Such assessment is optimistic because the rules will likely overfit the data. That is, the rules may perform well on the training data, but less well on subsequent data. To compensate for this, we can prune the rules. A rule is pruned by removing a conjunct (attribute test). We choose to prune a rule, R, if the pruned version of R has greater quality, as assessed on an independent set of tuples. As in decision tree pruning, we refer to this set as a *pruning set*. Various pruning strategies can be used, such as the pessimistic pruning approach described in the previous section. FOIL uses a simple yet effective method. Given a rule, R,

$$FOIL\_Prune(R) = \frac{pos - neg}{pos + neg}, \tag{6.23}$$

where *pos* and *neg* are the number of positive and negative tuples covered by R, respectively. This value will increase with the accuracy of R on a pruning set. Therefore, if the *FOIL_Prune* value is higher for the pruned version of R, then we prune R. By convention, RIPPER starts with the most recently added conjunct when considering pruning. Conjuncts are pruned one at a time as long as this results in an improvement.

6.6 Classification by Backpropagation

"What is backpropagation?" Backpropagation is a neural network learning algorithm. The field of neural networks was originally kindled by psychologists and neurobiologists who sought to develop and test computational analogues of neurons. Roughly speaking, a **neural network** is a set of connected input/output units in which each connection has a weight associated with it. During the learning phase, the network learns by adjusting the weights so as to be able to predict the correct class label of the input tuples. Neural network learning is also referred to as **connectionist learning** due to the connections between units.

Neural networks involve long training times and are therefore more suitable for applications where this is feasible. They require a number of parameters that are typically best determined empirically, such as the network topology or "structure." Neural networks have been criticized for their poor interpretability. For example, it is difficult for humans to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network. These features initially made neural networks less desirable for data mining.

Advantages of neural networks, however, include their high tolerance of noisy data as well as their ability to classify patterns on which they have not been trained. They can be used when you may have little knowledge of the relationships between attributes and classes. They are well-suited for continuous-valued inputs *and outputs*, unlike most decision tree algorithms. They have been successful on a wide array of real-world data, including handwritten character recognition, pathology and laboratory medicine, and training a computer to pronounce English text. Neural network algorithms are inherently parallel; parallelization techniques can be used to speed up the computation process. In addition, several techniques have recently been developed for the extraction of rules from trained neural networks. These factors contribute toward the usefulness of neural networks for classification and prediction in data mining.

There are many different kinds of neural networks and neural network algorithms. The most popular neural network algorithm is *backpropagation*, which gained repute in the 1980s. In Section 6.6.1 you will learn about multilayer feed-forward networks, the type of neural network on which the backpropagation algorithm performs. Section 6.6.2 discusses defining a network topology. The backpropagation algorithm is described in Section 6.6.3. Rule extraction from trained neural networks is discussed in Section 6.6.4.

6.6.1 A Multilayer Feed-Forward Neural Network

The backpropagation algorithm performs learning on a *multilayer feed-forward* neural network. It iteratively learns a set of weights for prediction of the class label of tuples. A **multilayer feed-forward** neural network consists of an *input layer*, one or more *hidden layers*, and an *output layer*. An example of a multilayer feed-forward network is shown in Figure 6.15.

Each layer is made up of units. The inputs to the network correspond to the attributes measured for each training tuple. The inputs are fed simultaneously into the units making up the **input layer**. These inputs pass through the input layer and are then weighted and fed simultaneously to a second layer of "neuronlike" units, known as a **hidden layer**. The outputs of the hidden layer units can be input to another hidden layer, and so on. The number of hidden layers is arbitrary, although in practice, usually only one is used. The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction for given tuples.

The units in the input layer are called **input units**. The units in the hidden layers and output layer are sometimes referred to as **neurodes**, due to their symbolic biological basis, or as **output units**. The multilayer neural network shown in Figure 6.15 has two layers

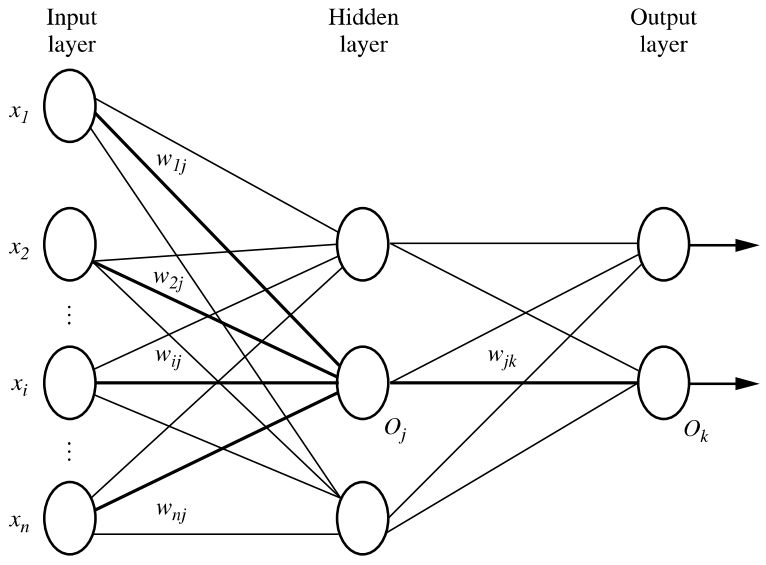


Figure 6.15 A multilayer feed-forward neural network.

of output units. Therefore, we say that it is a **two-layer** neural network. (The input layer is not counted because it serves only to pass the input values to the next layer.) Similarly, a network containing two hidden layers is called a *three-layer* neural network, and so on. The network is **feed-forward** in that none of the weights cycles back to an input unit or to an output unit of a previous layer. It is **fully connected** in that each unit provides input to each unit in the next forward layer.

Each output unit takes, as input, a weighted sum of the outputs from units in the previous layer (see Figure 6.17). It applies a nonlinear (activation) function to the weighted input. Multilayer feed-forward neural networks are able to model the class prediction as a nonlinear combination of the inputs. From a statistical point of view, they perform nonlinear regression. *Multilayer feed-forward networks, given enough hidden units and enough training samples, can closely approximate any function.*

6.6.2 Defining a Network Topology

"*How can I design the topology of the neural network?*" Before training can begin, the user must decide on the network topology by specifying the number of units in the input layer, the number of hidden layers (if more than one), the number of units in each hidden layer, and the number of units in the output layer.

Normalizing the input values for each attribute measured in the training tuples will help speed up the learning phase. Typically, input values are normalized so as to fall between 0.0 and 1.0. Discrete-valued attributes may be encoded such that there is one input unit per domain value. For example, if an attribute A has three possible or known values, namely $\{a_0, a_1, a_2\}$, then we may assign three input units to represent A. That is, we may have, say, I_0, I_1, I_2 as input units. Each unit is initialized to 0. If $A = a_0$, then I_0 is set to 1. If $A = a_1, I_1$ is set to 1, and so on. Neural networks can be used for both classification (to predict the class label of a given tuple) or prediction (to predict a continuous-valued output). For classification, one output unit may be used to represent two classes (where the value 1 represents one class, and the value 0 represents the other). If there are more than two classes, then one output unit per class is used.

There are no clear rules as to the "best" number of hidden layer units. Network design is a trial-and-error process and may affect the accuracy of the resulting trained network. The initial values of the weights may also affect the resulting accuracy. Once a network has been trained and its accuracy is not considered acceptable, it is common to repeat the training process with a different network topology or a different set of initial weights. Cross-validation techniques for accuracy estimation (described in Section 6.13) can be used to help decide when an acceptable network has been found. A number of automated techniques have been proposed that search for a "good" network structure. These typically use a hill-climbing approach that starts with an initial structure that is selectively modified.

6.6.3 Backpropagation

"*How does backpropagation work?*" Backpropagation learns by iteratively processing a data set of training tuples, comparing the network's prediction for each tuple with the

actual known *target* value. The target value may be the known class label of the training tuple (for classification problems) or a continuous value (for prediction). For each training tuple, the weights are modified so as to minimize the mean squared error between the network's prediction and the actual target value. These modifications are made in the "backwards" direction, that is, from the output layer, through each hidden layer down to the first hidden layer (hence the name *backpropagation*). Although it is not guaranteed, in general the weights will eventually converge, and the learning process stops. The algorithm is summarized in Figure 6.16. The steps involved are expressed in terms of inputs, outputs, and errors, and may seem awkward if this is your first look at neural network learning. However, once you become familiar with the process, you will see that each step is inherently simple. The steps are described below.

Algorithm: Backpropagation. Neural network learning for classification or prediction, using the backpropagation algorithm.

Input:

- D, a data set consisting of the training tuples and their associated target values;
- l, the learning rate;
- *network*, a multilayer feed-forward network.

Output: A trained neural network.

Method:

(1) Initialize all weights and biases in *network*;
(2) **while** terminating condition is not satisfied {
(3) **for** each training tuple $\boldsymbol{X}$ in D {
(4) // Propagate the inputs forward:
(5) **for** each input layer unit j {
(6) $O_j = I_j$; // output of an input unit is its actual input value
(7) **for** each hidden or output layer unit j {
(8) $I_j = \sum_i w_{ij} O_i + \theta_j$; //compute the net input of unit j with respect to the previous layer, i
(9) $O_j = \frac{1}{1+e^{-I_j}}$; } // compute the output of each unit j
(10) // Backpropagate the errors:
(11) **for** each unit j in the output layer
(12) $Err_j = O_j(1-O_j)(T_j - O_j)$; // compute the error
(13) **for** each unit j in the hidden layers, from the last to the first hidden layer
(14) $Err_j = O_j(1-O_j)\sum_k Err_k w_{jk}$; // compute the error with respect to the next higher layer, k
(15) **for** each weight w_{ij} in *network* {
(16) $\Delta w_{ij} = (l) Err_j O_i$; // weight increment
(17) $w_{ij} = w_{ij} + \Delta w_{ij}$; } // weight update
(18) **for** each bias θ_j in *network* {
(19) $\Delta\theta_j = (l) Err_j$; // bias increment
(20) $\theta_j = \theta_j + \Delta\theta_j$; } // bias update
(21) } }

Figure 6.16 Backpropagation algorithm.

Initialize the weights: The weights in the network are initialized to small random numbers (e.g., ranging from −1.0 to 1.0, or −0.5 to 0.5). Each unit has a *bias* associated with it, as explained below. The biases are similarly initialized to small random numbers.

Each training tuple, $\boldsymbol{X}$, is processed by the following steps.

Propagate the inputs forward: First, the training tuple is fed to the input layer of the network. The inputs pass through the input units, unchanged. That is, for an input unit, j, its output, O_j, is equal to its input value, I_j. Next, the net input and output of each unit in the hidden and output layers are computed. The net input to a unit in the hidden or output layers is computed as a linear combination of its inputs. To help illustrate this point, a hidden layer or output layer unit is shown in Figure 6.17. Each such unit has a number of inputs to it that are, in fact, the outputs of the units connected to it in the previous layer. Each connection has a weight. To compute the net input to the unit, each input connected to the unit is multiplied by its corresponding weight, and this is summed. Given a unit j in a hidden or output layer, the net input, I_j, to unit j is

$$I_j = \sum_i w_{ij} O_i + \theta_j, \tag{6.24}$$

where w_{ij} is the weight of the connection from unit i in the previous layer to unit j; O_i is the output of unit i from the previous layer; and θ_j is the **bias** of the unit. The bias acts as a threshold in that it serves to vary the activity of the unit.

Each unit in the hidden and output layers takes its net input and then applies an **activation** function to it, as illustrated in Figure 6.17. The function symbolizes the activation

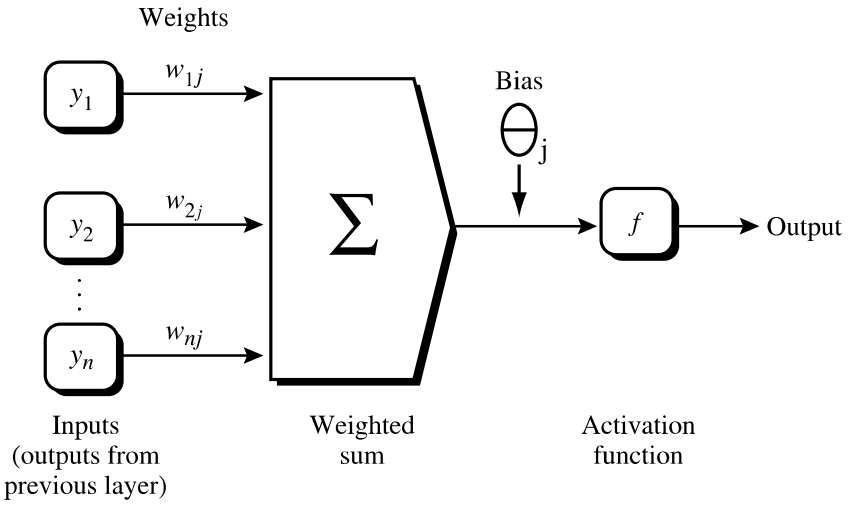


Figure 6.17 A hidden or output layer unit j: The inputs to unit j are outputs from the previous layer. These are multiplied by their corresponding weights in order to form a weighted sum, which is added to the bias associated with unit j. A nonlinear activation function is applied to the net input. (For ease of explanation, the inputs to unit j are labeled $y_1, y_2, \ldots, y_n$. If unit j were in the first hidden layer, then these inputs would correspond to the input tuple $(x_1, x_2, \ldots, x_n)$.)

of the neuron represented by the unit. The **logistic**, or **sigmoid,** function is used. Given the net input I_j to unit j, then O_j, the output of unit j, is computed as

$$O_j = \frac{1}{1+e^{-I_j}}. \tag{6.25}$$

This function is also referred to as a *squashing function*, because it maps a large input domain onto the smaller range of 0 to 1. The logistic function is nonlinear and differentiable, allowing the backpropagation algorithm to model classification problems that are linearly inseparable.

We compute the output values, O_j, for each hidden layer, up to and including the output layer, which gives the network's prediction. In practice, it is a good idea to cache (i.e., save) the intermediate output values at each unit as they are required again later, when backpropagating the error. This trick can substantially reduce the amount of computation required.

Backpropagate the error: The error is propagated backward by updating the weights and biases to reflect the error of the network's prediction. For a unit j in the output layer, the error Err_j is computed by

$$Err_j = O_j(1-O_j)(T_j - O_j), \tag{6.26}$$

where O_j is the actual output of unit j, and T_j is the known target value of the given training tuple. Note that $O_j(1-O_j)$ is the derivative of the logistic function.

To compute the error of a hidden layer unit j, the weighted sum of the errors of the units connected to unit j in the next layer are considered. The error of a hidden layer unit j is

$$Err_j = O_j(1-O_j)\sum_k Err_k w_{jk}, \tag{6.27}$$

where w_{jk} is the weight of the connection from unit j to a unit k in the next higher layer, and Err_k is the error of unit k.

The weights and biases are updated to reflect the propagated errors. Weights are updated by the following equations, where Δw_{ij} is the change in weight w_{ij}:

$$\Delta w_{ij} = (l) Err_j O_i \tag{6.28}$$

$$w_{ij} = w_{ij} + \Delta w_{ij} \tag{6.29}$$

"*What is the 'l' in Equation (6.28)?*" The variable l is the **learning rate**, a constant typically having a value between 0.0 and 1.0. Backpropagation learns using a method of gradient descent to search for a set of weights that fits the training data so as to minimize the mean squared distance between the network's class prediction and the known target value of the tuples.[8] The learning rate helps avoid getting stuck at a local minimum

[8]A method of gradient descent was also used for training Bayesian belief networks, as described in Section 6.4.4.

in decision space (i.e., where the weights appear to converge, but are not the optimum solution) and encourages finding the global minimum. If the learning rate is too small, then learning will occur at a very slow pace. If the learning rate is too large, then oscillation between inadequate solutions may occur. A rule of thumb is to set the learning rate to $1/t$, where t is the number of iterations through the training set so far.

Biases are updated by the following equations below, where $\Delta\theta_j$ is the change in bias θ_j:

$$\Delta\theta_j = (l)Err_j \tag{6.30}$$

$$\theta_j = \theta_j + \Delta\theta_j \tag{6.31}$$

Note that here we are updating the weights and biases after the presentation of each tuple. This is referred to as **case updating**. Alternatively, the weight and bias increments could be accumulated in variables, so that the weights and biases are updated after all of the tuples in the training set have been presented. This latter strategy is called **epoch updating**, where one iteration through the training set is an **epoch**. In theory, the mathematical derivation of backpropagation employs epoch updating, yet in practice, case updating is more common because it tends to yield more accurate results.

Terminating condition: Training stops when

- All Δw_{ij} in the previous epoch were so small as to be below some specified threshold, or
- The percentage of tuples misclassified in the previous epoch is below some threshold, or
- A prespecified number of epochs has expired.

In practice, several hundreds of thousands of epochs may be required before the weights will converge.

"How efficient is backpropagation?" The computational efficiency depends on the time spent training the network. Given $|D|$ tuples and w weights, each epoch requires $O(|D| \times w)$ time. However, in the worst-case scenario, the number of epochs can be exponential in n, the number of inputs. In practice, the time required for the networks to converge is highly variable. A number of techniques exist that help speed up the training time. For example, a technique known as *simulated annealing* can be used, which also ensures convergence to a global optimum.

Example 6.9 **Sample calculations for learning by the backpropagation algorithm.** Figure 6.18 shows a multilayer feed-forward neural network. Let the learning rate be 0.9. The initial weight and bias values of the network are given in Table 6.3, along with the first training tuple, $\boldsymbol{X} = (1, 0, 1)$, whose class label is 1.

This example shows the calculations for backpropagation, given the first training tuple, $\boldsymbol{X}$. The tuple is fed into the network, and the net input and output of each unit are computed. These values are shown in Table 6.4. The error of each unit is computed

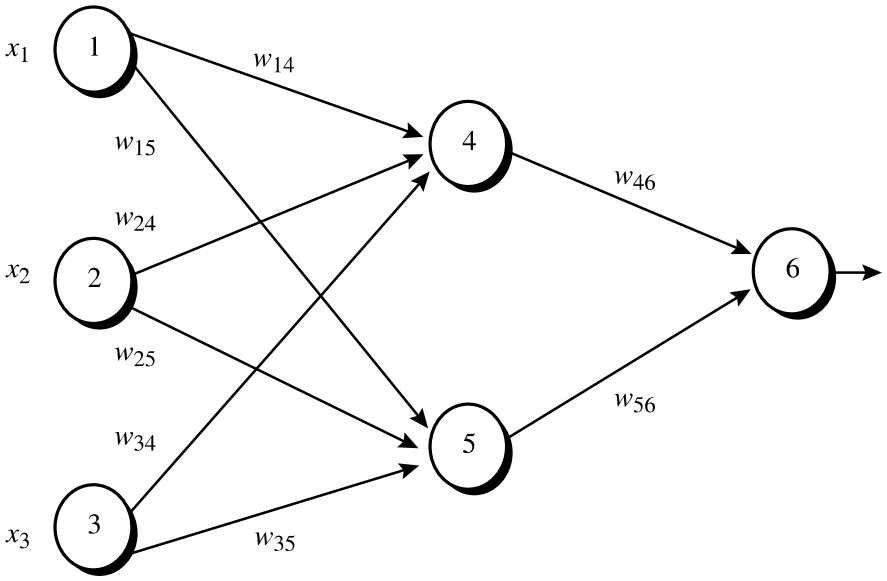


Figure 6.18 An example of a multilayer feed-forward neural network.

Table 6.3 Initial input, weight, and bias values.

x_1	x_2	x_3	w_{14}	w_{15}	w_{24}	w_{25}	w_{34}	w_{35}	w_{46}	w_{56}	θ_4	θ_5	θ_6
1	0	1	0.2	−0.3	0.4	0.1	−0.5	0.2	−0.3	−0.2	−0.4	0.2	0.1

Table 6.4 The net input and output calculations.

Unit j	*Net input,* I_j	*Output,* O_j
4	$0.2+0-0.5-0.4=-0.7$	$1/(1+e^{0.7})=0.332$
5	$-0.3+0+0.2+0.2=0.1$	$1/(1+e^{-0.1})=0.525$
6	$(-0.3)(0.332)-(0.2)(0.525)+0.1=-0.105$	$1/(1+e^{0.105})=0.474$

and propagated backward. The error values are shown in Table 6.5. The weight and bias updates are shown in Table 6.6. ■

Several variations and alternatives to the backpropagation algorithm have been proposed for classification in neural networks. These may involve the dynamic adjustment of the network topology and of the learning rate or other parameters, or the use of different error functions.

6.6.4 Inside the Black Box: Backpropagation and Interpretability

"Neural networks are like a black box. How can I 'understand' what the backpropagation network has learned?" A major disadvantage of neural networks lies in their knowledge

Table 6.5 Calculation of the error at each node.

Unit j	Err_j
6	$(0.474)(1-0.474)(1-0.474) = 0.1311$
5	$(0.525)(1-0.525)(0.1311)(-0.2) = -0.0065$
4	$(0.332)(1-0.332)(0.1311)(-0.3) = -0.0087$

Table 6.6 Calculations for weight and bias updating.

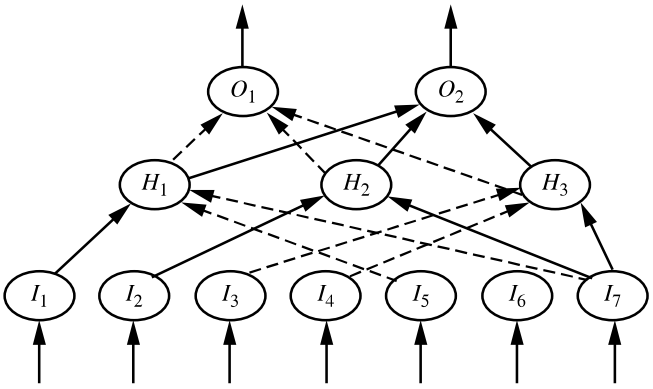
Weight or bias	*New value*
w_{46}	$-0.3 + (0.9)(0.1311)(0.332) = -0.261$
w_{56}	$-0.2 + (0.9)(0.1311)(0.525) = -0.138$
w_{14}	$0.2 + (0.9)(-0.0087)(1) = 0.192$
w_{15}	$-0.3 + (0.9)(-0.0065)(1) = -0.306$
w_{24}	$0.4 + (0.9)(-0.0087)(0) = 0.4$
w_{25}	$0.1 + (0.9)(-0.0065)(0) = 0.1$
w_{34}	$-0.5 + (0.9)(-0.0087)(1) = -0.508$
w_{35}	$0.2 + (0.9)(-0.0065)(1) = 0.194$
θ_6	$0.1 + (0.9)(0.1311) = 0.218$
θ_5	$0.2 + (0.9)(-0.0065) = 0.194$
θ_4	$-0.4 + (0.9)(-0.0087) = -0.408$

representation. Acquired knowledge in the form of a network of units connected by weighted links is difficult for humans to interpret. This factor has motivated research in extracting the knowledge embedded in trained neural networks and in representing that knowledge symbolically. Methods include extracting rules from networks and sensitivity analysis.

Various algorithms for the extraction of rules have been proposed. The methods typically impose restrictions regarding procedures used in training the given neural network, the network topology, and the discretization of input values.

Fully connected networks are difficult to articulate. Hence, often the first step toward extracting rules from neural networks is **network pruning**. This consists of simplifying the network structure by removing weighted links that have the least effect on the trained network. For example, a weighted link may be deleted if such removal does not result in a decrease in the classification accuracy of the network.

Once the trained network has been pruned, some approaches will then perform link, unit, or activation value clustering. In one method, for example, clustering is used to find the set of common activation values for each hidden unit in a given trained two-layer neural network (Figure 6.19). The combinations of these activation values for each hidden unit are analyzed. Rules are derived relating combinations of activation values with corresponding output unit values. Similarly, the sets of input



Identify sets of common activation values for each hidden node, H_i:
for H_1: (–1,0,1)
for H_2: (0.1)
for H_3: (–1,0.24,1)

Derive rules relating common activation values with output nodes, O_j:
IF ($H_2 = 0$ AND $H_3 = -1$) OR
($H_1 = -1$ AND $H_2 = 1$ AND $H_3 = -1$) OR
($H_1 = -1$ AND $H_2 = 0$ AND $H_3 = 0.24$)
THEN $O_1 = 1$, $O_2 = 0$
ELSE $O_1 = 0$, $O_2 = 1$

Derive rules relating input nodes, I_j, to output nodes, O_j:
IF ($I_2 = 0$ AND $I_7 = 0$) THEN $H_2 = 0$
IF ($I_4 = 1$ AND $I_6 = 1$) THEN $H_3 = -1$
IF ($I_5 = 0$) THEN $H_3 = -1$

Obtain rules relating inputs and output classes:
IF ($I_2 = 0$ AND $I_7 = 0$ AND $I_4 = 1$ AND $I_6 = 1$) THEN class = 1
IF ($I_2 = 0$ AND $I_7 = 0$ AND $I_5 = 0$) THEN class = 1

Figure 6.19 Rules can be extracted from training neural networks. Adapted from [LSL95].

values and activation values are studied to derive rules describing the relationship between the input and hidden unit layers. Finally, the two sets of rules may be combined to form IF-THEN rules. Other algorithms may derive rules of other forms, including *M*-of-*N* rules (where *M* out of a given *N* conditions in the rule antecedent must be true in order for the rule consequent to be applied), decision trees with *M*-of-*N* tests, fuzzy rules, and finite automata.

Sensitivity analysis is used to assess the impact that a given input variable has on a network output. The input to the variable is varied while the remaining input variables are fixed at some value. Meanwhile, changes in the network output are monitored. The knowledge gained from this form of analysis can be represented in rules such as "*IF X decreases* 5% *THEN Y increases* 8%."

6.7 Support Vector Machines

In this section, we study **Support Vector Machines**, a promising new method for the classification of both linear and nonlinear data. In a nutshell, a support vector machine (or **SVM**) is an algorithm that works as follows. It uses a nonlinear mapping to transform the original training data into a higher dimension. Within this new dimension, it searches for the linear optimal separating hyperplane (that is, a "decision boundary" separating the tuples of one class from another). With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane. The SVM finds this hyperplane using *support vectors* ("essential" training tuples) and *margins* (defined by the support vectors). We will delve more into these new concepts further below.

"*I've heard that SVMs have attracted a great deal of attention lately. Why?*" The first paper on support vector machines was presented in 1992 by Vladimir Vapnik and colleagues Bernhard Boser and Isabelle Guyon, although the groundwork for SVMs has been around since the 1960s (including early work by Vapnik and Alexei Chervonenkis on statistical learning theory). Although the training time of even the fastest SVMs can be extremely slow, they are highly accurate, owing to their ability to model complex nonlinear decision boundaries. They are much less prone to overfitting than other methods. The support vectors found also provide a compact description of the learned model. SVMs can be used for prediction as well as classification. They have been applied to a number of areas, including handwritten digit recognition, object recognition, and speaker identification, as well as benchmark time-series prediction tests.

6.7.1 The Case When the Data Are Linearly Separable

To explain the mystery of SVMs, let's first look at the simplest case—a two-class problem where the classes are linearly separable. Let the data set D be given as $(\boldsymbol{X}_1, y_1)$, $(\boldsymbol{X}_2, y_2), \ldots, (\boldsymbol{X}_{|D|}, y_{|D|})$, where $\boldsymbol{X}_i$ is the set of training tuples with associated class labels, y_i. Each y_i can take one of two values, either $+1$ or -1 (i.e., $y_i \in \{+1, -1\}$), corresponding to the classes *buys_computer* = *yes* and *buys_computer* = *no*, respectively. To aid in visualization, let's consider an example based on two input attributes, A_1 and A_2, as shown in Figure 6.20. From the graph, we see that the 2-D data are **linearly separable** (or "linear," for short) because a straight line can be drawn to separate all of the tuples of class $+1$ from all of the tuples of class -1. There are an infinite number of separating lines that could be drawn. We want to find the "best" one, that is, one that (we hope) will have the minimum classification error on previously unseen tuples. How can we find this best line? Note that if our data were 3-D (i.e., with three attributes), we would want to find the best separating *plane*. Generalizing to n dimensions, we want to find the best *hyperplane*. We will use the term "hyperplane" to refer to the decision boundary that we are seeking, regardless of the number of input attributes. So, in other words, how can we find the best hyperplane?

An SVM approaches this problem by searching for the **maximum marginal hyperplane**. Consider Figure 6.21, which shows two possible separating hyperplanes and