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`

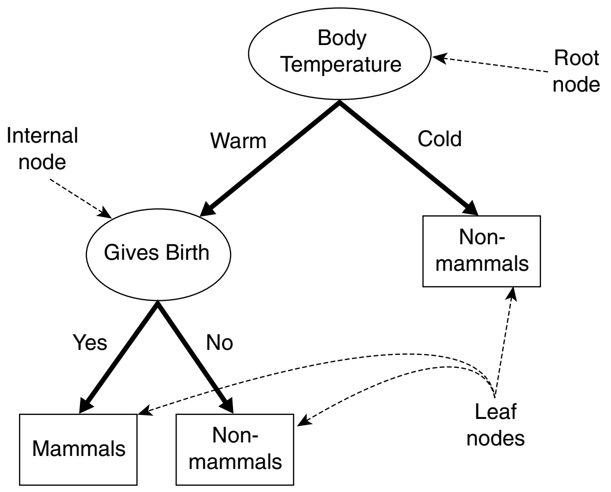


Figure 4.4. A decision tree for the mammal classification problem.

`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-

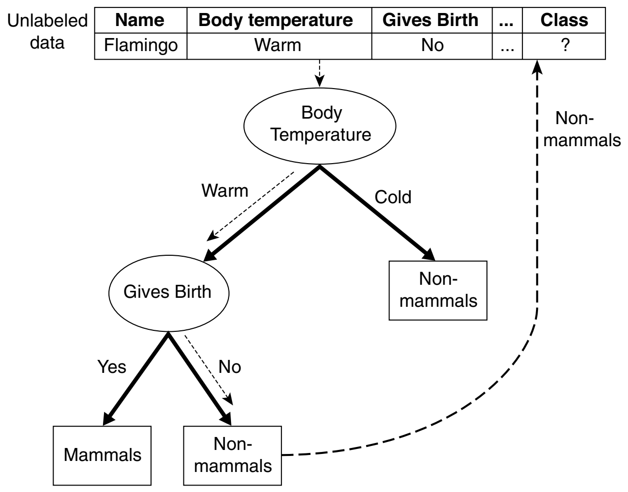


Figure 4.5. Classifying an unlabeled vertebrate. The dashed lines represent the outcomes of applying various attribute test conditions on the unlabeled vertebrate. The vertebrate is eventually assigned to the `Non-mammal` class.

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).

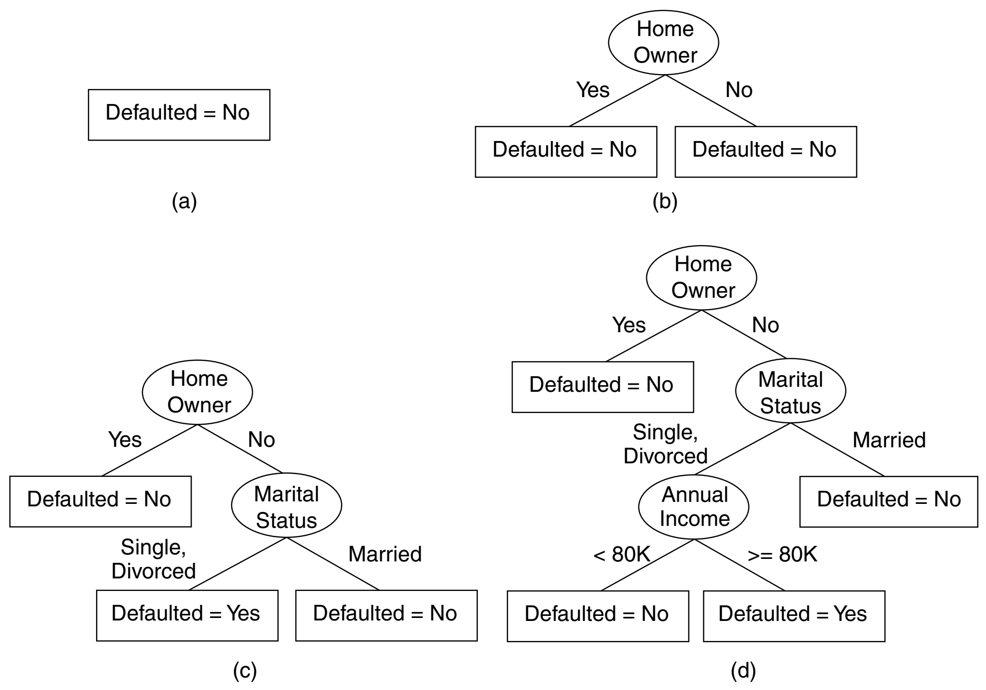


Figure 4.7. Hunt's algorithm for inducing decision trees.

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.

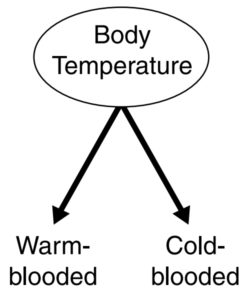


Figure 4.8. Test condition for binary attributes.

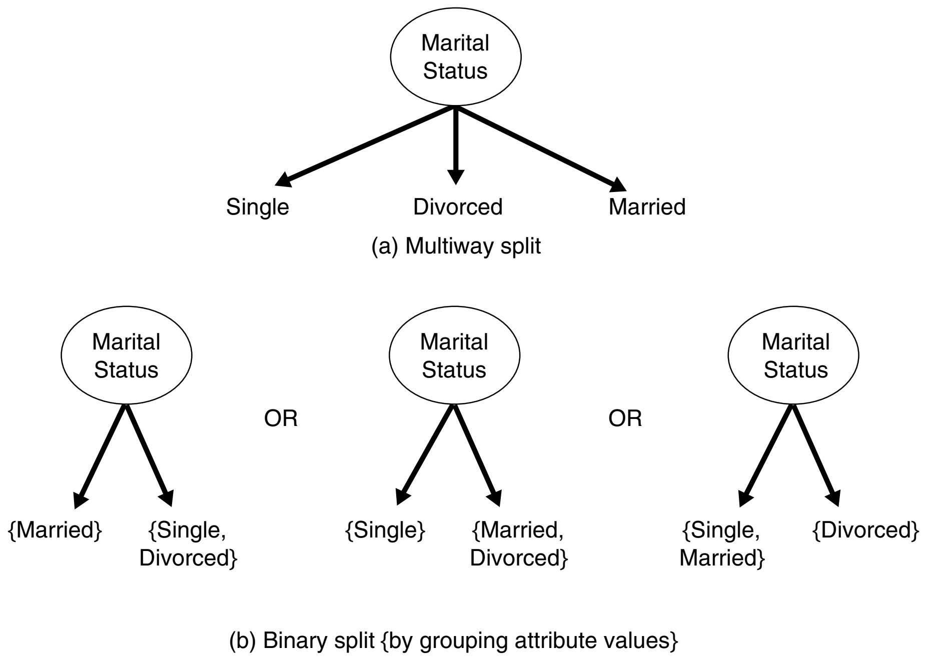


Figure 4.9. Test conditions for nominal attributes.

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

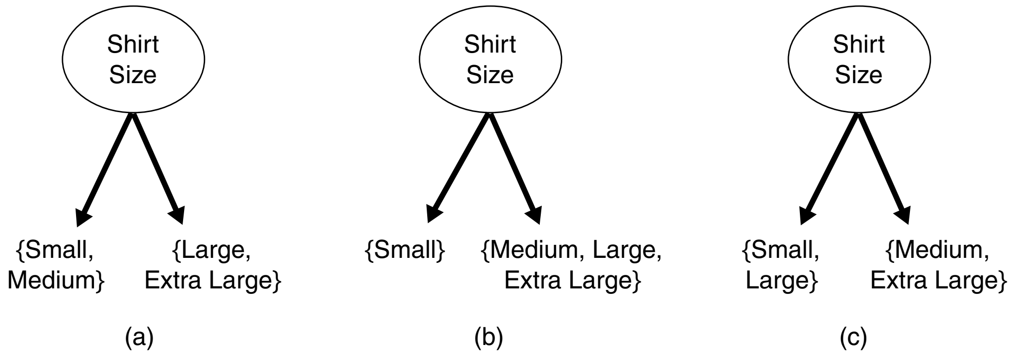


Figure 4.10. Different ways of grouping ordinal attribute values.

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.

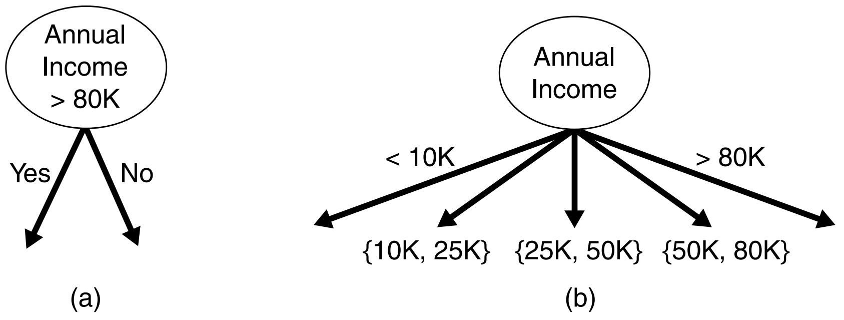


Figure 4.11. Test condition for continuous attributes.

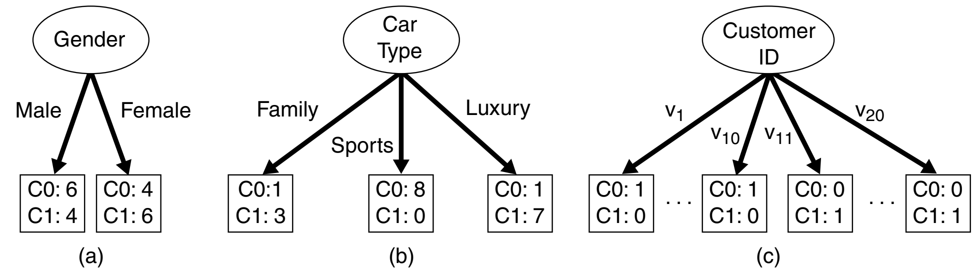


Figure 4.12. Multiway versus binary splits.

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

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

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

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

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

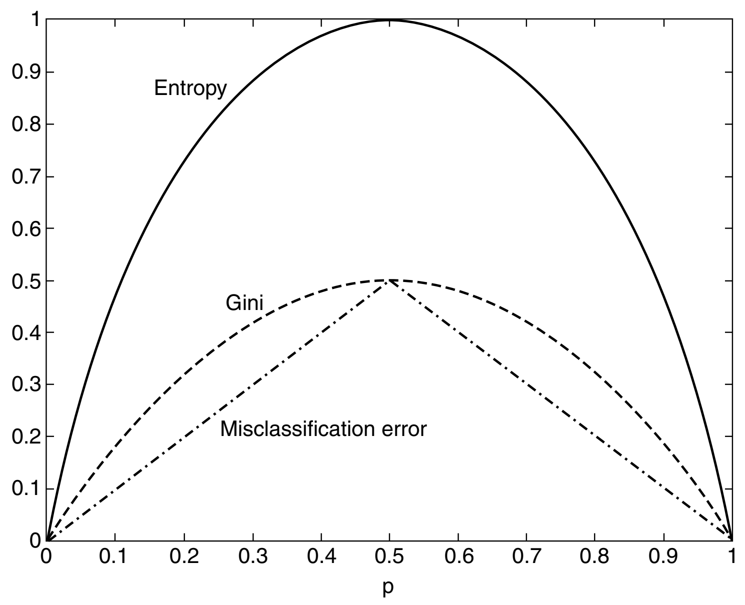


Figure 4.13. Comparison among the impurity measures for binary classification problems.

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

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

Node N_2	Count
Class=0	1
Class=1	5

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

Node N_3	Count
Class=0	3
Class=1	3

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

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:

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

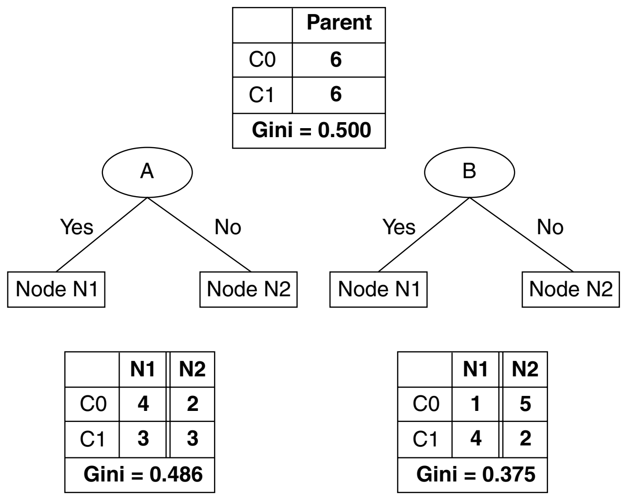
where $I(\cdot)$ is the impurity measure of a given node, N is the total number of records at the parent node, k is the number of attribute values, and $N(v_j)$ is the number of records associated with the child node, v_j. Decision tree induction algorithms often choose a test condition that maximizes 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,`

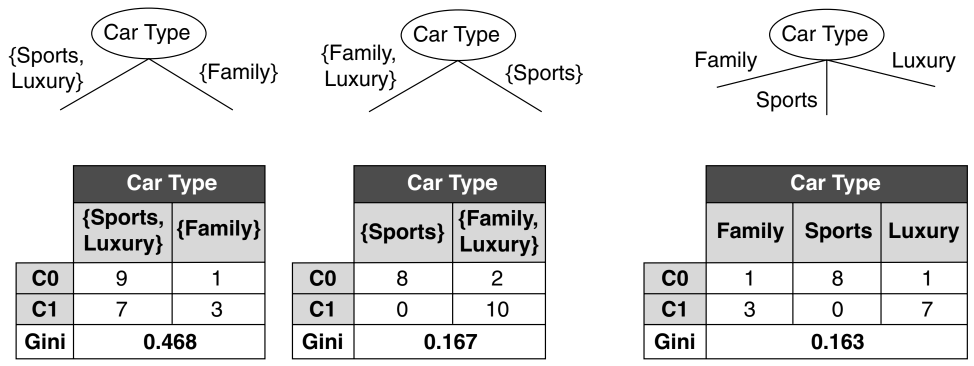


	Parent
C0	6
C1	6
Gini = 0.500	

	N1	N2
C0	4	2
C1	3	3
Gini = 0.486		

	N1	N2
C0	1	5
C1	4	2
Gini = 0.375		

Figure 4.14. Splitting binary attributes.



	Car Type	
	{Sports, Luxury}	{Family}
C0	9	1
C1	7	3
Gini	0.468	

	Car Type	
	{Sports}	{Family, Luxury}
C0	8	2
C1	0	10
Gini	0.167	

(a) Binary split

	Car Type		
	Family	Sports	Luxury
C0	1	8	1
C1	3	0	7
Gini	0.163		

(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
	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.

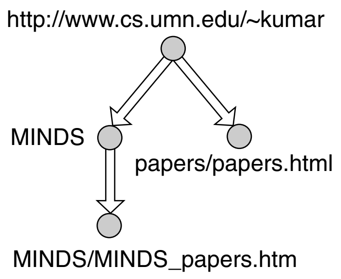
3. The `Classify()` function determines the class label to be assigned to a leaf node. For each leaf node t, let $p(i|t)$ denote the fraction of training records from class i associated with the node t. In most cases, the leaf node is assigned to the class that has the majority number of training records:
$$leaf.label = \underset{i}{\operatorname{argmax}}\ p(i|t), \tag{4.8}$$
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.

```
Decision Tree:
depth = 1:
| breadth> 7 :   class 1
| breadth<= 7:
| | breadth <= 3:
| | | ImagePages> 0.375:   class 0
| | | ImagePages<= 0.375:
| | | | totalPages<= 6:   class 1
| | | | totalPages> 6:
| | | | | breadth <= 1:   class 1
| | | | | breadth > 1:   class 0
| | width > 3:
| | | MultiIP = 0:
| | | | ImagePages<= 0.1333:   class 1
| | | | ImagePages> 0.1333:
| | | | breadth <= 6:   class 0
| | | | breadth > 6:   class 1
| | | MultiIP = 1:
| | | | TotalTime <= 361:   class 0
| | | | TotalTime > 361:   class 1
depth> 1:
| MultiAgent = 0:
| | depth > 2:   class 0
| | depth < 2:
| | | MultiIP = 1:   class 0
| | | MultiIP = 0:
| | | | breadth <= 6:   class 0
| | | | breadth > 6:
| | | | | RepeatedAccess <= 0.322:   class 0
| | | | | RepeatedAccess > 0.322:   class 1
| MultiAgent = 1:
| | totalPages <= 81:   class 0
| | totalPages > 81:   class 1
```

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.

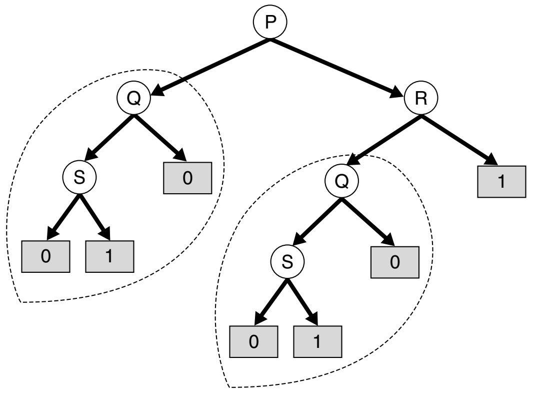


Figure 4.19. Tree replication problem. The same subtree can appear at different branches.

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

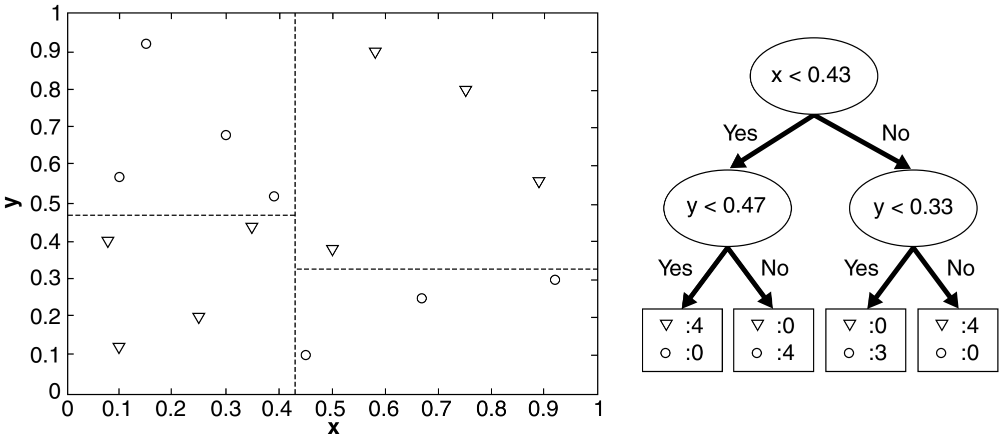


Figure 4.20. Example of a decision tree and its decision boundaries for a two-dimensional data set.

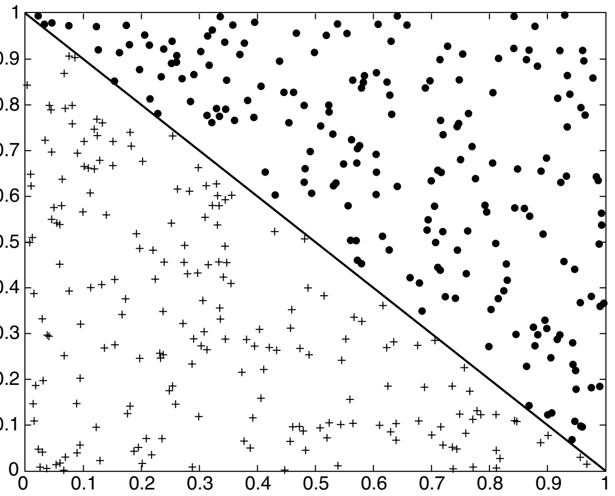


Figure 4.21. Example of data set that cannot be partitioned optimally using test conditions involving single attributes.

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

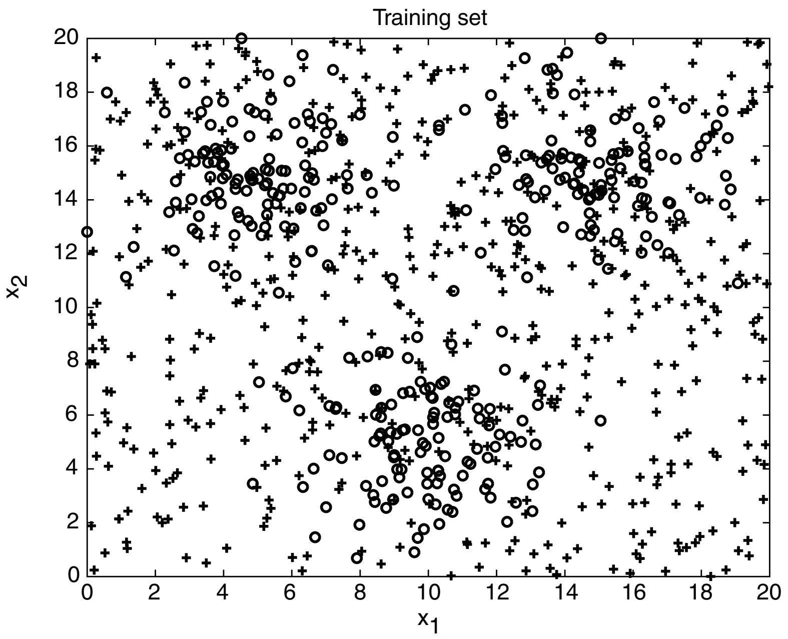


Figure 4.22. Example of a data set with binary classes.

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.

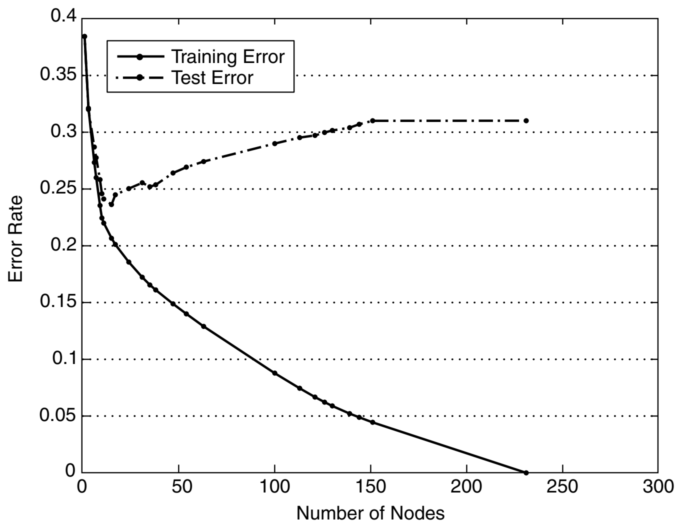
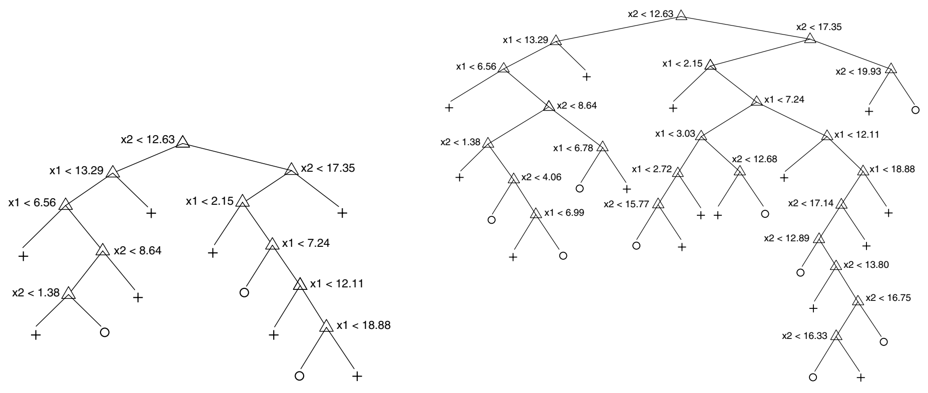


Figure 4.23. Training and test error rates.

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

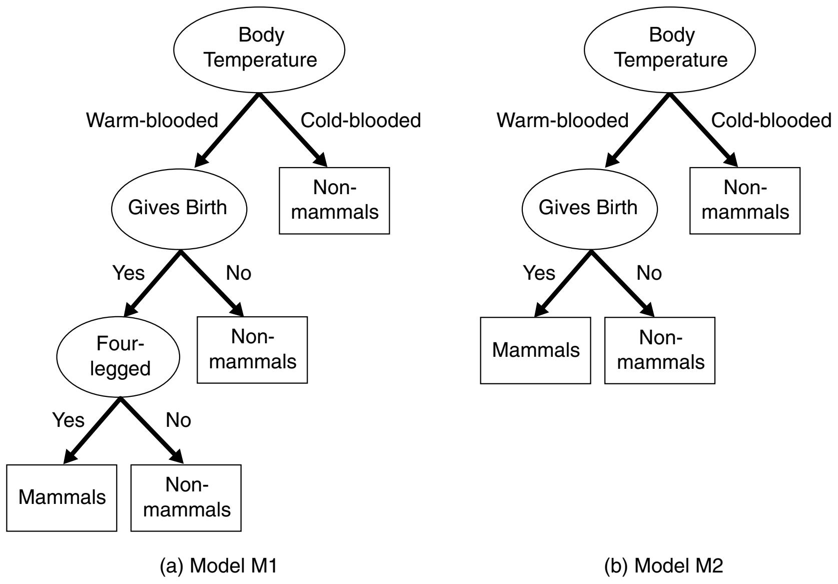


Figure 4.25. Decision tree induced from the data set shown in Table 4.3.

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.

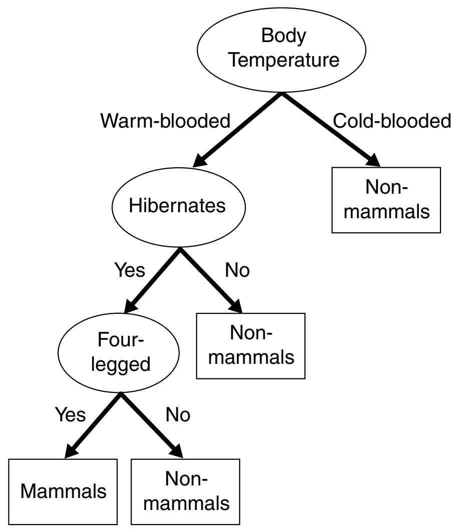


Figure 4.26. Decision tree induced from the data set shown in Table 4.5.

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

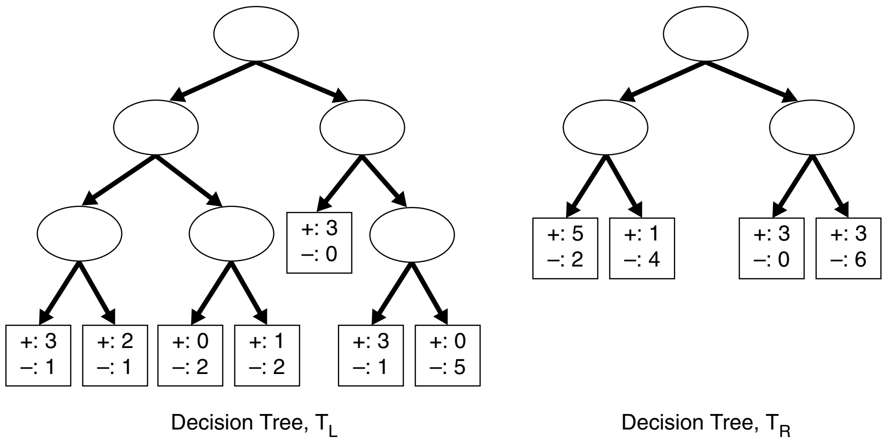


Figure 4.27. Example of two decision trees generated from the same training data.

$e(T_R) = 6/24 = 0.25$. 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

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

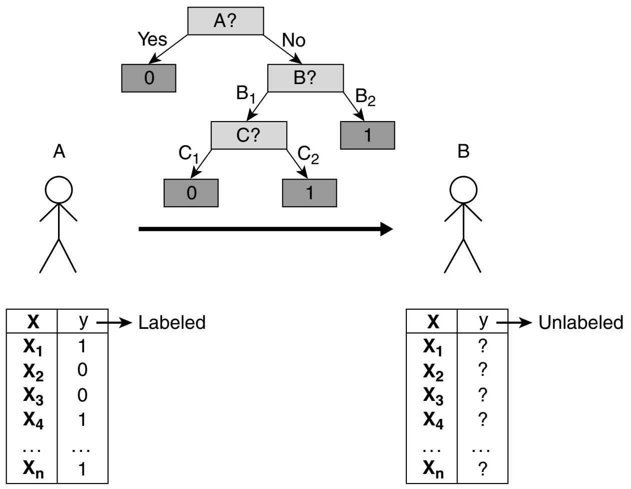


Figure 4.28. The minimum description length (MDL) principle.

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

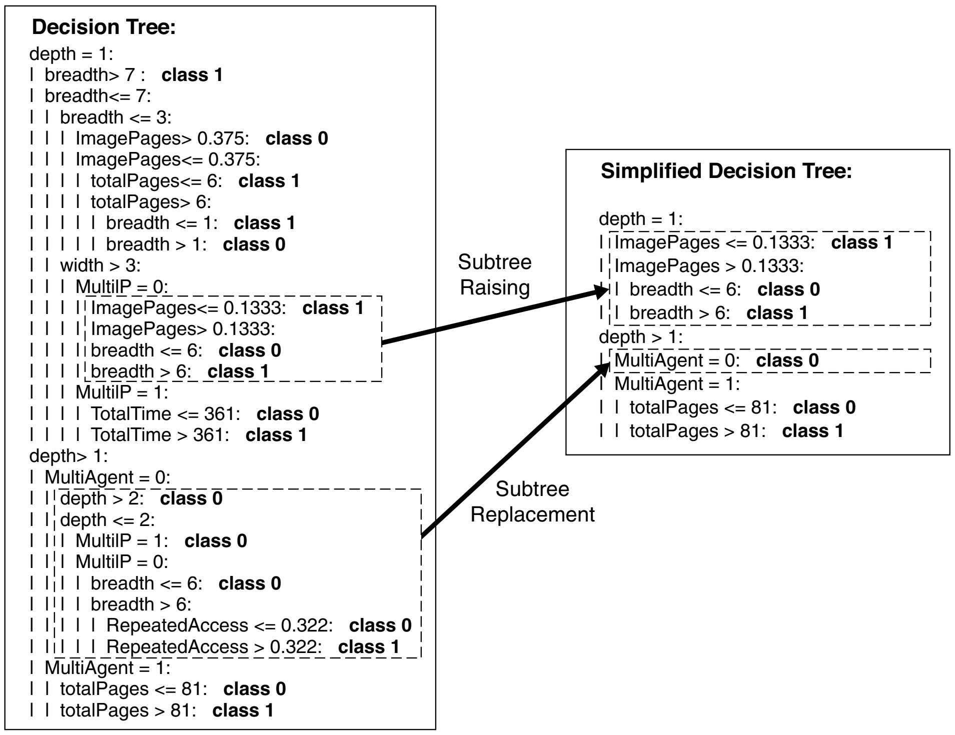
In this approach, instead of using the training set to estimate the generalization error, the original training data is divided into two smaller subsets. One of the subsets is used for training, while the other, known as the validation set, is used for estimating the generalization error. Typically, 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,



```
Decision Tree:
depth = 1:
| breadth> 7 :  class 1
| breadth<= 7:
| | breadth <= 3:
| | | ImagePages> 0.375:  class 0
| | | ImagePages<= 0.375:
| | | | totalPages<= 6:  class 1
| | | | totalPages> 6:
| | | | | breadth <= 1:  class 1
| | | | | breadth > 1:  class 0
| | width > 3:
| | | MultiIP = 0:
| | | | ImagePages<= 0.1333:  class 1
| | | | ImagePages> 0.1333:
| | | | breadth <= 6:  class 0
| | | | breadth > 6:  class 1
| | | MultiIP = 1:
| | | | TotalTime <= 361:  class 0
| | | | TotalTime > 361:  class 1
depth> 1:
| MultiAgent = 0:
| | depth > 2:  class 0
| | depth <= 2:
| | | MultiIP = 1:  class 0
| | | MultiIP = 0:
| | | | breadth <= 6:  class 0
| | | | breadth > 6:
| | | | | RepeatedAccess <= 0.322:  class 0
| | | | | RepeatedAccess > 0.322:  class 1
| MultiAgent = 1:
| | totalPages <= 81:  class 0
| | totalPages > 81:  class 1
```

```
Simplified Decision Tree:

depth = 1:
| ImagePages <= 0.1333:  class 1
| ImagePages > 0.1333:
| | breadth <= 6:  class 0
| | breadth > 6:  class 1
depth > 1:
| MultiAgent = 0:  class 0
| MultiAgent = 1:
| | totalPages <= 81:  class 0
| | totalPages > 81:  class 1
```

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:

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

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:

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

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 treatment 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], Cant*ú*-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.

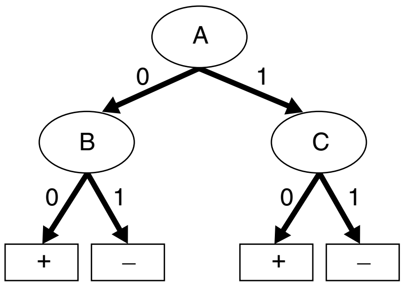
(e) Use the results in parts (c) and (d) to conclude about the greedy nature of the decision tree induction algorithm.

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:

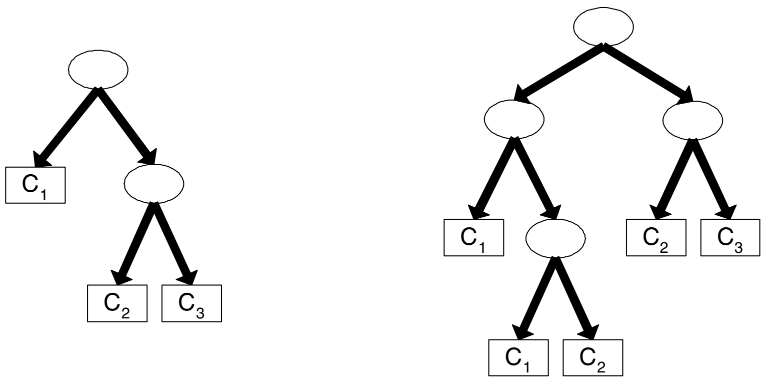
Instance	A	B	C	Class
1	0	0	0	+
2	0	0	1	+
3	0	1	0	+
4	0	1	1	–
5	1	0	0	+
6	1	0	0	+
7	1	1	0	–
8	1	0	1	+
9	1	1	0	–
10	1	1	0	–

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 $\times$ 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	Hiber-nates
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	Hiber-nates	Class Labe
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	Amphibia
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	Amphibia

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	Hiber-nates
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.

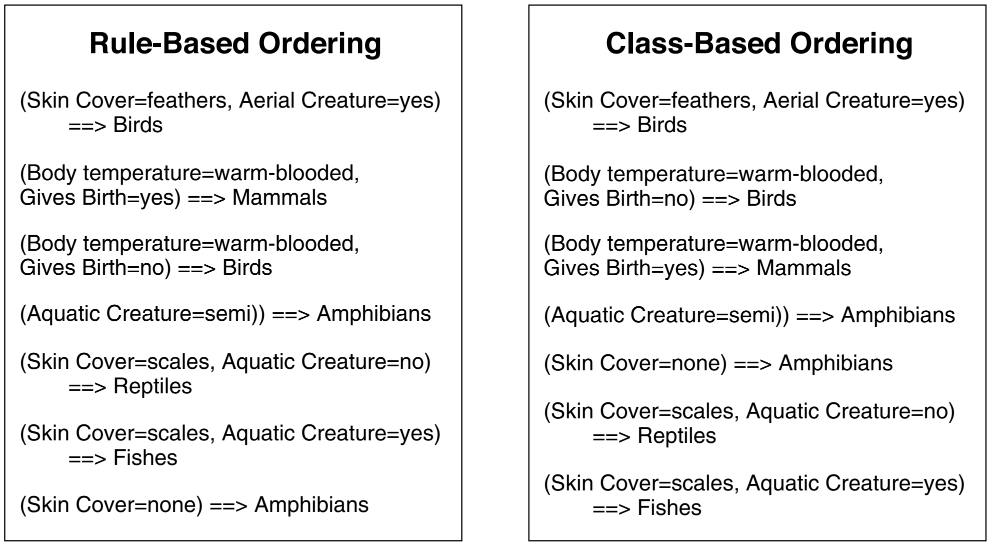
5.1.2 Rule-Ordering Schemes

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.



Rule-Based Ordering

(Skin Cover=feathers, Aerial Creature=yes)
==> Birds

(Body temperature=warm-blooded,
Gives Birth=yes) ==> Mammals

(Body temperature=warm-blooded,
Gives Birth=no) ==> Birds

(Aquatic Creature=semi)) ==> Amphibians

(Skin Cover=scales, Aquatic Creature=no)
==> Reptiles

(Skin Cover=scales, Aquatic Creature=yes)
==> Fishes

(Skin Cover=none) ==> Amphibians

Class-Based Ordering

(Skin Cover=feathers, Aerial Creature=yes)
==> Birds

(Body temperature=warm-blooded,
Gives Birth=no) ==> Birds

(Body temperature=warm-blooded,
Gives Birth=yes) ==> Mammals

(Aquatic Creature=semi)) ==> Amphibians

(Skin Cover=none) ==> Amphibians

(Skin Cover=scales, Aquatic Creature=no)
==> Reptiles

(Skin Cover=scales, Aquatic Creature=yes)
==> Fishes

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 $R2$.

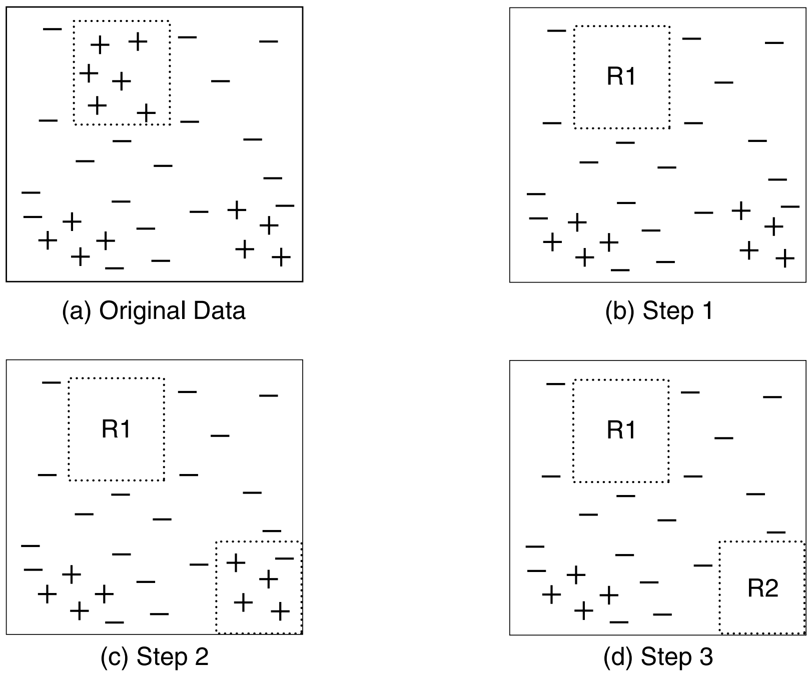


Figure 5.2. An example of the sequential covering algorithm.

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

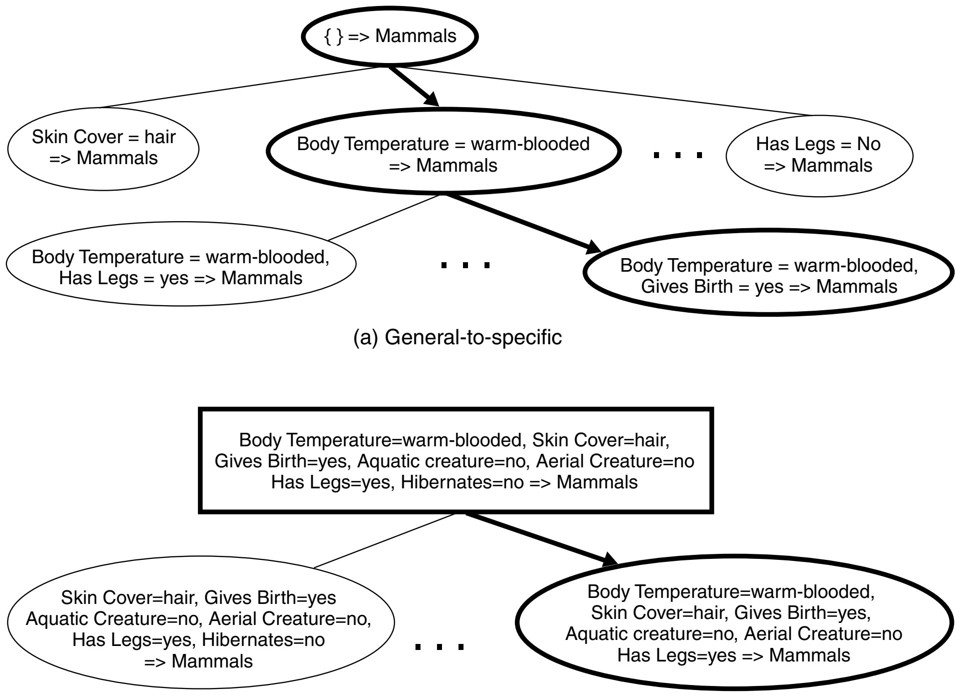

{ } => Mammals
Skin Cover = hair => Mammals
Body Temperature = warm-blooded => Mammals
. . .
Has Legs = No => Mammals
Body Temperature = warm-blooded, Has Legs = yes => Mammals
. . .
Body Temperature = warm-blooded, Gives Birth = yes => Mammals
(a) General-to-specific
Body Temperature=warm-blooded, Skin Cover=hair, Gives Birth=yes, Aquatic creature=no, Aerial Creature=no Has Legs=yes, Hibernates=no => Mammals
Skin Cover=hair, Gives Birth=yes Aquatic Creature=no, Aerial Creature=no, Has Legs=yes, Hibernates=no => Mammals
. . .
Body Temperature=warm-blooded, Skin Cover=hair, Gives Birth=yes, Aquatic creature=no, Aerial Creature=no Has Legs=yes => Mammals
(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:

$$\text{Laplace} = \frac{f_+ + 1}{n+k}, \quad (5.4)$$

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

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.

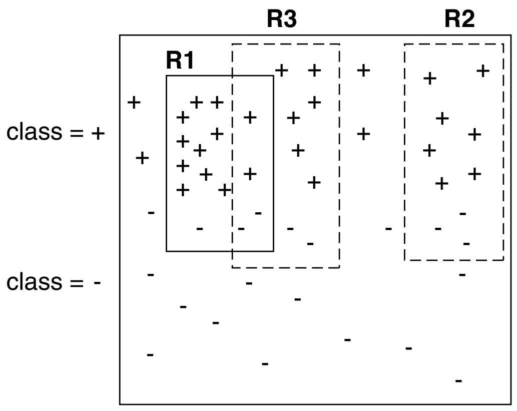


Figure 5.4. Elimination of training records by the sequential covering algorithm. $R1$, $R2$, and $R3$ represent regions covered by three different rules.

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 $(y_1, y_2, \dots, y_c)$ 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%.

RIPPER also performs additional optimization steps to determine whether some of the existing rules in the rule set can be replaced by better alternative rules. Readers who are interested in the details of the optimization method may refer to the reference cited at the end of this chapter.

5.1.5 Indirect Methods for Rule Extraction

This section presents a method for generating a rule set from a decision tree. In principle, every path from the root node to the leaf node of a decision tree can be expressed as a classification rule. The test conditions encountered along the path form the conjuncts of the rule antecedent, while the class label at the leaf node is assigned to the rule consequent. Figure 5.5 shows an example of a rule set generated from a decision tree. Notice that the rule set is exhaustive and contains mutually exclusive rules. However, some of the rules can be simplified as shown in the next example.

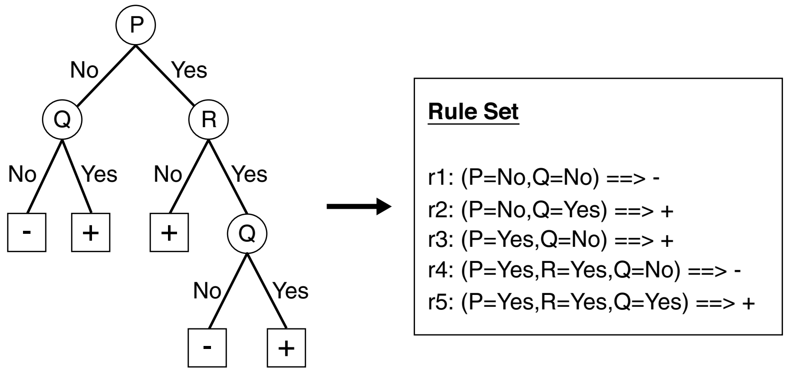


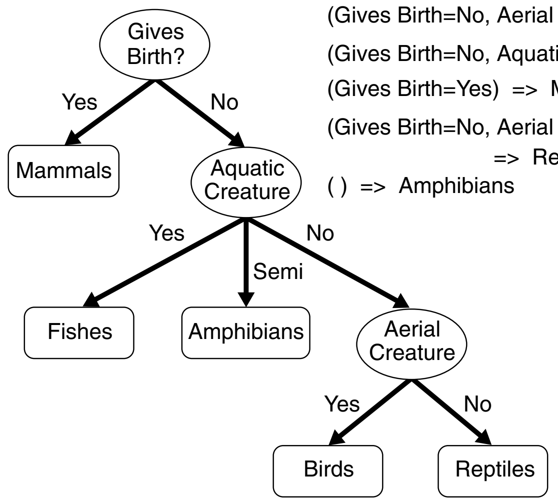
Figure 5.5. Converting a decision tree into classification rules.

Example 5.2. Consider the following three rules from Figure 5.5:

$r2 : (\text{P} = \text{No}) \wedge (\text{Q} = \text{Yes}) \longrightarrow +$
$r3 : (\text{P} = \text{Yes}) \wedge (\text{R} = \text{No}) \longrightarrow +$
$r5 : (\text{P} = \text{Yes}) \wedge (\text{R} = \text{Yes}) \wedge (\text{Q} = \text{Yes}) \longrightarrow +$

Observe that the rule set always predicts a positive class when the value of Q is Yes. Therefore, we may simplify the rules as follows:

$r2'$: $(\text{Q} = \text{Yes}) \longrightarrow +$
$r3$: $(\text{P} = \text{Yes}) \wedge (\text{R} = \text{No}) \longrightarrow +.$



Rule-Based Classifier:

(Gives Birth=No, Aerial Creature=Yes) => Birds

(Gives Birth=No, Aquatic Creature=Yes) => Fishes

(Gives Birth=Yes) => Mammals

(Gives Birth=No, Aerial Creature=No, Aquatic Creature=No) => Reptiles

( ) => Amphibians

Figure 5.6. Classification rules extracted from a decision tree for the vertebrate classification problem.

r_3 is retained to cover the remaining instances of the positive class. Although the rules obtained after simplification are no longer mutually exclusive, they are less complex and are easier to interpret. ■

In the following, we describe an approach used by the C4.5rules algorithm to generate a rule set from a decision tree. Figure 5.6 shows the decision tree and resulting classification rules obtained for the data set given in Table 5.2.

Rule Generation Classification rules are extracted for every path from the root to one of the leaf nodes in the decision tree. Given a classification rule $r : A \longrightarrow y$, we consider a simplified rule, $r' : A' \longrightarrow y$, where A' is obtained by removing one of the conjuncts in A. The simplified rule with the lowest pessimistic error rate is retained provided its error rate is less than that of the original rule. The rule-pruning step is repeated until the pessimistic error of the rule cannot be improved further. Because some of the rules may become identical after pruning, the duplicate rules must be discarded.

Rule Ordering After generating the rule set, C4.5rules uses the class-based ordering scheme to order the extracted rules. Rules that predict the same class are grouped together into the same subset. The total description length for each subset is computed, and the classes are arranged in increasing order of their total description length. The class that has the smallest description length is given the highest priority because it is expected to contain the best set of rules. The total description length for a class is given by $L_{\text{exception}} + g \times L_{\text{model}}$, where $L_{\text{exception}}$ is the number of bits needed to encode the misclassified examples, L_{model} is the number of bits needed to encode the model, and g is a tuning parameter whose default value is 0.5. The tuning parameter depends on the number of redundant attributes present in the model. The value of the tuning parameter is small if the model contains many redundant attributes.

5.1.6 Characteristics of Rule-Based Classifiers

A rule-based classifier has the following characteristics:

- The expressiveness of a rule set is almost equivalent to that of a decision tree because a decision tree can be represented by a set of mutually exclusive and exhaustive rules. Both rule-based and decision tree classifiers create rectilinear partitions of the attribute space and assign a class to each partition. Nevertheless, if the rule-based classifier allows multiple rules to be triggered for a given record, then a more complex decision boundary can be constructed.

- Rule-based classifiers are generally used to produce descriptive models that are easier to interpret, but gives comparable performance to the decision tree classifier.

- The class-based ordering approach adopted by many rule-based classifiers (such as RIPPER) is well suited for handling data sets with imbalanced class distributions.

5.2 Nearest-Neighbor classifiers

The classification framework shown in Figure 4.3 involves a two-step process: (1) an inductive step for constructing a classification model from data, and (2) a deductive step for applying the model to test examples. Decision tree and rule-based classifiers are examples of **eager learners** because they are designed to learn a model that maps the input attributes to the class label as soon as the training data becomes available. An opposite strategy would be to delay the process of modeling the training data until it is needed to classify the test examples. Techniques that employ this strategy are known as **lazy learners**. An example of a lazy learner is the **Rote classifier**, which memorizes the entire training data and performs classification only if the attributes of a test instance match one of the training examples exactly. An obvious drawback of

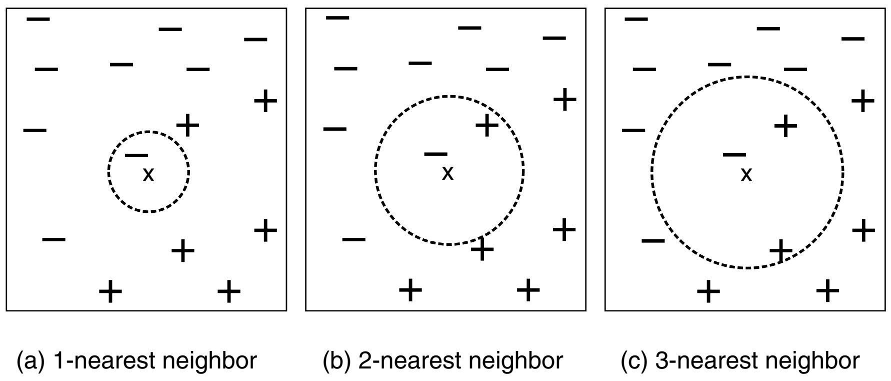


Figure 5.7. The 1-, 2-, and 3-nearest neighbors of an instance.

this approach is that some test records may not be classified because they do not match any training example.

One way to make this approach more flexible is to find all the training examples that are relatively similar to the attributes of the test example. These examples, which are known as **nearest neighbors**, can be used to determine the class label of the test example. The justification for using nearest neighbors is best exemplified by the following saying: *"If it walks like a duck, quacks like a duck, and looks like a duck, then it's probably a duck."* A nearest-neighbor classifier represents each example as a data point in a d-dimensional space, where d is the number of attributes. Given a test example, we compute its proximity to the rest of the data points in the training set, using one of the proximity measures described in Section 2.4 on page 65. The k-nearest neighbors of a given example z refer to the k points that are closest to z.

Figure 5.7 illustrates the 1-, 2-, and 3-nearest neighbors of a data point located at the center of each circle. The data point is classified based on the class labels of its neighbors. In the case where the neighbors have more than one label, the data point is assigned to the majority class of its nearest neighbors. In Figure 5.7(a), the 1-nearest neighbor of the data point is a negative example. Therefore the data point is assigned to the negative class. If the number of nearest neighbors is three, as shown in Figure 5.7(c), then the neighborhood contains two positive examples and one negative example. Using the majority voting scheme, the data point is assigned to the positive class. In the case where there is a tie between the classes (see Figure 5.7(b)), we may randomly choose one of them to classify the data point.

The preceding discussion underscores the importance of choosing the right value for k. If k is too small, then the nearest-neighbor classifier may be

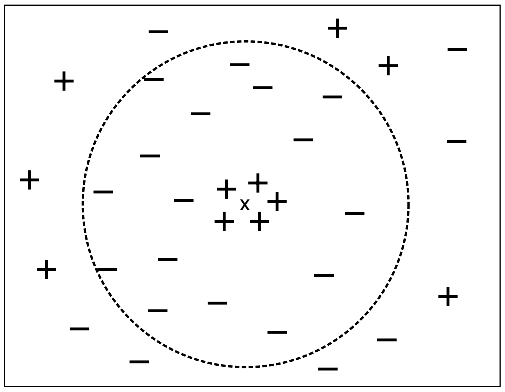


Figure 5.8. k-nearest neighbor classification with large k.

susceptible to overfitting because of noise in the training data. On the other hand, if k is too large, the nearest-neighbor classifier may misclassify the test instance because its list of nearest neighbors may include data points that are located far away from its neighborhood (see Figure 5.8).

5.2.1 Algorithm

A high-level summary of the nearest-neighbor classification method is given in Algorithm 5.2. The algorithm computes the distance (or similarity) between each test example $z = (\mathbf{x}', y')$ and all the training examples $(\mathbf{x}, y) \in D$ to determine its nearest-neighbor list, D_z. Such computation can be costly if the number of training examples is large. However, efficient indexing techniques are available to reduce the amount of computations needed to find the nearest neighbors of a test example.

Algorithm 5.2 The k-nearest neighbor classification algorithm.

```
1: Let $k$ be the number of nearest neighbors and $D$ be the set of training examples.
2: for each test example $z = (\mathbf{x}', y')$ do
3:     Compute $d(\mathbf{x}', \mathbf{x})$, the distance between $z$ and every example, $(\mathbf{x}, y) \in D$.
4:     Select $D_z \subseteq D$, the set of $k$ closest training examples to $z$.
5:     $y' = \underset{v}{\operatorname{argmax}} \sum_{(\mathbf{x}_i, y_i) \in D_z} I(v = y_i)$
6: end for
```

Once the nearest-neighbor list is obtained, the test example is classified based on the majority class of its nearest neighbors:

$$\text{Majority Voting: } y' = \underset{v}{\operatorname{argmax}} \sum_{(\mathbf{x}_i, y_i) \in D_z} I(v = y_i), \tag{5.7}$$

where v is a class label, y_i is the class label for one of the nearest neighbors, and $I(\cdot)$ is an indicator function that returns the value 1 if its argument is true and 0 otherwise.

In the majority voting approach, every neighbor has the same impact on the classification. This makes the algorithm sensitive to the choice of k, as shown in Figure 5.7. One way to reduce the impact of k is to weight the influence of each nearest neighbor $\mathbf{x}_i$ according to its distance: $w_i = 1/d(\mathbf{x}', \mathbf{x}_i)^2$. As a result, training examples that are located far away from z have a weaker impact on the classification compared to those that are located close to z. Using the distance-weighted voting scheme, the class label can be determined as follows:

$$\text{Distance-Weighted Voting: } y' = \underset{v}{\operatorname{argmax}} \sum_{(\mathbf{x}_i, y_i) \in D_z} w_i \times I(v = y_i). \tag{5.8}$$

5.2.2 Characteristics of Nearest-Neighbor Classifiers

The characteristics of the nearest-neighbor classifier are summarized below:

- Nearest-neighbor classification is part of a more general technique known as instance-based learning, which uses specific training instances to make predictions without having to maintain an abstraction (or model) derived from data. Instance-based learning algorithms require a proximity measure to determine the similarity or distance between instances and a classification function that returns the predicted class of a test instance based on its proximity to other instances.

- Lazy learners such as nearest-neighbor classifiers do not require model building. However, classifying a test example can be quite expensive because we need to compute the proximity values individually between the test and training examples. In contrast, eager learners often spend the bulk of their computing resources for model building. Once a model has been built, classifying a test example is extremely fast.

- Nearest-neighbor classifiers make their predictions based on local information, whereas decision tree and rule-based classifiers attempt to find a global model that fits the entire input space. Because the classification decisions are made locally, nearest-neighbor classifiers (with small values of k) are quite susceptible to noise.

- Nearest-neighbor classifiers can produce arbitrarily shaped decision boundaries. Such boundaries provide a more flexible model representation compared to decision tree and rule-based classifiers that are often constrained to rectilinear decision boundaries. The decision boundaries of nearest-neighbor classifiers also have high variability because they depend on the composition of training examples. Increasing the number of nearest neighbors may reduce such variability.

- Nearest-neighbor classifiers can produce wrong predictions unless the appropriate proximity measure and data preprocessing steps are taken. For example, suppose we want to classify a group of people based on attributes such as height (measured in meters) and weight (measured in pounds). The height attribute has a low variability, ranging from 1.5 m to 1.85 m, whereas the weight attribute may vary from 90 lb. to 250 lb. If the scale of the attributes are not taken into consideration, the proximity measure may be dominated by differences in the weights of a person.

5.3 Bayesian Classifiers

In many applications the relationship between the attribute set and the class variable is non-deterministic. In other words, the class label of a test record cannot be predicted with certainty even though its attribute set is identical to some of the training examples. This situation may arise because of noisy data or the presence of certain confounding factors that affect classification but are not included in the analysis. For example, consider the task of predicting whether a person is at risk for heart disease based on the person's diet and workout frequency. Although most people who eat healthily and exercise regularly have less chance of developing heart disease, they may still do so because of other factors such as heredity, excessive smoking, and alcohol abuse. Determining whether a person's diet is healthy or the workout frequency is sufficient is also subject to interpretation, which in turn may introduce uncertainties into the learning problem.

This section presents an approach for modeling probabilistic relationships between the attribute set and the class variable. The section begins with an introduction to the **Bayes theorem**, a statistical principle for combining prior knowledge of the classes with new evidence gathered from data. The use of the Bayes theorem for solving classification problems will be explained, followed by a description of two implementations of Bayesian classifiers: naïve Bayes and the Bayesian belief network.

5.3.1 Bayes Theorem

> *Consider a football game between two rival teams: Team 0 and Team 1. Suppose Team 0 wins* 65% *of the time and Team 1 wins the remaining matches. Among the games won by Team 0, only* 30% *of them come from playing on Team 1's football field. On the other hand,* 75% *of the victories for Team 1 are obtained while playing at home. If Team 1 is to host the next match between the two teams, which team will most likely emerge as the winner?*

This question can be answered by using the well-known Bayes theorem. For completeness, we begin with some basic definitions from probability theory. Readers who are unfamiliar with concepts in probability may refer to Appendix C for a brief review of this topic.

Let X and Y be a pair of random variables. Their joint probability, $P(X = x, Y = y)$, refers to the probability that variable X will take on the value x and variable Y will take on the value y. A conditional probability is the probability that a random variable will take on a particular value given that the outcome for another random variable is known. For example, the conditional probability $P(Y = y|X = x)$ refers to the probability that the variable Y will take on the value y, given that the variable X is observed to have the value x. The joint and conditional probabilities for X and Y are related in the following way:

$$P(X, Y) = P(Y|X) \times P(X) = P(X|Y) \times P(Y). \tag{5.9}$$

Rearranging the last two expressions in Equation 5.9 leads to the following formula, known as the Bayes theorem:

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}. \tag{5.10}$$

The Bayes theorem can be used to solve the prediction problem stated at the beginning of this section. For notational convenience, let X be the random variable that represents the team hosting the match and Y be the random variable that represents the winner of the match. Both X and Y can take on values from the set $\{0, 1\}$. We can summarize the information given in the problem as follows:

Probability Team 0 wins is $P(Y = 0) = 0.65$.
Probability Team 1 wins is $P(Y = 1) = 1 - P(Y = 0) = 0.35$.
Probability Team 1 hosted the match it won is $P(X = 1|Y = 1) = 0.75$.
Probability Team 1 hosted the match won by Team 0 is $P(X = 1|Y = 0) = 0.3$.

Our objective is to compute $P(Y = 1|X = 1)$, which is the conditional probability that Team 1 wins the next match it will be hosting, and compares it against $P(Y = 0|X = 1)$. Using the Bayes theorem, we obtain

$$\begin{aligned}
P(Y = 1|X = 1) &= \frac{P(X = 1|Y = 1) \times P(Y = 1)}{P(X = 1)} \\
&= \frac{P(X = 1|Y = 1) \times P(Y = 1)}{P(X = 1, Y = 1) + P(X = 1, Y = 0)} \\
&= \frac{P(X = 1|Y = 1) \times P(Y = 1)}{P(X = 1|Y = 1)P(Y = 1) + P(X = 1|Y = 0)P(Y = 0)} \\
&= \frac{0.75 \times 0.35}{0.75 \times 0.35 + 0.3 \times 0.65} \\
&= 0.5738,
\end{aligned}$$

where the law of total probability (see Equation C.5 on page 722) was applied in the second line. Furthermore, $P(Y = 0|X = 1) = 1 - P(Y = 1|X = 1) = 0.4262$. Since $P(Y = 1|X = 1) > P(Y = 0|X = 1)$, Team 1 has a better chance than Team 0 of winning the next match.

5.3.2 Using the Bayes Theorem for Classification

Before describing how the Bayes theorem can be used for classification, let us formalize the classification problem from a statistical perspective. Let $\mathbf{X}$ denote the attribute set and Y denote the class variable. If the class variable has a non-deterministic relationship with the attributes, then we can treat $\mathbf{X}$ and Y as random variables and capture their relationship probabilistically using $P(Y|\mathbf{X})$. This conditional probability is also known as the **posterior probability** for Y, as opposed to its **prior probability**, $P(Y)$.

During the training phase, we need to learn the posterior probabilities $P(Y|\mathbf{X})$ for every combination of $\mathbf{X}$ and Y based on information gathered from the training data. By knowing these probabilities, a test record $\mathbf{X}'$ can be classified by finding the class Y' that maximizes the posterior probability,

$P(Y'|\mathbf{X}')$. To illustrate this approach, consider the task of predicting whether a loan borrower will default on their payments. Figure 5.9 shows a training set with the following attributes: `Home Owner`, `Marital Status`, and `Annual Income`. Loan borrowers who defaulted on their payments are classified as `Yes`, while those who repaid their loans are classified as `No`.

	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 5.9. Training set for predicting the loan default problem.

Suppose we are given a test record with the following attribute set: $\mathbf{X} =$ (`Home Owner` $=$ `No`, `Marital Status` $=$ `Married`, `Annual Income` $=$ \$120K). To classify the record, we need to compute the posterior probabilities $P(\texttt{Yes}|\mathbf{X})$ and $P(\texttt{No}|\mathbf{X})$ based on information available in the training data. If $P(\texttt{Yes}|\mathbf{X}) > P(\texttt{No}|\mathbf{X})$, then the record is classified as `Yes`; otherwise, it is classified as `No`.

Estimating the posterior probabilities accurately for every possible combination of class label and attribute value is a difficult problem because it requires a very large training set, even for a moderate number of attributes. The Bayes theorem is useful because it allows us to express the posterior probability in terms of the prior probability $P(Y)$, the **class-conditional** probability $P(\mathbf{X}|Y)$, and the evidence, $P(\mathbf{X})$:

$$P(Y|\mathbf{X}) = \frac{P(\mathbf{X}|Y) \times P(Y)}{P(\mathbf{X})}. \tag{5.11}$$

When comparing the posterior probabilities for different values of Y, the denominator term, $P(\mathbf{X})$, is always constant, and thus, can be ignored. The prior probability $P(Y)$ can be easily estimated from the training set by computing the fraction of training records that belong to each class. To estimate the class-conditional probabilities $P(\mathbf{X}|Y)$, we present two implementations of Bayesian classification methods: the naïve Bayes classifier and the Bayesian belief network. These implementations are described in Sections 5.3.3 and 5.3.5, respectively.

5.3.3 Naïve Bayes Classifier

A naïve Bayes classifier estimates the class-conditional probability by assuming that the attributes are conditionally independent, given the class label y. The conditional independence assumption can be formally stated as follows:

$$P(\mathbf{X}|Y = y) = \prod_{i=1}^{d} P(X_i|Y = y), \tag{5.12}$$

where each attribute set $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ consists of d attributes.

Conditional Independence

Before delving into the details of how a naïve Bayes classifier works, let us examine the notion of conditional independence. Let $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ denote three sets of random variables. The variables in $\mathbf{X}$ are said to be conditionally independent of $\mathbf{Y}$, given $\mathbf{Z}$, if the following condition holds:

$$P(\mathbf{X}|\mathbf{Y}, \mathbf{Z}) = P(\mathbf{X}|\mathbf{Z}). \tag{5.13}$$

An example of conditional independence is the relationship between a person's arm length and his or her reading skills. One might observe that people with longer arms tend to have higher levels of reading skills. This relationship can be explained by the presence of a confounding factor, which is age. A young child tends to have short arms and lacks the reading skills of an adult. If the age of a person is fixed, then the observed relationship between arm length and reading skills disappears. Thus, we can conclude that arm length and reading skills are conditionally independent when the age variable is fixed.

The conditional independence between $\mathbf{X}$ and $\mathbf{Y}$ can also be written into a form that looks similar to Equation 5.12:

$$\begin{aligned}
P(\mathbf{X},\mathbf{Y}|\mathbf{Z}) &= \frac{P(\mathbf{X},\mathbf{Y},\mathbf{Z})}{P(\mathbf{Z})} \\
&= \frac{P(\mathbf{X},\mathbf{Y},\mathbf{Z})}{P(\mathbf{Y},\mathbf{Z})} \times \frac{P(\mathbf{Y},\mathbf{Z})}{P(\mathbf{Z})} \\
&= P(\mathbf{X}|\mathbf{Y},\mathbf{Z}) \times P(\mathbf{Y}|\mathbf{Z}) \\
&= P(\mathbf{X}|\mathbf{Z}) \times P(\mathbf{Y}|\mathbf{Z}), \qquad (5.14)
\end{aligned}$$

where Equation 5.13 was used to obtain the last line of Equation 5.14.

How a Naïve Bayes Classifier Works

With the conditional independence assumption, instead of computing the class-conditional probability for every combination of $\mathbf{X}$, we only have to estimate the conditional probability of each X_i, given Y. The latter approach is more practical because it does not require a very large training set to obtain a good estimate of the probability.

To classify a test record, the naïve Bayes classifier computes the posterior probability for each class Y:

$$P(Y|\mathbf{X}) = \frac{P(Y)\prod_{i=1}^{d} P(X_i|Y)}{P(\mathbf{X})}. \qquad (5.15)$$

Since $P(\mathbf{X})$ is fixed for every Y, it is sufficient to choose the class that maximizes the numerator term, $P(Y)\prod_{i=1}^{d} P(X_i|Y)$. In the next two subsections, we describe several approaches for estimating the conditional probabilities $P(X_i|Y)$ for categorical and continuous attributes.

Estimating Conditional Probabilities for Categorical Attributes

For a categorical attribute X_i, the conditional probability $P(X_i = x_i|Y = y)$ is estimated according to the fraction of training instances in class y that take on a particular attribute value x_i. For example, in the training set given in Figure 5.9, three out of the seven people who repaid their loans also own a home. As a result, the conditional probability for $P(\texttt{Home Owner}{=}\texttt{Yes}|\texttt{No})$ is equal to 3/7. Similarly, the conditional probability for defaulted borrowers who are single is given by $P(\texttt{Marital Status} = \texttt{Single}|\texttt{Yes}) = 2/3$.

Estimating Conditional Probabilities for Continuous Attributes

There are two ways to estimate the class-conditional probabilities for continuous attributes in naïve Bayes classifiers:

1. We can discretize each continuous attribute and then replace the continuous attribute value with its corresponding discrete interval. This approach transforms the continuous attributes into ordinal attributes. The conditional probability $P(X_i|Y = y)$ is estimated by computing the fraction of training records belonging to class y that falls within the corresponding interval for X_i. The estimation error depends on the discretization strategy (as described in Section 2.3.6 on page 57), as well as the number of discrete intervals. If the number of intervals is too large, there are too few training records in each interval to provide a reliable estimate for $P(X_i|Y)$. On the other hand, if the number of intervals is too small, then some intervals may aggregate records from different classes and we may miss the correct decision boundary.

2. We can assume a certain form of probability distribution for the continuous variable and estimate the parameters of the distribution using the training data. A Gaussian distribution is usually chosen to represent the class-conditional probability for continuous attributes. The distribution is characterized by two parameters, its mean, μ, and variance, σ^2. For each class y_j, the class-conditional probability for attribute X_i is

$$P(X_i = x_i|Y = y_j) = \frac{1}{\sqrt{2\pi}\sigma_{ij}} \exp^{-\frac{(x_i-\mu_{ij})^2}{2\sigma_{ij}^2}}. \tag{5.16}$$

   The parameter μ_{ij} can be estimated based on the sample mean of X_i ($\overline{x}$) for all training records that belong to the class y_j. Similarly, σ_{ij}^2 can be estimated from the sample variance (s^2) of such training records. For example, consider the annual income attribute shown in Figure 5.9. The sample mean and variance for this attribute with respect to the class `No` are

$$\begin{aligned}
\overline{x} &= \frac{125 + 100 + 70 + \ldots + 75}{7} = 110 \\
s^2 &= \frac{(125-110)^2 + (100-110)^2 + \ldots + (75-110)^2}{7(6)} = 2975 \\
s &= \sqrt{2975} = 54.54.
\end{aligned}$$

Given a test record with taxable income equal to \$120K, we can compute its class-conditional probability as follows:

$$P(\texttt{Income=120}|\texttt{No}) = \frac{1}{\sqrt{2\pi}(54.54)} \exp^{-\frac{(120-110)^2}{2\times 2975}} = 0.0072.$$

Note that the preceding interpretation of class-conditional probability is somewhat misleading. The right-hand side of Equation 5.16 corresponds to a **probability density function**, $f(X_i; \mu_{ij}, \sigma_{ij})$. Since the function is continuous, the probability that the random variable X_i takes a particular value is zero. Instead, we should compute the conditional probability that X_i lies within some interval, x_i and $x_i + \epsilon$, where ϵ is a small constant:

$$\begin{aligned} P(x_i \leq X_i \leq x_i + \epsilon | Y = y_j) &= \int_{x_i}^{x_i+\epsilon} f(X_i; \mu_{ij}, \sigma_{ij}) dX_i \\ &\approx f(x_i; \mu_{ij}, \sigma_{ij}) \times \epsilon. \qquad (5.17) \end{aligned}$$

Since ϵ appears as a constant multiplicative factor for each class, it cancels out when we normalize the posterior probability for $P(Y|\mathbf{X})$. Therefore, we can still apply Equation 5.16 to approximate the class-conditional probability $P(X_i|Y)$.

Example of the Naïve Bayes Classifier

Consider the data set shown in Figure 5.10(a). We can compute the class-conditional probability for each categorical attribute, along with the sample mean and variance for the continuous attribute using the methodology described in the previous subsections. These probabilities are summarized in Figure 5.10(b).

To predict the class label of a test record $\mathbf{X} =$ (`Home Owner`=`No`, `Marital Status` = `Married`, `Income` = \$120K), we need to compute the posterior probabilities $P(\texttt{No}|\mathbf{X})$ and $P(\texttt{Yes}|\mathbf{X})$. Recall from our earlier discussion that these posterior probabilities can be estimated by computing the product between the prior probability $P(Y)$ and the class-conditional probabilities $\prod_i P(X_i|Y)$, which corresponds to the numerator of the right-hand side term in Equation 5.15.

The prior probabilities of each class can be estimated by calculating the fraction of training records that belong to each class. Since there are three records that belong to the class `Yes` and seven records that belong to the 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**

(a)

P(Home Owner=Yes|No) = 3/7
P(Home Owner=No|No) = 4/7
P(Home Owner=Yes|Yes) = 0
P(Home Owner=No|Yes) = 1
P(Marital Status=Single|No) = 2/7
P(Marital Status=Divorced|No) = 1/7
P(Marital Status=Married|No) = 4/7
P(Marital Status=Single|Yes) = 2/3
P(Marital Status=Divorced|Yes) = 1/3
P(Marital Status=Married|Yes) = 0

For Annual Income:
If class=No: sample mean=110
sample variance=2975
If class=Yes: sample mean=90
sample variance=25

(b)

Figure 5.10. The naïve Bayes classifier for the loan classification problem.

No, $P(\texttt{Yes}) = 0.3$ and $P(\texttt{No}) = 0.7$. Using the information provided in Figure 5.10(b), the class-conditional probabilities can be computed as follows:

$$\begin{aligned} P(\mathbf{X}|\texttt{No}) &= P(\texttt{Home Owner} = \texttt{No}|\texttt{No}) \times P(\texttt{Status} = \texttt{Married}|\texttt{No}) \\ &\quad \times P(\texttt{Annual Income} = \$120\text{K}|\texttt{No}) \\ &= 4/7 \times 4/7 \times 0.0072 = 0.0024. \end{aligned}$$

$$\begin{aligned} P(\mathbf{X}|\texttt{Yes}) &= P(\texttt{Home Owner} = \texttt{No}|\texttt{Yes}) \times P(\texttt{Status} = \texttt{Married}|\texttt{Yes}) \\ &\quad \times P(\texttt{Annual Income} = \$120\text{K}|\texttt{Yes}) \\ &= 1 \times 0 \times 1.2 \times 10^{-9} = 0. \end{aligned}$$

Putting them together, the posterior probability for class No is $P(\texttt{No}|\mathbf{X}) = \alpha \times 7/10 \times 0.0024 = 0.0016\alpha$, where $\alpha = 1/P(\mathbf{X})$ is a constant term. Using a similar approach, we can show that the posterior probability for class Yes is zero because its class-conditional probability is zero. Since $P(\texttt{No}|\mathbf{X}) > P(\texttt{Yes}|\mathbf{X})$, the record is classified as No.

M-estimate of Conditional Probability

The preceding example illustrates a potential problem with estimating posterior probabilities from training data. If the class-conditional probability for one of the attributes is zero, then the overall posterior probability for the class vanishes. This approach of estimating class-conditional probabilities using simple fractions may seem too brittle, especially when there are few training examples available and the number of attributes is large.

In a more extreme case, if the training examples do not cover many of the attribute values, we may not be able to classify some of the test records. For example, if $P(\texttt{Marital Status} = \texttt{Divorced}|\texttt{No})$ is zero instead of 1/7, then a record with attribute set $\mathbf{X} = (\texttt{Home Owner} = \texttt{Yes}, \texttt{Marital Status} = \texttt{Divorced}, \texttt{Income} = \$120\text{K})$ has the following class-conditional probabilities:

$$P(\mathbf{X}|\texttt{No}) = 3/7 \times 0 \times 0.0072 = 0.$$
$$P(\mathbf{X}|\texttt{Yes}) = 0 \times 1/3 \times 1.2 \times 10^{-9} = 0.$$

The naïve Bayes classifier will not be able to classify the record. This problem can be addressed by using the m-estimate approach for estimating the conditional probabilities:

$$P(x_i|y_j) = \frac{n_c + mp}{n + m}, \tag{5.18}$$

where n is the total number of instances from class y_j, n_c is the number of training examples from class y_j that take on the value x_i, m is a parameter known as the equivalent sample size, and p is a user-specified parameter. If there is no training set available (i.e., $n = 0$), then $P(x_i|y_j) = p$. Therefore p can be regarded as the prior probability of observing the attribute value x_i among records with class y_j. The equivalent sample size determines the tradeoff between the prior probability p and the observed probability n_c/n.

In the example given in the previous section, the conditional probability $P(\texttt{Status} = \texttt{Married}|\texttt{Yes}) = 0$ because none of the training records for the class has the particular attribute value. Using the m-estimate approach with $m = 3$ and $p = 1/3$, the conditional probability is no longer zero:

$$P(\texttt{Marital Status} = \texttt{Married}|\texttt{Yes}) = (0 + 3 \times 1/3)/(3 + 3) = 1/6.$$

If we assume $p = 1/3$ for all attributes of class Yes and $p = 2/3$ for all attributes of class No, then

$$\begin{aligned} P(\mathbf{X}|\texttt{No}) &= P(\texttt{Home Owner} = \texttt{No}|\texttt{No}) \times P(\texttt{Status} = \texttt{Married}|\texttt{No}) \\ &\quad \times P(\texttt{Annual Income} = \$120\text{K}|\texttt{No}) \\ &= 6/10 \times 6/10 \times 0.0072 = 0.0026. \end{aligned}$$

$$\begin{aligned} P(\mathbf{X}|\texttt{Yes}) &= P(\texttt{Home Owner} = \texttt{No}|\texttt{Yes}) \times P(\texttt{Status} = \texttt{Married}|\texttt{Yes}) \\ &\quad \times P(\texttt{Annual Income} = \$120\text{K}|\texttt{Yes}) \\ &= 4/6 \times 1/6 \times 1.2 \times 10^{-9} = 1.3 \times 10^{-10}. \end{aligned}$$

The posterior probability for class No is $P(\texttt{No}|\mathbf{X}) = \alpha \times 7/10 \times 0.0026 = 0.0018\alpha$, while the posterior probability for class Yes is $P(\texttt{Yes}|\mathbf{X}) = \alpha \times 3/10 \times 1.3 \times 10^{-10} = 4.0 \times 10^{-11}\alpha$. Although the classification decision has not changed, the m-estimate approach generally provides a more robust way for estimating probabilities when the number of training examples is small.

Characteristics of Naïve Bayes Classifiers

Naïve Bayes classifiers generally have the following characteristics:

- They are robust to isolated noise points because such points are averaged out when estimating conditional probabilities from data. Naïve Bayes classifiers can also handle missing values by ignoring the example during model building and classification.
- They are robust to irrelevant attributes. If X_i is an irrelevant attribute, then $P(X_i|Y)$ becomes almost uniformly distributed. The class-conditional probability for X_i has no impact on the overall computation of the posterior probability.
- Correlated attributes can degrade the performance of naïve Bayes classifiers because the conditional independence assumption no longer holds for such attributes. For example, consider the following probabilities:

$$\begin{aligned} P(A = 0|Y = 0) = 0.4, \quad P(A = 1|Y = 0) = 0.6, \\ P(A = 0|Y = 1) = 0.6, \quad P(A = 1|Y = 1) = 0.4, \end{aligned}$$

  where A is a binary attribute and Y is a binary class variable. Suppose there is another binary attribute B that is perfectly correlated with A

when $Y = 0$, but is independent of A when $Y = 1$. For simplicity, assume that the class-conditional probabilities for B are the same as for A. Given a record with attributes $A = 0, B = 0$, we can compute its posterior probabilities as follows:

$$\begin{aligned} P(Y=0|A=0,B=0) &= \frac{P(A=0|Y=0)P(B=0|Y=0)P(Y=0)}{P(A=0,B=0)} \\ &= \frac{0.16 \times P(Y=0)}{P(A=0,B=0)}. \end{aligned}$$

$$\begin{aligned} P(Y=1|A=0,B=0) &= \frac{P(A=0|Y=1)P(B=0|Y=1)P(Y=1)}{P(A=0,B=0)} \\ &= \frac{0.36 \times P(Y=1)}{P(A=0,B=0)}. \end{aligned}$$

If $P(Y = 0) = P(Y = 1)$, then the naïve Bayes classifier would assign the record to class 1. However, the truth is,

$$P(A=0,B=0|Y=0) = P(A=0|Y=0) = 0.4,$$

because A and B are perfectly correlated when $Y = 0$. As a result, the posterior probability for $Y = 0$ is

$$\begin{aligned} P(Y=0|A=0,B=0) &= \frac{P(A=0,B=0|Y=0)P(Y=0)}{P(A=0,B=0)} \\ &= \frac{0.4 \times P(Y=0)}{P(A=0,B=0)}, \end{aligned}$$

which is larger than that for $Y = 1$. The record should have been classified as class 0.

5.3.4 Bayes Error Rate

Suppose we know the true probability distribution that governs $P(\mathbf{X}|Y)$. The Bayesian classification method allows us to determine the ideal decision boundary for the classification task, as illustrated in the following example.

Example 5.3. Consider the task of identifying alligators and crocodiles based on their respective lengths. The average length of an adult crocodile is about 15 feet, while the average length of an adult alligator is about 12 feet. Assuming

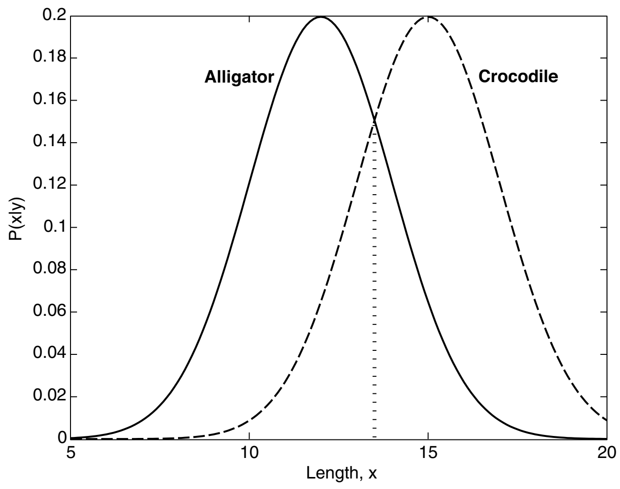


Figure 5.11. Comparing the likelihood functions of a crocodile and an alligator.

that their length x follows a Gaussian distribution with a standard deviation equal to 2 feet, we can express their class-conditional probabilities as follows:

$$P(X|\texttt{Crocodile}) = \frac{1}{\sqrt{2\pi}\cdot 2}\exp\left[-\frac{1}{2}\left(\frac{X-15}{2}\right)^2\right] \tag{5.19}$$

$$P(X|\texttt{Alligator}) = \frac{1}{\sqrt{2\pi}\cdot 2}\exp\left[-\frac{1}{2}\left(\frac{X-12}{2}\right)^2\right] \tag{5.20}$$

Figure 5.11 shows a comparison between the class-conditional probabilities for a crocodile and an alligator. Assuming that their prior probabilities are the same, the ideal decision boundary is located at some length $\hat{x}$ such that

$$P(X=\hat{x}|\texttt{Crocodile}) = P(X=\hat{x}|\texttt{Alligator}).$$

Using Equations 5.19 and 5.20, we obtain

$$\left(\frac{\hat{x}-15}{2}\right)^2 = \left(\frac{\hat{x}-12}{2}\right)^2,$$

which can be solved to yield $\hat{x} = 13.5$. The decision boundary for this example is located halfway between the two means. ■

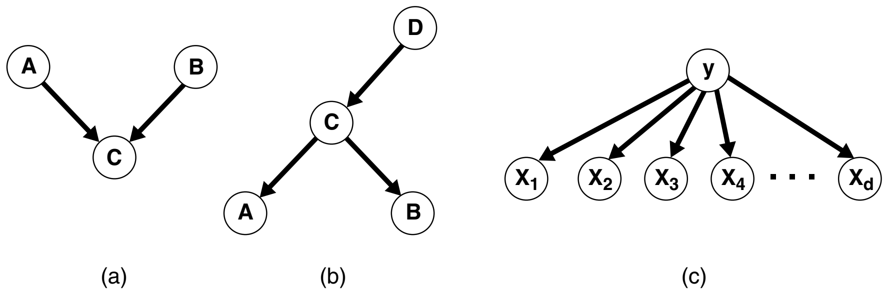


Figure 5.12. Representing probabilistic relationships using directed acyclic graphs.

When the prior probabilities are different, the decision boundary shifts toward the class with lower prior probability (see Exercise 10 on page 319). Furthermore, the minimum error rate attainable by any classifier on the given data can also be computed. The ideal decision boundary in the preceding example classifies all creatures whose lengths are less than $\hat{x}$ as alligators and those whose lengths are greater than $\hat{x}$ as crocodiles. The error rate of the classifier is given by the sum of the area under the posterior probability curve for crocodiles (from length 0 to $\hat{x}$) and the area under the posterior probability curve for alligators (from $\hat{x}$ to ∞):

$$\text{Error} = \int_0^{\hat{x}} P(\texttt{Crocodile}|X)dX + \int_{\hat{x}}^{\infty} P(\texttt{Alligator}|X)dX.$$

The total error rate is known as the **Bayes error rate**.

5.3.5 Bayesian Belief Networks

The conditional independence assumption made by naïve Bayes classifiers may seem too rigid, especially for classification problems in which the attributes are somewhat correlated. This section presents a more flexible approach for modeling the class-conditional probabilities $P(\mathbf{X}|Y)$. Instead of requiring all the attributes to be conditionally independent given the class, this approach allows us to specify which pair of attributes are conditionally independent. We begin with a discussion on how to represent and build such a probabilistic model, followed by an example of how to make inferences from the model.

Model Representation

A Bayesian belief network (BBN), or simply, Bayesian network, provides a graphical representation of the probabilistic relationships among a set of random variables. There are two key elements of a Bayesian network:

1. A directed acyclic graph (dag) encoding the dependence relationships among a set of variables.

2. A probability table associating each node to its immediate parent nodes.

Consider three random variables, A, B, and C, in which A and B are independent variables and each has a direct influence on a third variable, C. The relationships among the variables can be summarized into the directed acyclic graph shown in Figure 5.12(a). Each node in the graph represents a variable, and each arc asserts the dependence relationship between the pair of variables. If there is a directed arc from X to Y, then X is the **parent** of Y and Y is the **child** of X. Furthermore, if there is a directed path in the network from X to Z, then X is an **ancestor** of Z, while Z is a **descendant** of X. For example, in the diagram shown in Figure 5.12(b), A is a descendant of D and D is an ancestor of B. Both B and D are also non-descendants of A. An important property of the Bayesian network can be stated as follows:

Property 1 (Conditional Independence). *A node in a Bayesian network is conditionally independent of its non-descendants, if its parents are known.*

In the diagram shown in Figure 5.12(b), A is conditionally independent of both B and D given C because the nodes for B and D are non-descendants of node A. The conditional independence assumption made by a naïve Bayes classifier can also be represented using a Bayesian network, as shown in Figure 5.12(c), where y is the target class and $\{X_1, X_2, \ldots, X_d\}$ is the attribute set.

Besides the conditional independence conditions imposed by the network topology, each node is also associated with a probability table.

1. If a node X does not have any parents, then the table contains only the prior probability $P(X)$.

2. If a node X has only one parent, Y, then the table contains the conditional probability $P(X|Y)$.

3. If a node X has multiple parents, $\{Y_1, Y_2, \ldots, Y_k\}$, then the table contains the conditional probability $P(X|Y_1, Y_2, \ldots, Y_k)$.

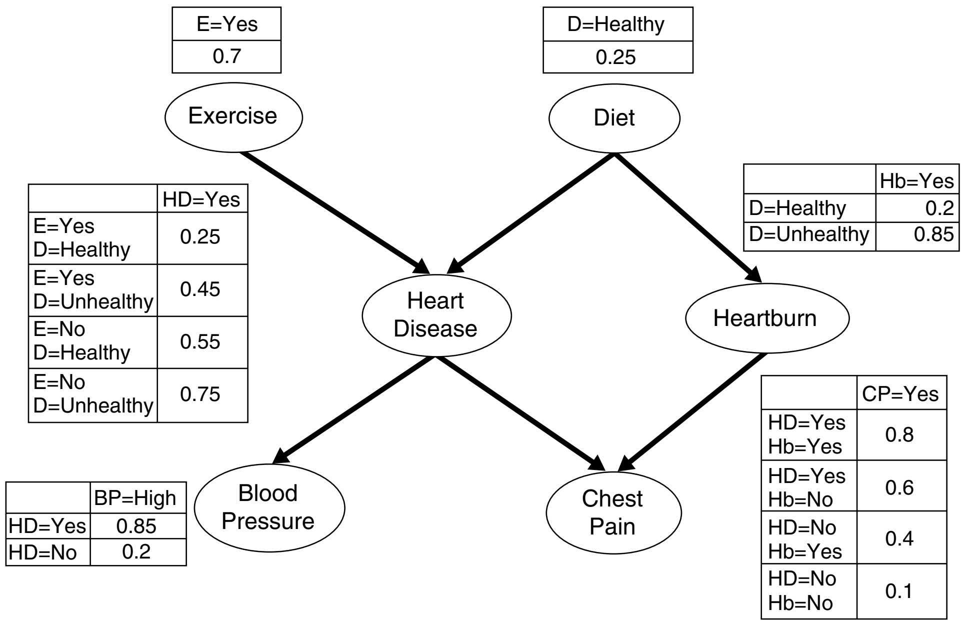


Figure 5.13. A Bayesian belief network for detecting heart disease and heartburn in patients.

Figure 5.13 shows an example of a Bayesian network for modeling patients with heart disease or heartburn problems. Each variable in the diagram is assumed to be binary-valued. The parent nodes for heart disease (HD) correspond to risk factors that may affect the disease, such as exercise (E) and diet (D). The child nodes for heart disease correspond to symptoms of the disease, such as chest pain (CP) and high blood pressure (BP). For example, the diagram shows that heartburn (Hb) may result from an unhealthy diet and may lead to chest pain.

The nodes associated with the risk factors contain only the prior probabilities, whereas the nodes for heart disease, heartburn, and their corresponding symptoms contain the conditional probabilities. To save space, some of the probabilities have been omitted from the diagram. The omitted probabilities can be recovered by noting that $P(X = \overline{x}) = 1 - P(X = x)$ and $P(X = \overline{x}|Y) = 1 - P(X = x|Y)$, where $\overline{x}$ denotes the opposite outcome of x. For example, the conditional probability

$$\begin{aligned} & P(\texttt{Heart Disease} = \texttt{No}|\texttt{Exercise} = \texttt{No}, \texttt{Diet} = \texttt{Healthy}) \\ = \; & 1 - P(\texttt{Heart Disease} = \texttt{Yes}|\texttt{Exercise} = \texttt{No}, \texttt{Diet} = \texttt{Healthy}) \\ = \; & 1 - 0.55 = 0.45. \end{aligned}$$

Model Building

Model building in Bayesian networks involves two steps: (1) creating the structure of the network, and (2) estimating the probability values in the tables associated with each node. The network topology can be obtained by encoding the subjective knowledge of domain experts. Algorithm 5.3 presents a systematic procedure for inducing the topology of a Bayesian network.

Algorithm 5.3 Algorithm for generating the topology of a Bayesian network.

```
1: Let $T = (X_1, X_2, \ldots, X_d)$ denote a total order of the variables.
2: for $j = 1$ to $d$ do
3:     Let $X_{T(j)}$ denote the $j^{th}$ highest order variable in $T$.
4:     Let $\pi(X_{T(j)}) = \{X_{T(1)}, X_{T(2)}, \ldots, X_{T(j-1)}\}$ denote the set of variables preceding $X_{T(j)}$.
5:     Remove the variables from $\pi(X_{T(j)})$ that do not affect $X_j$ (using prior knowledge).
6:     Create an arc between $X_{T(j)}$ and the remaining variables in $\pi(X_{T(j)})$.
7: end for
```

Example 5.4. Consider the variables shown in Figure 5.13. After performing Step 1, let us assume that the variables are ordered in the following way: (E, D, HD, Hb, CP, BP). From Steps 2 to 7, starting with variable D, we obtain the following conditional probabilities:

- $P(D|E)$ is simplified to $P(D)$.
- $P(HD|E, D)$ cannot be simplified.
- $P(Hb|HD, E, D)$ is simplified to $P(Hb|D)$.
- $P(CP|Hb, HD, E, D)$ is simplified to $P(CP|Hb, HD)$.
- $P(BP|CP, Hb, HD, E, D)$ is simplified to $P(BP|HD)$.

Based on these conditional probabilities, we can create arcs between the nodes (E, HD), (D, HD), (D, Hb), (HD, CP), (Hb, CP), and (HD, BP). These arcs result in the network structure shown in Figure 5.13. ■

Algorithm 5.3 guarantees a topology that does not contain any cycles. The proof for this is quite straightforward. If a cycle exists, then there must be at least one arc connecting the lower-ordered nodes to the higher-ordered nodes, and at least another arc connecting the higher-ordered nodes to the lower-ordered nodes. Since Algorithm 5.3 prevents any arc from connecting the lower-ordered nodes to the higher-ordered nodes, there cannot be any cycles in the topology.

Nevertheless, the network topology may change if we apply a different ordering scheme to the variables. Some topology may be inferior because it produces many arcs connecting between different pairs of nodes. In principle, we may have to examine all $d!$ possible orderings to determine the most appropriate topology, a task that can be computationally expensive. An alternative approach is to divide the variables into causal and effect variables, and then draw the arcs from each causal variable to its corresponding effect variables. This approach eases the task of building the Bayesian network structure.

Once the right topology has been found, the probability table associated with each node is determined. Estimating such probabilities is fairly straightforward and is similar to the approach used by naïve Bayes classifiers.

Example of Inferencing Using BBN

Suppose we are interested in using the BBN shown in Figure 5.13 to diagnose whether a person has heart disease. The following cases illustrate how the diagnosis can be made under different scenarios.

Case 1: No Prior Information

Without any prior information, we can determine whether the person is likely to have heart disease by computing the prior probabilities $P(\texttt{HD} = \texttt{Yes})$ and $P(\texttt{HD} = \texttt{No})$. To simplify the notation, let $\alpha \in \{\texttt{Yes}, \texttt{No}\}$ denote the binary values of `Exercise` and $\beta \in \{\texttt{Healthy}, \texttt{Unhealthy}\}$ denote the binary values of `Diet`.

$$\begin{aligned}
P(\texttt{HD} = \texttt{Yes}) &= \sum_\alpha \sum_\beta P(\texttt{HD} = \texttt{Yes}|E = \alpha, D = \beta)P(E = \alpha, D = \beta) \\
&= \sum_\alpha \sum_\beta P(\texttt{HD} = \texttt{Yes}|E = \alpha, D = \beta)P(E = \alpha)P(D = \beta) \\
&= 0.25 \times 0.7 \times 0.25 + 0.45 \times 0.7 \times 0.75 + 0.55 \times 0.3 \times 0.25 \\
&\quad + 0.75 \times 0.3 \times 0.75 \\
&= 0.49.
\end{aligned}$$

Since $P(\texttt{HD} = \texttt{no}) = 1 - P(\texttt{HD} = \texttt{yes}) = 0.51$, the person has a slightly higher chance of not getting the disease.

Case 2: High Blood Pressure

If the person has high blood pressure, we can make a diagnosis about heart disease by comparing the posterior probabilities, $P(\texttt{HD} = \texttt{Yes}|\texttt{BP} = \texttt{High})$ against $P(\texttt{HD} = \texttt{No}|\texttt{BP} = \texttt{High})$. To do this, we must compute $P(\texttt{BP} = \texttt{High})$:

$$\begin{aligned} P(\texttt{BP} = \texttt{High}) &= \sum_{\gamma} P(\texttt{BP} = \texttt{High}|\texttt{HD} = \gamma)P(\texttt{HD} = \gamma) \\ &= 0.85 \times 0.49 + 0.2 \times 0.51 = 0.5185. \end{aligned}$$

where $\gamma \in \{\texttt{Yes}, \texttt{No}\}$. Therefore, the posterior probability the person has heart disease is

$$\begin{aligned} P(\texttt{HD} = \texttt{Yes}|\texttt{BP} = \texttt{High}) &= \frac{P(\texttt{BP} = \texttt{High}|\texttt{HD} = \texttt{Yes})P(\texttt{HD} = \texttt{Yes})}{P(\texttt{BP} = \texttt{High})} \\ &= \frac{0.85 \times 0.49}{0.5185} = 0.8033. \end{aligned}$$

Similarly, $P(\texttt{HD} = \texttt{No}|\texttt{BP} = \texttt{High}) = 1 - 0.8033 = 0.1967$. Therefore, when a person has high blood pressure, it increases the risk of heart disease.

Case 3: High Blood Pressure, Healthy Diet, and Regular Exercise

Suppose we are told that the person exercises regularly and eats a healthy diet. How does the new information affect our diagnosis? With the new information, the posterior probability that the person has heart disease is

$$\begin{aligned} & P(\texttt{HD} = \texttt{Yes}|\texttt{BP} = \texttt{High}, D = \texttt{Healthy}, E = \texttt{Yes}) \\ = & \left[\frac{P(\texttt{BP} = \texttt{High}|\texttt{HD} = \texttt{Yes}, D = \texttt{Healthy}, E = \texttt{Yes})}{P(\texttt{BP} = \texttt{High}|D = \texttt{Healthy}, E = \texttt{Yes})}\right] \\ & \qquad \times P(\texttt{HD} = \texttt{Yes}|D = \texttt{Healthy}, E = \texttt{Yes}) \\ = & \frac{P(\texttt{BP} = \texttt{High}|\texttt{HD} = \texttt{Yes})P(\texttt{HD} = \texttt{Yes}|D = \texttt{Healthy}, E = \texttt{Yes})}{\sum_{\gamma} P(\texttt{BP} = \texttt{High}|\texttt{HD} = \gamma)P(\texttt{HD} = \gamma|D = \texttt{Healthy}, E = \texttt{Yes})} \\ = & \frac{0.85 \times 0.25}{0.85 \times 0.25 + 0.2 \times 0.75} \\ = & 0.5862, \end{aligned}$$

while the probability that the person does not have heart disease is

$$P(\texttt{HD} = \texttt{No}|\texttt{BP} = \texttt{High}, D = \texttt{Healthy}, E = \texttt{Yes}) = 1 - 0.5862 = 0.4138.$$

The model therefore suggests that eating healthily and exercising regularly may reduce a person's risk of getting heart disease.

Characteristics of BBN

Following are some of the general characteristics of the BBN method:

1. BBN provides an approach for capturing the prior knowledge of a particular domain using a graphical model. The network can also be used to encode causal dependencies among variables.

2. Constructing the network can be time consuming and requires a large amount of effort. However, once the structure of the network has been determined, adding a new variable is quite straightforward.

3. Bayesian networks are well suited to dealing with incomplete data. Instances with missing attributes can be handled by summing or integrating the probabilities over all possible values of the attribute.

4. Because the data is combined probabilistically with prior knowledge, the method is quite robust to model overfitting.

5.4 Artificial Neural Network (ANN)

The study of artificial neural networks (ANN) was inspired by attempts to simulate biological neural systems. The human brain consists primarily of nerve cells called **neurons**, linked together with other neurons via strands of fiber called **axons**. Axons are used to transmit nerve impulses from one neuron to another whenever the neurons are stimulated. A neuron is connected to the axons of other neurons via **dendrites**, which are extensions from the cell body of the neuron. The contact point between a dendrite and an axon is called a **synapse**. Neurologists have discovered that the human brain learns by changing the strength of the synaptic connection between neurons upon repeated stimulation by the same impulse.

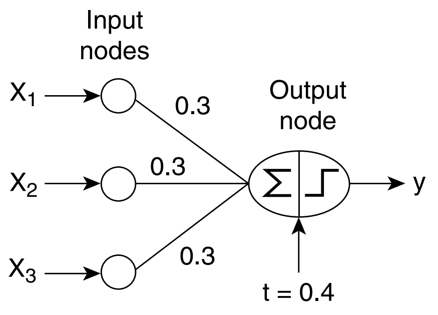
Analogous to human brain structure, an ANN is composed of an interconnected assembly of nodes and directed links. In this section, we will examine a family of ANN models, starting with the simplest model called **perceptron**, and show how the models can be trained to solve classification problems.

5.4.1 Perceptron

Consider the diagram shown in Figure 5.14. The table on the left shows a data set containing three boolean variables (x_1, x_2, x_3) and an output variable, y, that takes on the value -1 if at least two of the three inputs are zero, and $+1$ if at least two of the inputs are greater than zero.

X_1	X_2	X_3	y
1	0	0	–1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	–1
0	1	0	–1
0	1	1	1
0	0	0	–1

(a) Data set.



(b) Perceptron.

Figure 5.14. Modeling a boolean function using a perceptron.

Figure 5.14(b) illustrates a simple neural network architecture known as a perceptron. The perceptron consists of two types of nodes: input nodes, which are used to represent the input attributes, and an output node, which is used to represent the model output. The nodes in a neural network architecture are commonly known as neurons or units. In a perceptron, each input node is connected via a weighted link to the output node. The weighted link is used to emulate the strength of synaptic connection between neurons. As in biological neural systems, training a perceptron model amounts to adapting the weights of the links until they fit the input-output relationships of the underlying data.

A perceptron computes its output value, $\hat{y}$, by performing a weighted sum on its inputs, subtracting a bias factor t from the sum, and then examining the sign of the result. The model shown in Figure 5.14(b) has three input nodes, each of which has an identical weight of 0.3 to the output node and a bias factor of $t = 0.4$. The output computed by the model is

$$\hat{y} = \begin{cases} 1, & \text{if } 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 > 0; \\ -1, & \text{if } 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 < 0. \end{cases} \tag{5.21}$$

For example, if $x_1 = 1, x_2 = 1, x_3 = 0$, then $\hat{y} = +1$ because $0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4$ is positive. On the other hand, if $x_1 = 0, x_2 = 1, x_3 = 0$, then $\hat{y} = -1$ because the weighted sum subtracted by the bias factor is negative.

Note the difference between the input and output nodes of a perceptron. An input node simply transmits the value it receives to the outgoing link without performing any transformation. The output node, on the other hand, is a mathematical device that computes the weighted sum of its inputs, subtracts the bias term, and then produces an output that depends on the sign of the resulting sum. More specifically, the output of a perceptron model can be expressed mathematically as follows:

$$\hat{y} = sign\big(w_d x_d + w_{d-1} x_{d-1} + \ldots + w_2 x_2 + w_1 x_1 - t\big), \tag{5.22}$$

where $w_1, w_2, \ldots, w_d$ are the weights of the input links and $x_1, x_2, \ldots, x_d$ are the input attribute values. The sign function, which acts as an **activation function** for the output neuron, outputs a value $+1$ if its argument is positive and -1 if its argument is negative. The perceptron model can be written in a more compact form as follows:

$$\hat{y} = sign[w_d x_d + w_{d-1} x_{d-1} + \ldots + w_1 x_1 + w_0 x_0] = sign(\mathbf{w} \cdot \mathbf{x}), \tag{5.23}$$

where $w_0 = -t$, $x_0 = 1$, and $\mathbf{w} \cdot \mathbf{x}$ is the dot product between the weight vector $\mathbf{w}$ and the input attribute vector $\mathbf{x}$.

Learning Perceptron Model

During the training phase of a perceptron model, the weight parameters $\mathbf{w}$ are adjusted until the outputs of the perceptron become consistent with the true outputs of training examples. A summary of the perceptron learning algorithm is given in Algorithm 5.4.

The key computation for this algorithm is the weight update formula given in Step 7 of the algorithm:

$$w_j^{(k+1)} = w_j^{(k)} + \lambda\big(y_i - \hat{y}_i^{(k)}\big) x_{ij}, \tag{5.24}$$

where $w^{(k)}$ is the weight parameter associated with the i^{th} input link after the k^{th} iteration, λ is a parameter known as the **learning rate**, and x_{ij} is the value of the j^{th} attribute of the training example $\mathbf{x}_i$. The justification for the weight update formula is rather intuitive. Equation 5.24 shows that the new weight $w^{(k+1)}$ is a combination of the old weight $w^{(k)}$ and a term proportional

Algorithm 5.4 Perceptron learning algorithm.

```
1: Let $D = \{(\mathbf{x}_i, y_i) \mid i = 1, 2, \ldots, N\}$ be the set of training examples.
2: Initialize the weight vector with random values, $\mathbf{w}^{(0)}$
3: repeat
4:   for each training example $(\mathbf{x}_i, y_i) \in D$ do
5:     Compute the predicted output $\hat{y}_i^{(k)}$
6:     for each weight $w_j$ do
7:       Update the weight, $w_j^{(k+1)} = w_j^{(k)} + \lambda\big(y_i - \hat{y}_i^{(k)}\big)x_{ij}$.
8:     end for
9:   end for
10: until stopping condition is met
```

to the prediction error, $(y - \hat{y})$. If the prediction is correct, then the weight remains unchanged. Otherwise, it is modified in the following ways:

- If $y = +1$ and $\hat{y} = -1$, then the prediction error is $(y - \hat{y}) = 2$. To compensate for the error, we need to increase the value of the predicted output by increasing the weights of all links with positive inputs and decreasing the weights of all links with negative inputs.

- If $y_i = -1$ and $\hat{y} = +1$, then $(y - \hat{y}) = -2$. To compensate for the error, we need to decrease the value of the predicted output by decreasing the weights of all links with positive inputs and increasing the weights of all links with negative inputs.

In the weight update formula, links that contribute the most to the error term are the ones that require the largest adjustment. However, the weights should not be changed too drastically because the error term is computed only for the current training example. Otherwise, the adjustments made in earlier iterations will be undone. The learning rate λ, a parameter whose value is between 0 and 1, can be used to control the amount of adjustments made in each iteration. If λ is close to 0, then the new weight is mostly influenced by the value of the old weight. On the other hand, if λ is close to 1, then the new weight is sensitive to the amount of adjustment performed in the current iteration. In some cases, an adaptive λ value can be used; initially, λ is moderately large during the first few iterations and then gradually decreases in subsequent iterations.

The perceptron model shown in Equation 5.23 is linear in its parameters $\mathbf{w}$ and attributes $\mathbf{x}$. Because of this, the decision boundary of a perceptron, which is obtained by setting $\hat{y} = 0$, is a linear hyperplane that separates the data into two classes, -1 and $+1$. Figure 5.15 shows the decision boundary

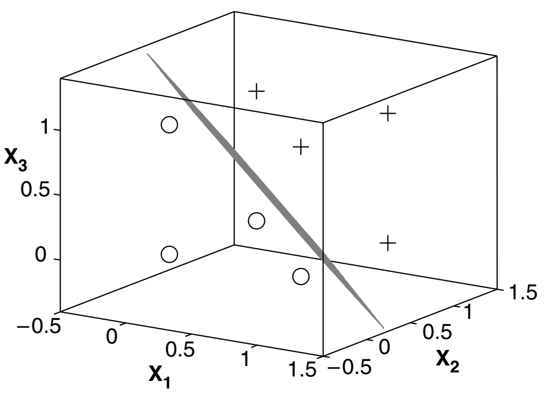


Figure 5.15. Perceptron decision boundary for the data given in Figure 5.14.

obtained by applying the perceptron learning algorithm to the data set given in Figure 5.14. The perceptron learning algorithm is guaranteed to converge to an optimal solution (as long as the learning rate is sufficiently small) for linearly separable classification problems. If the problem is not linearly separable, the algorithm fails to converge. Figure 5.16 shows an example of nonlinearly separable data given by the XOR function. Perceptron cannot find the right solution for this data because there is no linear hyperplane that can perfectly separate the training instances.

X_1	X_2	y
0	0	−1
1	0	1
0	1	1
1	1	−1

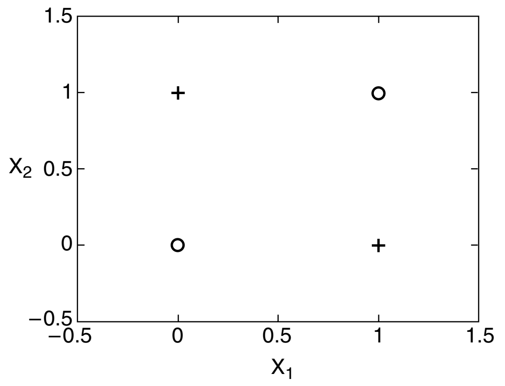


Figure 5.16. XOR classification problem. No linear hyperplane can separate the two classes.

5.4.2 Multilayer Artificial Neural Network

An artificial neural network has a more complex structure than that of a perceptron model. The additional complexities may arise in a number of ways:

1. The network may contain several intermediary layers between its input and output layers. Such intermediary layers are called **hidden layers** and the nodes embedded in these layers are called **hidden nodes**. The resulting structure is known as a multilayer neural network (see Figure 5.17). In a **feed-forward** neural network, the nodes in one layer are connected only to the nodes in the next layer. The perceptron is a single-layer, feed-forward neural network because it has only one layer of nodes—the output layer—that performs complex mathematical operations. In a **recurrent** neural network, the links may connect nodes within the same layer or nodes from one layer to the previous layers.

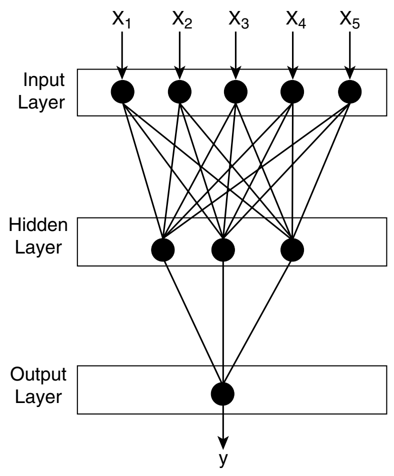


Figure 5.17. Example of a multilayer feed-forward artificial neural network (ANN).

2. The network may use types of activation functions other than the sign function. Examples of other activation functions include linear, sigmoid (logistic), and hyperbolic tangent functions, as shown in Figure 5.18. These activation functions allow the hidden and output nodes to produce output values that are nonlinear in their input parameters.

These additional complexities allow multilayer neural networks to model more complex relationships between the input and output variables. For ex-

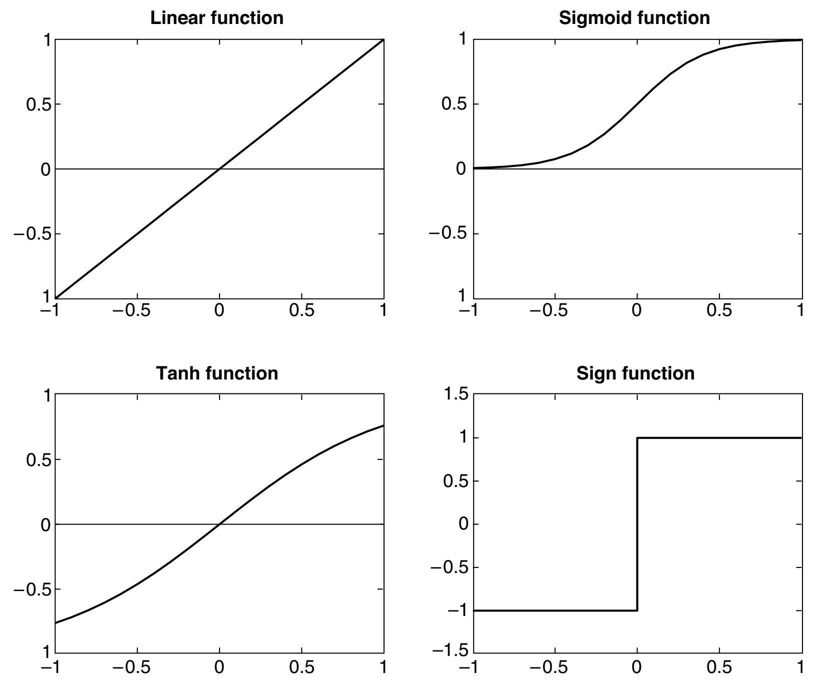
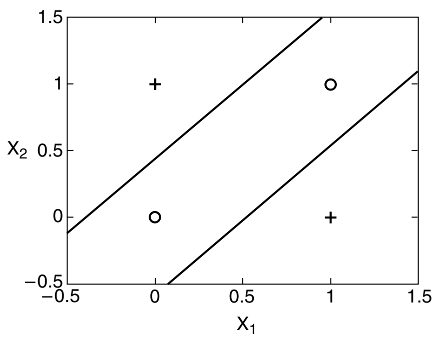


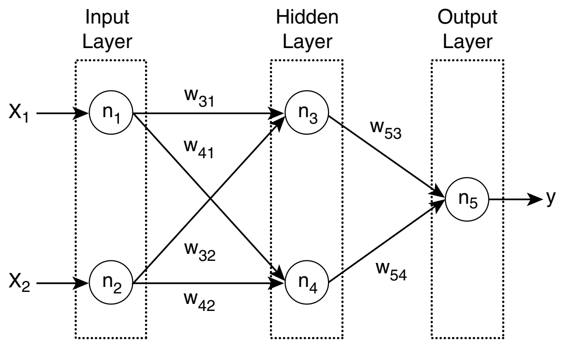
Figure 5.18. Types of activation functions in artificial neural networks.

ample, consider the XOR problem described in the previous section. The instances can be classified using two hyperplanes that partition the input space into their respective classes, as shown in Figure 5.19(a). Because a perceptron can create only one hyperplane, it cannot find the optimal solution. This problem can be addressed using a two-layer, feed-forward neural network, as shown in Figure 5.19(b). Intuitively, we can think of each hidden node as a perceptron that tries to construct one of the two hyperplanes, while the output node simply combines the results of the perceptrons to yield the decision boundary shown in Figure 5.19(a).

To learn the weights of an ANN model, we need an efficient algorithm that converges to the right solution when a sufficient amount of training data is provided. One approach is to treat each hidden node or output node in the network as an independent perceptron unit and to apply the same weight update formula as Equation 5.24. Obviously, this approach will not work because we lack *a priori* knowledge about the true outputs of the hidden nodes. This makes it difficult to determine the error term, $(y - \hat{y})$, associated



(a) Decision boundary.



(b) Neural network topology.

Figure 5.19. A two-layer, feed-forward neural network for the XOR problem.

with each hidden node. A methodology for learning the weights of a neural network based on the gradient descent approach is presented next.

Learning the ANN Model

The goal of the ANN learning algorithm is to determine a set of weights $\mathbf{w}$ that minimize the total sum of squared errors:

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2. \tag{5.25}$$

Note that the sum of squared errors depends on $\mathbf{w}$ because the predicted class $\hat{y}$ is a function of the weights assigned to the hidden and output nodes. Figure 5.20 shows an example of the error surface as a function of its two parameters, w_1 and w_2. This type of error surface is typically encountered when $\hat{y}_i$ is a linear function of its parameters, $\mathbf{w}$. If we replace $\hat{y} = \mathbf{w} \cdot \mathbf{x}$ into Equation 5.25, then the error function becomes quadratic in its parameters and a global minimum solution can be easily found.

In most cases, the output of an ANN is a nonlinear function of its parameters because of the choice of its activation functions (e.g., sigmoid or tanh function). As a result, it is no longer straightforward to derive a solution for $\mathbf{w}$ that is guaranteed to be globally optimal. Greedy algorithms such as those based on the gradient descent method have been developed to efficiently solve the optimization problem. The weight update formula used by the gradient

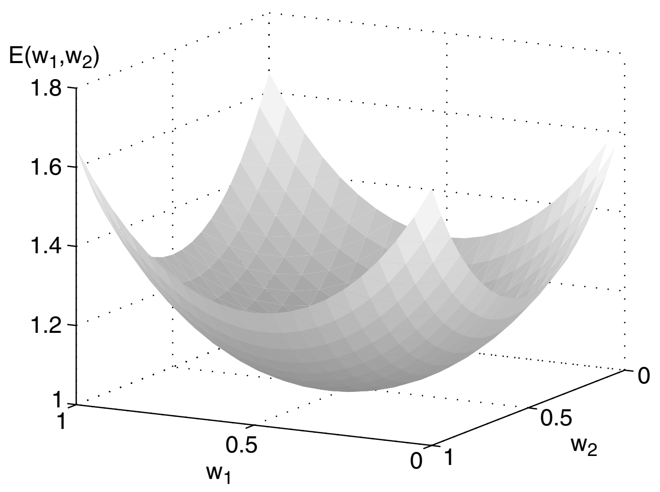


Figure 5.20. Error surface $E(w_1, w_2)$ for a two-parameter model.

descent method can be written as follows:

$$w_j \longleftarrow w_j - \lambda \frac{\partial E(\mathbf{w})}{\partial w_j}, \tag{5.26}$$

where λ is the learning rate. The second term states that the weight should be increased in a direction that reduces the overall error term. However, because the error function is nonlinear, it is possible that the gradient descent method may get trapped in a local minimum.

The gradient descent method can be used to learn the weights of the output and hidden nodes of a neural network. For hidden nodes, the computation is not trivial because it is difficult to assess their error term, $\partial E/\partial w_j$, without knowing what their output values should be. A technique known as **back-propagation** has been developed to address this problem. There are two phases in each iteration of the algorithm: the forward phase and the backward phase. During the forward phase, the weights obtained from the previous iteration are used to compute the output value of each neuron in the network. The computation progresses in the forward direction; i.e., outputs of the neurons at level k are computed prior to computing the outputs at level $k + 1$. During the backward phase, the weight update formula is applied in the reverse direction. In other words, the weights at level $k + 1$ are updated before the weights at level k are updated. This back-propagation approach allows us to use the errors for neurons at layer $k + 1$ to estimate the errors for neurons at layer k.

Design Issues in ANN Learning

Before we train a neural network to learn a classification task, the following design issues must be considered.

1. The number of nodes in the input layer should be determined. Assign an input node to each numerical or binary input variable. If the input variable is categorical, we could either create one node for each categorical value or encode the k-ary variable using $\lceil \log_2 k \rceil$ input nodes.

2. The number of nodes in the output layer should be established. For a two-class problem, it is sufficient to use a single output node. For a k-class problem, there are k output nodes.

3. The network topology (e.g., the number of hidden layers and hidden nodes, and feed-forward or recurrent network architecture) must be selected. Note that the target function representation depends on the weights of the links, the number of hidden nodes and hidden layers, biases in the nodes, and type of activation function. Finding the right topology is not an easy task. One way to do this is to start from a fully connected network with a sufficiently large number of nodes and hidden layers, and then repeat the model-building procedure with a smaller number of nodes. This approach can be very time consuming. Alternatively, instead of repeating the model-building procedure, we could remove some of the nodes and repeat the model evaluation procedure to select the right model complexity.

4. The weights and biases need to be initialized. Random assignments are usually acceptable.

5. Training examples with missing values should be removed or replaced with most likely values.

5.4.3 Characteristics of ANN

Following is a summary of the general characteristics of an artificial neural network:

1. Multilayer neural networks with at least one hidden layer are **universal approximators**; i.e., they can be used to approximate any target functions. Since an ANN has a very expressive hypothesis space, it is important to choose the appropriate network topology for a given problem to avoid model overfitting.

2. ANN can handle redundant features because the weights are automatically learned during the training step. The weights for redundant features tend to be very small.

3. Neural networks are quite sensitive to the presence of noise in the training data. One approach to handling noise is to use a validation set to determine the generalization error of the model. Another approach is to decrease the weight by some factor at each iteration.

4. The gradient descent method used for learning the weights of an ANN often converges to some local minimum. One way to escape from the local minimum is to add a momentum term to the weight update formula.

5. Training an ANN is a time consuming process, especially when the number of hidden nodes is large. Nevertheless, test examples can be classified rapidly.

5.5 Support Vector Machine (SVM)

A classification technique that has received considerable attention is support vector machine (SVM). This technique has its roots in statistical learning theory and has shown promising empirical results in many practical applications, from handwritten digit recognition to text categorization. SVM also works very well with high-dimensional data and avoids the curse of dimensionality problem. Another unique aspect of this approach is that it represents the decision boundary using a subset of the training examples, known as the **support vectors**.

To illustrate the basic idea behind SVM, we first introduce the concept of a **maximal margin hyperplane** and explain the rationale of choosing such a hyperplane. We then describe how a linear SVM can be trained to explicitly look for this type of hyperplane in linearly separable data. We conclude by showing how the SVM methodology can be extended to non-linearly separable data.

5.5.1 Maximum Margin Hyperplanes

Figure 5.21 shows a plot of a data set containing examples that belong to two different classes, represented as squares and circles. The data set is also linearly separable; i.e., we can find a hyperplane such that all the squares reside on one side of the hyperplane and all the circles reside on the other

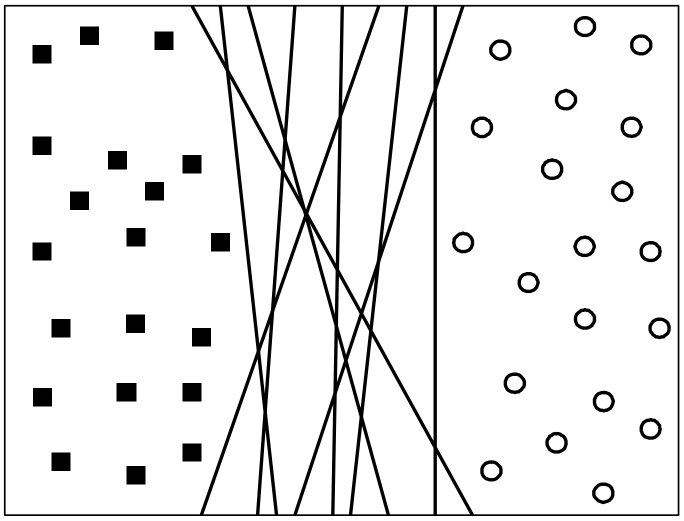


Figure 5.21. Possible decision boundaries for a linearly separable data set.

side. However, as shown in Figure 5.21, there are infinitely many such hyperplanes possible. Although their training errors are zero, there is no guarantee that the hyperplanes will perform equally well on previously unseen examples. The classifier must choose one of these hyperplanes to represent its decision boundary, based on how well they are expected to perform on test examples.

To get a clearer picture of how the different choices of hyperplanes affect the generalization errors, consider the two decision boundaries, B_1 and B_2, shown in Figure 5.22. Both decision boundaries can separate the training examples into their respective classes without committing any misclassification errors. Each decision boundary B_i is associated with a pair of hyperplanes, denoted as b_{i1} and b_{i2}, respectively. b_{i1} is obtained by moving a parallel hyperplane away from the decision boundary until it touches the closest square(s), whereas b_{i2} is obtained by moving the hyperplane until it touches the closest circle(s). The distance between these two hyperplanes is known as the margin of the classifier. From the diagram shown in Figure 5.22, notice that the margin for B_1 is considerably larger than that for B_2. In this example, B_1 turns out to be the maximum margin hyperplane of the training instances.

Rationale for Maximum Margin

Decision boundaries with large margins tend to have better generalization errors than those with small margins. Intuitively, if the margin is small, then

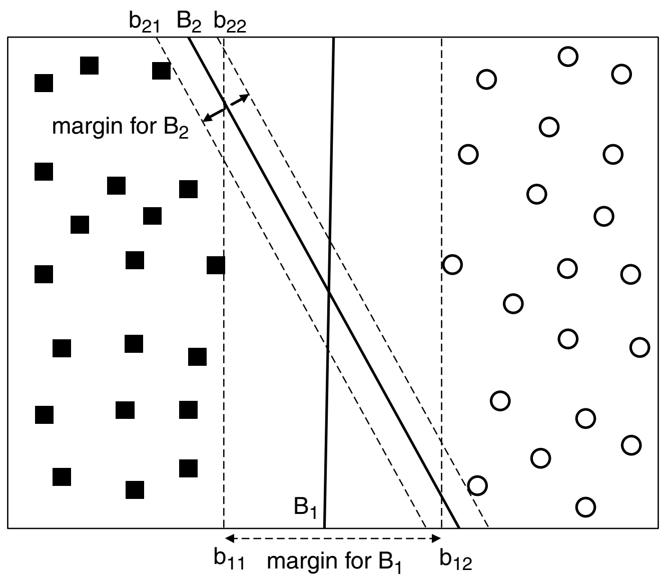


Figure 5.22. Margin of a decision boundary.

any slight perturbations to the decision boundary can have quite a significant impact on its classification. Classifiers that produce decision boundaries with small margins are therefore more susceptible to model overfitting and tend to generalize poorly on previously unseen examples.

A more formal explanation relating the margin of a linear classifier to its generalization error is given by a statistical learning principle known as **structural risk minimization** (SRM). This principle provides an upper bound to the generalization error of a classifier (R) in terms of its training error (R_e), the number of training examples (N), and the model complexity, otherwise known as its **capacity** (h). More specifically, with a probability of $1-\eta$, the generalization error of the classifier can be at worst

$$R \leq R_e + \varphi\left(\frac{h}{N}, \frac{\log(\eta)}{N}\right), \tag{5.27}$$

where φ is a monotone increasing function of the capacity h. The preceding inequality may seem quite familiar to the readers because it resembles the equation given in Section 4.4.4 (on page 179) for the minimum description length (MDL) principle. In this regard, SRM is another way to express generalization error as a tradeoff between training error and model complexity.

The capacity of a linear model is inversely related to its margin. Models with small margins have higher capacities because they are more flexible and can fit many training sets, unlike models with large margins. However, according to the SRM principle, as the capacity increases, the generalization error bound will also increase. Therefore, it is desirable to design linear classifiers that maximize the margins of their decision boundaries in order to ensure that their worst-case generalization errors are minimized. One such classifier is the **linear SVM**, which is explained in the next section.

5.5.2 Linear SVM: Separable Case

A linear SVM is a classifier that searches for a hyperplane with the largest margin, which is why it is often known as a **maximal margin classifier**. To understand how SVM learns such a boundary, we begin with some preliminary discussion about the decision boundary and margin of a linear classifier.

Linear Decision Boundary

Consider a binary classification problem consisting of N training examples. Each example is denoted by a tuple $(\mathbf{x_i}, y_i)$ $(i = 1, 2, \ldots, N)$, where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{id})^T$ corresponds to the attribute set for the i^{th} example. By convention, let $y_i \in \{-1, 1\}$ denote its class label. The decision boundary of a linear classifier can be written in the following form:

$$\mathbf{w} \cdot \mathbf{x} + b = 0, \tag{5.28}$$

where $\mathbf{w}$ and b are parameters of the model.

Figure 5.23 shows a two-dimensional training set consisting of squares and circles. A decision boundary that bisects the training examples into their respective classes is illustrated with a solid line. Any example located along the decision boundary must satisfy Equation 5.28. For example, if $\mathbf{x}_a$ and $\mathbf{x}_b$ are two points located on the decision boundary, then

$$\mathbf{w} \cdot \mathbf{x}_a + b = 0,$$
$$\mathbf{w} \cdot \mathbf{x}_b + b = 0.$$

Subtracting the two equations will yield the following:

$$\mathbf{w} \cdot (\mathbf{x}_b - \mathbf{x}_a) = 0,$$

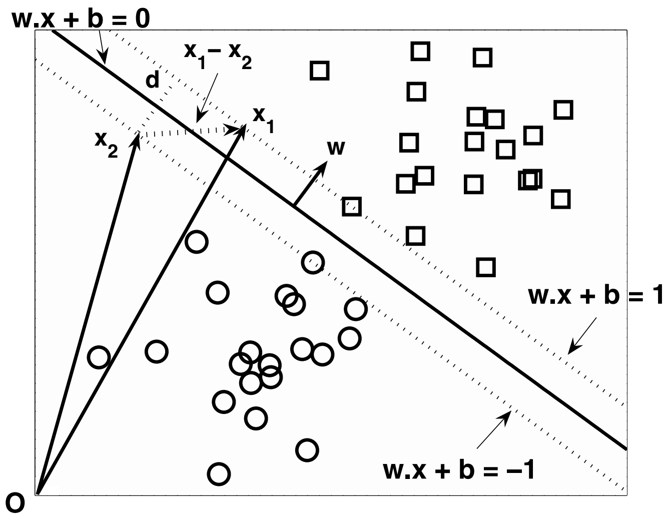


Figure 5.23. Decision boundary and margin of SVM.

where $\mathbf{x}_b - \mathbf{x}_a$ is a vector parallel to the decision boundary and is directed from $\mathbf{x}_a$ to $\mathbf{x}_b$. Since the dot product is zero, the direction for $\mathbf{w}$ must be perpendicular to the decision boundary, as shown in Figure 5.23.

For any square $\mathbf{x}_s$ located above the decision boundary, we can show that

$$\mathbf{w} \cdot \mathbf{x}_s + b = k, \tag{5.29}$$

where $k > 0$. Similarly, for any circle $\mathbf{x}_c$ located below the decision boundary, we can show that

$$\mathbf{w} \cdot \mathbf{x}_c + b = k', \tag{5.30}$$

where $k' < 0$. If we label all the squares as class $+1$ and all the circles as class -1, then we can predict the class label y for any test example $\mathbf{z}$ in the following way:

$$y = \begin{cases} 1, & \text{if } \mathbf{w} \cdot \mathbf{z} + b > 0; \\ -1, & \text{if } \mathbf{w} \cdot \mathbf{z} + b < 0. \end{cases} \tag{5.31}$$

Margin of a Linear Classifier

Consider the square and the circle that are closest to the decision boundary. Since the square is located above the decision boundary, it must satisfy Equation 5.29 for some positive value k, whereas the circle must satisfy Equation

5.30 for some negative value k'. We can rescale the parameters $\mathbf{w}$ and b of the decision boundary so that the two parallel hyperplanes b_{i1} and b_{i2} can be expressed as follows:

$$b_{i1}: \ \mathbf{w} \cdot \mathbf{x} + b = 1, \tag{5.32}$$
$$b_{i2}: \ \mathbf{w} \cdot \mathbf{x} + b = -1. \tag{5.33}$$

The margin of the decision boundary is given by the distance between these two hyperplanes. To compute the margin, let $\mathbf{x}_1$ be a data point located on b_{i1} and $\mathbf{x}_2$ be a data point on b_{i2}, as shown in Figure 5.23. Upon substituting these points into Equations 5.32 and 5.33, the margin d can be computed by subtracting the second equation from the first equation:

$$\begin{aligned} &\mathbf{w} \cdot (\mathbf{x}_1 - \mathbf{x}_2) = 2 \\ &\|\mathbf{w}\| \times d = 2 \\ &\therefore d = \frac{2}{\|\mathbf{w}\|}. \end{aligned} \tag{5.34}$$

Learning a Linear SVM Model

The training phase of SVM involves estimating the parameters $\mathbf{w}$ and b of the decision boundary from the training data. The parameters must be chosen in such a way that the following two conditions are met:

$$\begin{aligned} \mathbf{w} \cdot \mathbf{x_i} + b &\geq \ \ 1 \text{ if } y_i = 1, \\ \mathbf{w} \cdot \mathbf{x_i} + b &\leq -1 \text{ if } y_i = -1. \end{aligned} \tag{5.35}$$

These conditions impose the requirements that all training instances from class $y = 1$ (i.e., the squares) must be located on or above the hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 1$, while those instances from class $y = -1$ (i.e., the circles) must be located on or below the hyperplane $\mathbf{w} \cdot \mathbf{x} + b = -1$. Both inequalities can be summarized in a more compact form as follows:

$$y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1, \quad i = 1, 2, \ldots, N. \tag{5.36}$$

Although the preceding conditions are also applicable to any linear classifiers (including perceptrons), SVM imposes an additional requirement that the margin of its decision boundary must be maximal. Maximizing the margin, however, is equivalent to minimizing the following objective function:

$$f(\mathbf{w}) = \frac{\|\mathbf{w}\|^2}{2}. \tag{5.37}$$

Definition 5.1 (Linear SVM: Separable Case). The learning task in SVM can be formalized as the following constrained optimization problem:

$$\min_{\mathbf{w}} \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \qquad y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1, \quad i = 1, 2, \ldots, N.$$

Since the objective function is quadratic and the constraints are linear in the parameters $\mathbf{w}$ and b, this is known as a **convex** optimization problem, which can be solved using the standard **Lagrange multiplier** method. Following is a brief sketch of the main ideas for solving the optimization problem. A more detailed discussion is given in Appendix E.

First, we must rewrite the objective function in a form that takes into account the constraints imposed on its solutions. The new objective function is known as the Lagrangian for the optimization problem:

$$L_P = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \lambda_i \Big(y_i(\mathbf{w} \cdot \mathbf{x_i} + b) - 1 \Big), \tag{5.38}$$

where the parameters λ_i are called the Lagrange multipliers. The first term in the Lagrangian is the same as the original objective function, while the second term captures the inequality constraints. To understand why the objective function must be modified, consider the original objective function given in Equation 5.37. It is easy to show that the function is minimized when $\mathbf{w} = \mathbf{0}$, a null vector whose components are all zeros. Such a solution, however, violates the constraints given in Definition 5.1 because there is no feasible solution for b. The solutions for $\mathbf{w}$ and b are infeasible if they violate the inequality constraints; i.e., if $y_i(\mathbf{w}\cdot\mathbf{x_i}+b)-1 < 0$. The Lagrangian given in Equation 5.38 incorporates this constraint by subtracting the term from its original objective function. Assuming that $\lambda_i \geq 0$, it is clear that any infeasible solution may only increase the value of the Lagrangian.

To minimize the Lagrangian, we must take the derivative of L_P with respect to $\mathbf{w}$ and b and set them to zero:

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Longrightarrow \mathbf{w} = \sum_{i=1}^{N} \lambda_i y_i \mathbf{x}_i, \tag{5.39}$$

$$\frac{\partial L_p}{\partial b} = 0 \Longrightarrow \sum_{i=1}^{N} \lambda_i y_i = 0. \tag{5.40}$$

Because the Lagrange multipliers are unknown, we still cannot solve for $\mathbf{w}$ and b. If Definition 5.1 contains only equality instead of inequality constraints, then we can use the N equations from equality constraints along with Equations 5.39 and 5.40 to find the feasible solutions for $\mathbf{w}$, b, and λ_i. Note that the Lagrange multipliers for equality constraints are free parameters that can take any values.

One way to handle the inequality constraints is to transform them into a set of equality constraints. This is possible as long as the Lagrange multipliers are restricted to be non-negative. Such transformation leads to the following constraints on the Lagrange multipliers, which are known as the Karush-Kuhn-Tucker (KKT) conditions:

$$\lambda_i \geq 0, \tag{5.41}$$

$$\lambda_i \big[y_i(\mathbf{w} \cdot \mathbf{x}_i + b) - 1 \big] = 0. \tag{5.42}$$

At first glance, it may seem that there are as many Lagrange multipliers as there are training instances. It turns out that many of the Lagrange multipliers become zero after applying the constraint given in Equation 5.42. The constraint states that the Lagrange multiplier λ_i must be zero unless the training instance $\mathbf{x}_i$ satisfies the equation $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$. Such training instance, with $\lambda_i > 0$, lies along the hyperplanes b_{i1} or b_{i2} and is known as a support vector. Training instances that do not reside along these hyperplanes have $\lambda_i = 0$. Equations 5.39 and 5.42 also suggest that the parameters $\mathbf{w}$ and b, which define the decision boundary, depend only on the support vectors.

Solving the preceding optimization problem is still quite a daunting task because it involves a large number of parameters: $\mathbf{w}$, b, and λ_i. The problem can be simplified by transforming the Lagrangian into a function of the Lagrange multipliers only (this is known as the dual problem). To do this, we first substitute Equations 5.39 and 5.40 into Equation 5.38. This will lead to the following dual formulation of the optimization problem:

$$L_D = \sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \mathbf{x_i} \cdot \mathbf{x_j}. \tag{5.43}$$

The key differences between the dual and primary Lagrangians are as follows:

1. The dual Lagrangian involves only the Lagrange multipliers and the training data, while the primary Lagrangian involves the Lagrange multipliers as well as parameters of the decision boundary. Nevertheless, the solutions for both optimization problems are equivalent.

2. The quadratic term in Equation 5.43 has a negative sign, which means that the original minimization problem involving the primary Lagrangian, L_P, has turned into a maximization problem involving the dual Lagrangian, L_D.

For large data sets, the dual optimization problem can be solved using numerical techniques such as quadratic programming, a topic that is beyond the scope of this book. Once the λ_i's are found, we can use Equations 5.39 and 5.42 to obtain the feasible solutions for $\mathbf{w}$ and b. The decision boundary can be expressed as follows:

$$\left(\sum_{i=1}^{N} \lambda_i y_i \mathbf{x_i} \cdot \mathbf{x}\right) + b = 0. \tag{5.44}$$

b is obtained by solving Equation 5.42 for the support vectors. Because the λ_i's are calculated numerically and can have numerical errors, the value computed for b may not be unique. Instead it depends on the support vector used in Equation 5.42. In practice, the average value for b is chosen to be the parameter of the decision boundary.

Example 5.5. Consider the two-dimensional data set shown in Figure 5.24, which contains eight training instances. Using quadratic programming, we can solve the optimization problem stated in Equation 5.43 to obtain the Lagrange multiplier λ_i for each training instance. The Lagrange multipliers are depicted in the last column of the table. Notice that only the first two instances have non-zero Lagrange multipliers. These instances correspond to the support vectors for this data set.

Let $\mathbf{w} = (w_1, w_2)$ and b denote the parameters of the decision boundary. Using Equation 5.39, we can solve for w_1 and w_2 in the following way:

$$\begin{aligned} w_1 &= \sum_i \lambda_i y_i x_{i1} = 65.5621 \times 1 \times 0.3858 + 65.5621 \times -1 \times 0.4871 = -6.64. \\ w_2 &= \sum_i \lambda_i y_i x_{i2} = 65.5621 \times 1 \times 0.4687 + 65.5621 \times -1 \times 0.611 = -9.32. \end{aligned}$$

The bias term b can be computed using Equation 5.42 for each support vector:

$$\begin{aligned} b^{(1)} &= 1 - \mathbf{w} \cdot \mathbf{x}_1 = 1 - (-6.64)(0.3858) - (-9.32)(0.4687) = 7.9300. \\ b^{(2)} &= -1 - \mathbf{w} \cdot \mathbf{x}_2 = -1 - (-6.64)(0.4871) - (-9.32)(0.611) = 7.9289. \end{aligned}$$

Averaging these values, we obtain $b = 7.93$. The decision boundary corresponding to these parameters is shown in Figure 5.24. ■

x_1	x_2	y	Lagrange Multiplier
0.3858	0.4687	1	65.5261
0.4871	0.611	–1	65.5261
0.9218	0.4103	–1	0
0.7382	0.8936	–1	0
0.1763	0.0579	1	0
0.4057	0.3529	1	0
0.9355	0.8132	–1	0
0.2146	0.0099	1	0

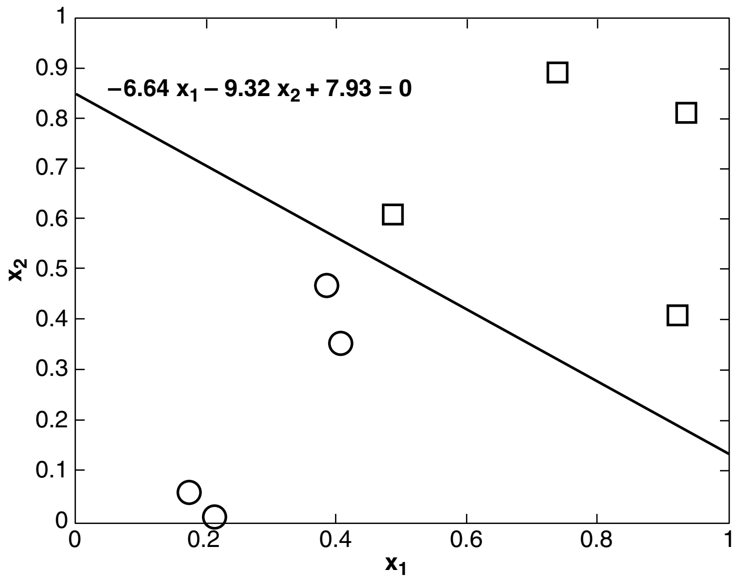


Figure 5.24. Example of a linearly separable data set.

Once the parameters of the decision boundary are found, a test instance $\mathbf{z}$ is classified as follows:

$$f(\mathbf{z}) = sign\big(\mathbf{w}\cdot\mathbf{z} + b\big) = sign\bigg(\sum_{i=1}^{N} \lambda_i y_i \mathbf{x_i}\cdot\mathbf{z} + b\bigg).$$

If $f(\mathbf{z}) = 1$, then the test instance is classified as a positive class; otherwise, it is classified as a negative class.

5.5.3 Linear SVM: Nonseparable Case

Figure 5.25 shows a data set that is similar to Figure 5.22, except it has two new examples, P and Q. Although the decision boundary B_1 misclassifies the new examples, while B_2 classifies them correctly, this does not mean that B_2 is a better decision boundary than B_1 because the new examples may correspond to noise in the training data. B_1 should still be preferred over B_2 because it has a wider margin, and thus, is less susceptible to overfitting. However, the SVM formulation presented in the previous section constructs only decision boundaries that are mistake-free. This section examines how the formulation can be modified to learn a decision boundary that is tolerable to small training errors using a method known as the **soft margin** approach. More importantly, the method presented in this section allows SVM to construct a linear decision boundary even in situations where the classes are not linearly separable. To do this, the learning algorithm in SVM must consider the trade-off between the width of the margin and the number of training errors committed by the linear decision boundary.

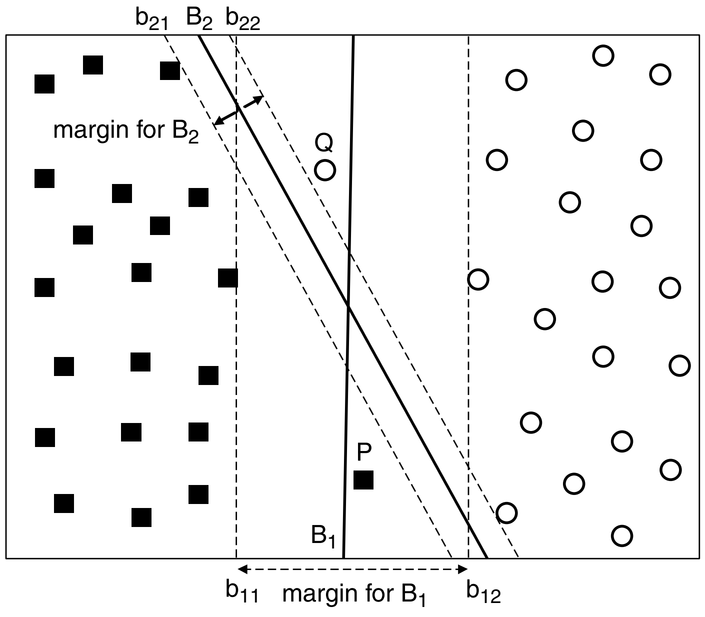


Figure 5.25. Decision boundary of SVM for the nonseparable case.

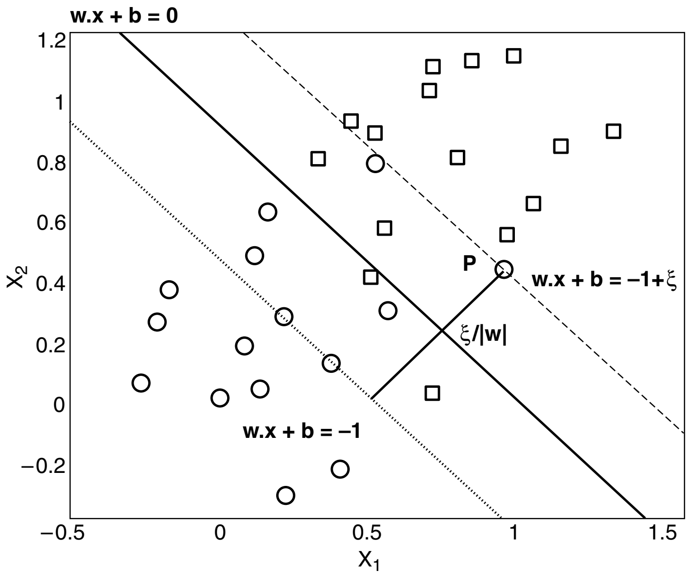


Figure 5.26. Slack variables for nonseparable data.

While the original objective function given in Equation 5.37 is still applicable, the decision boundary B_1 no longer satisfies all the constraints given in Equation 5.36. The inequality constraints must therefore be relaxed to accommodate the nonlinearly separable data. This can be done by introducing positive-valued **slack variables** (ξ) into the constraints of the optimization problem, as shown in the following equations:

$$\begin{aligned} \mathbf{w} \cdot \mathbf{x_i} + b &\geq 1 - \xi_i \quad \text{if } y_i = 1, \\ \mathbf{w} \cdot \mathbf{x_i} + b &\leq -1 + \xi_i \quad \text{if } y_i = -1, \end{aligned} \tag{5.45}$$

where $\forall i: \ \xi_i > 0$.

To interpret the meaning of the slack variables ξ_i, consider the diagram shown in Figure 5.26. The circle **P** is one of the instances that violates the constraints given in Equation 5.35. Let $\mathbf{w} \cdot \mathbf{x} + b = -1 + \xi$ denote a line that is parallel to the decision boundary and passes through the point **P**. It can be shown that the distance between this line and the hyperplane $\mathbf{w} \cdot \mathbf{x} + b = -1$ is $\xi/\|\mathbf{w}\|$. Thus, ξ provides an estimate of the error of the decision boundary on the training example **P**.

In principle, we can apply the same objective function as before and impose the conditions given in Equation 5.45 to find the decision boundary. However,

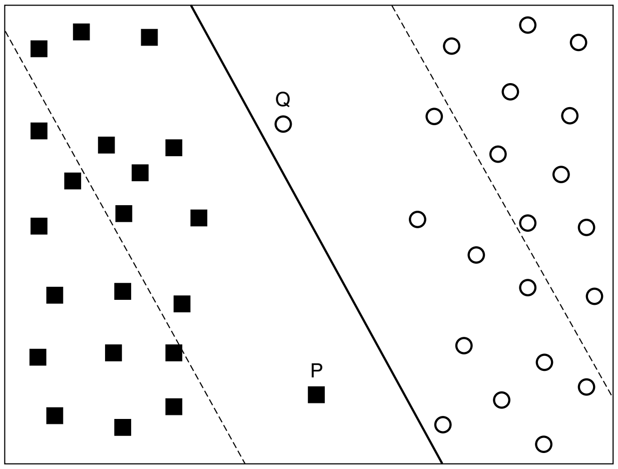


Figure 5.27. A decision boundary that has a wide margin but large training error.

since there are no constraints on the number of mistakes the decision boundary can make, the learning algorithm may find a decision boundary with a very wide margin but misclassifies many of the training examples, as shown in Figure 5.27. To avoid this problem, the objective function must be modified to penalize a decision boundary with large values of slack variables. The modified objective function is given by the following equation:

$$f(\mathbf{w}) = \frac{\|\mathbf{w}\|^2}{2} + C(\sum_{i=1}^{N} \xi_i)^k,$$

where C and k are user-specified parameters representing the penalty of misclassifying the training instances. For the remainder of this section, we assume $k = 1$ to simplify the problem. The parameter C can be chosen based on the model's performance on the validation set.

It follows that the Lagrangian for this constrained optimization problem can be written as follows:

$$L_P = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \lambda_i \{y_i(\mathbf{w} \cdot \mathbf{x_i} + b) - 1 + \xi_i\} - \sum_{i=1}^{N} \mu_i \xi_i, \quad (5.46)$$

where the first two terms are the objective function to be minimized, the third term represents the inequality constraints associated with the slack variables, and the last term is the result of the non-negativity requirements on the values of ξ_i's. Furthermore, the inequality constraints can be transformed into equality constraints using the following KKT conditions:

$$\xi_i \geq 0, \quad \lambda_i \geq 0, \quad \mu_i \geq 0, \tag{5.47}$$

$$\lambda_i\{y_i(\mathbf{w}\cdot\mathbf{x}_i + b) - 1 + \xi_i\} = 0, \tag{5.48}$$

$$\mu_i\xi_i = 0. \tag{5.49}$$

Note that the Lagrange multiplier λ_i given in Equation 5.48 is non-vanishing only if the training instance resides along the lines $\mathbf{w}\cdot\mathbf{x}_i + b = \pm 1$ or has $\xi_i > 0$. On the other hand, the Lagrange multipliers μ_i given in Equation 5.49 are zero for any training instances that are misclassified (i.e., having $\xi_i > 0$).

Setting the first-order derivative of L with respect to $\mathbf{w}$, b, and ξ_i to zero would result in the following equations:

$$\frac{\partial L}{\partial w_j} = w_j - \sum_{i=1}^{N}\lambda_i y_i x_{ij} = 0 \implies w_j = \sum_{i=1}^{N}\lambda_i y_i x_{ij}. \tag{5.50}$$

$$\frac{\partial L}{\partial b} = -\sum_{i=1}^{N}\lambda_i y_i = 0 \implies \sum_{i=1}^{N}\lambda_i y_i = 0. \tag{5.51}$$

$$\frac{\partial L}{\partial \xi_i} = C - \lambda_i - \mu_i = 0 \implies \lambda_i + \mu_i = C. \tag{5.52}$$

Substituting Equations 5.50, 5.51, and 5.52 into the Lagrangian will produce the following dual Lagrangian:

$$\begin{aligned} L_D &= \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x}_i\cdot\mathbf{x}_j + C\sum_i \xi_i \\ &\quad -\sum_i \lambda_i\{y_i(\sum_j \lambda_j y_j \mathbf{x}_i\cdot\mathbf{x}_j + b) - 1 + \xi_i\} \\ &\quad -\sum_i (C-\lambda_i)\xi_i \\ &= \sum_{i=1}^{N}\lambda_i - \frac{1}{2}\sum_{i,j}\lambda_i\lambda_j y_i y_j \mathbf{x_i}\cdot\mathbf{x_j}, \end{aligned} \tag{5.53}$$

which turns out to be identical to the dual Lagrangian for linearly separable data (see Equation 5.40 on page 262). Nevertheless, the constraints imposed on the Lagrange multipliers λ_i's are slightly different those in the linearly separable case. In the linearly separable case, the Lagrange multipliers must be non-negative, i.e., $\lambda_i \geq 0$. On the other hand, Equation 5.52 suggests that λ_i should not exceed C (since both μ_i and λ_i are non-negative). Therefore, the Lagrange multipliers for nonlinearly separable data are restricted to $0 \leq \lambda_i \leq C$.

The dual problem can then be solved numerically using quadratic programming techniques to obtain the Lagrange multipliers λ_i. These multipliers can be replaced into Equation 5.50 and the KKT conditions to obtain the parameters of the decision boundary.

5.5.4 Nonlinear SVM

The SVM formulations described in the previous sections construct a linear decision boundary to separate the training examples into their respective classes. This section presents a methodology for applying SVM to data sets that have nonlinear decision boundaries. The trick here is to transform the data from its original coordinate space in $\mathbf{x}$ into a new space $\Phi(\mathbf{x})$ so that a linear decision boundary can be used to separate the instances in the transformed space. After doing the transformation, we can apply the methodology presented in the previous sections to find a linear decision boundary in the transformed space.

Attribute Transformation

To illustrate how attribute transformation can lead to a linear decision boundary, Figure 5.28(a) shows an example of a two-dimensional data set consisting of squares (classified as $y = 1$) and circles (classified as $y = -1$). The data set is generated in such a way that all the circles are clustered near the center of the diagram and all the squares are distributed farther away from the center. Instances of the data set can be classified using the following equation:

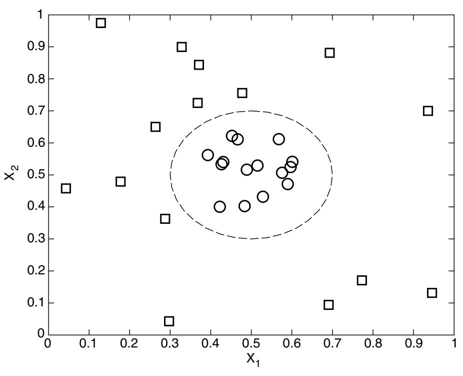
$$y(x_1, x_2) = \begin{cases} 1 & \text{if } \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} > 0.2, \\ -1 & \text{otherwise.} \end{cases} \tag{5.54}$$

The decision boundary for the data can therefore be written as follows:

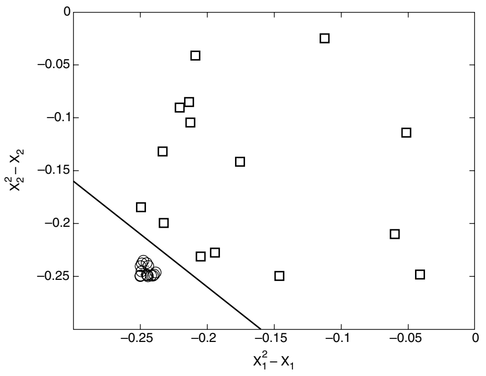
$$\sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} = 0.2,$$

which can be further simplified into the following quadratic equation:

$$x_1^2 - x_1 + x_2^2 - x_2 = -0.46.$$



(a) Decision boundary in the original two-dimensional space.



(b) Decision boundary in the transformed space.

Figure 5.28. Classifying data with a nonlinear decision boundary.

A nonlinear transformation Φ is needed to map the data from its original feature space into a new space where the decision boundary becomes linear. Suppose we choose the following transformation:

$$\Phi : (x_1, x_2) \longrightarrow (x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, 1). \tag{5.55}$$

In the transformed space, we can find the parameters $\mathbf{w} = (w_0, w_1, \ldots, w_4)$ such that:

$$w_4 x_1^2 + w_3 x_2^2 + w_2\sqrt{2}x_1 + w_1\sqrt{2}x_2 + w_0 = 0.$$

For illustration purposes, let us plot the graph of $x_2^2 - x_2$ versus $x_1^2 - x_1$ for the previously given instances. Figure 5.28(b) shows that in the transformed space, all the circles are located in the lower right-hand side of the diagram. A linear decision boundary can therefore be constructed to separate the instances into their respective classes.

One potential problem with this approach is that it may suffer from the curse of dimensionality problem often associated with high-dimensional data. We will show how nonlinear SVM avoids this problem (using a method known as the kernel trick) later in this section.

Learning a Nonlinear SVM Model

Although the attribute transformation approach seems promising, it raises several implementation issues. First, it is not clear what type of mapping function should be used to ensure that a linear decision boundary can be constructed in the transformed space. One possibility is to transform the data into an infinite dimensional space, but such a high-dimensional space may not be that easy to work with. Second, even if the appropriate mapping function is known, solving the constrained optimization problem in the high-dimensional feature space is a computationally expensive task.

To illustrate these issues and examine the ways they can be addressed, let us assume that there is a suitable function, $\Phi(\mathbf{x})$, to transform a given data set. After the transformation, we need to construct a linear decision boundary that will separate the instances into their respective classes. The linear decision boundary in the transformed space has the following form: $\mathbf{w} \cdot \Phi(\mathbf{x}) + b = 0$.

Definition 5.2 (Nonlinear SVM). The learning task for a nonlinear SVM can be formalized as the following optimization problem:

$$\min_{\mathbf{w}} \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \quad y_i(\mathbf{w} \cdot \Phi(\mathbf{x}_i) + b) \geq 1, \quad i = 1, 2, \ldots, N.$$

Note the similarity between the learning task of a nonlinear SVM to that of a linear SVM (see Definition 5.1 on page 262). The main difference is that, instead of using the original attributes $\mathbf{x}$, the learning task is performed on the transformed attributes $\Phi(\mathbf{x})$. Following the approach taken in Sections 5.5.2 and 5.5.3 for linear SVM, we may derive the following dual Lagrangian for the constrained optimization problem:

$$L_D = \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j) \tag{5.56}$$

Once the λ_i's are found using quadratic programming techniques, the parameters $\mathbf{w}$ and b can be derived using the following equations:

$$\mathbf{w} = \sum_{i} \lambda_i y_i \Phi(\mathbf{x}_i) \tag{5.57}$$

$$\lambda_i \{ y_i (\sum_{j} \lambda_j y_j \Phi(\mathbf{x}_j) \cdot \Phi(\mathbf{x}_i) + b) - 1 \} = 0, \tag{5.58}$$

which are analogous to Equations 5.39 and 5.40 for linear SVM. Finally, a test instance z can be classified using the following equation:

$$f(\mathbf{z}) = sign\big(\mathbf{w} \cdot \Phi(\mathbf{z}) + b\big) = sign\bigg(\sum_{i=1}^{n} \lambda_i y_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{z}) + b\bigg). \tag{5.59}$$

Except for Equation 5.57, note that the rest of the computations (Equations 5.58 and 5.59) involve calculating the dot product (i.e., similarity) between pairs of vectors in the transformed space, $\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$. Such computation can be quite cumbersome and may suffer from the curse of dimensionality problem. A breakthrough solution to this problem comes in the form of a method known as the **kernel trick**.

Kernel Trick

The dot product is often regarded as a measure of similarity between two input vectors. For example, the cosine similarity described in Section 2.4.5 on page 73 can be defined as the dot product between two vectors that are normalized to unit length. Analogously, the dot product $\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$ can also be regarded as a measure of similarity between two instances, $\mathbf{x}_i$ and $\mathbf{x}_j$, in the transformed space.

The kernel trick is a method for computing similarity in the transformed space using the original attribute set. Consider the mapping function Φ given in Equation 5.55. The dot product between two input vectors $\mathbf{u}$ and $\mathbf{v}$ in the transformed space can be written as follows:

$$\begin{aligned} \Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) &= (u_1^2, u_2^2, \sqrt{2}u_1, \sqrt{2}u_2, 1) \cdot (v_1^2, v_2^2, \sqrt{2}v_1, \sqrt{2}v_2, 1) \\ &= u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 v_1 + 2u_2 v_2 + 1 \\ &= (\mathbf{u} \cdot \mathbf{v} + 1)^2. \end{aligned} \tag{5.60}$$

This analysis shows that the dot product in the transformed space can be expressed in terms of a similarity function in the original space:

$$K(\mathbf{u}, \mathbf{v}) = \Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^2. \tag{5.61}$$

The similarity function, K, which is computed in the original attribute space, is known as the **kernel function**. The kernel trick helps to address some of the concerns about how to implement nonlinear SVM. First, we do not have to know the exact form of the mapping function Φ because the kernel functions used in nonlinear SVM must satisfy a mathematical principle known as **Mercer's theorem**. This principle ensures that the kernel functions can always be expressed as the dot product between two input vectors in some high-dimensional space. The transformed space of the SVM kernels is called a **reproducing kernel Hilbert space** (RKHS). Second, computing the dot products using kernel functions is considerably cheaper than using the transformed attribute set $\Phi(\mathbf{x})$. Third, since the computations are performed in the original space, issues associated with the curse of dimensionality problem can be avoided.

Figure 5.29 shows the nonlinear decision boundary obtained by SVM using the polynomial kernel function given in Equation 5.61. A test instance $\mathbf{x}$ is classified according to the following equation:

$$\begin{aligned} f(\mathbf{z}) &= sign(\sum_{i=1}^{n} \lambda_i y_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{z}) + b) \\ &= sign(\sum_{i=1}^{n} \lambda_i y_i K(\mathbf{x}_i, \mathbf{z}) + b) \\ &= sign(\sum_{i=1}^{n} \lambda_i y_i (\mathbf{x}_i \cdot \mathbf{z} + 1)^2 + b), \end{aligned} \tag{5.62}$$

where b is the parameter obtained using Equation 5.58. The decision boundary obtained by nonlinear SVM is quite close to the true decision boundary shown in Figure 5.28(a).

Mercer's Theorem

The main requirement for the kernel function used in nonlinear SVM is that there must exist a corresponding transformation such that the kernel function computed for a pair of vectors is equivalent to the dot product between the vectors in the transformed space. This requirement can be formally stated in the form of Mercer's theorem.

Theorem 5.1 (Mercer's Theorem). *A kernel function K can be expressed as*

$$K(\boldsymbol{u}, \boldsymbol{v}) = \Phi(\boldsymbol{u}) \cdot \Phi(\boldsymbol{v})$$

if and only if, for any function $g(x)$ such that $\int g(\boldsymbol{x})^2 d\boldsymbol{x}$ is finite, then

$$\int K(\boldsymbol{x}, \boldsymbol{y})\ g(\boldsymbol{x})\ g(\boldsymbol{y})\ d\boldsymbol{x}\ d\boldsymbol{y} \geq 0.$$

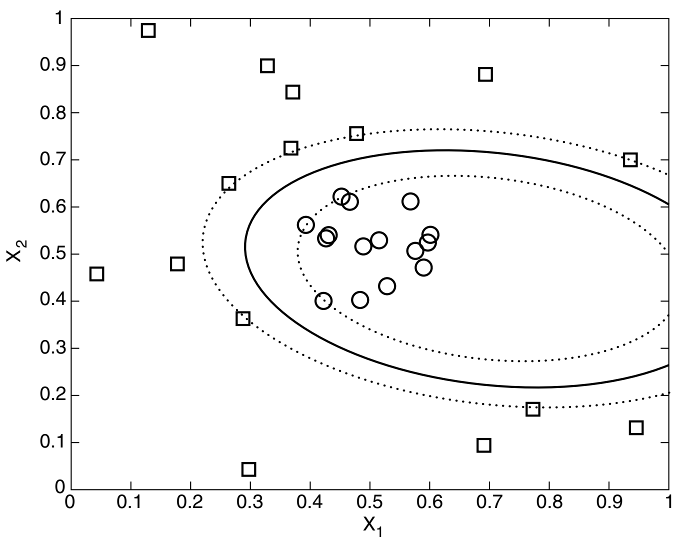


Figure 5.29. Decision boundary produced by a nonlinear SVM with polynomial kernel.

Kernel functions that satisfy Theorem 5.1 are called positive definite kernel functions. Examples of such functions are listed below:

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}\cdot\mathbf{y}+1)^p \tag{5.63}$$

$$K(\mathbf{x},\mathbf{y}) = e^{-\|\mathbf{x}-\mathbf{y}\|^2/(2\sigma^2)} \tag{5.64}$$

$$K(\mathbf{x},\mathbf{y}) = \tanh(k\mathbf{x}\cdot\mathbf{y}-\delta) \tag{5.65}$$

Example 5.6. Consider the polynomial kernel function given in Equation 5.63. Let $g(x)$ be a function that has a finite L_2 norm, i.e., $\int g(\mathbf{x})^2 d\mathbf{x} < \infty$.

$$\begin{aligned}
& \int (\mathbf{x}\cdot\mathbf{y}+1)^p g(\mathbf{x})g(\mathbf{y})d\mathbf{x}d\mathbf{y} \\
= & \int \sum_{i=0}^{p} \binom{p}{i} (\mathbf{x}\cdot\mathbf{y})^i g(\mathbf{x})g(\mathbf{y})d\mathbf{x}d\mathbf{y} \\
= & \sum_{i=0}^{p} \binom{p}{i} \int \sum_{\alpha_1,\alpha_2,\ldots} \binom{i}{\alpha_1\alpha_2\ldots} \Big[(x_1y_1)^{\alpha_1}(x_2y_2)^{\alpha_2}(x_3y_3)^{\alpha_3}\ldots\Big] \\
& \qquad g(x_1,x_2,\ldots)\ g(y_1,y_2,\ldots)dx_1dx_2\ldots dy_1dy_2\ldots
\end{aligned}$$

$$= \sum_{i=0}^{p} \sum_{\alpha_1,\alpha_2,\ldots} \binom{p}{i} \binom{i}{\alpha_1\alpha_2\ldots} \left[\int x_1^{\alpha_1} x_2^{\alpha_2} \ldots g(x_1, x_2, \ldots) dx_1 dx_2 \ldots \right]^2.$$

Because the result of the integration is non-negative, the polynomial kernel function therefore satisfies Mercer's theorem. ■

5.5.5 Characteristics of SVM

SVM has many desirable qualities that make it one of the most widely used classification algorithms. Following is a summary of the general characteristics of SVM:

1. The SVM learning problem can be formulated as a convex optimization problem, in which efficient algorithms are available to find the global minimum of the objective function. Other classification methods, such as rule-based classifiers and artificial neural networks, employ a greedy-based strategy to search the hypothesis space. Such methods tend to find only locally optimum solutions.

2. SVM performs capacity control by maximizing the margin of the decision boundary. Nevertheless, the user must still provide other parameters such as the type of kernel function to use and the cost function C for introducing each slack variable.

3. SVM can be applied to categorical data by introducing dummy variables for each categorical attribute value present in the data. For example, if `Marital Status` has three values {`Single`, `Married`, `Divorced`}, we can introduce a binary variable for each of the attribute values.

4. The SVM formulation presented in this chapter is for binary class problems. Some of the methods available to extend SVM to multiclass problems are presented in Section 5.8.

5.6 Ensemble Methods

The classification techniques we have seen so far in this chapter, with the exception of the nearest-neighbor method, predict the class labels of unknown examples using a single classifier induced from training data. This section presents techniques for improving classification accuracy by aggregating the predictions of multiple classifiers. These techniques are known as the **ensemble** or **classifier combination** methods. An ensemble method constructs a set of **base classifiers** from training data and performs classification by taking a vote on the predictions made by each base classifier. This section explains why ensemble methods tend to perform better than any single classifier and presents techniques for constructing the classifier ensemble.

5.6.1 Rationale for Ensemble Method

The following example illustrates how an ensemble method can improve a classifier's performance.

Example 5.7. Consider an ensemble of twenty-five binary classifiers, each of which has an error rate of $\epsilon = 0.35$. The ensemble classifier predicts the class label of a test example by taking a majority vote on the predictions made by the base classifiers. If the base classifiers are identical, then the ensemble will misclassify the same examples predicted incorrectly by the base classifiers. Thus, the error rate of the ensemble remains 0.35. On the other hand, if the base classifiers are independent—i.e., their errors are uncorrelated—then the ensemble makes a wrong prediction only if more than half of the base classifiers predict incorrectly. In this case, the error rate of the ensemble classifier is

$$e_{\text{ensemble}} = \sum_{i=13}^{25} \binom{25}{i} \epsilon^i (1-\epsilon)^{25-i} = 0.06, \tag{5.66}$$

which is considerably lower than the error rate of the base classifiers. ■

Figure 5.30 shows the error rate of an ensemble of twenty-five binary classifiers (e_{ensemble}) for different base classifier error rates (ϵ). The diagonal line represents the case in which the base classifiers are identical, while the solid line represents the case in which the base classifiers are independent. Observe that the ensemble classifier performs worse than the base classifiers when ϵ is larger than 0.5.

The preceding example illustrates two necessary conditions for an ensemble classifier to perform better than a single classifier: (1) the base classifiers should be independent of each other, and (2) the base classifiers should do better than a classifier that performs random guessing. In practice, it is difficult to ensure total independence among the base classifiers. Nevertheless, improvements in classification accuracies have been observed in ensemble methods in which the base classifiers are slightly correlated.

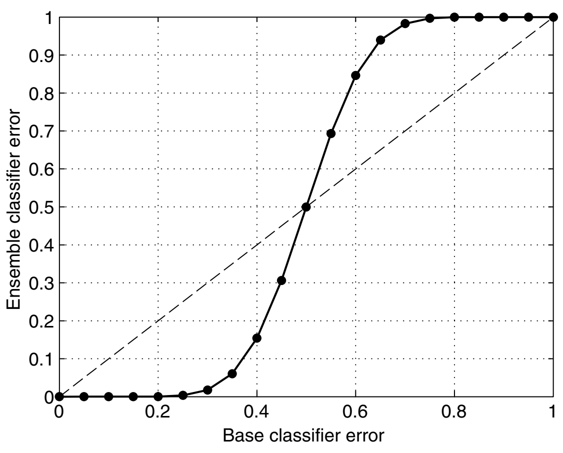


Figure 5.30. Comparison between errors of base classifiers and errors of the ensemble classifier.

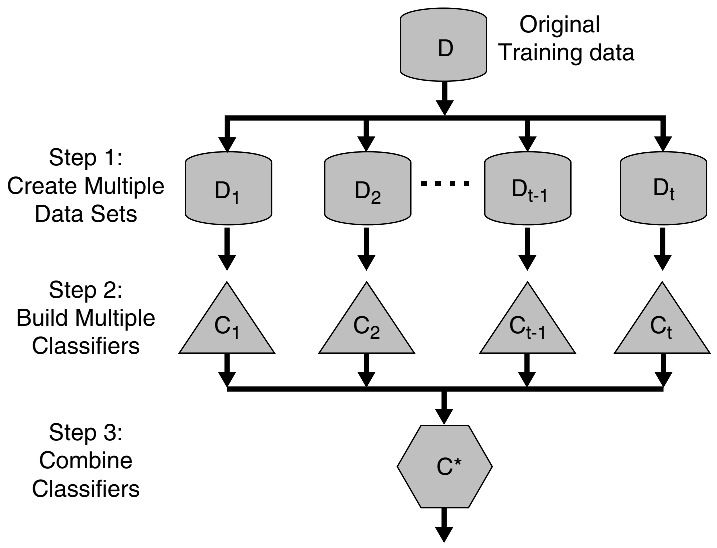

D
Original Training data
Step 1: Create Multiple Data Sets
D_1
D_2
D_{t-1}
D_t
Step 2: Build Multiple Classifiers
C_1
C_2
C_{t-1}
C_t
Step 3: Combine Classifiers
C*

Figure 5.31. A logical view of the ensemble learning method.

5.6.2 Methods for Constructing an Ensemble Classifier

A logical view of the ensemble method is presented in Figure 5.31. The basic idea is to construct multiple classifiers from the original data and then aggregate their predictions when classifying unknown examples. The ensemble of classifiers can be constructed in many ways:

1. **By manipulating the training set.** In this approach, multiple training sets are created by resampling the original data according to some sampling distribution. The sampling distribution determines how likely it is that an example will be selected for training, and it may vary from one trial to another. A classifier is then built from each training set using a particular learning algorithm. **Bagging** and **boosting** are two examples of ensemble methods that manipulate their training sets. These methods are described in further detail in Sections 5.6.4 and 5.6.5.

2. **By manipulating the input features.** In this approach, a subset of input features is chosen to form each training set. The subset can be either chosen randomly or based on the recommendation of domain experts. Some studies have shown that this approach works very well with data sets that contain highly redundant features. **Random forest**, which is described in Section 5.6.6, is an ensemble method that manipulates its input features and uses decision trees as its base classifiers.

3. **By manipulating the class labels.** This method can be used when the number of classes is sufficiently large. The training data is transformed into a binary class problem by randomly partitioning the class labels into two disjoint subsets, A_0 and A_1. Training examples whose class label belongs to the subset A_0 are assigned to class 0, while those that belong to the subset A_1 are assigned to class 1. The relabeled examples are then used to train a base classifier. By repeating the class-relabeling and model-building steps multiple times, an ensemble of base classifiers is obtained. When a test example is presented, each base classifier C_i is used to predict its class label. If the test example is predicted as class 0, then all the classes that belong to A_0 will receive a vote. Conversely, if it is predicted to be class 1, then all the classes that belong to A_1 will receive a vote. The votes are tallied and the class that receives the highest vote is assigned to the test example. An example of this approach is the **error-correcting output coding** method described on page 307.

4. **By manipulating the learning algorithm.** Many learning algorithms can be manipulated in such a way that applying the algorithm several times on the same training data may result in different models. For example, an artificial neural network can produce different models by changing its network topology or the initial weights of the links between neurons. Similarly, an ensemble of decision trees can be constructed by injecting randomness into the tree-growing procedure. For

example, instead of choosing the best splitting attribute at each node, we can randomly choose one of the top k attributes for splitting.

The first three approaches are generic methods that are applicable to any classifiers, whereas the fourth approach depends on the type of classifier used. The base classifiers for most of these approaches can be generated sequentially (one after another) or in parallel (all at once). Algorithm 5.5 shows the steps needed to build an ensemble classifier in a sequential manner. The first step is to create a training set from the original data D. Depending on the type of ensemble method used, the training sets are either identical to or slight modifications of D. The size of the training set is often kept the same as the original data, but the distribution of examples may not be identical; i.e., some examples may appear multiple times in the training set, while others may not appear even once. A base classifier C_i is then constructed from each training set D_i. Ensemble methods work better with **unstable classifiers**, i.e., base classifiers that are sensitive to minor perturbations in the training set. Examples of unstable classifiers include decision trees, rule-based classifiers, and artificial neural networks. As will be discussed in Section 5.6.3, the variability among training examples is one of the primary sources of errors in a classifier. By aggregating the base classifiers built from different training sets, this may help to reduce such types of errors.

Finally, a test example $\mathbf{x}$ is classified by combining the predictions made by the base classifiers $C_i(\mathbf{x})$:

$$C^*(\mathbf{x}) = Vote(C_1(\mathbf{x}), C_2(\mathbf{x}), \ldots, C_k(\mathbf{x})).$$

The class can be obtained by taking a majority vote on the individual predictions or by weighting each prediction with the accuracy of the base classifier.

Algorithm 5.5 General procedure for ensemble method.

```
1: Let $D$ denote the original training data, $k$ denote the number of base classifiers,
   and $T$ be the test data.
2: for $i = 1$ to $k$ do
3:    Create training set, $D_i$ from $D$.
4:    Build a base classifier $C_i$ from $D_i$.
5: end for
6: for each test record $x \in T$ do
7:    $C^*(x) = Vote(C_1(\mathbf{x}), C_2(\mathbf{x}), \ldots, C_k(\mathbf{x}))$
8: end for
```

5.6.3 Bias-Variance Decomposition

Bias-variance decomposition is a formal method for analyzing the prediction error of a predictive model. The following example gives an intuitive explanation for this method.

Figure 5.32 shows the trajectories of a projectile launched at a particular angle. Suppose the projectile hits the floor surface at some location x, at a distance d away from the target position t. Depending on the force applied to the projectile, the observed distance may vary from one trial to another. The observed distance can be decomposed into several components. The first component, which is known as **bias**, measures the average distance between the target position and the location where the projectile hits the floor. The amount of bias depends on the angle of the projectile launcher. The second component, which is known as **variance**, measures the deviation between x and the average position $\overline{x}$ where the projectile hits the floor. The variance can be explained as a result of changes in the amount of force applied to the projectile. Finally, if the target is not stationary, then the observed distance is also affected by changes in the location of the target. This is considered the **noise** component associated with variability in the target position. Putting these components together, the average distance can be expressed as:

$$d_{f,\theta}(y,t) \;=\; \text{Bias}_\theta + \; \text{Variance}_f + \; \text{Noise}_t, \tag{5.67}$$

where f refers to the amount of force applied and θ is the angle of the launcher.

The task of predicting the class label of a given example can be analyzed using the same approach. For a given classifier, some predictions may turn out to be correct, while others may be completely off the mark. We can decompose the expected error of a classifier as a sum of the three terms given in Equation 5.67, where expected error is the probability that the classifier misclassifies a

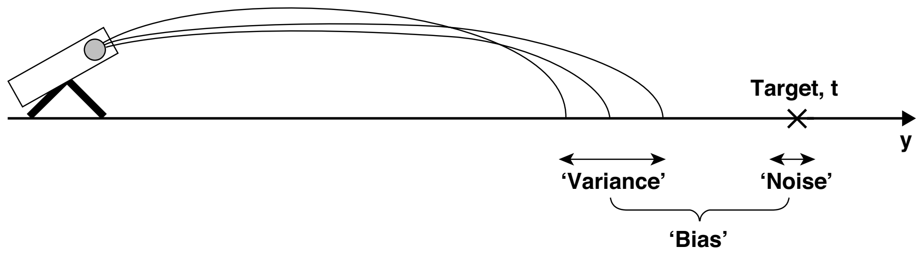


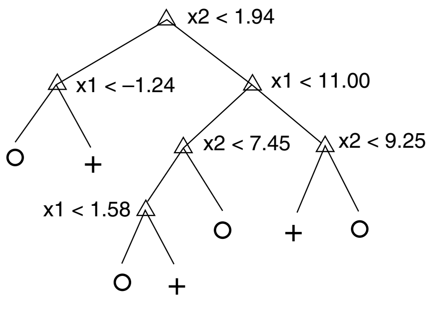
Figure 5.32. Bias-variance decomposition.

given example. The remainder of this section examines the meaning of bias, variance, and noise in the context of classification.

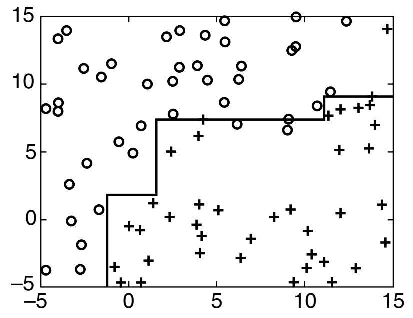
A classifier is usually trained to minimize its training error. However, to be useful, the classifier must be able to make an informed guess about the class labels of examples it has never seen before. This requires the classifier to generalize its decision boundary to regions where there are no training examples available—a decision that depends on the design choice of the classifier. For example, a key design issue in decision tree induction is the amount of pruning needed to obtain a tree with low expected error. Figure 5.33 shows two decision trees, T_1 and T_2, that are generated from the same training data, but have different complexities. T_2 is obtained by pruning T_1 until a tree with maximum depth of two is obtained. T_1, on the other hand, performs very little pruning on its decision tree. These design choices will introduce a bias into the classifier that is analogous to the bias of the projectile launcher described in the previous example. In general, the stronger the assumptions made by a classifier about the nature of its decision boundary, the larger the classifier's bias will be. T_2 therefore has a larger bias because it makes stronger assumptions about its decision boundary (which is reflected by the size of the tree) compared to T_1. Other design choices that may introduce a bias into a classifier include the network topology of an artificial neural network and the number of neighbors considered by a nearest-neighbor classifier.

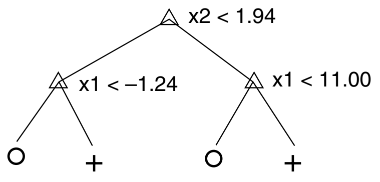
The expected error of a classifier is also affected by variability in the training data because different compositions of the training set may lead to different decision boundaries. This is analogous to the variance in x when different amounts of force are applied to the projectile. The last component of the expected error is associated with the intrinsic noise in the target class. The target class for some domains can be non-deterministic; i.e., instances with the same attribute values can have different class labels. Such errors are unavoidable even when the true decision boundary is known.

The amount of bias and variance contributing to the expected error depend on the type of classifier used. Figure 5.34 compares the decision boundaries produced by a decision tree and a 1-nearest neighbor classifier. For each classifier, we plot the decision boundary obtained by "averaging" the models induced from 100 training sets, each containing 100 examples. The true decision boundary from which the data is generated is also plotted using a dashed line. The difference between the true decision boundary and the "averaged" decision boundary reflects the bias of the classifier. After averaging the models, observe that the difference between the true decision boundary and the decision boundary produced by the 1-nearest neighbor classifier is smaller than



(a) Decision tree T_1





(b) Decision tree T_2

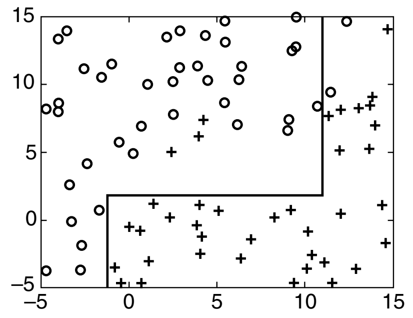


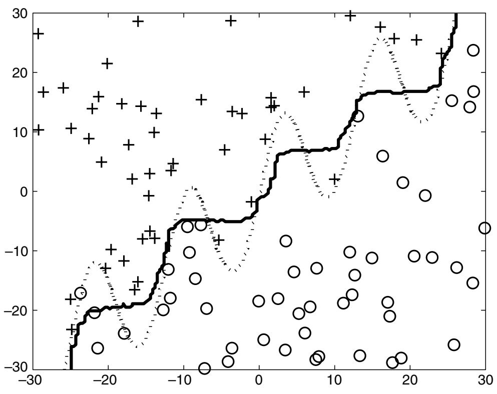
Figure 5.33. Two decision trees with different complexities induced from the same training data.

the observed difference for a decision tree classifier. This result suggests that the bias of a 1-nearest neighbor classifier is lower than the bias of a decision tree classifier.

On the other hand, the 1-nearest neighbor classifier is more sensitive to the composition of its training examples. If we examine the models induced from different training sets, there is more variability in the decision boundary of a 1-nearest neighbor classifier than a decision tree classifier. Therefore, the decision boundary of a decision tree classifier has a lower variance than the 1-nearest neighbor classifier.

5.6.4 Bagging

Bagging, which is also known as bootstrap aggregating, is a technique that repeatedly samples (with replacement) from a data set according to a uniform probability distribution. Each bootstrap sample has the same size as the original data. Because the sampling is done with replacement, some instances may appear several times in the same training set, while others may be omitted from the training set. On average, a bootstrap sample D_i contains approxi-


(a) Decision boundary for decision tree.

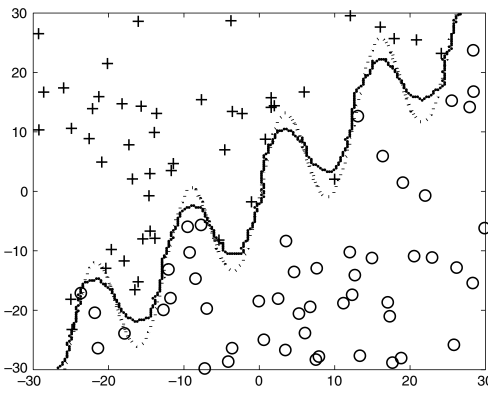

(b) Decision boundary for 1-nearest neighbor.

Figure 5.34. Bias of decision tree and 1-nearest neighbor classifiers.

Algorithm 5.6 Bagging algorithm.

```
1: Let $k$ be the number of bootstrap samples.
2: for $i = 1$ to $k$ do
3:     Create a bootstrap sample of size $N$, $D_i$.
4:     Train a base classifier $C_i$ on the bootstrap sample $D_i$.
5: end for
6: $C^*(x) = \underset{y}{\text{argmax}} \sum_i \delta\big(C_i(x) = y\big)$.
   $\{\delta(\cdot) = 1$ if its argument is true and 0 otherwise$\}$.
```

mately 63% of the original training data because each sample has a probability $1 - (1 - 1/N)^N$ of being selected in each D_i. If N is sufficiently large, this probability converges to $1 - 1/e \simeq 0.632$. The basic procedure for bagging is summarized in Algorithm 5.6. After training the k classifiers, a test instance is assigned to the class that receives the highest number of votes.

To illustrate how bagging works, consider the data set shown in Table 5.4. Let x denote a one-dimensional attribute and y denote the class label. Suppose we apply a classifier that induces only one-level binary decision trees, with a test condition $x \leq k$, where k is a split point chosen to minimize the entropy of the leaf nodes. Such a tree is also known as a **decision stump**.

Without bagging, the best decision stump we can produce splits the records at either $x \leq 0.35$ or $x \leq 0.75$. Either way, the accuracy of the tree is at

Table 5.4. Example of data set used to construct an ensemble of bagging classifiers.

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

most 70%. Suppose we apply the bagging procedure on the data set using ten bootstrap samples. The examples chosen for training in each bagging round are shown in Figure 5.35. On the right-hand side of each table, we also illustrate the decision boundary produced by the classifier.

We classify the entire data set given in Table 5.4 by taking a majority vote among the predictions made by each base classifier. The results of the predictions are shown in Figure 5.36. Since the class labels are either -1 or $+1$, taking the majority vote is equivalent to summing up the predicted values of y and examining the sign of the resulting sum (refer to the second to last row in Figure 5.36). Notice that the ensemble classifier perfectly classifies all ten examples in the original data.

The preceding example illustrates another advantage of using ensemble methods in terms of enhancing the representation of the target function. Even though each base classifier is a decision stump, combining the classifiers can lead to a decision tree of depth 2.

Bagging improves generalization error by reducing the variance of the base classifiers. The performance of bagging depends on the stability of the base classifier. If a base classifier is unstable, bagging helps to reduce the errors associated with random fluctuations in the training data. If a base classifier is stable, i.e., robust to minor perturbations in the training set, then the error of the ensemble is primarily caused by bias in the base classifier. In this situation, bagging may not be able to improve the performance of the base classifiers significantly. It may even degrade the classifier's performance because the effective size of each training set is about 37% smaller than the original data.

Finally, since every sample has an equal probability of being selected, bagging does not focus on any particular instance of the training data. It is therefore less susceptible to model overfitting when applied to noisy data.

5.6.5 Boosting

Boosting is an iterative procedure used to adaptively change the distribution of training examples so that the base classifiers will focus on examples that are hard to classify. Unlike bagging, boosting assigns a weight to each training

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Round 2:

x	0.1	0.2	0.3	0.4	0.5	0.8	0.9	1	1	1
y	1	1	1	-1	-1	1	1	1	1	1

x <= 0.65 ==> y = 1
x > 0.65 ==> y = 1

Bagging Round 3:

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Round 4:

x	0.1	0.1	0.2	0.4	0.4	0.5	0.5	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.3 ==> y = 1
x > 0.3 ==> y = -1

Bagging Round 5:

x	0.1	0.1	0.2	0.5	0.6	0.6	0.6	1	1	1
y	1	1	1	-1	-1	-1	-1	1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Round 6:

x	0.2	0.4	0.5	0.6	0.7	0.7	0.7	0.8	0.9	1
y	1	-1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 7:

x	0.1	0.4	0.4	0.6	0.7	0.8	0.9	0.9	0.9	1
y	1	-1	-1	-1	-1	1	1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 8:

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 9:

x	0.1	0.3	0.4	0.4	0.6	0.7	0.7	0.8	1	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 10:

x	0.1	0.1	0.1	0.1	0.3	0.3	0.8	0.8	0.9	0.9
y	1	1	1	1	1	1	1	1	1	1

x <= 0.05 ==> y = -1
x > 0.05 ==> y = 1

Figure 5.35. Example of bagging.

example and may adaptively change the weight at the end of each boosting round. The weights assigned to the training examples can be used in the following ways:

1. They can be used as a sampling distribution to draw a set of bootstrap samples from the original data.
2. They can be used by the base classifier to learn a model that is biased toward higher-weight examples.

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	1	1	1	-1	-1	-1	-1	-1	-1	-1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	-1
5	1	1	1	-1	-1	-1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1	1	1	1
7	-1	-1	-1	-1	-1	-1	-1	1	1	1
8	-1	-1	-1	-1	-1	-1	-1	1	1	1
9	-1	-1	-1	-1	-1	-1	-1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
Sum	2	2	2	-6	-6	-6	-6	2	2	2
Sign	1	1	1	-1	-1	-1	-1	1	1	1
True Class	1	1	1	-1	-1	-1	-1	1	1	1

Figure 5.36. Example of combining classifiers constructed using the bagging approach.

This section describes an algorithm that uses weights of examples to determine the sampling distribution of its training set. Initially, the examples are assigned equal weights, $1/N$, so that they are equally likely to be chosen for training. A sample is drawn according to the sampling distribution of the training examples to obtain a new training set. Next, a classifier is induced from the training set and used to classify all the examples in the original data. The weights of the training examples are updated at the end of each boosting round. Examples that are classified incorrectly will have their weights increased, while those that are classified correctly will have their weights decreased. This forces the classifier to focus on examples that are difficult to classify in subsequent iterations.

The following table shows the examples chosen during each boosting round.

Boosting (Round 1):	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2):	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3):	4	4	8	10	4	5	4	6	3	4

Initially, all the examples are assigned the same weights. However, some examples may be chosen more than once, e.g., examples 3 and 7, because the sampling is done with replacement. A classifier built from the data is then used to classify all the examples. Suppose example 4 is difficult to classify. The weight for this example will be increased in future iterations as it gets misclassified repeatedly. Meanwhile, examples that were not chosen in the previous round, e.g., examples 1 and 5, also have a better chance of being selected in the next round since their predictions in the previous round were likely to be wrong. As the boosting rounds proceed, examples that are the hardest to classify tend to become even more prevalent. The final ensemble is obtained by aggregating the base classifiers obtained from each boosting round.

Over the years, several implementations of the boosting algorithm have been developed. These algorithms differ in terms of (1) how the weights of the training examples are updated at the end of each boosting round, and (2) how the predictions made by each classifier are combined. An implementation called AdaBoost is explored in the next section.

AdaBoost

Let $\{(\mathbf{x}_j, y_j) \mid j = 1, 2, \ldots, N\}$ denote a set of N training examples. In the AdaBoost algorithm, the importance of a base classifier C_i depends on its error rate, which is defined as

$$\epsilon_i = \frac{1}{N}\left[\sum_{j=1}^{N} w_j \; I\Big(C_i(\mathbf{x}_j) \neq y_j\Big)\right], \tag{5.68}$$

where $I(p) = 1$ if the predicate p is true, and 0 otherwise. The importance of a classifier C_i is given by the following parameter,

$$\alpha_i = \frac{1}{2}\ln\left(\frac{1-\epsilon_i}{\epsilon_i}\right).$$

Note that α_i has a large positive value if the error rate is close to 0 and a large negative value if the error rate is close to 1, as shown in Figure 5.37.

The α_i parameter is also used to update the weight of the training examples. To illustrate, let $w_i^{(j)}$ denote the weight assigned to example $(\mathbf{x}_i, y_i)$ during the j^{th} boosting round. The weight update mechanism for AdaBoost is given by the equation:

$$w_i^{(j+1)} \;=\; \frac{w_i^{(j)}}{Z_j} \times \begin{cases} \exp^{-\alpha_j} & \text{if } C_j(\mathbf{x_i}) = y_i \\ \exp^{\alpha_j} & \text{if } C_j(\mathbf{x_i}) \neq y_i \end{cases}, \tag{5.69}$$

where Z_j is the normalization factor used to ensure that $\sum_i w_i^{(j+1)} = 1$. The weight update formula given in Equation 5.69 increases the weights of incorrectly classified examples and decreases the weights of those classified correctly.

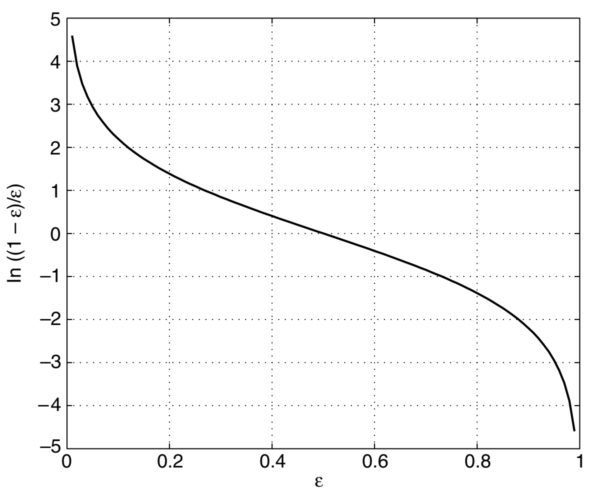


Figure 5.37. Plot of α as a function of training error ϵ.

Instead of using a majority voting scheme, the prediction made by each classifier C_j is weighted according to α_j. This approach allows AdaBoost to penalize models that have poor accuracy, e.g., those generated at the earlier boosting rounds. In addition, if any intermediate rounds produce an error rate higher than 50%, the weights are reverted back to their original uniform values, $w_i = 1/N$, and the resampling procedure is repeated. The AdaBoost algorithm is summarized in Algorithm 5.7.

Let us examine how the boosting approach works on the data set shown in Table 5.4. Initially, all the examples have identical weights. After three boosting rounds, the examples chosen for training are shown in Figure 5.38(a). The weights for each example are updated at the end of each boosting round using Equation 5.69.

Without boosting, the accuracy of the decision stump is, at best, 70%. With AdaBoost, the results of the predictions are given in Figure 5.39(b). The final prediction of the ensemble classifier is obtained by taking a weighted average of the predictions made by each base classifier, which is shown in the last row of Figure 5.39(b). Notice that AdaBoost perfectly classifies all the examples in the training data.

An important analytical result of boosting shows that the training error of the ensemble is bounded by the following expression:

$$e_{\text{ensemble}} \leq \prod_i \left[\sqrt{\epsilon_i(1-\epsilon_i)}\right], \qquad (5.70)$$

Algorithm 5.7 AdaBoost algorithm.

```
1: $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$.    {Initialize the weights for all $N$ examples.}
2: Let $k$ be the number of boosting rounds.
3: for $i = 1$ to $k$ do
4:    Create training set $D_i$ by sampling (with replacement) from $D$ according to $\mathbf{w}$.
5:    Train a base classifier $C_i$ on $D_i$.
6:    Apply $C_i$ to all examples in the original training set, $D$.
7:    $\epsilon_i = \frac{1}{N}\big[\sum_j w_j\ \delta\big(C_i(x_j) \neq y_j\big)\big]$    {Calculate the weighted error.}
8:    if $\epsilon_i > 0.5$ then
9:       $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \ldots, N\}$.    {Reset the weights for all $N$ examples.}
10:      Go back to Step 4.
11:   end if
12:   $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$.
13:   Update the weight of each example according to Equation 5.69.
14: end for
15: $C^*(\mathbf{x}) = \operatorname*{argmax}_y \sum_{j=1}^{T} \alpha_j \delta\big(C_j(\mathbf{x}) = y)\big)$.
```

where ϵ_i is the error rate of each base classifier i. If the error rate of the base classifier is less than 50%, we can write $\epsilon_i = 0.5 - \gamma_i$, where γ_i measures how much better the classifier is than random guessing. The bound on the training error of the ensemble becomes

$$e_{\text{ensemble}} \leq \prod_i \sqrt{1 - 4\gamma_i^2} \leq \exp\left(-2 \sum_i \gamma_i^2 \right). \tag{5.71}$$

If $\gamma_i < \gamma*$ for all i's, then the training error of the ensemble decreases exponentially, which leads to the fast convergence of the algorithm. Nevertheless, because of its tendency to focus on training examples that are wrongly classified, the boosting technique can be quite susceptible to overfitting.

5.6.6 Random Forests

Random forest is a class of ensemble methods specifically designed for decision tree classifiers. It combines the predictions made by multiple decision trees, where each tree is generated based on the values of an independent set of random vectors, as shown in Figure 5.40. The random vectors are generated from a fixed probability distribution, unlike the adaptive approach used in AdaBoost, where the probability distribution is varied to focus on examples that are hard to classify. Bagging using decision trees is a special case of random forests, where randomness is injected into the model-building process

Boosting Round 1:

x	0.1	0.4	0.5	0.6	0.6	0.7	0.7	0.7	0.8	1
y	1	-1	-1	-1	-1	-1	-1	-1	1	1

Boosting Round 2:

x	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.3
y	1	1	1	1	1	1	1	1	1	1

Boosting Round 3:

x	0.2	0.2	0.4	0.4	0.4	0.4	0.5	0.6	0.6	0.7
y	1	1	-1	-1	-1	-1	-1	-1	-1	-1

(a) Training records chosen during boosting

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
2	0.311	0.311	0.311	0.01	0.01	0.01	0.01	0.01	0.01	0.01
3	0.029	0.029	0.029	0.228	0.228	0.228	0.228	0.009	0.009	0.009

(b) Weights of training records

Figure 5.38. Example of boosting.

by randomly choosing N samples, with replacement, from the original training set. Bagging also uses the same uniform probability distribution to generate its bootstrapped samples throughout the entire model-building process.

It was theoretically proven that the upper bound for generalization error of random forests converges to the following expression, when the number of trees is sufficiently large.

$$\text{Generalization error } \leq \frac{\overline{\rho}(1-s^2)}{s^2}, \tag{5.72}$$

where $\overline{\rho}$ is the average correlation among the trees and s is a quantity that measures the "strength" of the tree classifiers. The strength of a set of classifiers refers to the average performance of the classifiers, where performance is measured probabilistically in terms of the classifier's margin:

$$\text{margin}, M(\mathbf{X}, Y) = P(\hat{Y}_\theta = Y) - \max_{Z \neq Y} P(\hat{Y}_\theta = Z), \tag{5.73}$$

where $\hat{Y}_\theta$ is the predicted class of $\mathbf{X}$ according to a classifier built from some random vector θ. The higher the margin is, the more likely it is that the

Round	Split Point	Left Class	Right Class	α
1	0.75	-1	1	1.738
2	0.05	1	1	2.7784
3	0.3	1	-1	4.1195

(a)

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	-1	-1	-1	-1	-1	-1	-1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
Sum	5.16	5.16	5.16	-3.08	-3.08	-3.08	-3.08	0.397	0.397	0.397
Sign	1	1	1	-1	-1	-1	-1	1	1	1

(b)

Figure 5.39. Example of combining classifiers constructed using the AdaBoost approach.

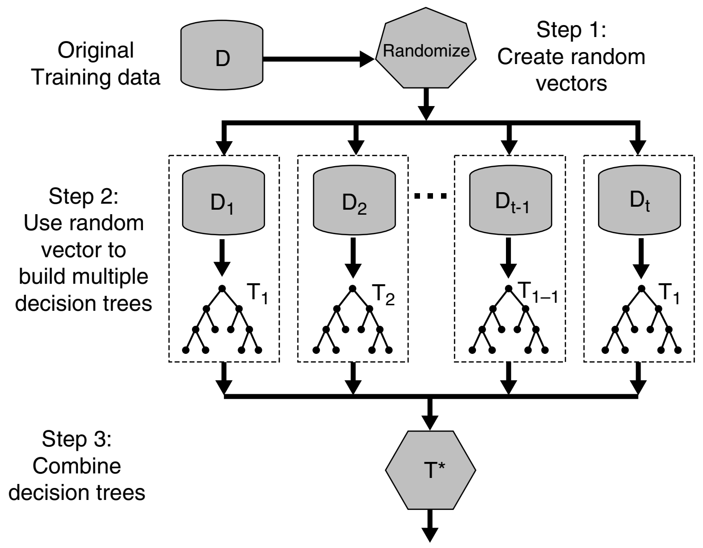

Original Training data
D
Randomize
Step 1: Create random vectors
Step 2: Use random vector to build multiple decision trees
D_1
D_2
D_{t-1}
D_t
T_1
T_2
T_{1-1}
T_1
Step 3: Combine decision trees
T*

Figure 5.40. Random forests.

classifier correctly predicts a given example $\mathbf{X}$. Equation 5.72 is quite intuitive; as the trees become more correlated or the strength of the ensemble decreases, the generalization error bound tends to increase. Randomization helps to reduce the correlation among decision trees so that the generalization error of the ensemble can be improved.

Each decision tree uses a random vector that is generated from some fixed probability distribution. A random vector can be incorporated into the tree-growing process in many ways. The first approach is to randomly select F input features to split at each node of the decision tree. As a result, instead of examining all the available features, the decision to split a node is determined from these selected F features. The tree is then grown to its entirety without any pruning. This may help reduce the bias present in the resulting tree. Once the trees have been constructed, the predictions are combined using a majority voting scheme. This approach is known as Forest-RI, where RI refers to random input selection. To increase randomness, bagging can also be used to generate bootstrap samples for Forest-RI. The strength and correlation of random forests may depend on the size of F. If F is sufficiently small, then the trees tend to become less correlated. On the other hand, the strength of the tree classifier tends to improve with a larger number of features, F. As a tradeoff, the number of features is commonly chosen to be $F = \log_2 d + 1$, where d is the number of input features. Since only a subset of the features needs to be examined at each node, this approach helps to significantly reduce the runtime of the algorithm.

If the number of original features d is too small, then it is difficult to choose an independent set of random features for building the decision trees. One way to increase the feature space is to create linear combinations of the input features. Specifically, at each node, a new feature is generated by randomly selecting L of the input features. The input features are linearly combined using coefficients generated from a uniform distribution in the range of $[-1, 1]$. At each node, F of such randomly combined new features are generated, and the best of them is subsequently selected to split the node. This approach is known as Forest-RC.

A third approach for generating the random trees is to randomly select one of the F best splits at each node of the decision tree. This approach may potentially generate trees that are more correlated than Forest-RI and Forest-RC, unless F is sufficiently large. It also does not have the runtime savings of Forest-RI and Forest-RC because the algorithm must examine all the splitting features at each node of the decision tree.

It has been shown empirically that the classification accuracies of random forests are quite comparable to the AdaBoost algorithm. It is also more robust to noise and runs much faster than the AdaBoost algorithm. The classification accuracies of various ensemble algorithms are compared in the next section.

Table 5.5. Comparing the accuracy of a decision tree classifier against three ensemble methods.

Data Set	Number of (Attributes, Classes, Records)	Decision Tree (%)	Bagging (%)	Boosting (%)	RF (%)
Anneal	(39, 6, 898)	92.09	94.43	95.43	95.43
Australia	(15, 2, 690)	85.51	87.10	85.22	85.80
Auto	(26, 7, 205)	81.95	85.37	85.37	84.39
Breast	(11, 2, 699)	95.14	96.42	97.28	96.14
Cleve	(14, 2, 303)	76.24	81.52	82.18	82.18
Credit	(16, 2, 690)	85.8	86.23	86.09	85.8
Diabetes	(9, 2, 768)	72.40	76.30	73.18	75.13
German	(21, 2, 1000)	70.90	73.40	73.00	74.5
Glass	(10, 7, 214)	67.29	76.17	77.57	78.04
Heart	(14, 2, 270)	80.00	81.48	80.74	83.33
Hepatitis	(20, 2, 155)	81.94	81.29	83.87	83.23
Horse	(23, 2, 368)	85.33	85.87	81.25	85.33
Ionosphere	(35, 2, 351)	89.17	92.02	93.73	93.45
Iris	(5, 3, 150)	94.67	94.67	94.00	93.33
Labor	(17, 2, 57)	78.95	84.21	89.47	84.21
Led7	(8, 10, 3200)	73.34	73.66	73.34	73.06
Lymphography	(19, 4, 148)	77.03	79.05	85.14	82.43
Pima	(9, 2, 768)	74.35	76.69	73.44	77.60
Sonar	(61, 2, 208)	78.85	78.85	84.62	85.58
Tic-tac-toe	(10, 2, 958)	83.72	93.84	98.54	95.82
Vehicle	(19, 4, 846)	71.04	74.11	78.25	74.94
Waveform	(22, 3, 5000)	76.44	83.30	83.90	84.04
Wine	(14, 3, 178)	94.38	96.07	97.75	97.75
Zoo	(17, 7, 101)	93.07	93.07	95.05	97.03

5.6.7 Empirical Comparison among Ensemble Methods

Table 5.5 shows the empirical results obtained when comparing the performance of a decision tree classifier against bagging, boosting, and random forest. The base classifiers used in each ensemble method consist of fifty decision trees. The classification accuracies reported in this table are obtained from ten-fold cross-validation. Notice that the ensemble classifiers generally outperform a single decision tree classifier on many of the data sets.

5.7 Class Imbalance Problem

Data sets with imbalanced class distributions are quite common in many real applications. For example, an automated inspection system that monitors products that come off a manufacturing assembly line may find that the number of defective products is significantly fewer than that of non-defective products. Similarly, in credit card fraud detection, fraudulent transactions are outnumbered by legitimate transactions. In both of these examples, there is a disproportionate number of instances that belong to different classes. The degree of imbalance varies from one application to another—a manufacturing plant operating under the six sigma principle may discover four defects in a million products shipped to their customers, while the amount of credit card fraud may be of the order of 1 in 100. Despite their infrequent occurrences, a correct classification of the rare class in these applications often has greater value than a correct classification of the majority class. However, because the class distribution is imbalanced, this presents a number of problems to existing classification algorithms.

The accuracy measure, which is used extensively to compare the performance of classifiers, may not be well suited for evaluating models derived from imbalanced data sets. For example, if 1% of the credit card transactions are fraudulent, then a model that predicts every transaction as legitimate has an accuracy of 99% even though it fails to detect any of the fraudulent activities. Additionally, measures that are used to guide the learning algorithm (e.g., information gain for decision tree induction) may need to be modified to focus on the rare class.

Detecting instances of the rare class is akin to finding a needle in a haystack. Because their instances occur infrequently, models that describe the rare class tend to be highly specialized. For example, in a rule-based classifier, the rules extracted for the rare class typically involve a large number of attributes and cannot be easily simplified into more general rules with broader coverage (unlike the rules for the majority class). Such models are also susceptible to the presence of noise in training data. As a result, many of the existing classification algorithms may not effectively detect instances of the rare class.

This section presents some of the methods developed for handling the class imbalance problem. First, alternative metrics besides accuracy are introduced, along with a graphical method called ROC analysis. We then describe how cost-sensitive learning and sampling-based methods may be used to improve the detection of rare classes.

5.7.1 Alternative Metrics

Since the accuracy measure treats every class as equally important, it may not be suitable for analyzing imbalanced data sets, where the rare class is considered more interesting than the majority class. For binary classification, the rare class is often denoted as the positive class, while the majority class is

Table 5.6. A confusion matrix for a binary classification problem in which the classes are not equally important.

		Predicted Class	
		$+$	$-$
Actual	$+$	f_{++} (TP)	f_{+-} (FN)
Class	$-$	f_{-+} (FP)	f_{--} (TN)

denoted as the negative class. A confusion matrix that summarizes the number of instances predicted correctly or incorrectly by a classification model is shown in Table 5.6.

The following terminology is often used when referring to the counts tabulated in a confusion matrix:

- True positive (TP) or f_{++}, which corresponds to the number of positive examples correctly predicted by the classification model.
- False negative (FN) or f_{+-}, which corresponds to the number of positive examples wrongly predicted as negative by the classification model.
- False positive (FP) or f_{-+}, which corresponds to the number of negative examples wrongly predicted as positive by the classification model.
- True negative (TN) or f_{--}, which corresponds to the number of negative examples correctly predicted by the classification model.

The counts in a confusion matrix can also be expressed in terms of percentages. The **true positive rate** (TPR) or **sensitivity** is defined as the fraction of positive examples predicted correctly by the model, i.e.,

$$TPR = TP/(TP + FN).$$

Similarly, the **true negative rate** (TNR) or **specificity** is defined as the fraction of negative examples predicted correctly by the model, i.e.,

$$TNR = TN/(TN + FP).$$

Finally, the **false positive rate** (FPR) is the fraction of negative examples predicted as a positive class, i.e.,

$$FPR = FP/(TN + FP),$$

while the **false negative rate** (FNR) is the fraction of positive examples predicted as a negative class, i.e.,

$$FNR = FN/(TP + FN).$$

Recall and **precision** are two widely used metrics employed in applications where successful detection of one of the classes is considered more significant than detection of the other classes. A formal definition of these metrics is given below.

$$\text{Precision, } p = \frac{TP}{TP + FP} \tag{5.74}$$

$$\text{Recall, } r = \frac{TP}{TP + FN} \tag{5.75}$$

Precision determines the fraction of records that actually turns out to be positive in the group the classifier has declared as a positive class. The higher the precision is, the lower the number of false positive errors committed by the classifier. Recall measures the fraction of positive examples correctly predicted by the classifier. Classifiers with large recall have very few positive examples misclassified as the negative class. In fact, the value of recall is equivalent to the true positive rate.

It is often possible to construct baseline models that maximize one metric but not the other. For example, a model that declares every record to be the positive class will have a perfect recall, but very poor precision. Conversely, a model that assigns a positive class to every test record that matches one of the positive records in the training set has very high precision, but low recall. Building a model that maximizes both precision and recall is the key challenge of classification algorithms.

Precision and recall can be summarized into another metric known as the F_1 measure.

$$F_1 = \frac{2rp}{r + p} = \frac{2 \times TP}{2 \times TP + FP + FN} \tag{5.76}$$

In principle, F_1 represents a harmonic mean between recall and precision, i.e.,

$$F_1 = \frac{2}{\frac{1}{r} + \frac{1}{p}}.$$

The harmonic mean of two numbers x and y tends to be closer to the smaller of the two numbers. Hence, a high value of F_1-measure ensures that both precision and recall are reasonably high. A comparison among harmonic, geometric, and arithmetic means is given in the next example.

Example 5.8. Consider two positive numbers $a = 1$ and $b = 5$. Their arithmetic mean is $\mu_a = (a + b)/2 = 3$ and their geometric mean is $\mu_g = \sqrt{ab} = 2.236$. Their harmonic mean is $\mu_h = (2\times1\times5)/6 = 1.667$, which is closer to the smaller value between a and b than the arithmetic and geometric means. ■

More generally, the F_β measure can be used to examine the tradeoff between recall and precision:

$$F_\beta = \frac{(\beta^2 + 1)rp}{r + \beta^2 p} = \frac{(\beta^2 + 1) \times TP}{(\beta^2 + 1)TP + \beta^2 FP + FN}. \tag{5.77}$$

Both precision and recall are special cases of F_β by setting $\beta = 0$ and $\beta = \infty$, respectively. Low values of β make F_β closer to precision, and high values make it closer to recall.

A more general metric that captures F_β as well as accuracy is the weighted accuracy measure, which is defined by the following equation:

$$\text{Weighted accuracy} = \frac{w_1 TP + w_4 TN}{w_1 TP + w_2 FP + w_3 FN + w_4 TN}. \tag{5.78}$$

The relationship between weighted accuracy and other performance metrics is summarized in the following table:

Measure	w_1	w_2	w_3	w_4
Recall	1	1	0	0
Precision	1	0	1	0
F_β	$\beta^2 + 1$	β^2	1	0
Accuracy	1	1	1	1

5.7.2 The Receiver Operating Characteristic Curve

A receiver operating characteristic (ROC) curve is a graphical approach for displaying the tradeoff between true positive rate and false positive rate of a classifier. In an ROC curve, the true positive rate (TPR) is plotted along the y axis and the false positive rate (FPR) is shown on the x axis. Each point along the curve corresponds to one of the models induced by the classifier. Figure 5.41 shows the ROC curves for a pair of classifiers, M_1 and M_2.

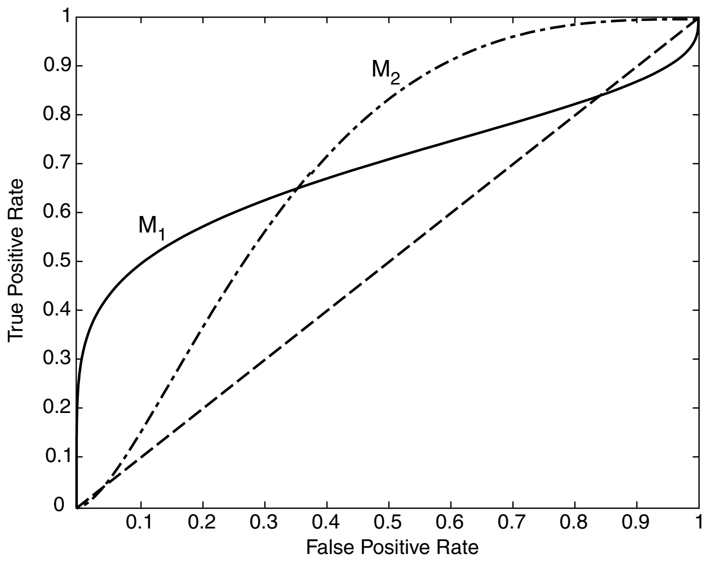


Figure 5.41. ROC curves for two different classifiers.

There are several critical points along an ROC curve that have well-known interpretations:

(TPR=0, FPR=0):	Model predicts every instance to be a negative class.
(TPR=1, FPR=1):	Model predicts every instance to be a positive class.
(TPR=1, FPR=0):	The ideal model.

A good classification model should be located as close as possible to the upper left corner of the diagram, while a model that makes random guesses should reside along the main diagonal, connecting the points $(TPR = 0, FPR = 0)$ and $(TPR = 1, FPR = 1)$. Random guessing means that a record is classified as a positive class with a fixed probability p, irrespective of its attribute set. For example, consider a data set that contains n_+ positive instances and n_- negative instances. The random classifier is expected to correctly classify pn_+ of the positive instances and to misclassify pn_- of the negative instances. Therefore, the TPR of the classifier is $(pn_+)/n_+ = p$, while its FPR is $(pn_-)/p = p$. Since the TPR and FPR are identical, the ROC curve for a random classifier always reside along the main diagonal.

An ROC curve is useful for comparing the relative performance among different classifiers. In Figure 5.41, M_1 is better than M_2 when FPR is less than 0.36, while M_2 is superior when FPR is greater than 0.36. Clearly, neither of these two classifiers dominates the other.

The area under the ROC curve (AUC) provides another approach for evaluating which model is better on average. If the model is perfect, then its area under the ROC curve would equal 1. If the model simply performs random guessing, then its area under the ROC curve would equal 0.5. A model that is strictly better than another would have a larger area under the ROC curve.

Generating an ROC curve

To draw an ROC curve, the classifier should be able to produce a continuous-valued output that can be used to rank its predictions, from the most likely record to be classified as a positive class to the least likely record. These outputs may correspond to the posterior probabilities generated by a Bayesian classifier or the numeric-valued outputs produced by an artificial neural network. The following procedure can then be used to generate an ROC curve:

1. Assuming that the continuous-valued outputs are defined for the positive class, sort the test records in increasing order of their output values.

2. Select the lowest ranked test record (i.e., the record with lowest output value). Assign the selected record and those ranked above it to the positive class. This approach is equivalent to classifying all the test records as positive class. Because all the positive examples are classified correctly and the negative examples are misclassified, $TPR = FPR = 1$.

3. Select the next test record from the sorted list. Classify the selected record and those ranked above it as positive, while those ranked below it as negative. Update the counts of TP and FP by examining the actual class label of the previously selected record. If the previously selected record is a positive class, the TP count is decremented and the FP count remains the same as before. If the previously selected record is a negative class, the FP count is decremented and TP count remains the same as before.

4. Repeat Step 3 and update the TP and FP counts accordingly until the highest ranked test record is selected.

5. Plot the TPR against FPR of the classifier.

Figure 5.42 shows an example of how to compute the ROC curve. There are five positive examples and five negative examples in the test set. The class