4.3 Decision Tree Induction

This section introduces a **decision tree** classifier, which is a simple yet widely used classification technique.

4.3.1 How a Decision Tree Works

To illustrate how classification with a decision tree works, consider a simpler version of the vertebrate classification problem described in the previous section. Instead of classifying the vertebrates into five distinct groups of species, we assign them to two categories: mammals and non-mammals.

Suppose a new species is discovered by scientists. How can we tell whether it is a mammal or a non-mammal? One approach is to pose a series of questions about the characteristics of the species. The first question we may ask is whether the species is cold- or warm-blooded. If it is cold-blooded, then it is definitely not a mammal. Otherwise, it is either a bird or a mammal. In the latter case, we need to ask a follow-up question: Do the females of the species give birth to their young? Those that do give birth are definitely mammals, while those that do not are likely to be non-mammals (with the exception of egg-laying mammals such as the platypus and spiny anteater).

The previous example illustrates how we can solve a classification problem by asking a series of carefully crafted questions about the attributes of the test record. Each time we receive an answer, a follow-up question is asked until we reach a conclusion about the class label of the record. The series of questions and their possible answers can be organized in the form of a decision tree, which is a hierarchical structure consisting of nodes and directed edges. Figure 4.4 shows the decision tree for the mammal classification problem. The tree has three types of nodes:

- A **root node** that has no incoming edges and zero or more outgoing edges.
- **Internal nodes**, each of which has exactly one incoming edge and two or more outgoing edges.
- **Leaf** or **terminal** nodes, each of which has exactly one incoming edge and no outgoing edges.

In a decision tree, each leaf node is assigned a class label. The **non-terminal** nodes, which include the root and other internal nodes, contain attribute test conditions to separate records that have different characteristics. For example, the root node shown in Figure 4.4 uses the attribute `Body`

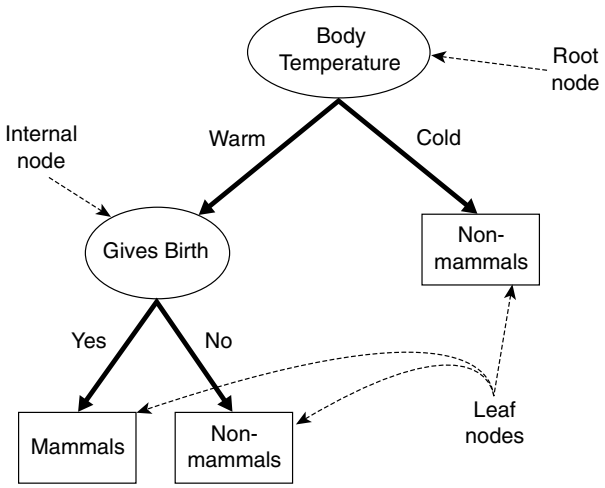


Figure 4.4. A decision tree for the mammal classification problem.

`Temperature` to separate warm-blooded from cold-blooded vertebrates. Since all cold-blooded vertebrates are non-mammals, a leaf node labeled `Non-mammals` is created as the right child of the root node. If the vertebrate is warm-blooded, a subsequent attribute, `Gives Birth`, is used to distinguish mammals from other warm-blooded creatures, which are mostly birds.

Classifying a test record is straightforward once a decision tree has been constructed. Starting from the root node, we apply the test condition to the record and follow the appropriate branch based on the outcome of the test. This will lead us either to another internal node, for which a new test condition is applied, or to a leaf node. The class label associated with the leaf node is then assigned to the record. As an illustration, Figure 4.5 traces the path in the decision tree that is used to predict the class label of a flamingo. The path terminates at a leaf node labeled `Non-mammals`.

4.3.2 How to Build a Decision Tree

In principle, there are exponentially many decision trees that can be constructed from a given set of attributes. While some of the trees are more accurate than others, finding the optimal tree is computationally infeasible because of the exponential size of the search space. Nevertheless, efficient algorithms have been developed to induce a reasonably accurate, albeit suboptimal, decision tree in a reasonable amount of time. These algorithms usually employ a greedy strategy that grows a decision tree by making a series of locally op-

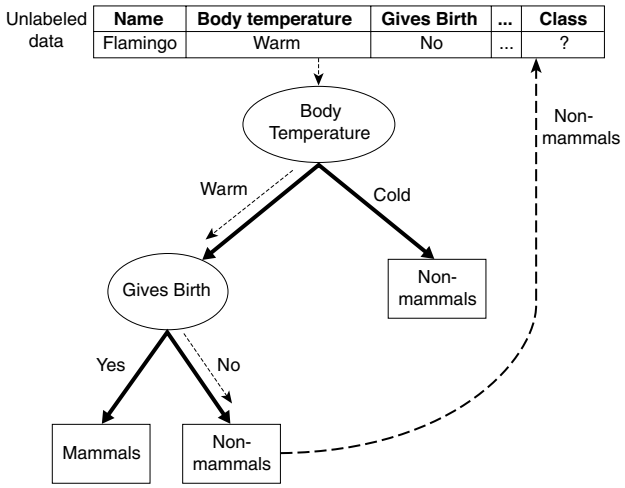


Figure 4.5. Classifying an unlabeled vertebrate. The dashed lines represent the outcomes of applying various attribute test conditions on the unlabeled vertebrate. The vertebrate is eventually assigned to the `Non-mammal` class.

timum decisions about which attribute to use for partitioning the data. One such algorithm is **Hunt's algorithm**, which is the basis of many existing decision tree induction algorithms, including ID3, C4.5, and CART. This section presents a high-level discussion of Hunt's algorithm and illustrates some of its design issues.

Hunt's Algorithm

In Hunt's algorithm, a decision tree is grown in a recursive fashion by partitioning the training records into successively purer subsets. Let D_t be the set of training records that are associated with node t and $y = \{y_1, y_2, \ldots, y_c\}$ be the class labels. The following is a recursive definition of Hunt's algorithm.

Step 1: If all the records in D_t belong to the same class y_t, then t is a leaf node labeled as y_t.

Step 2: If D_t contains records that belong to more than one class, an **attribute test condition** is selected to partition the records into smaller subsets. A child node is created for each outcome of the test condition and the records in D_t are distributed to the children based on the outcomes. The algorithm is then recursively applied to each child node.

	binary	categorical	continuous	class
Tid	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Figure 4.6. Training set for predicting borrowers who will default on loan payments.

To illustrate how the algorithm works, consider the problem of predicting whether a loan applicant will repay her loan obligations or become delinquent, subsequently defaulting on her loan. A training set for this problem can be constructed by examining the records of previous borrowers. In the example shown in Figure 4.6, each record contains the personal information of a borrower along with a class label indicating whether the borrower has defaulted on loan payments.

The initial tree for the classification problem contains a single node with class label `Defaulted = No` (see Figure 4.7(a)), which means that most of the borrowers successfully repaid their loans. The tree, however, needs to be refined since the root node contains records from both classes. The records are subsequently divided into smaller subsets based on the outcomes of the `Home Owner` test condition, as shown in Figure 4.7(b). The justification for choosing this attribute test condition will be discussed later. For now, we will assume that this is the best criterion for splitting the data at this point. Hunt's algorithm is then applied recursively to each child of the root node. From the training set given in Figure 4.6, notice that all borrowers who are home owners successfully repaid their loans. The left child of the root is therefore a leaf node labeled `Defaulted = No` (see Figure 4.7(b)). For the right child, we need to continue applying the recursive step of Hunt's algorithm until all the records belong to the same class. The trees resulting from each recursive step are shown in Figures 4.7(c) and (d).

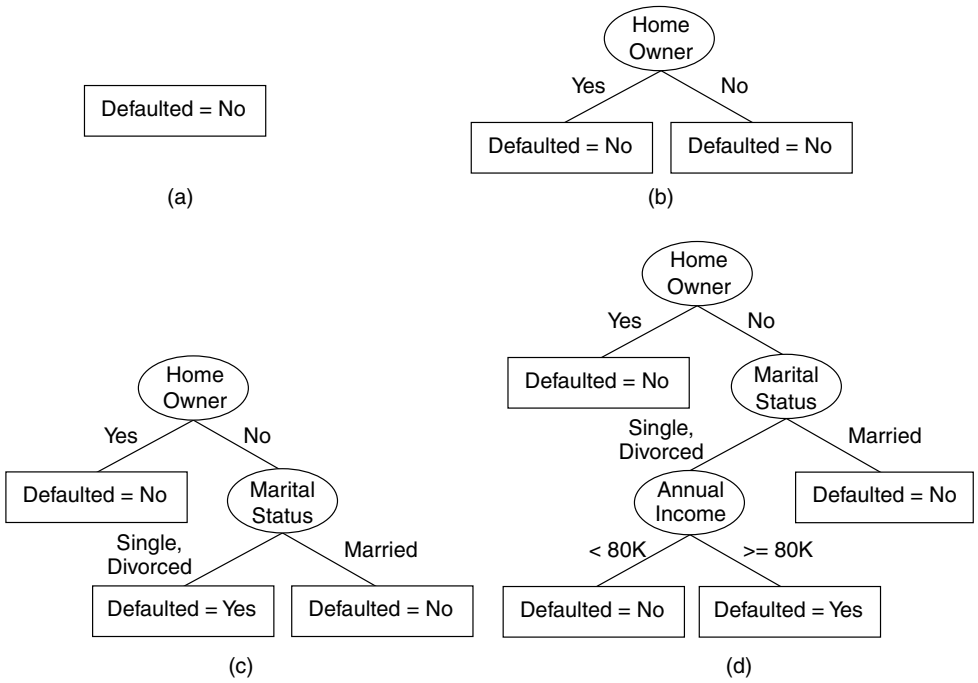


Figure 4.7. Hunt's algorithm for inducing decision trees.

Hunt's algorithm will work if every combination of attribute values is present in the training data and each combination has a unique class label. These assumptions are too stringent for use in most practical situations. Additional conditions are needed to handle the following cases:

1. It is possible for some of the child nodes created in Step 2 to be empty; i.e., there are no records associated with these nodes. This can happen if none of the training records have the combination of attribute values associated with such nodes. In this case the node is declared a leaf node with the same class label as the majority class of training records associated with its parent node.

2. In Step 2, if all the records associated with D_t have identical attribute values (except for the class label), then it is not possible to split these records any further. In this case, the node is declared a leaf node with the same class label as the majority class of training records associated with this node.

Design Issues of Decision Tree Induction

A learning algorithm for inducing decision trees must address the following two issues.

1. **How should the training records be split?** Each recursive step of the tree-growing process must select an attribute test condition to divide the records into smaller subsets. To implement this step, the algorithm must provide a method for specifying the test condition for different attribute types as well as an objective measure for evaluating the goodness of each test condition.

2. **How should the splitting procedure stop?** A stopping condition is needed to terminate the tree-growing process. A possible strategy is to continue expanding a node until either all the records belong to the same class or all the records have identical attribute values. Although both conditions are sufficient to stop any decision tree induction algorithm, other criteria can be imposed to allow the tree-growing procedure to terminate earlier. The advantages of early termination will be discussed later in Section 4.4.5.

4.3.3 Methods for Expressing Attribute Test Conditions

Decision tree induction algorithms must provide a method for expressing an attribute test condition and its corresponding outcomes for different attribute types.

Binary Attributes The test condition for a binary attribute generates two potential outcomes, as shown in Figure 4.8.

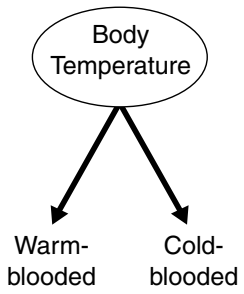


Figure 4.8. Test condition for binary attributes.

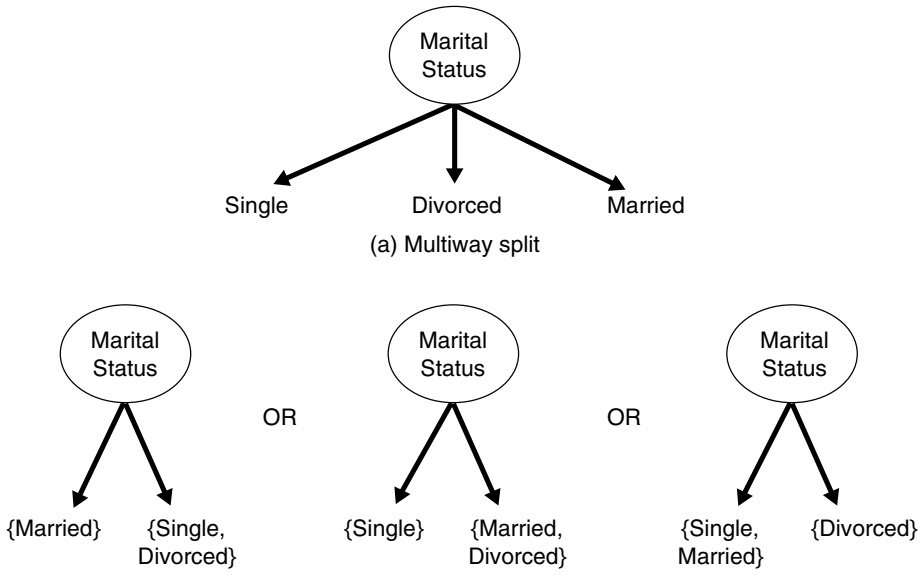


Figure 4.9. Test conditions for nominal attributes.

Nominal Attributes Since a nominal attribute can have many values, its test condition can be expressed in two ways, as shown in Figure 4.9. For a multiway split (Figure 4.9(a)), the number of outcomes depends on the number of distinct values for the corresponding attribute. For example, if an attribute such as marital status has three distinct values—single, married, or divorced—its test condition will produce a three-way split. On the other hand, some decision tree algorithms, such as CART, produce only binary splits by considering all $2^{k-1} - 1$ ways of creating a binary partition of k attribute values. Figure 4.9(b) illustrates three different ways of grouping the attribute values for marital status into two subsets.

Ordinal Attributes Ordinal attributes can also produce binary or multiway splits. Ordinal attribute values can be grouped as long as the grouping does not violate the order property of the attribute values. Figure 4.10 illustrates various ways of splitting training records based on the `Shirt Size` attribute. The groupings shown in Figures 4.10(a) and (b) preserve the order among the attribute values, whereas the grouping shown in Figure 4.10(c) violates this property because it combines the attribute values `Small` and `Large` into

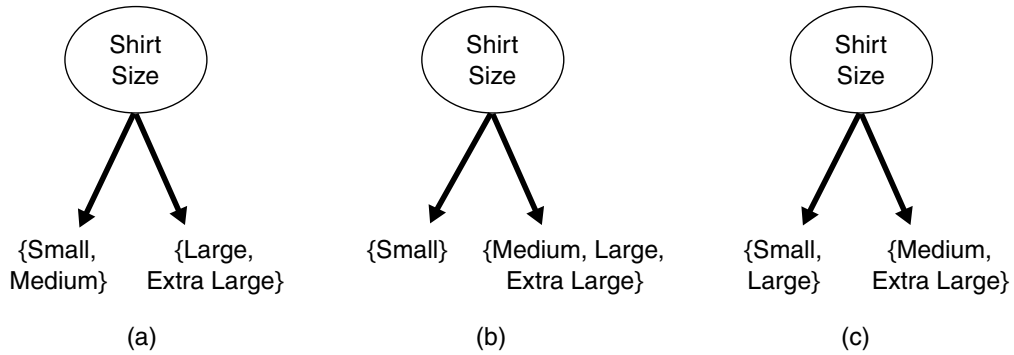


Figure 4.10. Different ways of grouping ordinal attribute values.

the same partition while `Medium` and `Extra Large` are combined into another partition.

Continuous Attributes For continuous attributes, the test condition can be expressed as a comparison test $(A < v)$ or $(A \geq v)$ with binary outcomes, or a range query with outcomes of the form $v_i \leq A < v_{i+1}$, for $i = 1, \ldots, k$. The difference between these approaches is shown in Figure 4.11. For the binary case, the decision tree algorithm must consider all possible split positions v, and it selects the one that produces the best partition. For the multiway split, the algorithm must consider all possible ranges of continuous values. One approach is to apply the discretization strategies described in Section 2.3.6 on page 57. After discretization, a new ordinal value will be assigned to each discretized interval. Adjacent intervals can also be aggregated into wider ranges as long as the order property is preserved.

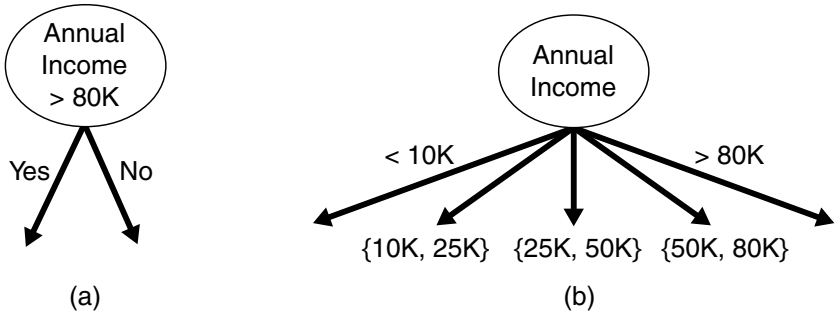


Figure 4.11. Test condition for continuous attributes.

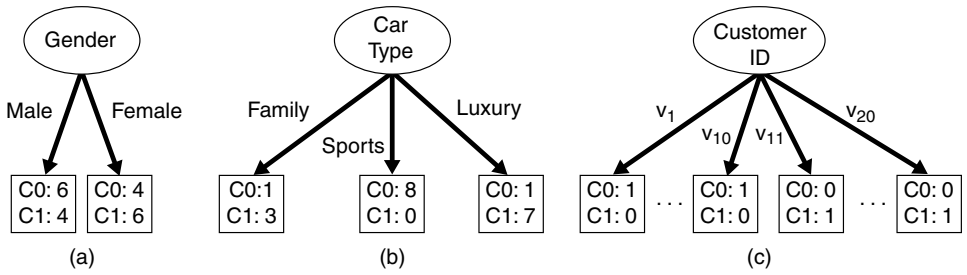


Figure 4.12. Multiway versus binary splits.

4.3.4 Measures for Selecting the Best Split

There are many measures that can be used to determine the best way to split the records. These measures are defined in terms of the class distribution of the records before and after splitting.

Let $p(i|t)$ denote the fraction of records belonging to class i at a given node t. We sometimes omit the reference to node t and express the fraction as p_i. In a two-class problem, the class distribution at any node can be written as (p_0, p_1), where $p_1 = 1 - p_0$. To illustrate, consider the test conditions shown in Figure 4.12. The class distribution before splitting is $(0.5, 0.5)$ because there are an equal number of records from each class. If we split the data using the `Gender` attribute, then the class distributions of the child nodes are $(0.6, 0.4)$ and $(0.4, 0.6)$, respectively. Although the classes are no longer evenly distributed, the child nodes still contain records from both classes. Splitting on the second attribute, `Car Type`, will result in purer partitions.

The measures developed for selecting the best split are often based on the degree of impurity of the child nodes. The smaller the degree of impurity, the more skewed the class distribution. For example, a node with class distribution $(0, 1)$ has zero impurity, whereas a node with uniform class distribution $(0.5, 0.5)$ has the highest impurity. Examples of impurity measures include

$$\text{Entropy}(t) = -\sum_{i=0}^{c-1} p(i|t) \log_2 p(i|t), \tag{4.3}$$

$$\text{Gini}(t) = 1 - \sum_{i=0}^{c-1} [p(i|t)]^2, \tag{4.4}$$

$$\text{Classification error}(t) = 1 - \max_i [p(i|t)], \tag{4.5}$$

where c is the number of classes and $0 \log_2 0 = 0$ in entropy calculations.

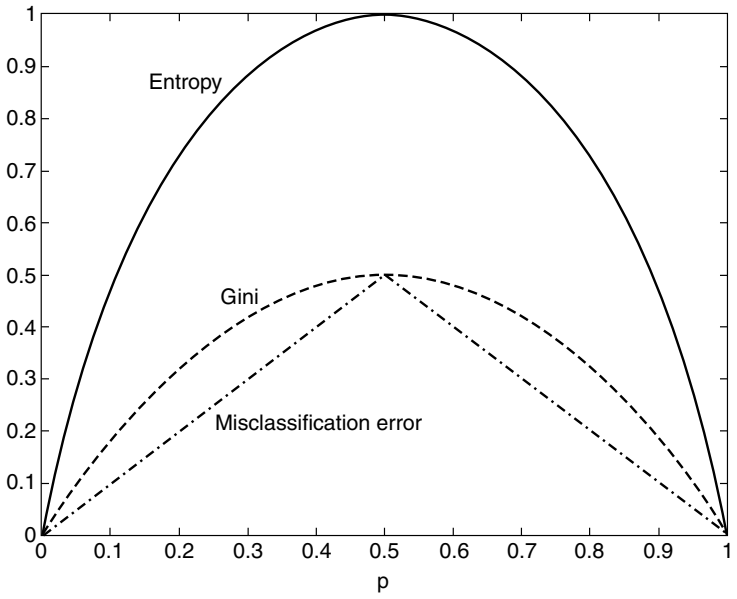


Figure 4.13. Comparison among the impurity measures for binary classification problems.

Figure 4.13 compares the values of the impurity measures for binary classification problems. p refers to the fraction of records that belong to one of the two classes. Observe that all three measures attain their maximum value when the class distribution is uniform (i.e., when $p = 0.5$). The minimum values for the measures are attained when all the records belong to the same class (i.e., when p equals 0 or 1). We next provide several examples of computing the different impurity measures.

Node N_1	Count
Class=0	0
Class=1	6

Gini $= 1 - (0/6)^2 - (6/6)^2 = 0$
Entropy $= -(0/6)\log_2(0/6) - (6/6)\log_2(6/6) = 0$
Error $= 1 - \max[0/6, 6/6] = 0$

Node N_2	Count
Class=0	1
Class=1	5

Gini $= 1 - (1/6)^2 - (5/6)^2 = 0.278$
Entropy $= -(1/6)\log_2(1/6) - (5/6)\log_2(5/6) = 0.650$
Error $= 1 - \max[1/6, 5/6] = 0.167$

Node N_3	Count
Class=0	3
Class=1	3

Gini $= 1 - (3/6)^2 - (3/6)^2 = 0.5$
Entropy $= -(3/6)\log_2(3/6) - (3/6)\log_2(3/6) = 1$
Error $= 1 - \max[3/6, 3/6] = 0.5$

The preceding examples, along with Figure 4.13, illustrate the consistency among different impurity measures. Based on these calculations, node N_1 has the lowest impurity value, followed by N_2 and N_3. Despite their consistency, the attribute chosen as the test condition may vary depending on the choice of impurity measure, as will be shown in Exercise 3 on page 198.

To determine how well a test condition performs, we need to compare the degree of impurity of the parent node (before splitting) with the degree of impurity of the child nodes (after splitting). The larger their difference, the better the test condition. The gain, Δ, is a criterion that can be used to determine the goodness of a split:

$$\Delta = I(\text{parent}) - \sum_{j=1}^{k} \frac{N(v_j)}{N} I(v_j), \tag{4.6}$$

where $I(\cdot)$ is the impurity measure of a given node, N is the total number of records at the parent node, k is the number of attribute values, and $N(v_j)$ is the number of records associated with the child node, v_j. Decision tree induction algorithms often choose a test condition that maximizes the gain Δ. Since $I(\text{parent})$ is the same for all test conditions, maximizing the gain is equivalent to minimizing the weighted average impurity measures of the child nodes. Finally, when entropy is used as the impurity measure in Equation 4.6, the difference in entropy is known as the **information gain**, Δ_{info}.

Splitting of Binary Attributes

Consider the diagram shown in Figure 4.14. Suppose there are two ways to split the data into smaller subsets. Before splitting, the Gini index is 0.5 since there are an equal number of records from both classes. If attribute A is chosen to split the data, the Gini index for node N1 is 0.4898, and for node N2, it is 0.480. The weighted average of the Gini index for the descendent nodes is $(7/12) \times 0.4898 + (5/12) \times 0.480 = 0.486$. Similarly, we can show that the weighted average of the Gini index for attribute B is 0.375. Since the subsets for attribute B have a smaller Gini index, it is preferred over attribute A.

Splitting of Nominal Attributes

As previously noted, a nominal attribute can produce either binary or multiway splits, as shown in Figure 4.15. The computation of the Gini index for a binary split is similar to that shown for determining binary attributes. For the first binary grouping of the `Car Type` attribute, the Gini index of {`Sports,`

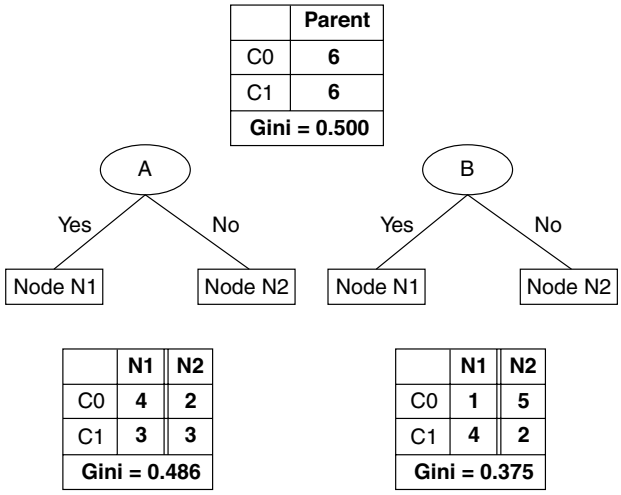
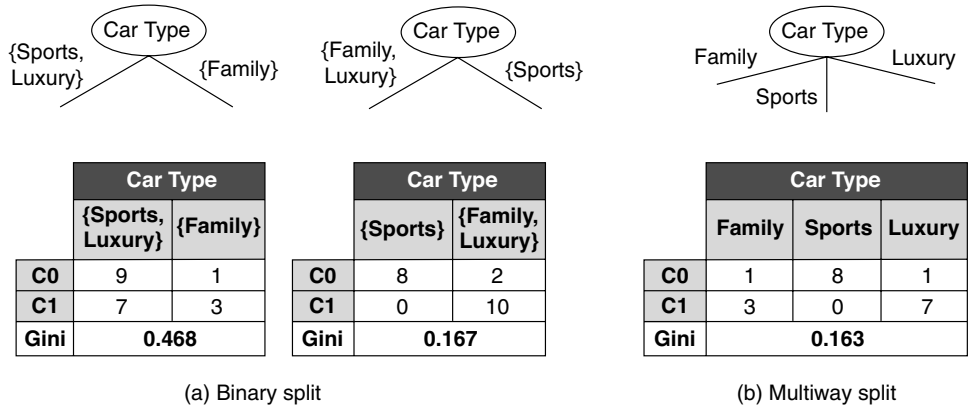


Figure 4.14. Splitting binary attributes.



(a) Binary split

(b) Multiway split

Figure 4.15. Splitting nominal attributes.

`Luxury`} is 0.4922 and the Gini index of {`Family`} is 0.3750. The weighted average Gini index for the grouping is equal to

$$16/20 \times 0.4922 + 4/20 \times 0.3750 = 0.468.$$

Similarly, for the second binary grouping of {`Sports`} and {`Family, Luxury`}, the weighted average Gini index is 0.167. The second grouping has a lower Gini index because its corresponding subsets are much purer.

Class	No		No		No		Yes		Yes		Yes		No		No		No		No		No	
	Annual Income																					
Sorted Values →	60		70		75		85		90		95		100		120		125		220			
Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		*0.300*		0.343		0.375		0.400		0.420	

Figure 4.16. Splitting continuous attributes.

For the multiway split, the Gini index is computed for every attribute value. Since Gini({`Family`}) = 0.375, Gini({`Sports`}) = 0, and Gini({`Luxury`}) = 0.219, the overall Gini index for the multiway split is equal to

$$4/20 \times 0.375 + 8/20 \times 0 + 8/20 \times 0.219 = 0.163.$$

The multiway split has a smaller Gini index compared to both two-way splits. This result is not surprising because the two-way split actually merges some of the outcomes of a multiway split, and thus, results in less pure subsets.

Splitting of Continuous Attributes

Consider the example shown in Figure 4.16, in which the test condition `Annual Income` $\leq v$ is used to split the training records for the loan default classification problem. A brute-force method for finding v is to consider every value of the attribute in the N records as a candidate split position. For each candidate v, the data set is scanned once to count the number of records with annual income less than or greater than v. We then compute the Gini index for each candidate and choose the one that gives the lowest value. This approach is computationally expensive because it requires $O(N)$ operations to compute the Gini index at each candidate split position. Since there are N candidates, the overall complexity of this task is $O(N^2)$. To reduce the complexity, the training records are sorted based on their annual income, a computation that requires $O(N \log N)$ time. Candidate split positions are identified by taking the midpoints between two adjacent sorted values: 55, 65, 72, and so on. However, unlike the brute-force approach, we do not have to examine all N records when evaluating the Gini index of a candidate split position.

For the first candidate, $v = 55$, none of the records has annual income less than \$55K. As a result, the Gini index for the descendent node with `Annual`

`Income` $<$ \$55K is zero. On the other hand, the number of records with annual income greater than or equal to \$55K is 3 (for class `Yes`) and 7 (for class `No`), respectively. Thus, the Gini index for this node is 0.420. The overall Gini index for this candidate split position is equal to $0 \times 0 + 1 \times 0.420 = 0.420$.

For the second candidate, $v = 65$, we can determine its class distribution by updating the distribution of the previous candidate. More specifically, the new distribution is obtained by examining the class label of the record with the lowest annual income (i.e., \$60K). Since the class label for this record is `No`, the count for class `No` is increased from 0 to 1 (for `Annual Income` $\leq$ \$65K) and is decreased from 7 to 6 (for `Annual Income` $>$ \$65K). The distribution for class `Yes` remains unchanged. The new weighted-average Gini index for this candidate split position is 0.400.

This procedure is repeated until the Gini index values for all candidates are computed, as shown in Figure 4.16. The best split position corresponds to the one that produces the smallest Gini index, i.e., $v = 97$. This procedure is less expensive because it requires a constant amount of time to update the class distribution at each candidate split position. It can be further optimized by considering only candidate split positions located between two adjacent records with different class labels. For example, because the first three sorted records (with annual incomes \$60K, \$70K, and \$75K) have identical class labels, the best split position should not reside between \$60K and \$75K. Therefore, the candidate split positions at $v =$ \$55K, \$65K, \$72K, \$87K, \$92K, \$110K, \$122K, \$172K, and \$230K are ignored because they are located between two adjacent records with the same class labels. This approach allows us to reduce the number of candidate split positions from 11 to 2.

Gain Ratio

Impurity measures such as entropy and Gini index tend to favor attributes that have a large number of distinct values. Figure 4.12 shows three alternative test conditions for partitioning the data set given in Exercise 2 on page 198. Comparing the first test condition, `Gender`, with the second, `Car Type`, it is easy to see that `Car Type` seems to provide a better way of splitting the data since it produces purer descendent nodes. However, if we compare both conditions with `Customer ID`, the latter appears to produce purer partitions. Yet `Customer ID` is not a predictive attribute because its value is unique for each record. Even in a less extreme situation, a test condition that results in a large number of outcomes may not be desirable because the number of records associated with each partition is too small to enable us to make any reliable predictions.

There are two strategies for overcoming this problem. The first strategy is to restrict the test conditions to binary splits only. This strategy is employed by decision tree algorithms such as CART. Another strategy is to modify the splitting criterion to take into account the number of outcomes produced by the attribute test condition. For example, in the C4.5 decision tree algorithm, a splitting criterion known as **gain ratio** is used to determine the goodness of a split. This criterion is defined as follows:

$$\text{Gain ratio} = \frac{\Delta_{\text{info}}}{\text{Split Info}}. \tag{4.7}$$

Here, Split Info $= -\sum_{i=1}^{k} P(v_i) \log_2 P(v_i)$ and k is the total number of splits. For example, if each attribute value has the same number of records, then $\forall i : P(v_i) = 1/k$ and the split information would be equal to $\log_2 k$. This example suggests that if an attribute produces a large number of splits, its split information will also be large, which in turn reduces its gain ratio.

4.3.5 Algorithm for Decision Tree Induction

A skeleton decision tree induction algorithm called `TreeGrowth` is shown in Algorithm 4.1. The input to this algorithm consists of the training records E and the attribute set F. The algorithm works by recursively selecting the best attribute to split the data (Step 7) and expanding the leaf nodes of the

Algorithm 4.1 A skeleton decision tree induction algorithm.

`TreeGrowth` (E, F)
1: **if** `stopping_cond`(E,F) = *true* **then**
2: $leaf$ = `createNode`().
3: $leaf.label$ = `Classify`(E).
4: return $leaf$.
5: **else**
6: $root$ = `createNode`().
7: $root.test\_cond$ = `find_best_split`(E, F).
8: let $V = \{v | v$ is a possible outcome of $root.test\_cond$ $\}$.
9: **for** each $v \in V$ **do**
10: $E_v = \{e \mid root.test\_cond(e) = v$ and $e \in E\}$.
11: $child$ = `TreeGrowth`(E_v, F).
12: add $child$ as descendent of $root$ and label the edge ($root \rightarrow child$) as v.
13: **end for**
14: **end if**
15: return $root$.

tree (Steps 11 and 12) until the stopping criterion is met (Step 1). The details of this algorithm are explained below:

1. The `createNode`() function extends the decision tree by creating a new node. A node in the decision tree has either a test condition, denoted as *node.test_cond*, or a class label, denoted as *node.label*.

2. The `find_best_split`() function determines which attribute should be selected as the test condition for splitting the training records. As previously noted, the choice of test condition depends on which impurity measure is used to determine the goodness of a split. Some widely used measures include entropy, the Gini index, and the χ^2 statistic.

3. The `Classify`() function determines the class label to be assigned to a leaf node. For each leaf node t, let $p(i|t)$ denote the fraction of training records from class i associated with the node t. In most cases, the leaf node is assigned to the class that has the majority number of training records:

$$leaf.label = \underset{i}{\text{argmax}}\ p(i|t), \tag{4.8}$$

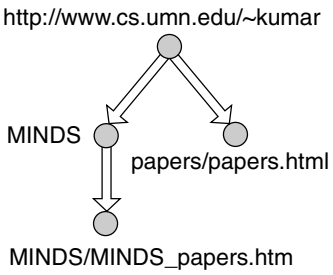
   where the argmax operator returns the argument i that maximizes the expression $p(i|t)$. Besides providing the information needed to determine the class label of a leaf node, the fraction $p(i|t)$ can also be used to estimate the probability that a record assigned to the leaf node t belongs to class i. Sections 5.7.2 and 5.7.3 describe how such probability estimates can be used to determine the performance of a decision tree under different cost functions.

4. The `stopping_cond`() function is used to terminate the tree-growing process by testing whether all the records have either the same class label or the same attribute values. Another way to terminate the recursive function is to test whether the number of records have fallen below some minimum threshold.

After building the decision tree, a **tree-pruning** step can be performed to reduce the size of the decision tree. Decision trees that are too large are susceptible to a phenomenon known as **overfitting**. Pruning helps by trimming the branches of the initial tree in a way that improves the generalization capability of the decision tree. The issues of overfitting and tree pruning are discussed in more detail in Section 4.4.

Session	IP Address	Timestamp	Request Method	Requested Web Page	Protocol	Status	Number of Bytes	Referrer	User Agent
1	160.11.11.11	08/Aug/2004 10:15:21	GET	http://www.cs.umn.edu/~kumar	HTTP/1.1	200	6424		Mozilla/4.0 (compatible; MSIE 6.0; Windows NT 5.0)
1	160.11.11.11	08/Aug/2004 10:15:34	GET	http://www.cs.umn.edu/~kumar/MINDS	HTTP/1.1	200	41378	http://www.cs.umn.edu/~kumar	Mozilla/4.0 (compatible; MSIE 6.0; Windows NT 5.0)
1	160.11.11.11	08/Aug/2004 10:15:41	GET	http://www.cs.umn.edu/~kumar/MINDS/MINDS_papers.htm	HTTP/1.1	200	1018516	http://www.cs.umn.edu/~kumar/MINDS	Mozilla/4.0 (compatible; MSIE 6.0; Windows NT 5.0)
1	160.11.11.11	08/Aug/2004 10:16:11	GET	http://www.cs.umn.edu/~kumar/papers/papers.html	HTTP/1.1	200	7463	http://www.cs.umn.edu/~kumar	Mozilla/4.0 (compatible; MSIE 6.0; Windows NT 5.0)
2	35.9.2.2	08/Aug/2004 10:16:15	GET	http://www.cs.umn.edu/~steinbac	HTTP/1.0	200	3149		Mozilla/5.0 (Windows; U; Windows NT 5.1; en-US; rv:1.7) Gecko/20040616

(a) Example of a Web server log.



(b) Graph of a Web session.

Attribute Name	Description
totalPages	Total number of pages retrieved in a Web session
ImagePages	Total number of image pages retrieved in a Web session
TotalTime	Total amount of time spent by Web site visitor
RepeatedAccess	The same page requested more than once in a Web session
ErrorRequest	Errors in requesting for Web pages
GET	Percentage of requests made using GET method
POST	Percentage of requests made using POST method
HEAD	Percentage of requests made using HEAD method
Breadth	Breadth of Web traversal
Depth	Depth of Web traversal
MultiIP	Session with multiple IP addresses
MultiAgent	Session with multiple user agents

(c) Derived attributes for Web robot detection.

Figure 4.17. Input data for Web robot detection.

4.3.6 An Example: Web Robot Detection

Web usage mining is the task of applying data mining techniques to extract useful patterns from Web access logs. These patterns can reveal interesting characteristics of site visitors; e.g., people who repeatedly visit a Web site and view the same product description page are more likely to buy the product if certain incentives such as rebates or free shipping are offered.

In Web usage mining, it is important to distinguish accesses made by human users from those due to Web robots. A Web robot (also known as a Web crawler) is a software program that automatically locates and retrieves information from the Internet by following the hyperlinks embedded in Web pages. These programs are deployed by search engine portals to gather the documents necessary for indexing the Web. Web robot accesses must be discarded before applying Web mining techniques to analyze human browsing behavior.

This section describes how a decision tree classifier can be used to distinguish between accesses by human users and those by Web robots. The input data was obtained from a Web server log, a sample of which is shown in Figure 4.17(a). Each line corresponds to a single page request made by a Web client (a user or a Web robot). The fields recorded in the Web log include the IP address of the client, timestamp of the request, Web address of the requested document, size of the document, and the client's identity (via the user agent field). A Web session is a sequence of requests made by a client during a single visit to a Web site. Each Web session can be modeled as a directed graph, in which the nodes correspond to Web pages and the edges correspond to hyperlinks connecting one Web page to another. Figure 4.17(b) shows a graphical representation of the first Web session given in the Web server log.

To classify the Web sessions, features are constructed to describe the characteristics of each session. Figure 4.17(c) shows some of the features used for the Web robot detection task. Among the notable features include the `depth` and `breadth` of the traversal. `Depth` determines the maximum distance of a requested page, where distance is measured in terms of the number of hyperlinks away from the entry point of the Web site. For example, the home page `http://www.cs.umn.edu/~kumar` is assumed to be at depth 0, whereas `http://www.cs.umn.edu/kumar/MINDS/MINDS_papers.htm` is located at depth 2. Based on the Web graph shown in Figure 4.17(b), the `depth` attribute for the first session is equal to two. The `breadth` attribute measures the width of the corresponding Web graph. For example, the `breadth` of the Web session shown in Figure 4.17(b) is equal to two.

The data set for classification contains 2916 records, with equal numbers of sessions due to Web robots (class 1) and human users (class 0). 10% of the data were reserved for training while the remaining 90% were used for testing. The induced decision tree model is shown in Figure 4.18. The tree has an error rate equal to 3.8% on the training set and 5.3% on the test set.

The model suggests that Web robots can be distinguished from human users in the following way:

1. Accesses by Web robots tend to be broad but shallow, whereas accesses by human users tend to be more focused (narrow but deep).

2. Unlike human users, Web robots seldom retrieve the image pages associated with a Web document.

3. Sessions due to Web robots tend to be long and contain a large number of requested pages.

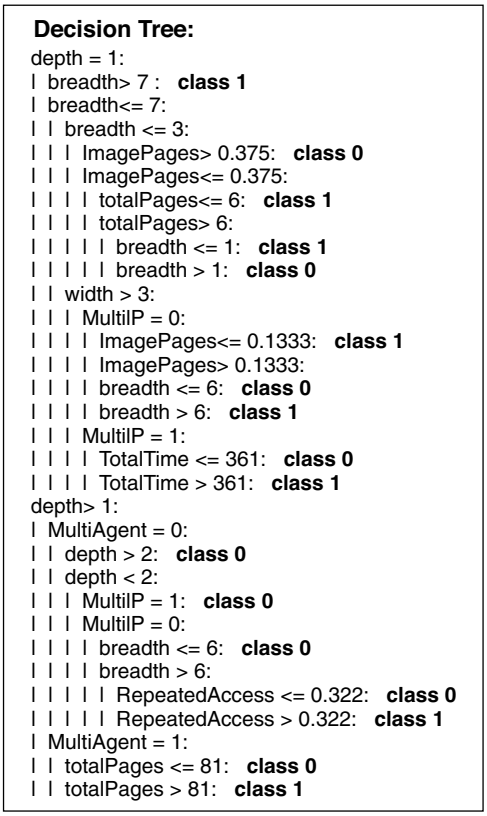


Figure 4.18. Decision tree model for Web robot detection.

4. Web robots are more likely to make repeated requests for the same document since the Web pages retrieved by human users are often cached by the browser.

4.3.7 Characteristics of Decision Tree Induction

The following is a summary of the important characteristics of decision tree induction algorithms.

1. Decision tree induction is a nonparametric approach for building classification models. In other words, it does not require any prior assumptions regarding the type of probability distributions satisfied by the class and other attributes (unlike some of the techniques described in Chapter 5).

2. Finding an optimal decision tree is an NP-complete problem. Many decision tree algorithms employ a heuristic-based approach to guide their search in the vast hypothesis space. For example, the algorithm presented in Section 4.3.5 uses a greedy, top-down, recursive partitioning strategy for growing a decision tree.

3. Techniques developed for constructing decision trees are computationally inexpensive, making it possible to quickly construct models even when the training set size is very large. Furthermore, once a decision tree has been built, classifying a test record is extremely fast, with a worst-case complexity of $O(w)$, where w is the maximum depth of the tree.

4. Decision trees, especially smaller-sized trees, are relatively easy to interpret. The accuracies of the trees are also comparable to other classification techniques for many simple data sets.

5. Decision trees provide an expressive representation for learning discrete-valued functions. However, they do not generalize well to certain types of Boolean problems. One notable example is the parity function, whose value is 0 (1) when there is an odd (even) number of Boolean attributes with the value $True$. Accurate modeling of such a function requires a full decision tree with 2^d nodes, where d is the number of Boolean attributes (see Exercise 1 on page 198).

6. Decision tree algorithms are quite robust to the presence of noise, especially when methods for avoiding overfitting, as described in Section 4.4, are employed.

7. The presence of redundant attributes does not adversely affect the accuracy of decision trees. An attribute is redundant if it is strongly correlated with another attribute in the data. One of the two redundant attributes will not be used for splitting once the other attribute has been chosen. However, if the data set contains many irrelevant attributes, i.e., attributes that are not useful for the classification task, then some of the irrelevant attributes may be accidently chosen during the tree-growing process, which results in a decision tree that is larger than necessary. Feature selection techniques can help to improve the accuracy of decision trees by eliminating the irrelevant attributes during preprocessing. We will investigate the issue of too many irrelevant attributes in Section 4.4.3.

8. Since most decision tree algorithms employ a top-down, recursive partitioning approach, the number of records becomes smaller as we traverse down the tree. At the leaf nodes, the number of records may be too small to make a statistically significant decision about the class representation of the nodes. This is known as the **data fragmentation** problem. One possible solution is to disallow further splitting when the number of records falls below a certain threshold.

9. A subtree can be replicated multiple times in a decision tree, as illustrated in Figure 4.19. This makes the decision tree more complex than necessary and perhaps more difficult to interpret. Such a situation can arise from decision tree implementations that rely on a single attribute test condition at each internal node. Since most of the decision tree algorithms use a divide-and-conquer partitioning strategy, the same test condition can be applied to different parts of the attribute space, thus leading to the subtree replication problem.

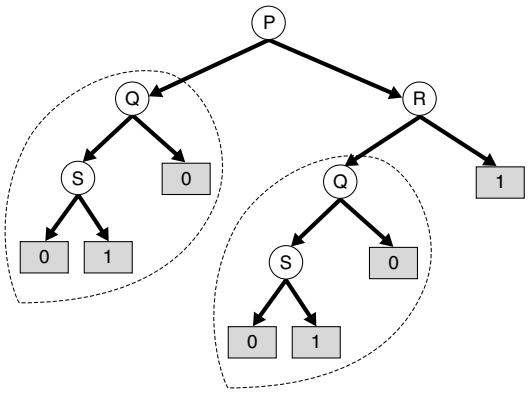


Figure 4.19. Tree replication problem. The same subtree can appear at different branches.

10. The test conditions described so far in this chapter involve using only a single attribute at a time. As a consequence, the tree-growing procedure can be viewed as the process of partitioning the attribute space into disjoint regions until each region contains records of the same class (see Figure 4.20). The border between two neighboring regions of different classes is known as a **decision boundary**. Since the test condition involves only a single attribute, the decision boundaries are rectilinear; i.e., parallel to the "coordinate axes." This limits the expressiveness of the

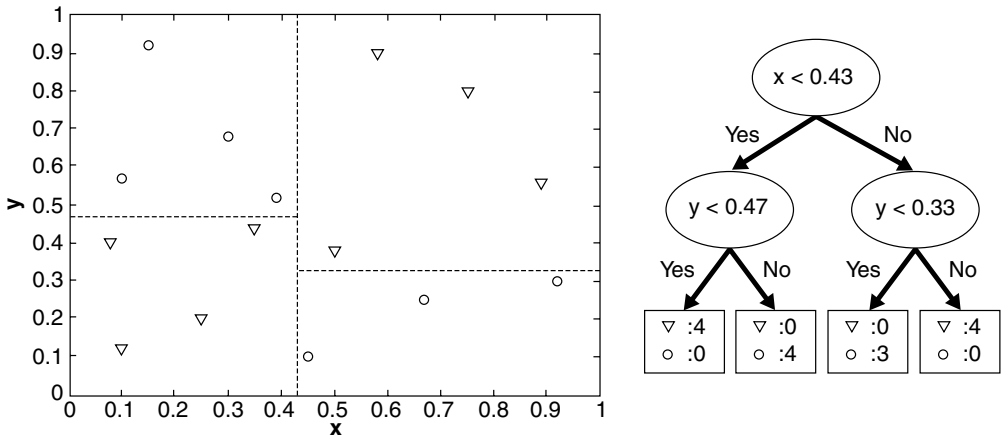


Figure 4.20. Example of a decision tree and its decision boundaries for a two-dimensional data set.

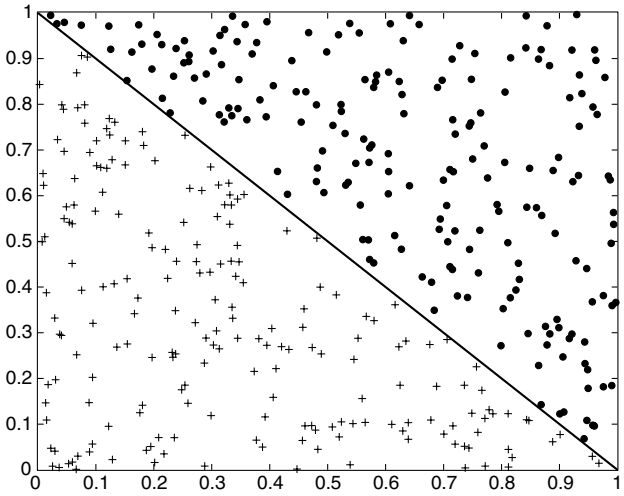


Figure 4.21. Example of data set that cannot be partitioned optimally using test conditions involving single attributes.

decision tree representation for modeling complex relationships among continuous attributes. Figure 4.21 illustrates a data set that cannot be classified effectively by a decision tree algorithm that uses test conditions involving only a single attribute at a time.

An **oblique decision tree** can be used to overcome this limitation because it allows test conditions that involve more than one attribute. The data set given in Figure 4.21 can be easily represented by an oblique decision tree containing a single node with test condition

$$x + y < 1.$$

Although such techniques are more expressive and can produce more compact trees, finding the optimal test condition for a given node can be computationally expensive.

Constructive induction provides another way to partition the data into homogeneous, nonrectangular regions (see Section 2.3.5 on page 57). This approach creates composite attributes representing an arithmetic or logical combination of the existing attributes. The new attributes provide a better discrimination of the classes and are augmented to the data set prior to decision tree induction. Unlike the oblique decision tree approach, constructive induction is less expensive because it identifies all the relevant combinations of attributes once, prior to constructing the decision tree. In contrast, an oblique decision tree must determine the right attribute combination dynamically, every time an internal node is expanded. However, constructive induction can introduce attribute redundancy in the data since the new attribute is a combination of several existing attributes.

11. Studies have shown that the choice of impurity measure has little effect on the performance of decision tree induction algorithms. This is because many impurity measures are quite consistent with each other, as shown in Figure 4.13 on page 159. Indeed, the strategy used to prune the tree has a greater impact on the final tree than the choice of impurity measure.

4.4 Model Overfitting

The errors committed by a classification model are generally divided into two types: **training errors** and **generalization errors**. Training error, also known as **resubstitution error** or **apparent error**, is the number of misclassification errors committed on training records, whereas generalization error is the expected error of the model on previously unseen records.

Recall from Section 4.2 that a good classification model must not only fit the training data well, it must also accurately classify records it has never

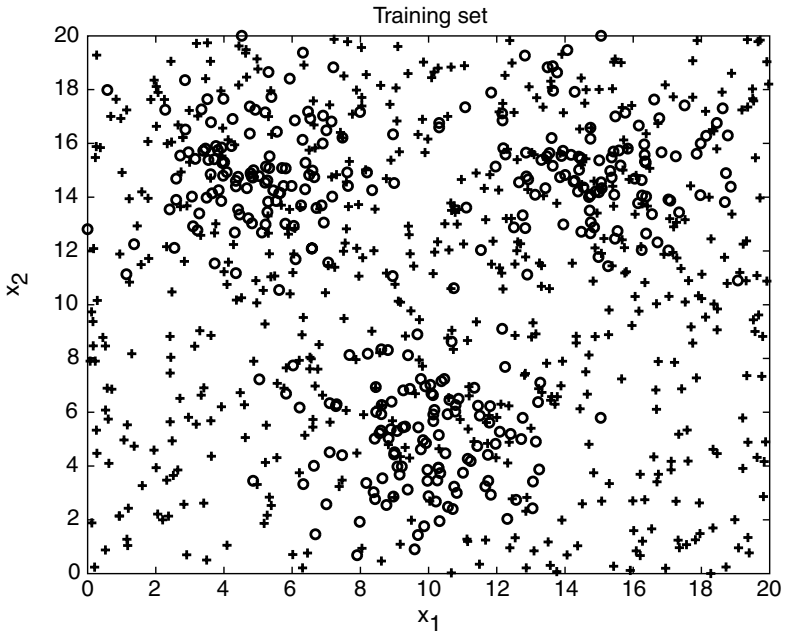


Figure 4.22. Example of a data set with binary classes.

seen before. In other words, a good model must have low training error as well as low generalization error. This is important because a model that fits the training data too well can have a poorer generalization error than a model with a higher training error. Such a situation is known as model overfitting.

Overfitting Example in Two-Dimensional Data For a more concrete example of the overfitting problem, consider the two-dimensional data set shown in Figure 4.22. The data set contains data points that belong to two different classes, denoted as class o and class +, respectively. The data points for the o class are generated from a mixture of three Gaussian distributions, while a uniform distribution is used to generate the data points for the + class. There are altogether 1200 points belonging to the o class and 1800 points belonging to the + class. 30% of the points are chosen for training, while the remaining 70% are used for testing. A decision tree classifier that uses the Gini index as its impurity measure is then applied to the training set. To investigate the effect of overfitting, different levels of pruning are applied to the initial, fully-grown tree. Figure 4.23(b) shows the training and test error rates of the decision tree.

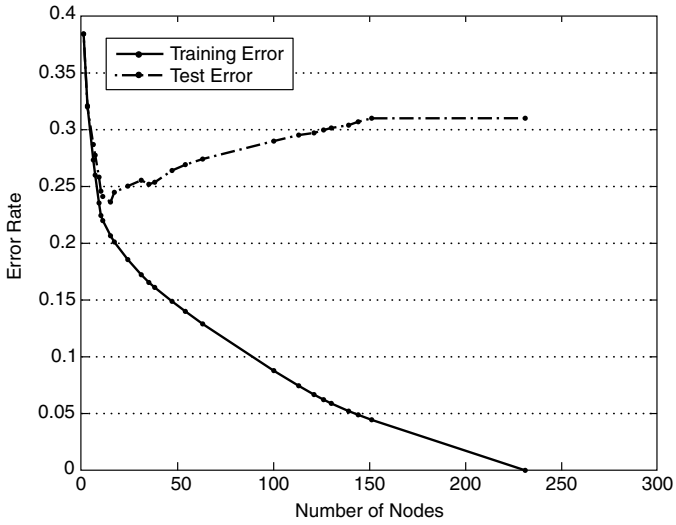
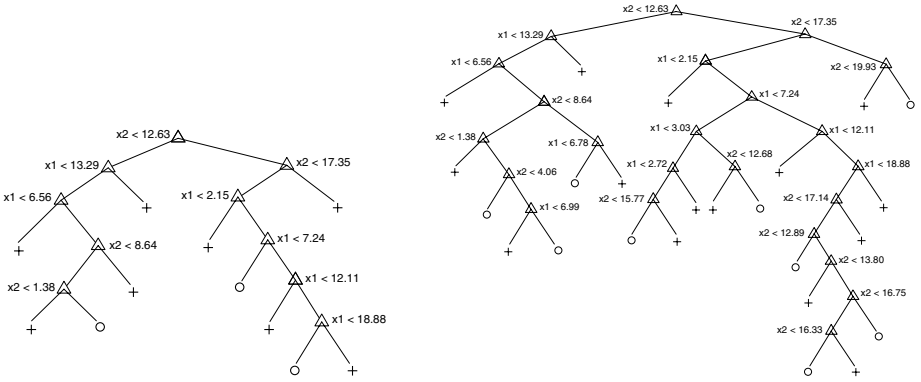


Figure 4.23. Training and test error rates.

Notice that the training and test error rates of the model are large when the size of the tree is very small. This situation is known as **model underfitting**. Underfitting occurs because the model has yet to learn the true structure of the data. As a result, it performs poorly on both the training and the test sets. As the number of nodes in the decision tree increases, the tree will have fewer training and test errors. However, once the tree becomes too large, its test error rate begins to increase even though its training error rate continues to decrease. This phenomenon is known as **model overfitting**.

To understand the overfitting phenomenon, note that the training error of a model can be reduced by increasing the model complexity. For example, the leaf nodes of the tree can be expanded until it perfectly fits the training data. Although the training error for such a complex tree is zero, the test error can be large because the tree may contain nodes that accidently fit some of the noise points in the training data. Such nodes can degrade the performance of the tree because they do not generalize well to the test examples. Figure 4.24 shows the structure of two decision trees with different number of nodes. The tree that contains the smaller number of nodes has a higher training error rate, but a lower test error rate compared to the more complex tree.

Overfitting and underfitting are two pathologies that are related to the model complexity. The remainder of this section examines some of the potential causes of model overfitting.



(a) Decision tree with 11 leaf nodes.

(b) Decision tree with 24 leaf nodes.

Figure 4.24. Decision trees with different model complexities.

4.4.1 Overfitting Due to Presence of Noise

Consider the training and test sets shown in Tables 4.3 and 4.4 for the mammal classification problem. Two of the ten training records are mislabeled: bats and whales are classified as non-mammals instead of mammals.

A decision tree that perfectly fits the training data is shown in Figure 4.25(a). Although the training error for the tree is zero, its error rate on

Table 4.3. An example training set for classifying mammals. Class labels with asterisk symbols represent mislabeled records.

Name	Body Temperature	Gives Birth	Four-legged	Hibernates	Class Label
porcupine	warm-blooded	yes	yes	yes	yes
cat	warm-blooded	yes	yes	no	yes
bat	warm-blooded	yes	no	yes	no*
whale	warm-blooded	yes	no	no	no*
salamander	cold-blooded	no	yes	yes	no
komodo dragon	cold-blooded	no	yes	no	no
python	cold-blooded	no	no	yes	no
salmon	cold-blooded	no	no	no	no
eagle	warm-blooded	no	no	no	no
guppy	cold-blooded	yes	no	no	no

Table 4.4. An example test set for classifying mammals.

Name	Body Temperature	Gives Birth	Four-legged	Hibernates	Class Label
human	warm-blooded	yes	no	no	yes
pigeon	warm-blooded	no	no	no	no
elephant	warm-blooded	yes	yes	no	yes
leopard shark	cold-blooded	yes	no	no	no
turtle	cold-blooded	no	yes	no	no
penguin	cold-blooded	no	no	no	no
eel	cold-blooded	no	no	no	no
dolphin	warm-blooded	yes	no	no	yes
spiny anteater	warm-blooded	no	yes	yes	yes
gila monster	cold-blooded	no	yes	yes	no

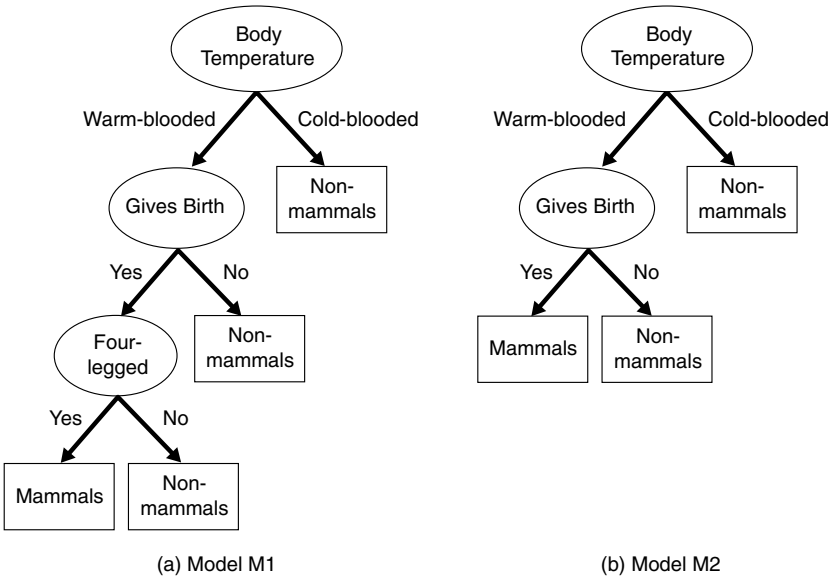


Figure 4.25. Decision tree induced from the data set shown in Table 4.3.

the test set is 30%. Both humans and dolphins were misclassified as non-mammals because their attribute values for `Body Temperature`, `Gives Birth`, and `Four-legged` are identical to the mislabeled records in the training set. Spiny anteaters, on the other hand, represent an exceptional case in which the class label of a test record contradicts the class labels of other similar records in the training set. Errors due to exceptional cases are often unavoidable and establish the minimum error rate achievable by any classifier.

In contrast, the decision tree $M2$ shown in Figure 4.25(b) has a lower test error rate (10%) even though its training error rate is somewhat higher (20%). It is evident that the first decision tree, $M1$, has overfitted the training data because there is a simpler model with lower error rate on the test set. The `Four-legged` attribute test condition in model $M1$ is spurious because it fits the mislabeled training records, which leads to the misclassification of records in the test set.

4.4.2 Overfitting Due to Lack of Representative Samples

Models that make their classification decisions based on a small number of training records are also susceptible to overfitting. Such models can be generated because of lack of representative samples in the training data and learning algorithms that continue to refine their models even when few training records are available. We illustrate these effects in the example below.

Consider the five training records shown in Table 4.5. All of these training records are labeled correctly and the corresponding decision tree is depicted in Figure 4.26. Although its training error is zero, its error rate on the test set is 30%.

Table 4.5. An example training set for classifying mammals.

Name	Body Temperature	Gives Birth	Four-legged	Hibernates	Class Label
salamander	cold-blooded	no	yes	yes	no
guppy	cold-blooded	yes	no	no	no
eagle	warm-blooded	no	no	no	no
poorwill	warm-blooded	no	no	yes	no
platypus	warm-blooded	no	yes	yes	yes

Humans, elephants, and dolphins are misclassified because the decision tree classifies all warm-blooded vertebrates that do not hibernate as non-mammals. The tree arrives at this classification decision because there is only one training record, which is an eagle, with such characteristics. This example clearly demonstrates the danger of making wrong predictions when there are not enough representative examples at the leaf nodes of a decision tree.

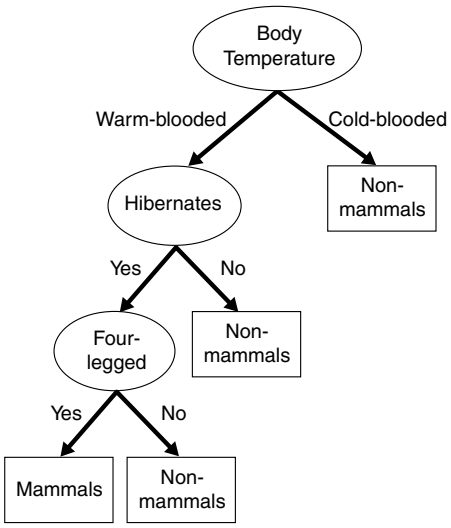


Figure 4.26. Decision tree induced from the data set shown in Table 4.5.

4.4.3 Overfitting and the Multiple Comparison Procedure

Model overfitting may arise in learning algorithms that employ a methodology known as multiple comparison procedure. To understand multiple comparison procedure, consider the task of predicting whether the stock market will rise or fall in the next ten trading days. If a stock analyst simply makes random guesses, the probability that her prediction is correct on any trading day is 0.5. However, the probability that she will predict correctly at least eight out of the ten times is

$$\frac{\binom{10}{8} + \binom{10}{9} + \binom{10}{10}}{2^{10}} = 0.0547,$$

which seems quite unlikely.

Suppose we are interested in choosing an investment advisor from a pool of fifty stock analysts. Our strategy is to select the analyst who makes the most correct predictions in the next ten trading days. The flaw in this strategy is that even if all the analysts had made their predictions in a random fashion, the probability that at least one of them makes at least eight correct predictions is

$$1 - (1 - 0.0547)^{50} = 0.9399,$$

which is very high. Although each analyst has a low probability of predicting at least eight times correctly, putting them together, we have a high probability of finding an analyst who can do so. Furthermore, there is no guarantee in the

future that such an analyst will continue to make accurate predictions through random guessing.

How does the multiple comparison procedure relate to model overfitting? Many learning algorithms explore a set of independent alternatives, $\{\gamma_i\}$, and then choose an alternative, $\gamma_{\max}$, that maximizes a given criterion function. The algorithm will add $\gamma_{\max}$ to the current model in order to improve its overall performance. This procedure is repeated until no further improvement is observed. As an example, during decision tree growing, multiple tests are performed to determine which attribute can best split the training data. The attribute that leads to the best split is chosen to extend the tree as long as the observed improvement is statistically significant.

Let T_0 be the initial decision tree and T_x be the new tree after inserting an internal node for attribute x. In principle, x can be added to the tree if the observed gain, $\Delta(T_0, T_x)$, is greater than some predefined threshold α. If there is only one attribute test condition to be evaluated, then we can avoid inserting spurious nodes by choosing a large enough value of α. However, in practice, more than one test condition is available and the decision tree algorithm must choose the best attribute $x_{\max}$ from a set of candidates, $\{x_1, x_2, \ldots, x_k\}$, to partition the data. In this situation, the algorithm is actually using a multiple comparison procedure to decide whether a decision tree should be extended. More specifically, it is testing for $\Delta(T_0, T_{x_{\max}}) > \alpha$ instead of $\Delta(T_0, T_x) > \alpha$. As the number of alternatives, k, increases, so does our chance of finding $\Delta(T_0, T_{x_{\max}}) > \alpha$. Unless the gain function Δ or threshold α is modified to account for k, the algorithm may inadvertently add spurious nodes to the model, which leads to model overfitting.

This effect becomes more pronounced when the number of training records from which $x_{\max}$ is chosen is small, because the variance of $\Delta(T_0, T_{x_{\max}})$ is high when fewer examples are available for training. As a result, the probability of finding $\Delta(T_0, T_{x_{\max}}) > \alpha$ increases when there are very few training records. This often happens when the decision tree grows deeper, which in turn reduces the number of records covered by the nodes and increases the likelihood of adding unnecessary nodes into the tree. Failure to compensate for the large number of alternatives or the small number of training records will therefore lead to model overfitting.

4.4.4 Estimation of Generalization Errors

Although the primary reason for overfitting is still a subject of debate, it is generally agreed that the complexity of a model has an impact on model overfitting, as was illustrated in Figure 4.23. The question is, how do we

determine the right model complexity? The ideal complexity is that of a model that produces the lowest generalization error. The problem is that the learning algorithm has access only to the training set during model building (see Figure 4.3). It has no knowledge of the test set, and thus, does not know how well the tree will perform on records it has never seen before. The best it can do is to estimate the generalization error of the induced tree. This section presents several methods for doing the estimation.

Using Resubstitution Estimate

The resubstitution estimate approach assumes that the training set is a good representation of the overall data. Consequently, the training error, otherwise known as resubstitution error, can be used to provide an optimistic estimate for the generalization error. Under this assumption, a decision tree induction algorithm simply selects the model that produces the lowest training error rate as its final model. However, the training error is usually a poor estimate of generalization error.

Example 4.1. Consider the binary decision trees shown in Figure 4.27. Assume that both trees are generated from the same training data and both make their classification decisions at each leaf node according to the majority class. Note that the left tree, T_L, is more complex because it expands some of the leaf nodes in the right tree, T_R. The training error rate for the left tree is $e(T_L) = 4/24 = 0.167$, while the training error rate for the right tree is

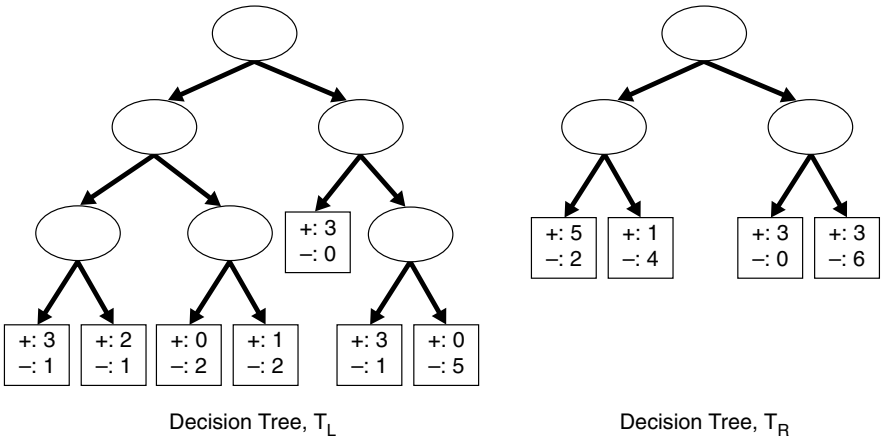


Figure 4.27. Example of two decision trees generated from the same training data.

$e(T_R) = 6/24 = 0.25$. Based on their resubstitution estimate, the left tree is considered better than the right tree. ■

Incorporating Model Complexity

As previously noted, the chance for model overfitting increases as the model becomes more complex. For this reason, we should prefer simpler models, a strategy that agrees with a well-known principle known as **Occam's razor** or the **principle of parsimony**:

Definition 4.2. Occam's Razor: Given two models with the same generalization errors, the simpler model is preferred over the more complex model.

Occam's razor is intuitive because the additional components in a complex model stand a greater chance of being fitted purely by chance. In the words of Einstein, "Everything should be made as simple as possible, but not simpler." Next, we present two methods for incorporating model complexity into the evaluation of classification models.

Pessimistic Error Estimate The first approach explicitly computes generalization error as the sum of training error and a penalty term for model complexity. The resulting generalization error can be considered its pessimistic error estimate. For instance, let $n(t)$ be the number of training records classified by node t and $e(t)$ be the number of misclassified records. The pessimistic error estimate of a decision tree T, $e_g(T)$, can be computed as follows:

$$e_g(T) = \frac{\sum_{i=1}^{k}[e(t_i) + \Omega(t_i)]}{\sum_{i=1}^{k} n(t_i)} = \frac{e(T) + \Omega(T)}{N_t},$$

where k is the number of leaf nodes, $e(T)$ is the overall training error of the decision tree, N_t is the number of training records, and $\Omega(t_i)$ is the penalty term associated with each node t_i.

Example 4.2. Consider the binary decision trees shown in Figure 4.27. If the penalty term is equal to 0.5, then the pessimistic error estimate for the left tree is

$$e_g(T_L) = \frac{4 + 7 \times 0.5}{24} = \frac{7.5}{24} = 0.3125$$

and the pessimistic error estimate for the right tree is

$$e_g(T_R) = \frac{6 + 4 \times 0.5}{24} = \frac{8}{24} = 0.3333.$$

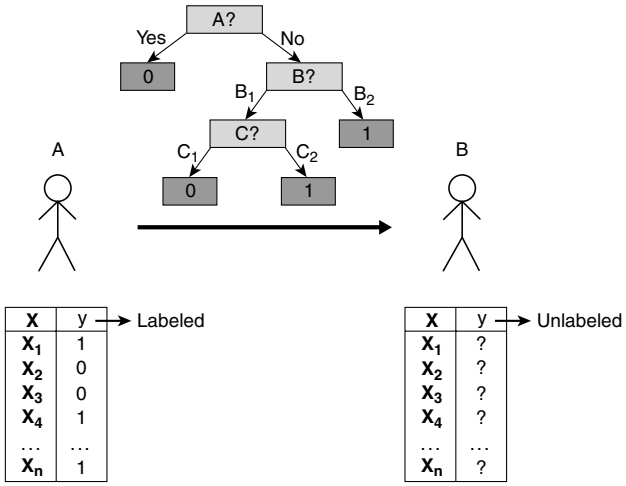


Figure 4.28. The minimum description length (MDL) principle.

Thus, the left tree has a better pessimistic error rate than the right tree. For binary trees, a penalty term of 0.5 means a node should always be expanded into its two child nodes as long as it improves the classification of at least one training record because expanding a node, which is equivalent to adding 0.5 to the overall error, is less costly than committing one training error.

If $\Omega(t) = 1$ for all the nodes t, the pessimistic error estimate for the left tree is $e_g(T_L) = 11/24 = 0.458$, while the pessimistic error estimate for the right tree is $e_g(T_R) = 10/24 = 0.417$. The right tree therefore has a better pessimistic error rate than the left tree. Thus, a node should not be expanded into its child nodes unless it reduces the misclassification error for more than one training record. ■

Minimum Description Length Principle Another way to incorporate model complexity is based on an information-theoretic approach known as the minimum description length or MDL principle. To illustrate this principle, consider the example shown in Figure 4.28. In this example, both `A` and `B` are given a set of records with known attribute values $\mathbf{x}$. In addition, person `A` knows the exact class label for each record, while person `B` knows none of this information. `B` can obtain the classification of each record by requesting that `A` transmits the class labels sequentially. Such a message would require $\Theta(n)$ bits of information, where n is the total number of records.

Alternatively, `A` may decide to build a classification model that summarizes the relationship between $\mathbf{x}$ and y. The model can be encoded in a compact

form before being transmitted to B. If the model is 100% accurate, then the cost of transmission is equivalent to the cost of encoding the model. Otherwise, A must also transmit information about which record is classified incorrectly by the model. Thus, the overall cost of transmission is

$$Cost(model, data) = Cost(model) + Cost(data|model), \tag{4.9}$$

where the first term on the right-hand side is the cost of encoding the model, while the second term represents the cost of encoding the mislabeled records. According to the MDL principle, we should seek a model that minimizes the overall cost function. An example showing how to compute the total description length of a decision tree is given by Exercise 9 on page 202.

Estimating Statistical Bounds

The generalization error can also be estimated as a statistical correction to the training error. Since generalization error tends to be larger than training error, the statistical correction is usually computed as an upper bound to the training error, taking into account the number of training records that reach a particular leaf node. For instance, in the C4.5 decision tree algorithm, the number of errors committed by each leaf node is assumed to follow a binomial distribution. To compute its generalization error, we must determine the upper bound limit to the observed training error, as illustrated in the next example.

Example 4.3. Consider the left-most branch of the binary decision trees shown in Figure 4.27. Observe that the left-most leaf node of T_R has been expanded into two child nodes in T_L. Before splitting, the error rate of the node is $2/7 = 0.286$. By approximating a binomial distribution with a normal distribution, the following upper bound of the error rate e can be derived:

$$e_{upper}(N, e, \alpha) = \frac{e + \frac{z^2_{\alpha/2}}{2N} + z_{\alpha/2}\sqrt{\frac{e(1-e)}{N} + \frac{z^2_{\alpha/2}}{4N^2}}}{1 + \frac{z^2_{\alpha/2}}{N}}, \tag{4.10}$$

where α is the confidence level, $z_{\alpha/2}$ is the standardized value from a standard normal distribution, and N is the total number of training records used to compute e. By replacing $\alpha = 25\%$, $N = 7$, and $e = 2/7$, the upper bound for the error rate is $e_{upper}(7, 2/7, 0.25) = 0.503$, which corresponds to $7 \times 0.503 = 3.521$ errors. If we expand the node into its child nodes as shown in T_L, the training error rates for the child nodes are $1/4 = 0.250$ and $1/3 = 0.333$,

respectively. Using Equation 4.10, the upper bounds of these error rates are $e_{upper}(4, 1/4, 0.25) = 0.537$ and $e_{upper}(3, 1/3, 0.25) = 0.650$, respectively. The overall training error of the child nodes is $4 \times 0.537 + 3 \times 0.650 = 4.098$, which is larger than the estimated error for the corresponding node in T_R. ■

Using a Validation Set

In this approach, instead of using the training set to estimate the generalization error, the original training data is divided into two smaller subsets. One of the subsets is used for training, while the other, known as the validation set, is used for estimating the generalization error. Typically, two-thirds of the training set is reserved for model building, while the remaining one-third is used for error estimation.

This approach is typically used with classification techniques that can be parameterized to obtain models with different levels of complexity. The complexity of the best model can be estimated by adjusting the parameter of the learning algorithm (e.g., the pruning level of a decision tree) until the empirical model produced by the learning algorithm attains the lowest error rate on the validation set. Although this approach provides a better way for estimating how well the model performs on previously unseen records, less data is available for training.

4.4.5 Handling Overfitting in Decision Tree Induction

In the previous section, we described several methods for estimating the generalization error of a classification model. Having a reliable estimate of generalization error allows the learning algorithm to search for an accurate model without overfitting the training data. This section presents two strategies for avoiding model overfitting in the context of decision tree induction.

Prepruning (Early Stopping Rule) In this approach, the tree-growing algorithm is halted before generating a fully grown tree that perfectly fits the entire training data. To do this, a more restrictive stopping condition must be used; e.g., stop expanding a leaf node when the observed gain in impurity measure (or improvement in the estimated generalization error) falls below a certain threshold. The advantage of this approach is that it avoids generating overly complex subtrees that overfit the training data. Nevertheless, it is difficult to choose the right threshold for early termination. Too high of a threshold will result in underfitted models, while a threshold that is set too low may not be sufficient to overcome the model overfitting problem. Furthermore,

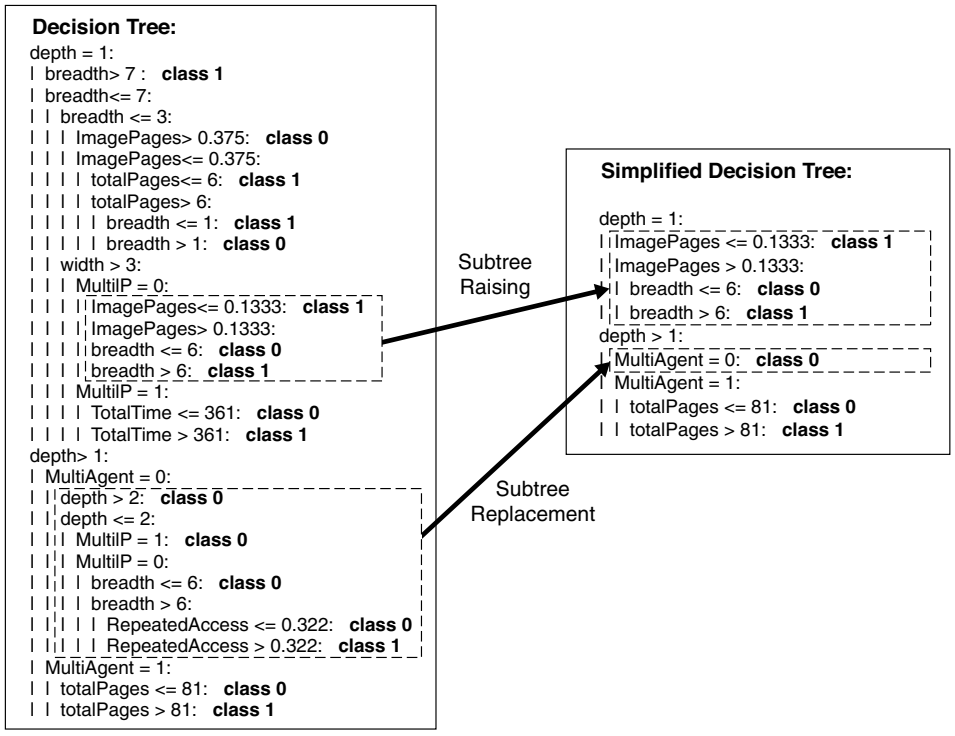


Figure 4.29. Post-pruning of the decision tree for Web robot detection.

even if no significant gain is obtained using one of the existing attribute test conditions, subsequent splitting may result in better subtrees.

Post-pruning In this approach, the decision tree is initially grown to its maximum size. This is followed by a tree-pruning step, which proceeds to trim the fully grown tree in a bottom-up fashion. Trimming can be done by replacing a subtree with (1) a new leaf node whose class label is determined from the majority class of records affiliated with the subtree, or (2) the most frequently used branch of the subtree. The tree-pruning step terminates when no further improvement is observed. Post-pruning tends to give better results than prepruning because it makes pruning decisions based on a fully grown tree, unlike prepruning, which can suffer from premature termination of the tree-growing process. However, for post-pruning, the additional computations needed to grow the full tree may be wasted when the subtree is pruned.

Figure 4.29 illustrates the simplified decision tree model for the Web robot detection example given in Section 4.3.6. Notice that the subtrees rooted at

depth = 1 have been replaced by one of the branches involving the attribute ImagePages. This approach is also known as **subtree raising**. The depth > 1 and MultiAgent = 0 subtree has been replaced by a leaf node assigned to class 0. This approach is known as **subtree replacement**. The subtree for depth > 1 and MultiAgent = 1 remains intact.

4.5 Evaluating the Performance of a Classifier

Section 4.4.4 described several methods for estimating the generalization error of a model during training. The estimated error helps the learning algorithm to do **model selection**; i.e., to find a model of the right complexity that is not susceptible to overfitting. Once the model has been constructed, it can be applied to the test set to predict the class labels of previously unseen records.

It is often useful to measure the performance of the model on the test set because such a measure provides an unbiased estimate of its generalization error. The accuracy or error rate computed from the test set can also be used to compare the relative performance of different classifiers on the same domain. However, in order to do this, the class labels of the test records must be known. This section reviews some of the methods commonly used to evaluate the performance of a classifier.

4.5.1 Holdout Method

In the holdout method, the original data with labeled examples is partitioned into two disjoint sets, called the training and the test sets, respectively. A classification model is then induced from the training set and its performance is evaluated on the test set. The proportion of data reserved for training and for testing is typically at the discretion of the analysts (e.g., 50-50 or two-thirds for training and one-third for testing). The accuracy of the classifier can be estimated based on the accuracy of the induced model on the test set.

The holdout method has several well-known limitations. First, fewer labeled examples are available for training because some of the records are withheld for testing. As a result, the induced model may not be as good as when all the labeled examples are used for training. Second, the model may be highly dependent on the composition of the training and test sets. The smaller the training set size, the larger the variance of the model. On the other hand, if the training set is too large, then the estimated accuracy computed from the smaller test set is less reliable. Such an estimate is said to have a wide confidence interval. Finally, the training and test sets are no longer independent

of each other. Because the training and test sets are subsets of the original data, a class that is overrepresented in one subset will be underrepresented in the other, and vice versa.

4.5.2 Random Subsampling

The holdout method can be repeated several times to improve the estimation of a classifier's performance. This approach is known as random subsampling. Let acc_i be the model accuracy during the i^{th} iteration. The overall accuracy is given by $acc_{\text{sub}} = \sum_{i=1}^{k} acc_i/k$. Random subsampling still encounters some of the problems associated with the holdout method because it does not utilize as much data as possible for training. It also has no control over the number of times each record is used for testing and training. Consequently, some records might be used for training more often than others.

4.5.3 Cross-Validation

An alternative to random subsampling is cross-validation. In this approach, each record is used the same number of times for training and exactly once for testing. To illustrate this method, suppose we partition the data into two equal-sized subsets. First, we choose one of the subsets for training and the other for testing. We then swap the roles of the subsets so that the previous training set becomes the test set and vice versa. This approach is called a two-fold cross-validation. The total error is obtained by summing up the errors for both runs. In this example, each record is used exactly once for training and once for testing. The k-fold cross-validation method generalizes this approach by segmenting the data into k equal-sized partitions. During each run, one of the partitions is chosen for testing, while the rest of them are used for training. This procedure is repeated k times so that each partition is used for testing exactly once. Again, the total error is found by summing up the errors for all k runs. A special case of the k-fold cross-validation method sets $k = N$, the size of the data set. In this so-called **leave-one-out** approach, each test set contains only one record. This approach has the advantage of utilizing as much data as possible for training. In addition, the test sets are mutually exclusive and they effectively cover the entire data set. The drawback of this approach is that it is computationally expensive to repeat the procedure N times. Furthermore, since each test set contains only one record, the variance of the estimated performance metric tends to be high.

4.5.4 Bootstrap

The methods presented so far assume that the training records are sampled without replacement. As a result, there are no duplicate records in the training and test sets. In the bootstrap approach, the training records are sampled with replacement; i.e., a record already chosen for training is put back into the original pool of records so that it is equally likely to be redrawn. If the original data has N records, it can be shown that, on average, a bootstrap sample of size N contains about 63.2% of the records in the original data. This approximation follows from the fact that the probability a record is chosen by a bootstrap sample is $1 - (1 - 1/N)^N$. When N is sufficiently large, the probability asymptotically approaches $1 - e^{-1} = 0.632$. Records that are not included in the bootstrap sample become part of the test set. The model induced from the training set is then applied to the test set to obtain an estimate of the accuracy of the bootstrap sample, ϵ_i. The sampling procedure is then repeated b times to generate b bootstrap samples.

There are several variations to the bootstrap sampling approach in terms of how the overall accuracy of the classifier is computed. One of the more widely used approaches is the **.632 bootstrap**, which computes the overall accuracy by combining the accuracies of each bootstrap sample (ϵ_i) with the accuracy computed from a training set that contains all the labeled examples in the original data (acc_s):

$$\text{Accuracy, } acc_{boot} = \frac{1}{b}\sum_{i=1}^{b}(0.632 \times \epsilon_i + 0.368 \times acc_s). \tag{4.11}$$

4.6 Methods for Comparing Classifiers

It is often useful to compare the performance of different classifiers to determine which classifier works better on a given data set. However, depending on the size of the data, the observed difference in accuracy between two classifiers may not be statistically significant. This section examines some of the statistical tests available to compare the performance of different models and classifiers.

For illustrative purposes, consider a pair of classification models, M_A and M_B. Suppose M_A achieves 85% accuracy when evaluated on a test set containing 30 records, while M_B achieves 75% accuracy on a different test set containing 5000 records. Based on this information, is M_A a better model than M_B?

The preceding example raises two key questions regarding the statistical significance of the performance metrics:

1. Although M_A has a higher accuracy than M_B, it was tested on a smaller test set. How much confidence can we place on the accuracy for M_A?

2. Is it possible to explain the difference in accuracy as a result of variations in the composition of the test sets?

The first question relates to the issue of estimating the confidence interval of a given model accuracy. The second question relates to the issue of testing the statistical significance of the observed deviation. These issues are investigated in the remainder of this section.

4.6.1 Estimating a Confidence Interval for Accuracy

To determine the confidence interval, we need to establish the probability distribution that governs the accuracy measure. This section describes an approach for deriving the confidence interval by modeling the classification task as a binomial experiment. Following is a list of characteristics of a binomial experiment:

1. The experiment consists of N independent trials, where each trial has two possible outcomes: success or failure.

2. The probability of success, p, in each trial is constant.

An example of a binomial experiment is counting the number of heads that turn up when a coin is flipped N times. If X is the number of successes observed in N trials, then the probability that X takes a particular value is given by a binomial distribution with mean Np and variance $Np(1-p)$:

$$P(X = v) = \binom{N}{p} p^v (1-p)^{N-v}.$$

For example, if the coin is fair ($p = 0.5$) and is flipped fifty times, then the probability that the head shows up 20 times is

$$P(X = 20) = \binom{50}{20} 0.5^{20}(1-0.5)^{30} = 0.0419.$$

If the experiment is repeated many times, then the average number of heads expected to show up is $50 \times 0.5 = 25$, while its variance is $50 \times 0.5 \times 0.5 = 12.5$.

The task of predicting the class labels of test records can also be considered as a binomial experiment. Given a test set that contains N records, let X be the number of records correctly predicted by a model and p be the true accuracy of the model. By modeling the prediction task as a binomial experiment, X has a binomial distribution with mean Np and variance $Np(1-p)$. It can be shown that the empirical accuracy, $acc = X/N$, also has a binomial distribution with mean p and variance $p(1-p)/N$ (see Exercise 12). Although the binomial distribution can be used to estimate the confidence interval for acc, it is often approximated by a normal distribution when N is sufficiently large. Based on the normal distribution, the following confidence interval for acc can be derived:

$$P\left(-Z_{\alpha/2} \leq \frac{acc - p}{\sqrt{p(1-p)/N}} \leq Z_{1-\alpha/2} \right) = 1 - \alpha, \tag{4.12}$$

where $Z_{\alpha/2}$ and $Z_{1-\alpha/2}$ are the upper and lower bounds obtained from a standard normal distribution at confidence level $(1-\alpha)$. Since a standard normal distribution is symmetric around $Z = 0$, it follows that $Z_{\alpha/2} = Z_{1-\alpha/2}$. Rearranging this inequality leads to the following confidence interval for p:

$$\frac{2 \times N \times acc + Z_{\alpha/2}^2 \pm Z_{\alpha/2}\sqrt{Z_{\alpha/2}^2 + 4Nacc - 4Nacc^2}}{2(N + Z_{\alpha/2}^2)}. \tag{4.13}$$

The following table shows the values of $Z_{\alpha/2}$ at different confidence levels:

$1-\alpha$	0.99	0.98	0.95	0.9	0.8	0.7	0.5
$Z_{\alpha/2}$	2.58	2.33	1.96	1.65	1.28	1.04	0.67

Example 4.4. Consider a model that has an accuracy of 80% when evaluated on 100 test records. What is the confidence interval for its true accuracy at a 95% confidence level? The confidence level of 95% corresponds to $Z_{\alpha/2} = 1.96$ according to the table given above. Inserting this term into Equation 4.13 yields a confidence interval between 71.1% and 86.7%. The following table shows the confidence interval when the number of records, N, increases:

N	20	50	100	500	1000	5000
Confidence Interval	0.584 − 0.919	0.670 − 0.888	0.711 − 0.867	0.763 − 0.833	0.774 − 0.824	0.789 − 0.811

Note that the confidence interval becomes tighter when N increases. ■

4.6.2 Comparing the Performance of Two Models

Consider a pair of models, M_1 and M_2, that are evaluated on two independent test sets, D_1 and D_2. Let n_1 denote the number of records in D_1 and n_2 denote the number of records in D_2. In addition, suppose the error rate for M_1 on D_1 is e_1 and the error rate for M_2 on D_2 is e_2. Our goal is to test whether the observed difference between e_1 and e_2 is statistically significant.

Assuming that n_1 and n_2 are sufficiently large, the error rates e_1 and e_2 can be approximated using normal distributions. If the observed difference in the error rate is denoted as $d = e_1 - e_2$, then d is also normally distributed with mean d_t, its true difference, and variance, σ_d^2. The variance of d can be computed as follows:

$$\sigma_d^2 \simeq \widehat{\sigma}_d^2 = \frac{e_1(1-e_1)}{n_1} + \frac{e_2(1-e_2)}{n_2}, \tag{4.14}$$

where $e_1(1-e_1)/n_1$ and $e_2(1-e_2)/n_2$ are the variances of the error rates. Finally, at the $(1-\alpha)\%$ confidence level, it can be shown that the confidence interval for the true difference d_t is given by the following equation:

$$d_t = d \pm z_{\alpha/2}\widehat{\sigma}_d. \tag{4.15}$$

Example 4.5. Consider the problem described at the beginning of this section. Model M_A has an error rate of $e_1 = 0.15$ when applied to $N_1 = 30$ test records, while model M_B has an error rate of $e_2 = 0.25$ when applied to $N_2 = 5000$ test records. The observed difference in their error rates is $d = |0.15 - 0.25| = 0.1$. In this example, we are performing a two-sided test to check whether $d_t = 0$ or $d_t \neq 0$. The estimated variance of the observed difference in error rates can be computed as follows:

$$\widehat{\sigma}_d^2 = \frac{0.15(1-0.15)}{30} + \frac{0.25(1-0.25)}{5000} = 0.0043$$

or $\widehat{\sigma}_d = 0.0655$. Inserting this value into Equation 4.15, we obtain the following confidence interval for d_t at 95% confidence level:

$$d_t = 0.1 \pm 1.96 \times 0.0655 = 0.1 \pm 0.128.$$

As the interval spans the value zero, we can conclude that the observed difference is not statistically significant at a 95% confidence level. ■

At what confidence level can we reject the hypothesis that $d_t = 0$? To do this, we need to determine the value of $Z_{\alpha/2}$ such that the confidence interval for d_t does not span the value zero. We can reverse the preceding computation and look for the value $Z_{\alpha/2}$ such that $d > Z_{\alpha/2}\widehat{\sigma}_d$. Replacing the values of d and $\widehat{\sigma}_d$ gives $Z_{\alpha/2} < 1.527$. This value first occurs when $(1-\alpha) \lesssim 0.936$ (for a two-sided test). The result suggests that the null hypothesis can be rejected at confidence level of 93.6% or lower.

4.6.3 Comparing the Performance of Two Classifiers

Suppose we want to compare the performance of two classifiers using the k-fold cross-validation approach. Initially, the data set D is divided into k equal-sized partitions. We then apply each classifier to construct a model from $k-1$ of the partitions and test it on the remaining partition. This step is repeated k times, each time using a different partition as the test set.

Let M_{ij} denote the model induced by classification technique L_i during the j^{th} iteration. Note that each pair of models M_{1j} and M_{2j} are tested on the same partition j. Let e_{1j} and e_{2j} be their respective error rates. The difference between their error rates during the j^{th} fold can be written as $d_j = e_{1j} - e_{2j}$. If k is sufficiently large, then d_j is normally distributed with mean d_t^{cv}, which is the true difference in their error rates, and variance σ^{cv}. Unlike the previous approach, the overall variance in the observed differences is estimated using the following formula:

$$\widehat{\sigma}^2_{d^{cv}} = \frac{\sum_{j=1}^{k}(d_j - \overline{d})^2}{k(k-1)}, \tag{4.16}$$

where $\overline{d}$ is the average difference. For this approach, we need to use a t-distribution to compute the confidence interval for d_t^{cv}:

$$d_t^{cv} = \overline{d} \pm t_{(1-\alpha),k-1}\widehat{\sigma}_{d^{cv}}.$$

The coefficient $t_{(1-\alpha),k-1}$ is obtained from a probability table with two input parameters, its confidence level $(1-\alpha)$ and the number of degrees of freedom, $k-1$. The probability table for the t-distribution is shown in Table 4.6.

Example 4.6. Suppose the estimated difference in the accuracy of models generated by two classification techniques has a mean equal to 0.05 and a standard deviation equal to 0.002. If the accuracy is estimated using a 30-fold cross-validation approach, then at a 95% confidence level, the true accuracy difference is

$$d_t^{cv} = 0.05 \pm 2.04 \times 0.002. \tag{4.17}$$

Table 4.6. Probability table for t-distribution.

	$(1-\alpha)$				
$k-1$	0.99	0.98	0.95	0.9	0.8
1	3.08	6.31	12.7	31.8	63.7
2	1.89	2.92	4.30	6.96	9.92
4	1.53	2.13	2.78	3.75	4.60
9	1.38	1.83	2.26	2.82	3.25
14	1.34	1.76	2.14	2.62	2.98
19	1.33	1.73	2.09	2.54	2.86
24	1.32	1.71	2.06	2.49	2.80
29	1.31	1.70	2.04	2.46	2.76

Since the confidence interval does not span the value zero, the observed difference between the techniques is statistically significant. ■

4.7 Bibliographic Notes

Early classification systems were developed to organize a large collection of objects. For example, the Dewey Decimal and Library of Congress classification systems were designed to catalog and index the vast number of library books. The categories are typically identified in a manual fashion, with the help of domain experts.

Automated classification has been a subject of intensive research for many years. The study of classification in classical statistics is sometimes known as **discriminant analysis**, where the objective is to predict the group membership of an object based on a set of predictor variables. A well-known classical method is Fisher's linear discriminant analysis [117], which seeks to find a linear projection of the data that produces the greatest discrimination between objects that belong to different classes.

Many pattern recognition problems also require the discrimination of objects from different classes. Examples include speech recognition, handwritten character identification, and image classification. Readers who are interested in the application of classification techniques for pattern recognition can refer to the survey articles by Jain et al. [122] and Kulkarni et al. [128] or classic pattern recognition books by Bishop [107], Duda et al. [114], and Fukunaga [118]. The subject of classification is also a major research topic in the fields of neural networks, statistical learning, and machine learning. An in-depth treat-

ment of various classification techniques is given in the books by Cherkassky and Mulier [112], Hastie et al. [120], Michie et al. [133], and Mitchell [136].

An overview of decision tree induction algorithms can be found in the survey articles by Buntine [110], Moret [137], Murthy [138], and Safavian et al. [147]. Examples of some well-known decision tree algorithms include CART [108], ID3 [143], C4.5 [145], and CHAID [125]. Both ID3 and C4.5 employ the entropy measure as their splitting function. An in-depth discussion of the C4.5 decision tree algorithm is given by Quinlan [145]. Besides explaining the methodology for decision tree growing and tree pruning, Quinlan [145] also described how the algorithm can be modified to handle data sets with missing values. The CART algorithm was developed by Breiman et al. [108] and uses the Gini index as its splitting function. CHAID [125] uses the statistical χ^2 test to determine the best split during the tree-growing process.

The decision tree algorithm presented in this chapter assumes that the splitting condition is specified one attribute at a time. An oblique decision tree can use multiple attributes to form the attribute test condition in the internal nodes [121, 152]. Breiman et al. [108] provide an option for using linear combinations of attributes in their CART implementation. Other approaches for inducing oblique decision trees were proposed by Heath et al. [121], Murthy et al. [139], Cantú-Paz and Kamath [111], and Utgoff and Brodley [152]. Although oblique decision trees help to improve the expressiveness of a decision tree representation, learning the appropriate test condition at each node is computationally challenging. Another way to improve the expressiveness of a decision tree without using oblique decision trees is to apply a method known as **constructive induction** [132]. This method simplifies the task of learning complex splitting functions by creating compound features from the original attributes.

Besides the top-down approach, other strategies for growing a decision tree include the bottom-up approach by Landeweerd et al. [130] and Pattipati and Alexandridis [142], as well as the bidirectional approach by Kim and Landgrebe [126]. Schuermann and Doster [150] and Wang and Suen [154] proposed using a **soft splitting criterion** to address the data fragmentation problem. In this approach, each record is assigned to different branches of the decision tree with different probabilities.

Model overfitting is an important issue that must be addressed to ensure that a decision tree classifier performs equally well on previously unknown records. The model overfitting problem has been investigated by many authors including Breiman et al. [108], Schaffer [148], Mingers [135], and Jensen and Cohen [123]. While the presence of noise is often regarded as one of the

primary reasons for overfitting [135, 140], Jensen and Cohen [123] argued that overfitting is the result of using incorrect hypothesis tests in a multiple comparison procedure.

Schapire [149] defined generalization error as "the probability of misclassifying a new example" and test error as "the fraction of mistakes on a newly sampled test set." Generalization error can therefore be considered as the expected test error of a classifier. Generalization error may sometimes refer to the true error [136] of a model, i.e., its expected error for randomly drawn data points from the same population distribution where the training set is sampled. These definitions are in fact equivalent if both the training and test sets are gathered from the same population distribution, which is often the case in many data mining and machine learning applications.

The Occam's razor principle is often attributed to the philosopher William of Occam. Domingos [113] cautioned against the pitfall of misinterpreting Occam's razor as comparing models with similar training errors, instead of generalization errors. A survey on decision tree-pruning methods to avoid overfitting is given by Breslow and Aha [109] and Esposito et al. [116]. Some of the typical pruning methods include reduced error pruning [144], pessimistic error pruning [144], minimum error pruning [141], critical value pruning [134], cost-complexity pruning [108], and error-based pruning [145]. Quinlan and Rivest proposed using the minimum description length principle for decision tree pruning in [146].

Kohavi [127] had performed an extensive empirical study to compare the performance metrics obtained using different estimation methods such as random subsampling, bootstrapping, and k-fold cross-validation. Their results suggest that the best estimation method is based on the ten-fold stratified cross-validation. Efron and Tibshirani [115] provided a theoretical and empirical comparison between cross-validation and a bootstrap method known as the 632+ rule.

Current techniques such as C4.5 require that the entire training data set fit into main memory. There has been considerable effort to develop parallel and scalable versions of decision tree induction algorithms. Some of the proposed algorithms include SLIQ by Mehta et al. [131], SPRINT by Shafer et al. [151], CMP by Wang and Zaniolo [153], CLOUDS by Alsabti et al. [106], RainForest by Gehrke et al. [119], and ScalParC by Joshi et al. [124]. A general survey of parallel algorithms for data mining is available in [129].

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4.8 Exercises

1. Draw the full decision tree for the parity function of four Boolean attributes, A, B, C, and D. Is it possible to simplify the tree?

2. Consider the training examples shown in Table 4.7 for a binary classification problem.

   (a) Compute the Gini index for the overall collection of training examples.

   (b) Compute the Gini index for the `Customer ID` attribute.

   (c) Compute the Gini index for the `Gender` attribute.

   (d) Compute the Gini index for the `Car Type` attribute using multiway split.

   (e) Compute the Gini index for the `Shirt Size` attribute using multiway split.

   (f) Which attribute is better, `Gender`, `Car Type`, or `Shirt Size`?

   (g) Explain why `Customer ID` should not be used as the attribute test condition even though it has the lowest Gini.

3. Consider the training examples shown in Table 4.8 for a binary classification problem.

   (a) What is the entropy of this collection of training examples with respect to the positive class?

Table 4.7. Data set for Exercise 2.

Customer ID	Gender	Car Type	Shirt Size	Class
1	M	Family	Small	C0
2	M	Sports	Medium	C0
3	M	Sports	Medium	C0
4	M	Sports	Large	C0
5	M	Sports	Extra Large	C0
6	M	Sports	Extra Large	C0
7	F	Sports	Small	C0
8	F	Sports	Small	C0
9	F	Sports	Medium	C0
10	F	Luxury	Large	C0
11	M	Family	Large	C1
12	M	Family	Extra Large	C1
13	M	Family	Medium	C1
14	M	Luxury	Extra Large	C1
15	F	Luxury	Small	C1
16	F	Luxury	Small	C1
17	F	Luxury	Medium	C1
18	F	Luxury	Medium	C1
19	F	Luxury	Medium	C1
20	F	Luxury	Large	C1

Table 4.8. Data set for Exercise 3.

Instance	a_1	a_2	a_3	Target Class
1	T	T	1.0	+
2	T	T	6.0	+
3	T	F	5.0	−
4	F	F	4.0	+
5	F	T	7.0	−
6	F	T	3.0	−
7	F	F	8.0	−
8	T	F	7.0	+
9	F	T	5.0	−

(b) What are the information gains of a_1 and a_2 relative to these training examples?

(c) For a_3, which is a continuous attribute, compute the information gain for every possible split.

(d) What is the best split (among a_1, a_2, and a_3) according to the information gain?

(e) What is the best split (between a_1 and a_2) according to the classification error rate?

(f) What is the best split (between a_1 and a_2) according to the Gini index?

4. Show that the entropy of a node never increases after splitting it into smaller successor nodes.

5. Consider the following data set for a binary class problem.

A	B	Class Label
T	F	+
T	T	+
T	T	+
T	F	−
T	T	+
F	F	−
F	F	−
F	F	−
T	T	−
T	F	−

(a) Calculate the information gain when splitting on A and B. Which attribute would the decision tree induction algorithm choose?

(b) Calculate the gain in the Gini index when splitting on A and B. Which attribute would the decision tree induction algorithm choose?

(c) Figure 4.13 shows that entropy and the Gini index are both monotonously increasing on the range [0, 0.5] and they are both monotonously decreasing on the range [0.5, 1]. Is it possible that information gain and the gain in the Gini index favor different attributes? Explain.

6. Consider the following set of training examples.

X	Y	Z	No. of Class C1 Examples	No. of Class C2 Examples
0	0	0	5	40
0	0	1	0	15
0	1	0	10	5
0	1	1	45	0
1	0	0	10	5
1	0	1	25	0
1	1	0	5	20
1	1	1	0	15

(a) Compute a two-level decision tree using the greedy approach described in this chapter. Use the classification error rate as the criterion for splitting. What is the overall error rate of the induced tree?

(b) Repeat part (a) using X as the first splitting attribute and then choose the best remaining attribute for splitting at each of the two successor nodes. What is the error rate of the induced tree?

(c) Compare the results of parts (a) and (b). Comment on the suitability of the greedy heuristic used for splitting attribute selection.

7. The following table summarizes a data set with three attributes A, B, C and two class labels $+$, $-$. Build a two-level decision tree.

A	B	C	Number of Instances	
			+	−
T	T	T	5	0
F	T	T	0	20
T	F	T	20	0
F	F	T	0	5
T	T	F	0	0
F	T	F	25	0
T	F	F	0	0
F	F	F	0	25

(a) According to the classification error rate, which attribute would be chosen as the first splitting attribute? For each attribute, show the contingency table and the gains in classification error rate.

(b) Repeat for the two children of the root node.

(c) How many instances are misclassified by the resulting decision tree?

(d) Repeat parts (a), (b), and (c) using C as the splitting attribute.

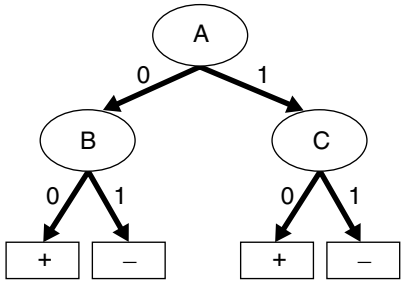
(e) Use the results in parts (c) and (d) to conclude about the greedy nature of the decision tree induction algorithm.

8. Consider the decision tree shown in Figure 4.30.

(a) Compute the generalization error rate of the tree using the optimistic approach.

(b) Compute the generalization error rate of the tree using the pessimistic approach. (For simplicity, use the strategy of adding a factor of 0.5 to each leaf node.)

(c) Compute the generalization error rate of the tree using the validation set shown above. This approach is known as **reduced error pruning**.



Training:

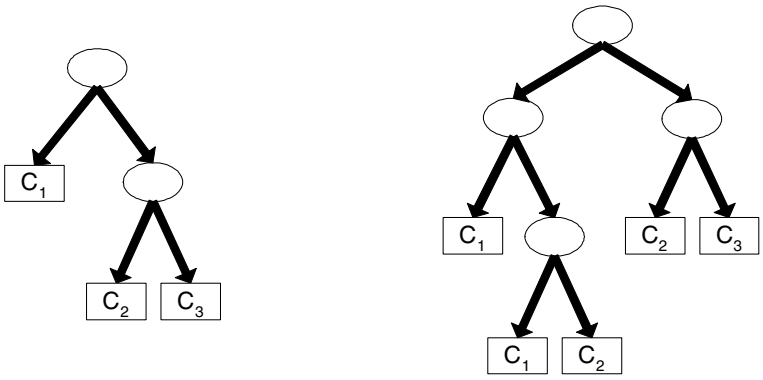
Instance	A	B	C	Class
1	0	0	0	+
2	0	0	1	+
3	0	1	0	+
4	0	1	1	–
5	1	0	0	+
6	1	0	0	+
7	1	1	0	–
8	1	0	1	+
9	1	1	0	–
10	1	1	0	–

Validation:

Instance	A	B	C	Class
11	0	0	0	+
12	0	1	1	+
13	1	1	0	+
14	1	0	1	–
15	1	0	0	+

Figure 4.30. Decision tree and data sets for Exercise 8.

9. Consider the decision trees shown in Figure 4.31. Assume they are generated from a data set that contains 16 binary attributes and 3 classes, C_1, C_2, and C_3.



(a) Decision tree with 7 errors

(b) Decision tree with 4 errors

Figure 4.31. Decision trees for Exercise 9.

Compute the total description length of each decision tree according to the minimum description length principle.

- The total description length of a tree is given by:

$$Cost(tree, data) = Cost(tree) + Cost(data|tree).$$

- Each internal node of the tree is encoded by the ID of the splitting attribute. If there are m attributes, the cost of encoding each attribute is $\log_2 m$ bits.
- Each leaf is encoded using the ID of the class it is associated with. If there are k classes, the cost of encoding a class is $\log_2 k$ bits.
- $Cost(tree)$ is the cost of encoding all the nodes in the tree. To simplify the computation, you can assume that the total cost of the tree is obtained by adding up the costs of encoding each internal node and each leaf node.
- $Cost(data|tree)$ is encoded using the classification errors the tree commits on the training set. Each error is encoded by $\log_2 n$ bits, where n is the total number of training instances.

Which decision tree is better, according to the MDL principle?

10. While the .632 bootstrap approach is useful for obtaining a reliable estimate of model accuracy, it has a known limitation [127]. Consider a two-class problem, where there are equal number of positive and negative examples in the data. Suppose the class labels for the examples are generated randomly. The classifier used is an unpruned decision tree (i.e., a perfect memorizer). Determine the accuracy of the classifier using each of the following methods.

    (a) The holdout method, where two-thirds of the data are used for training and the remaining one-third are used for testing.

    (b) Ten-fold cross-validation.

    (c) The .632 bootstrap method.

    (d) From the results in parts (a), (b), and (c), which method provides a more reliable evaluation of the classifier's accuracy?

11. Consider the following approach for testing whether a classifier A beats another classifier B. Let N be the size of a given data set, p_A be the accuracy of classifier A, p_B be the accuracy of classifier B, and $p = (p_A + p_B)/2$ be the average accuracy for both classifiers. To test whether classifier A is significantly better than B, the following Z-statistic is used:

$$Z = \frac{p_A - p_B}{\sqrt{\frac{2p(1-p)}{N}}}.$$

Classifier A is assumed to be better than classifier B if Z $>$ 1.96.

Table 4.9 compares the accuracies of three different classifiers, decision tree classifiers, naïve Bayes classifiers, and support vector machines, on various data sets. (The latter two classifiers are described in Chapter 5.)

Table 4.9. Comparing the accuracy of various classification methods.

Data Set	Size (N)	Decision Tree (%)	naïve Bayes (%)	Support vector machine (%)
Anneal	898	92.09	79.62	87.19
Australia	690	85.51	76.81	84.78
Auto	205	81.95	58.05	70.73
Breast	699	95.14	95.99	96.42
Cleve	303	76.24	83.50	84.49
Credit	690	85.80	77.54	85.07
Diabetes	768	72.40	75.91	76.82
German	1000	70.90	74.70	74.40
Glass	214	67.29	48.59	59.81
Heart	270	80.00	84.07	83.70
Hepatitis	155	81.94	83.23	87.10
Horse	368	85.33	78.80	82.61
Ionosphere	351	89.17	82.34	88.89
Iris	150	94.67	95.33	96.00
Labor	57	78.95	94.74	92.98
Led7	3200	73.34	73.16	73.56
Lymphography	148	77.03	83.11	86.49
Pima	768	74.35	76.04	76.95
Sonar	208	78.85	69.71	76.92
Tic-tac-toe	958	83.72	70.04	98.33
Vehicle	846	71.04	45.04	74.94
Wine	178	94.38	96.63	98.88
Zoo	101	93.07	93.07	96.04

Summarize the performance of the classifiers given in Table 4.9 using the following 3×3 table:

win-loss-draw	Decision tree	Naïve Bayes	Support vector machine
Decision tree	0 - 0 - 23		
Naïve Bayes		0 - 0 - 23	
Support vector machine			0 - 0 - 23

Each cell in the table contains the number of wins, losses, and draws when comparing the classifier in a given row to the classifier in a given column.

12. Let X be a binomial random variable with mean Np and variance $Np(1-p)$. Show that the ratio X/N also has a binomial distribution with mean p and variance $p(1-p)/N$.

5

Classification: Alternative Techniques

The previous chapter described a simple, yet quite effective, classification technique known as decision tree induction. Issues such as model overfitting and classifier evaluation were also discussed in great detail. This chapter presents alternative techniques for building classification models—from simple techniques such as rule-based and nearest-neighbor classifiers to more advanced techniques such as support vector machines and ensemble methods. Other key issues such as the class imbalance and multiclass problems are also discussed at the end of the chapter.

5.1 Rule-Based Classifier

A rule-based classifier is a technique for classifying records using a collection of "if . . .then. . ." rules. Table 5.1 shows an example of a model generated by a rule-based classifier for the vertebrate classification problem. The rules for the model are represented in a disjunctive normal form, $R = (r_1 \vee r_2 \vee \ldots r_k)$, where R is known as the **rule set** and r_i's are the classification rules or disjuncts.

Table 5.1. Example of a rule set for the vertebrate classification problem.

r_1:	(Gives Birth = no) $\wedge$ (Aerial Creature = yes) $\longrightarrow$ Birds
r_2:	(Gives Birth = no) $\wedge$ (Aquatic Creature = yes) $\longrightarrow$ Fishes
r_3:	(Gives Birth = yes) $\wedge$ (Body Temperature = warm-blooded) $\longrightarrow$ Mammals
r_4:	(Gives Birth = no) $\wedge$ (Aerial Creature = no) $\longrightarrow$ Reptiles
r_5:	(Aquatic Creature = semi) $\longrightarrow$ Amphibians

Each classification rule can be expressed in the following way:

$$r_i : \quad (Condition_i) \longrightarrow y_i. \tag{5.1}$$

The left-hand side of the rule is called the **rule antecedent** or **precondition**. It contains a conjunction of attribute tests:

$$Condition_i = (A_1 \; op \; v_1) \wedge (A_2 \; op \; v_2) \wedge \ldots (A_k \; op \; v_k), \tag{5.2}$$

where (A_j, v_j) is an attribute-value pair and op is a logical operator chosen from the set $\{=, \neq, <, >, \leq, \geq\}$. Each attribute test $(A_j \; op \; v_j)$ is known as a conjunct. The right-hand side of the rule is called the **rule consequent**, which contains the predicted class y_i.

A rule r covers a record x if the precondition of r matches the attributes of x. r is also said to be fired or triggered whenever it covers a given record. For an illustration, consider the rule r_1 given in Table 5.1 and the following attributes for two vertebrates: hawk and grizzly bear.

Name	Body Temperature	Skin Cover	Gives Birth	Aquatic Creature	Aerial Creature	Has Legs	Hibernates
hawk	warm-blooded	feather	no	no	yes	yes	no
grizzly bear	warm-blooded	fur	yes	no	no	yes	yes

r_1 covers the first vertebrate because its precondition is satisfied by the hawk's attributes. The rule does not cover the second vertebrate because grizzly bears give birth to their young and cannot fly, thus violating the precondition of r_1.

The quality of a classification rule can be evaluated using measures such as coverage and accuracy. Given a data set D and a classification rule $r : A \longrightarrow y$, the coverage of the rule is defined as the fraction of records in D that trigger the rule r. On the other hand, its accuracy or confidence factor is defined as the fraction of records triggered by r whose class labels are equal to y. The formal definitions of these measures are

$$\begin{aligned} \text{Coverage}(r) &= \frac{|A|}{|D|} \\ \text{Accuracy}(r) &= \frac{|A \cap y|}{|A|}, \end{aligned} \tag{5.3}$$

where $|A|$ is the number of records that satisfy the rule antecedent, $|A \cap y|$ is the number of records that satisfy both the antecedent and consequent, and $|D|$ is the total number of records.

Table 5.2. The vertebrate data set.

Name	Body Temperature	Skin Cover	Gives Birth	Aquatic Creature	Aerial Creature	Has Legs	Hibernates	Class Label
human	warm-blooded	hair	yes	no	no	yes	no	Mammals
python	cold-blooded	scales	no	no	no	no	yes	Reptiles
salmon	cold-blooded	scales	no	yes	no	no	no	Fishes
whale	warm-blooded	hair	yes	yes	no	no	no	Mammals
frog	cold-blooded	none	no	semi	no	yes	yes	Amphibian
komodo dragon	cold-blooded	scales	no	no	no	yes	no	Reptiles
bat	warm-blooded	hair	yes	no	yes	yes	yes	Mammals
pigeon	warm-blooded	feathers	no	no	yes	yes	no	Birds
cat	warm-blooded	fur	yes	no	no	yes	no	Mammals
guppy	cold-blooded	scales	yes	yes	no	no	no	Fishes
alligator	cold-blooded	scales	no	semi	no	yes	no	Reptiles
penguin	warm-blooded	feathers	no	semi	no	yes	no	Birds
porcupine	warm-blooded	quills	yes	no	no	yes	yes	Mammals
eel	cold-blooded	scales	no	yes	no	no	no	Fishes
salamander	cold-blooded	none	no	semi	no	yes	yes	Amphibian

Example 5.1. Consider the data set shown in Table 5.2. The rule

$$(\texttt{Gives Birth} = \texttt{yes}) \wedge (\texttt{Body Temperature} = \texttt{warm-blooded}) \longrightarrow \texttt{Mammals}$$

has a coverage of 33% since five of the fifteen records support the rule antecedent. The rule accuracy is 100% because all five vertebrates covered by the rule are mammals. ■

5.1.1 How a Rule-Based Classifier Works

A rule-based classifier classifies a test record based on the rule triggered by the record. To illustrate how a rule-based classifier works, consider the rule set shown in Table 5.1 and the following vertebrates:

Name	Body Temperature	Skin Cover	Gives Birth	Aquatic Creature	Aerial Creature	Has Legs	Hibernates
lemur	warm-blooded	fur	yes	no	no	yes	yes
turtle	cold-blooded	scales	no	semi	no	yes	no
dogfish shark	cold-blooded	scales	yes	yes	no	no	no

- The first vertebrate, which is a lemur, is warm-blooded and gives birth to its young. It triggers the rule r_3, and thus, is classified as a mammal.

- The second vertebrate, which is a turtle, triggers the rules r_4 and r_5. Since the classes predicted by the rules are contradictory (reptiles versus amphibians), their conflicting classes must be resolved.

- None of the rules are applicable to a dogfish shark. In this case, we need to ensure that the classifier can still make a reliable prediction even though a test record is not covered by any rule.

The previous example illustrates two important properties of the rule set generated by a rule-based classifier.

Mutually Exclusive Rules The rules in a rule set R are mutually exclusive if no two rules in R are triggered by the same record. This property ensures that every record is covered by at most one rule in R. An example of a mutually exclusive rule set is shown in Table 5.3.

Exhaustive Rules A rule set R has exhaustive coverage if there is a rule for each combination of attribute values. This property ensures that every record is covered by at least one rule in R. Assuming that `Body Temperature` and `Gives Birth` are binary variables, the rule set shown in Table 5.3 has exhaustive coverage.

Table 5.3. Example of a mutually exclusive and exhaustive rule set.

r_1: (Body Temperature = cold-blooded) $\longrightarrow$ Non-mammals
r_2: (Body Temperature = warm-blooded) $\wedge$ (Gives Birth = yes) $\longrightarrow$ Mammals
r_3: (Body Temperature = warm-blooded) $\wedge$ (Gives Birth = no) $\longrightarrow$ Non-mammals

Together, these properties ensure that every record is covered by exactly one rule. Unfortunately, many rule-based classifiers, including the one shown in Table 5.1, do not have such properties. If the rule set is not exhaustive, then a default rule, r_d : () $\longrightarrow y_d$, must be added to cover the remaining cases. A default rule has an empty antecedent and is triggered when all other rules have failed. y_d is known as the default class and is typically assigned to the majority class of training records not covered by the existing rules.

If the rule set is not mutually exclusive, then a record can be covered by several rules, some of which may predict conflicting classes. There are two ways to overcome this problem.

Ordered Rules In this approach, the rules in a rule set are ordered in decreasing order of their priority, which can be defined in many ways (e.g., based on accuracy, coverage, total description length, or the order in which the rules are generated). An ordered rule set is also known as a **decision list**. When a test record is presented, it is classified by the highest-ranked rule that covers the record. This avoids the problem of having conflicting classes predicted by multiple classification rules.

Unordered Rules This approach allows a test record to trigger multiple classification rules and considers the consequent of each rule as a vote for a particular class. The votes are then tallied to determine the class label of the test record. The record is usually assigned to the class that receives the highest number of votes. In some cases, the vote may be weighted by the rule's accuracy. Using unordered rules to build a rule-based classifier has both advantages and disadvantages. Unordered rules are less susceptible to errors caused by the wrong rule being selected to classify a test record (unlike classifiers based on ordered rules, which are sensitive to the choice of rule-ordering criteria). Model building is also less expensive because the rules do not have to be kept in sorted order. Nevertheless, classifying a test record can be quite an expensive task because the attributes of the test record must be compared against the precondition of every rule in the rule set.

In the remainder of this section, we will focus on rule-based classifiers that use ordered rules.

5.1.2 Rule-Ordering Schemes

Rule ordering can be implemented on a rule-by-rule basis or on a class-by-class basis. The difference between these schemes is illustrated in Figure 5.1.

Rule-Based Ordering Scheme This approach orders the individual rules by some rule quality measure. This ordering scheme ensures that every test record is classified by the "best" rule covering it. A potential drawback of this scheme is that lower-ranked rules are much harder to interpret because they assume the negation of the rules preceding them. For example, the fourth rule shown in Figure 5.1 for rule-based ordering,

$$\text{Aquatic Creature} = \text{semi} \longrightarrow \text{Amphibians},$$

has the following interpretation: If the vertebrate does not have any feathers or cannot fly, and is cold-blooded and semi-aquatic, then it is an amphibian.

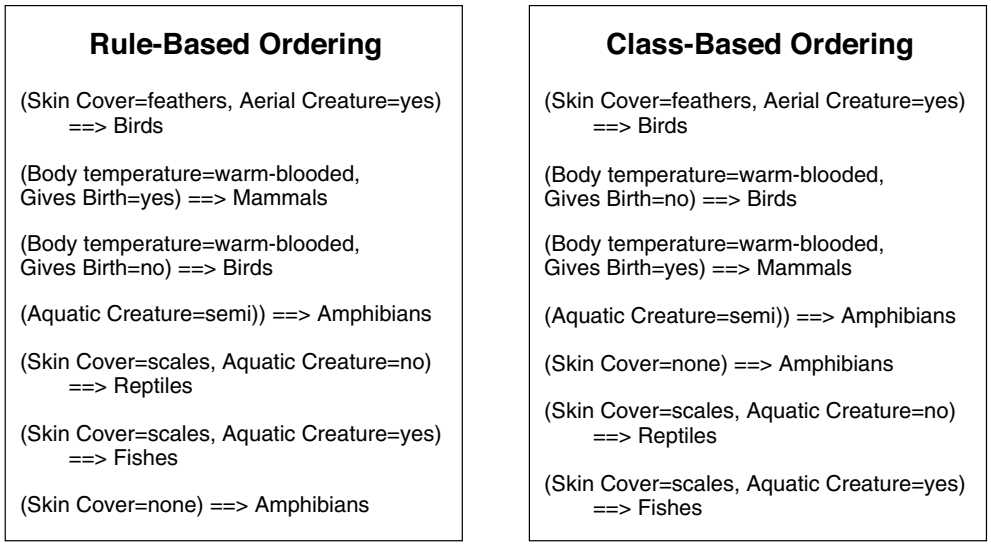


Figure 5.1. Comparison between rule-based and class-based ordering schemes.

The additional conditions (that the vertebrate does not have any feathers or cannot fly, and is cold-blooded) are due to the fact that the vertebrate does not satisfy the first three rules. If the number of rules is large, interpreting the meaning of the rules residing near the bottom of the list can be a cumbersome task.

Class-Based Ordering Scheme In this approach, rules that belong to the same class appear together in the rule set R. The rules are then collectively sorted on the basis of their class information. The relative ordering among the rules from the same class is not important; as long as one of the rules fires, the class will be assigned to the test record. This makes rule interpretation slightly easier. However, it is possible for a high-quality rule to be overlooked in favor of an inferior rule that happens to predict the higher-ranked class.

Since most of the well-known rule-based classifiers (such as C4.5rules and RIPPER) employ the class-based ordering scheme, the discussion in the remainder of this section focuses mainly on this type of ordering scheme.

5.1.3 How to Build a Rule-Based Classifier

To build a rule-based classifier, we need to extract a set of rules that identifies key relationships between the attributes of a data set and the class label.

There are two broad classes of methods for extracting classification rules: (1) direct methods, which extract classification rules directly from data, and (2) indirect methods, which extract classification rules from other classification models, such as decision trees and neural networks.

Direct methods partition the attribute space into smaller subspaces so that all the records that belong to a subspace can be classified using a single classification rule. Indirect methods use the classification rules to provide a succinct description of more complex classification models. Detailed discussions of these methods are presented in Sections 5.1.4 and 5.1.5, respectively.

5.1.4 Direct Methods for Rule Extraction

The **sequential covering** algorithm is often used to extract rules directly from data. Rules are grown in a greedy fashion based on a certain evaluation measure. The algorithm extracts the rules one class at a time for data sets that contain more than two classes. For the vertebrate classification problem, the sequential covering algorithm may generate rules for classifying birds first, followed by rules for classifying mammals, amphibians, reptiles, and finally, fishes (see Figure 5.1). The criterion for deciding which class should be generated first depends on a number of factors, such as the class prevalence (i.e., fraction of training records that belong to a particular class) or the cost of misclassifying records from a given class.

A summary of the sequential covering algorithm is given in Algorithm 5.1. The algorithm starts with an empty decision list, R. The Learn-One-Rule function is then used to extract the best rule for class y that covers the current set of training records. During rule extraction, all training records for class y are considered to be positive examples, while those that belong to

Algorithm 5.1 Sequential covering algorithm.

1: Let E be the training records and A be the set of attribute-value pairs, $\{(A_j, v_j)\}$.
2: Let Y_o be an ordered set of classes $\{y_1, y_2, \ldots, y_k\}$.
3: Let $R = \{\ \}$ be the initial rule list.
4: **for** each class $y \in Y_o - \{y_k\}$ **do**
5: **while** stopping condition is not met **do**
6: $r \leftarrow$ Learn-One-Rule (E, A, y).
7: Remove training records from E that are covered by r.
8: Add r to the bottom of the rule list: $R \longrightarrow R \vee r$.
9: **end while**
10: **end for**
11: Insert the default rule, $\{\} \longrightarrow y_k$, to the bottom of the rule list R.

other classes are considered to be negative examples. A rule is desirable if it covers most of the positive examples and none (or very few) of the negative examples. Once such a rule is found, the training records covered by the rule are eliminated. The new rule is added to the bottom of the decision list R. This procedure is repeated until the stopping criterion is met. The algorithm then proceeds to generate rules for the next class.

Figure 5.2 demonstrates how the sequential covering algorithm works for a data set that contains a collection of positive and negative examples. The rule $R1$, whose coverage is shown in Figure 5.2(b), is extracted first because it covers the largest fraction of positive examples. All the training records covered by $R1$ are subsequently removed and the algorithm proceeds to look for the next best rule, which is $R2$.

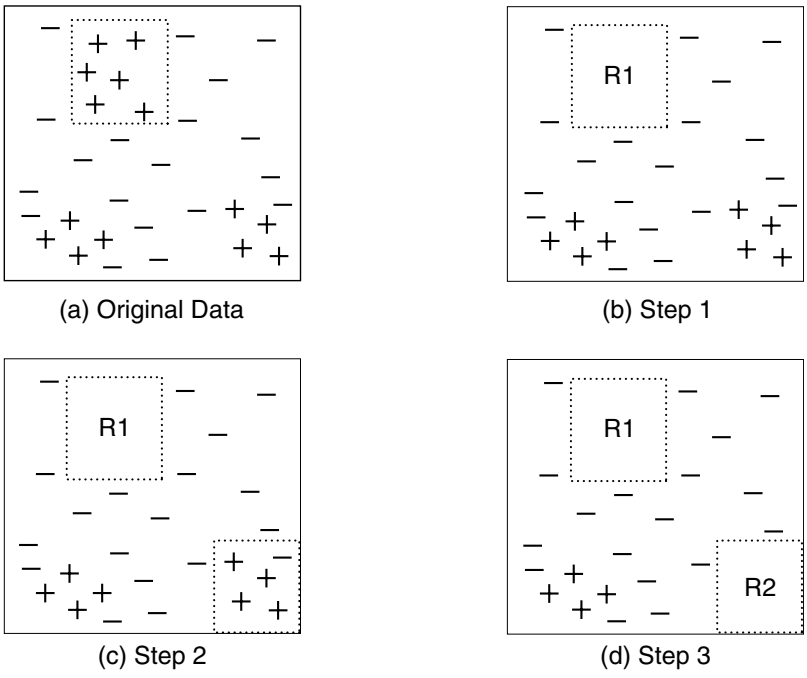
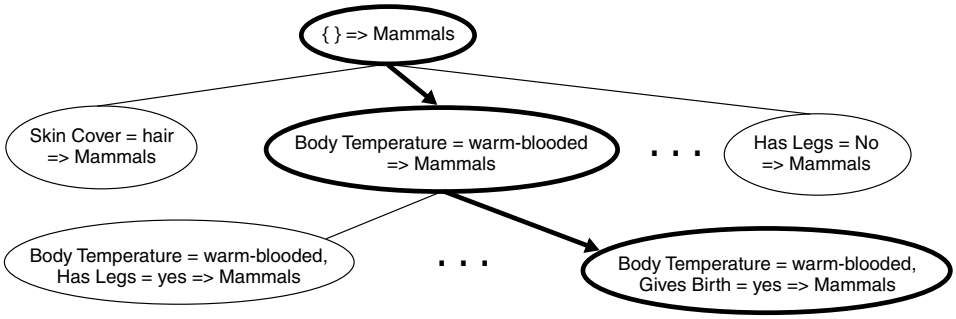


Figure 5.2. An example of the sequential covering algorithm.

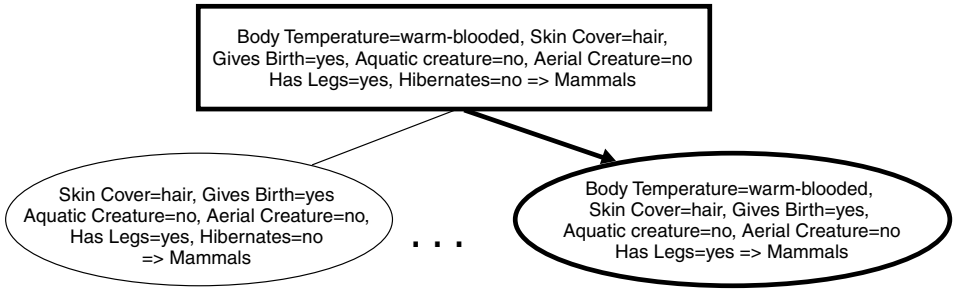
Learn-One-Rule Function

The objective of the Learn-One-Rule function is to extract a classification rule that covers many of the positive examples and none (or very few) of the negative examples in the training set. However, finding an optimal rule is computationally expensive given the exponential size of the search space. The Learn-One-Rule function addresses the exponential search problem by growing the rules in a greedy fashion. It generates an initial rule r and keeps refining the rule until a certain stopping criterion is met. The rule is then pruned to improve its generalization error.

Rule-Growing Strategy There are two common strategies for growing a classification rule: general-to-specific or specific-to-general. Under the general-to-specific strategy, an initial rule $r : \{\} \longrightarrow y$ is created, where the left-hand side is an empty set and the right-hand side contains the target class. The rule has poor quality because it covers all the examples in the training set. New



(a) General-to-specific



(b) Specific-to-general

Figure 5.3. General-to-specific and specific-to-general rule-growing strategies.

conjuncts are subsequently added to improve the rule's quality. Figure 5.3(a) shows the general-to-specific rule-growing strategy for the vertebrate classification problem. The conjunct `Body Temperature=warm-blooded` is initially chosen to form the rule antecedent. The algorithm then explores all the possible candidates and greedily chooses the next conjunct, `Gives Birth=yes`, to be added into the rule antecedent. This process continues until the stopping criterion is met (e.g., when the added conjunct does not improve the quality of the rule).

For the specific-to-general strategy, one of the positive examples is randomly chosen as the initial seed for the rule-growing process. During the refinement step, the rule is generalized by removing one of its conjuncts so that it can cover more positive examples. Figure 5.3(b) shows the specific-to-general approach for the vertebrate classification problem. Suppose a positive example for mammals is chosen as the initial seed. The initial rule contains the same conjuncts as the attribute values of the seed. To improve its coverage, the rule is generalized by removing the conjunct `Hibernate=no`. The refinement step is repeated until the stopping criterion is met, e.g., when the rule starts covering negative examples.

The previous approaches may produce suboptimal rules because the rules are grown in a greedy fashion. To avoid this problem, a beam search may be used, where k of the best candidate rules are maintained by the algorithm. Each candidate rule is then grown separately by adding (or removing) a conjunct from its antecedent. The quality of the candidates are evaluated and the k best candidates are chosen for the next iteration.

Rule Evaluation An evaluation metric is needed to determine which conjunct should be added (or removed) during the rule-growing process. Accuracy is an obvious choice because it explicitly measures the fraction of training examples classified correctly by the rule. However, a potential limitation of accuracy is that it does not take into account the rule's coverage. For example, consider a training set that contains 60 positive examples and 100 negative examples. Suppose we are given the following two candidate rules:

Rule r_1: covers 50 positive examples and 5 negative examples,
Rule r_2: covers 2 positive examples and no negative examples.

The accuracies for r_1 and r_2 are 90.9% and 100%, respectively. However, r_1 is the better rule despite its lower accuracy. The high accuracy for r_2 is potentially spurious because the coverage of the rule is too low.

The following approaches can be used to handle this problem.

1. A statistical test can be used to prune rules that have poor coverage. For example, we may compute the following likelihood ratio statistic:

$$R = 2 \sum_{i=1}^{k} f_i \log(f_i/e_i),$$

where k is the number of classes, f_i is the observed frequency of class i examples that are covered by the rule, and e_i is the expected frequency of a rule that makes random predictions. Note that R has a chi-square distribution with $k-1$ degrees of freedom. A large R value suggests that the number of correct predictions made by the rule is significantly larger than that expected by random guessing. For example, since r_1 covers 55 examples, the expected frequency for the positive class is $e_+ = 55 \times 60/160 = 20.625$, while the expected frequency for the negative class is $e_- = 55 \times 100/160 = 34.375$. Thus, the likelihood ratio for r_1 is

$$R(r_1) = 2 \times [50 \times \log_2(50/20.625) + 5 \times \log_2(5/34.375)] = 99.9.$$

Similarly, the expected frequencies for r_2 are $e_+ = 2 \times 60/160 = 0.75$ and $e_- = 2 \times 100/160 = 1.25$. The likelihood ratio statistic for r_2 is

$$R(r_2) = 2 \times [2 \times \log_2(2/0.75) + 0 \times \log_2(0/1.25)] = 5.66.$$

This statistic therefore suggests that r_1 is a better rule than r_2.

2. An evaluation metric that takes into account the rule coverage can be used. Consider the following evaluation metrics:

$$\text{Laplace} = \frac{f_+ + 1}{n + k}, \tag{5.4}$$

$$\text{m-estimate} = \frac{f_+ + kp_+}{n + k}, \tag{5.5}$$

where n is the number of examples covered by the rule, f_+ is the number of positive examples covered by the rule, k is the total number of classes, and p_+ is the prior probability for the positive class. Note that the m-estimate is equivalent to the Laplace measure by choosing $p_+ = 1/k$. Depending on the rule coverage, these measures capture the trade-off

between rule accuracy and the prior probability of the positive class. If the rule does not cover any training example, then the Laplace measure reduces to $1/k$, which is the prior probability of the positive class assuming a uniform class distribution. The m-estimate also reduces to the prior probability (p_+) when $n = 0$. However, if the rule coverage is large, then both measures asymptotically approach the rule accuracy, f_+/n. Going back to the previous example, the Laplace measure for r_1 is $51/57 = 89.47\%$, which is quite close to its accuracy. Conversely, the Laplace measure for r_2 (75%) is significantly lower than its accuracy because r_2 has a much lower coverage.

3. An evaluation metric that takes into account the support count of the rule can be used. One such metric is the **FOIL's information gain**. The support count of a rule corresponds to the number of positive examples covered by the rule. Suppose the rule $r: A \longrightarrow +$ covers p_0 positive examples and n_0 negative examples. After adding a new conjunct B, the extended rule $r': A \wedge B \longrightarrow +$ covers p_1 positive examples and n_1 negative examples. Given this information, the FOIL's information gain of the extended rule is defined as follows:

$$\text{FOIL's information gain} = p_1 \times \left(\log_2 \frac{p_1}{p_1 + n_1} - \log_2 \frac{p_0}{p_0 + n_0} \right). \quad (5.6)$$

Since the measure is proportional to p_1 and $p_1/(p_1 + n_1)$, it prefers rules that have high support count and accuracy. The FOIL's information gains for rules r_1 and r_2 given in the preceding example are 43.12 and 2, respectively. Therefore, r_1 is a better rule than r_2.

Rule Pruning The rules generated by the Learn-One-Rule function can be pruned to improve their generalization errors. To determine whether pruning is necessary, we may apply the methods described in Section 4.4 on page 172 to estimate the generalization error of a rule. For example, if the error on validation set decreases after pruning, we should keep the simplified rule. Another approach is to compare the pessimistic error of the rule before and after pruning (see Section 4.4.4 on page 179). The simplified rule is retained in place of the original rule if the pessimistic error improves after pruning.

Rationale for Sequential Covering

After a rule is extracted, the sequential covering algorithm must eliminate all the positive and negative examples covered by the rule. The rationale for doing this is given in the next example.

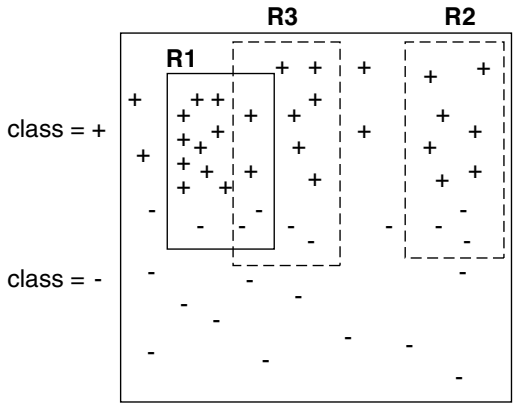


Figure 5.4. Elimination of training records by the sequential covering algorithm. $R1$, $R2$, and $R3$ represent regions covered by three different rules.

Figure 5.4 shows three possible rules, $R1$, $R2$, and $R3$, extracted from a data set that contains 29 positive examples and 21 negative examples. The accuracies of $R1$, $R2$, and $R3$ are 12/15 (80%), 7/10 (70%), and 8/12 (66.7%), respectively. $R1$ is generated first because it has the highest accuracy. After generating $R1$, it is clear that the positive examples covered by the rule must be removed so that the next rule generated by the algorithm is different than $R1$. Next, suppose the algorithm is given the choice of generating either $R2$ or $R3$. Even though $R2$ has higher accuracy than $R3$, $R1$ and $R3$ together cover 18 positive examples and 5 negative examples (resulting in an overall accuracy of 78.3%), whereas $R1$ and $R2$ together cover 19 positive examples and 6 negative examples (resulting in an overall accuracy of 76%). The incremental impact of $R2$ or $R3$ on accuracy is more evident when the positive and negative examples covered by $R1$ are removed before computing their accuracies. In particular, if positive examples covered by $R1$ are not removed, then we may overestimate the effective accuracy of $R3$, and if negative examples are not removed, then we may underestimate the accuracy of $R3$. In the latter case, we might end up preferring $R2$ over $R3$ even though half of the false positive errors committed by $R3$ have already been accounted for by the preceding rule, $R1$.

RIPPER Algorithm

To illustrate the direct method, we consider a widely used rule induction algorithm called RIPPER. This algorithm scales almost linearly with the number of training examples and is particularly suited for building models from data sets with imbalanced class distributions. RIPPER also works well with noisy data sets because it uses a validation set to prevent model overfitting.

For two-class problems, RIPPER chooses the majority class as its default class and learns the rules for detecting the minority class. For multiclass problems, the classes are ordered according to their frequencies. Let $(y_1, y_2, \ldots, y_c)$ be the ordered classes, where y_1 is the least frequent class and y_c is the most frequent class. During the first iteration, instances that belong to y_1 are labeled as positive examples, while those that belong to other classes are labeled as negative examples. The sequential covering method is used to generate rules that discriminate between the positive and negative examples. Next, RIPPER extracts rules that distinguish y_2 from other remaining classes. This process is repeated until we are left with y_c, which is designated as the default class.

Rule Growing RIPPER employs a general-to-specific strategy to grow a rule and the FOIL's information gain measure to choose the best conjunct to be added into the rule antecedent. It stops adding conjuncts when the rule starts covering negative examples. The new rule is then pruned based on its performance on the validation set. The following metric is computed to determine whether pruning is needed: $(p-n)/(p+n)$, where p (n) is the number of positive (negative) examples in the validation set covered by the rule. This metric is monotonically related to the rule's accuracy on the validation set. If the metric improves after pruning, then the conjunct is removed. Pruning is done starting from the last conjunct added to the rule. For example, given a rule $ABCD \longrightarrow y$, RIPPER checks whether D should be pruned first, followed by CD, BCD, etc. While the original rule covers only positive examples, the pruned rule may cover some of the negative examples in the training set.

Building the Rule Set After generating a rule, all the positive and negative examples covered by the rule are eliminated. The rule is then added into the rule set as long as it does not violate the stopping condition, which is based on the minimum description length principle. If the new rule increases the total description length of the rule set by at least d bits, then RIPPER stops adding rules into its rule set (by default, d is chosen to be 64 bits). Another stopping condition used by RIPPER is that the error rate of the rule on the validation set must not exceed 50%.