradictory conclusions by Occam's razor! For example, the function represented by the learned decision tree in Figure 3.1 could be represented as a tree with just one decision node, by a learner that uses the boolean attribute XYZ, where we define the attribute XYZ to

[†]Apparently while shaving.

be true for instances that are classified positive by the decision tree in Figure 3.1 and false otherwise. Thus, two learners, both applying Occam's razor, would generalize in different ways if one used the XYZ attribute to describe its examples and the other used only the attributes Outlook, Temperature, Humidity, and Wind.

This last argument shows that Occam's razor will produce two different hypotheses from the same training examples when it is applied by two learners that perceive these examples in terms of different internal representations. On this basis we might be tempted to reject Occam's razor altogether. However, consider the following scenario that examines the question of which internal representations might arise from a process of evolution and natural selection. Imagine a population of artificial learning agents created by a simulated evolutionary process involving reproduction, mutation, and natural selection of these agents. Let us assume that this evolutionary process can alter the perceptual systems of these agents from generation to generation, thereby changing the internal attributes by which they perceive their world. For the sake of argument, let us also assume that the learning agents employ a fixed learning algorithm (say ID3) that cannot be altered by evolution. It is reasonable to assume that over time evolution will produce internal representation that make these agents increasingly successful within their environment. Assuming that the success of an agent depends highly on its ability to generalize accurately, we would therefore expect evolution to develop internal representations that work well with whatever learning algorithm and inductive bias is present. If the species of agents employs a learning algorithm whose inductive bias is Occam's razor, then we expect evolution to produce internal representations for which Occam's razor is a successful strategy. The essence of the argument here is that evolution will create internal representations that make the learning algorithm's inductive bias a self-fulfilling prophecy, simply because it can alter the representation easier than it can alter the learning algorithm.

For now, we leave the debate regarding Occam's razor. We will revisit it in Chapter 6, where we discuss the Minimum Description Length principle, a version of Occam's razor that can be interpreted within a Bayesian framework.

3.7 ISSUES IN DECISION TREE LEARNING

Practical issues in learning decision trees include determining how deeply to grow the decision tree, handling continuous attributes, choosing an appropriate attribute selection measure, handling training data with missing attribute values, handling attributes with differing costs, and improving computational efficiency. Below we discuss each of these issues and extensions to the basic ID3 algorithm that address them. ID3 has itself been extended to address most of these issues, with the resulting system renamed C4.5 (Quinlan 1993).

3.7.1 Avoiding Overfitting the Data

The algorithm described in Table 3.1 grows each branch of the tree just deeply enough to perfectly classify the training examples. While this is sometimes a

reasonable st or when the i sample of the can produce

We will hypothesis the entire distribution

Definition training smaller over the

Figure 3 sion tree lear which medic indicates the structed. The The solid line whereas the bexamples (no over the train ever, the acc then decrease

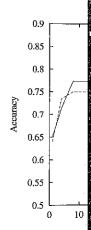


FIGURE 3.6
Overfitting in dethe tree measured a set of test exar Software and daweb at http://ww

reasonable strategy, in fact it can lead to difficulties when there is noise in the data, or when the number of training examples is too small to produce a representative sample of the true target function. In either of these cases, this simple algorithm can produce trees that *overfit* the training examples.

11

Įd

S

We will say that a hypothesis overfits the training examples if some other hypothesis that fits the training examples less well actually performs better over the entire distribution of instances (i.e., including instances beyond the training set).

Definition: Given a hypothesis space H, a hypothesis $h \in H$ is said to **overfit** the training data if there exists some alternative hypothesis $h' \in H$, such that h has smaller error than h' over the training examples, but h' has a smaller error than h over the entire distribution of instances.

Figure 3.6 illustrates the impact of overfitting in a typical application of decision tree learning. In this case, the ID3 algorithm is applied to the task of learning which medical patients have a form of diabetes. The horizontal axis of this plot indicates the total number of nodes in the decision tree, as the tree is being constructed. The vertical axis indicates the accuracy of predictions made by the tree. The solid line shows the accuracy of the decision tree over the training examples, whereas the broken line shows accuracy measured over an independent set of test examples (not included in the training set). Predictably, the accuracy of the tree over the training examples increases monotonically as the tree is grown. However, the accuracy measured over the independent test examples first increases, then decreases. As can be seen, once the tree size exceeds approximately 25 nodes,

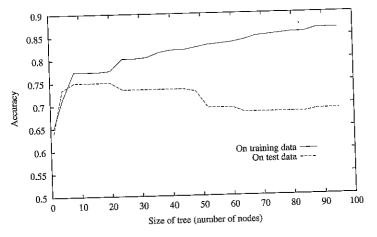


FIGURE 3.6 Overfitting in decision tree learning. As ID3 adds new nodes to grow the decision tree, the accuracy of the tree measured over the training examples increases monotonically. However, when measured over a set of test examples independent of the training examples, accuracy first increases, then decreases. Software and data for experimenting with variations on this plot are available on the World Wide Web at http://www.cs.cmu.edu/~tom/mlbook.html.