Learning Processes

2.1 INTRODUCTION

The property that is of primary significance for a neural network is the ability of the network to *learn* from its environment, and to *improve* its performance through learning. The improvement in performance takes place over time in accordance with some prescribed measure. A neural network learns about its environment through an interactive process of adjustments applied to its synaptic weights and bias levels. Ideally, the network becomes more knowledgeable about its environment after each iteration of the learning process.

There are too many activities associated with the notion of "learning" to justify defining it in a precise manner. Moreover, the process of learning is a matter of viewpoint, which makes it all the more difficult to agree on a precise definition of the term. For example, learning as viewed by a psychologist is quite different from learning in a classroom sense. Recognizing that our particular interest is in neural networks, we use a definition of learning that is adapted from Mendel and McClaren (1970).

We define learning in the context of neural networks as:

> *Learning is a process by which the free parameters of a neural network are adapted through a process of stimulation by the environment in which the network is embedded. The type of learning is determined by the manner in which the parameter changes take place.*

This definition of the learning process implies the following sequence of events:

1. The neural network is *stimulated* by an environment.
2. The neural network *undergoes changes* in its free parameters as a result of this stimulation.
3. The neural network *responds in a new way* to the environment because of the changes that have occurred in its internal structure.

A prescribed set of well-defined rules for the solution of a learning problem is called a *learning algorithm.*[1] As one would expect, there is no unique learning algorithm for the design of neural networks. Rather, we have a "kit of tools" represented by a diverse variety of learning algorithms, each of which offers advantages of its own. Basically, learning algorithms differ from each other in the way in which the adjust-

ment to a synaptic weight of a neuron is formulated. Another factor to be considered is the manner in which a neural network (learning machine), made up of a set of interconnected neurons, relates to its environment. In this latter context we speak of a *learning paradigm* that refers to a *model* of the environment in which the neural network operates.

Organization of the Chapter

The chapter is organized in four interrelated parts. In the first part, consisting of Sections 2.2 through 2.6, we discuss five basic learning rules: error-correction learning, memory-based learning, Hebbian learning, competitive learning, and Boltzmann learning. Error-correction learning is rooted in optimum filtering. Memory-based learning operates by memorizing the training data explicitly. Hebbian learning and competitive learning are both inspired by neurobiological considerations. Boltzmann learning is different because it is based on ideas borrowed from statistical mechanics.

The second part of the chapter explores learning paradigms. Section 2.7 discusses the credit-assignment problem, which is basic to the learning process. Sections 2.8 and 2.9 present overviews of the two fundamental learning paradigms: (1) learning *with* a teacher, and (2) learning *without* a teacher.

The third part of the chapter, consisting of Sections 2.10 through 2.12, examines the issues of learning tasks, memory, and adaptation.

The final part of the chapter, consisting of Sections 2.13 through 2.15, deals with probabilistic and statistical aspects of the learning process. Section 2.13 discusses the bias/variance dilemma. Section 2.14 discusses statistical learning theory, based on the notion of VC-dimension that provides a measure of machine capacity. Section 2.14 introduces another important concept: probably approximately correct (PAC) learning, which provides a conservative model for the learning process.

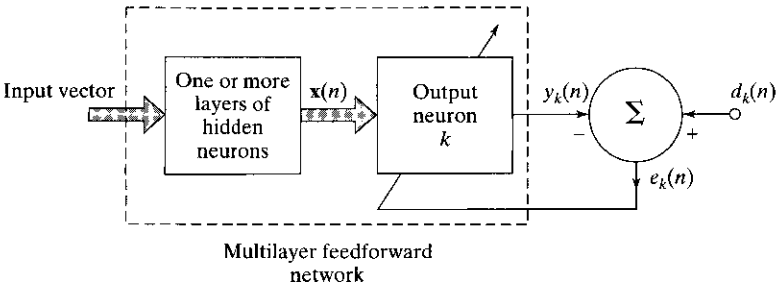
The chapter concludes with some final remarks in Section 2.16.

2.2 ERROR-CORRECTION LEARNING

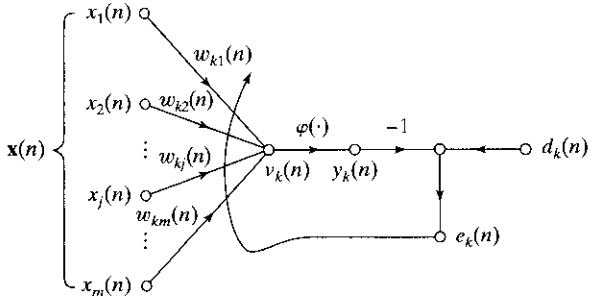
To illustrate our first learning rule, consider the simple case of a neuron k constituting the only computational node in the output layer of a feedforward neural network, as depicted in Fig. 2.1a. Neuron k is driven by a *signal vector* $\mathbf{x}(n)$ produced by one or more layers of hidden neurons, which are themselves driven by an input vector (stimulus) applied to the source nodes (i.e., input layer) of the neural network. The argument n denotes discrete time, or more precisely, the time step of an iterative process involved in adjusting the synaptic weights of neuron k. The *output signal* of neuron k is denoted by $y_k(n)$. This output signal, representing the only output of the neural network, is compared to a *desired response* or *target output,* denoted by $d_k(n)$. Consequently, an *error signal,* denoted by $e_k(n)$, is produced. By definition, we thus have

$$e_k(n) = d_k(n) - y_k(n) \tag{2.1}$$

The error signal $e_k(n)$ actuates a *control mechanism,* the purpose of which is to apply a sequence of corrective adjustments to the synaptic weights of neuron k. The corrective adjustments are designed to make the output signal $y_k(n)$ come closer to the desired



(a) Block diagram of a neural network, highlighting the only neuron in the output layer



(b) Signal-flow graph of output neuron

FIGURE 2.1 Illustrating error-correction learning.

response $d_k(n)$ in a step-by-step manner. This objective is achieved by minimizing a *cost function* or *index of performance*, $\mathscr{E}(n)$, defined in terms of the error signal $e_k(n)$ as:

$$\mathscr{E}(n) = \frac{1}{2} e_k^2(n) \tag{2.2}$$

That is, $\mathscr{E}(n)$ is the *instantaneous value of the error energy*. The step-by-step adjustments to the synaptic weights of neuron k are continued until the system reaches a *steady state* (i.e., the synaptic weights are essentially stabilized). At that point the learning process is terminated.

The learning process described herein is obviously referred to as *error-correction learning*. In particular, minimization of the cost function $\mathscr{E}(n)$ leads to a learning rule commonly referred to as the *delta rule* or *Widrow–Hoff rule*, named in honor of its originators (Widrow and Hoff, 1960). Let $w_{kj}(n)$ denote the value of synaptic weight w_{kj} of neuron k excited by element $x_j(n)$ of the signal vector $\mathbf{x}(n)$ at time step n. According to the delta rule, the adjustment $\Delta w_{kj}(n)$ applied to the synaptic weight w_{kj} at time step n is defined by

$$\Delta w_{kj}(n) = \eta e_k(n) x_j(n) \tag{2.3}$$

where η is a positive constant that determines the *rate of learning* as we proceed from one step in the learning process to another. It is therefore natural that we refer to η as the *learning-rate parameter*. In other words, the delta rule may be stated as:

The adjustment made to a synaptic weight of a neuron is proportional to the product of the error signal and the input signal of the synapse in question.

Keep in mind that the delta rule, as stated herein, presumes that the error signal is *directly measurable*. For this measurement to be feasible we clearly need a supply of desired response from some external source, which is directly accessible to neuron k. In other words, neuron k is *visible* to the outside world, as depicted in Fig. 2.1a. From this figure we also observe that error-correction learning is in fact *local* in nature. This is merely saying that the synaptic adjustments made by the delta rule are localized around neuron k.

Having computed the synaptic adjustment $\Delta w_{kj}(n)$, the updated value of synaptic weight w_{kj} is determined by

$$w_{kj}(n + 1) = w_{kj}(n) + \Delta w_{kj}(n) \tag{2.4}$$

In effect, $w_{kj}(n)$ and $w_{kj}(n + 1)$ may be viewed as the *old* and *new* values of synaptic weight w_{kj}, respectively. In computational terms we may also write

$$w_{kj}(n) = z^{-1}[w_{kj}(n + 1)] \tag{2.5}$$

where z^{-1} is the *unit-delay operator*. That is, z^{-1} represents a *storage element*.

Figure 2.1b shows a signal-flow graph representation of the error-correction learning process, focusing on the activity surrounding neuron k. The input signal x_j and induced local field v_k of neuron k are referred to as the *presynaptic* and *postsynaptic signals* of the jth synapse of neuron k, respectively. From Fig. 2.1b we see that error-correction learning is an example of a *closed-loop feedback system*. From control theory we know that the stability of such a system is determined by those parameters that constitute the feedback loops of the system. In our case we only have a single feedback loop, and one of those parameters of particular interest is the learning-rate parameter η. It is therefore important that η is carefully selected to ensure that the stability or convergence of the iterative learning process is achieved. The choice of η also has a profound influence on the accuracy and other aspects of the learning process. In short, the learning-rate parameter η plays a key role in determining the performance of error-correction learning in practice.

Error-correction learning is discussed in much greater detail in Chapter 3, which discusses single-layer feedforward networks and in Chapter 4, which details multilayer feedforward networks.

2.3 MEMORY-BASED LEARNING

In *memory-based learning*, all (or most) of the past experiences are explicitly stored in a large memory of correctly classified input–output examples: $\{(\mathbf{x}_i, d_i)\}_{i=1}^{N}$, where $\mathbf{x}_i$ denotes an input vector and d_i denotes the corresponding desired response. Without loss of generality, we have restricted the desired response to be a scalar. For example, in a binary pattern classification problem there are two classes/hypotheses, denoted by $\mathscr{C}_1$ and $\mathscr{C}_2$, to be considered. In this example, the desired response d_i takes the value 0 (or -1) for class $\mathscr{C}_1$ and the value 1 for class $\mathscr{C}_2$. When classification of a test vector $\mathbf{x}_{\text{test}}$ (not seen before) is required, the algorithm responds by retrieving and analyzing the training data in a "local neighborhood" of $\mathbf{x}_{\text{test}}$.

All memory-based learning algorithms involve two essential ingredients:

- Criterion used for defining the local neighborhood of the test vector $\mathbf{x}_{\text{test}}$.
- Learning rule applied to the training examples in the local neighborhood of $\mathbf{x}_{\text{test}}$.

The algorithms differ from each other in the way in which these two ingredients are defined.

In a simple yet effective type of memory-based learning known as the *nearest neighbor rule*,[2] the local neighborhood is defined as the training example that lies in the immediate neighborhood of the test vector $\mathbf{x}_{\text{test}}$. In particular, the vector

$$\mathbf{x}'_N \in \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\} \tag{2.6}$$

is said to be the nearest neighbor of $\mathbf{x}_{\text{test}}$ if

$$\min_i d(\mathbf{x}_i, \mathbf{x}_{\text{test}}) = d(\mathbf{x}'_N, \mathbf{x}_{\text{test}}) \tag{2.7}$$

where $d(\mathbf{x}_i, \mathbf{x}_{\text{test}})$ is the Euclidean distance between the vectors $\mathbf{x}_i$ and $\mathbf{x}_{\text{test}}$. The class associated with the minimum distance, that is, vector $\mathbf{x}'_N$, is reported as the classification of $\mathbf{x}_{\text{test}}$. This rule is independent of the underlying distribution responsible for generating the training examples.

Cover and Hart (1967) have formally studied the nearest neighbor rule as a tool for pattern classification. The analysis presented therein is based on two assumptions:

- The classified examples $(\mathbf{x}_i, d_i)$ are *independently and identically distributed (iid)*, according to the joint probability distribution of the example $(\mathbf{x}, d)$.
- The sample size N is infinitely large.

Under these two assumptions, it is shown that the probability of classification error incurred by the nearest neighbor rule is bounded above by twice the *Bayes probability of error*, that is, the minimum probability of error over all decision rules. Bayes probability of error is discussed in Chapter 3. In this sense, it may be said that half the classification information in a training set of infinite size is contained in the nearest neighbor, which is a surprising result.

A variant of the nearest neighbor classifier is the *k-nearest neighbor classifier*, which proceeds as follows:

- Identify the k classified patterns that lie nearest to the test vector $\mathbf{x}_{\text{test}}$ for some integer k.
- Assign $\mathbf{x}_{\text{test}}$ to the class (hypothesis) that is most frequently represented in the k nearest neighbors to $\mathbf{x}_{\text{test}}$ (i.e., use a majority vote to make the classification).

Thus the k-nearest neighbor classifier acts like an averaging device. In particular, it discriminates against a single outlier, as illustrated in Fig. 2.2 for $k = 3$. An *outlier* is an observation that is improbably large for a nominal model of interest.

In Chapter 5 we discuss another important type of memory-based classifier known as the radial-basis function network.

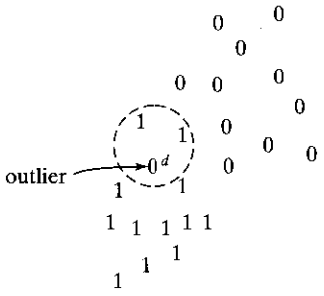


FIGURE 2.2 The area lying inside the dashed circle includes two points pertaining to class 1 and an outlier from class 0. The point *d* corresponds to the test vector $\mathbf{x}_{test}$. With $k = 3$, the *k-nearest* neighbor *classifier* assigns class 1 to point *d* even though it lies closest to the *outlier*.

2.4 HEBBIAN LEARNING

Hebb's postulate of learning is the oldest and most famous of all learning rules; it is named in honor of the neuropsychologist Hebb (1949). Quoting from Hebb's book, *The Organization of Behavior* (1949, p.62):

> When an axon of cell A is near enough to excite a cell B and repeatedly or persistently takes part in firing it, some growth process or metabolic changes take place in one or both cells such that A's efficiency as one of the cells firing B, is increased.

Hebb proposed this change as a basis of associative learning (at the cellular level), which would result in an enduring modification in the activity pattern of a spatially distributed "assembly of nerve cells."

This statement is made in a neurobiological context. We may expand and rephrase it as a two-part rule (Stent, 1973; Changeux and Danchin, 1976):

1. *If two neurons on either side of a synapse (connection) are activated simultaneously (i.e., synchronously), then the strength of that synapse is selectively increased.*
2. *If two neurons on either side of a synapse are activated asynchronously, then that synapse is selectively weakened or eliminated.*

Such a synapse is called a *Hebbian synapse.*[3] (The original Hebb rule did not contain part 2.) More precisely, we define a Hebbian synapse as a synapse that uses a *time-dependent, highly local, and strongly interactive mechanism to increase synaptic efficiency as a function of the correlation between the presynaptic and postsynaptic activities.* From this definition we may deduce the following four key mechanisms (properties) that characterize a Hebbian synapse (Brown et al., 1990):

1. *Time-dependent mechanism.* This mechanism refers to the fact that the modifications in a Hebbian synapse depend on the exact time of occurrence of the presynaptic and postsynaptic signals.

2. *Local mechanism.* By its very nature, a synapse is the transmission site where information-bearing signals (representing ongoing activity in the presynaptic and postsynaptic units) are in *spatiotemporal* contiguity. This locally available information is used by a Hebbian synapse to produce a local synaptic modification that is input specific.

3. *Interactive mechanism.* The occurrence of a change in a Hebbian synapse depends on signals on both sides of the synapse. That is, a Hebbian form of learning depends on a "true interaction" between presynaptic and postsynaptic signals in the sense that we cannot make a prediction from either one of these two activities by itself. Note also that this dependence or interaction may be deterministic or statistical in nature.

4. *Conjunctional* or *correlational mechanism.* One interpretation of Hebb's postulate of learning is that the condition for a change in synaptic efficiency is the conjunction of presynaptic and postsynaptic signals. Thus, according to this interpretation, the co-occurrence of presynaptic and postsynaptic signals (within a short interval of time) is sufficient to produce the synaptic modification. It is for this reason that a Hebbian synapse is sometimes referred to as a *conjunctional synapse.* For another interpretation of Hebb's postulate of learning, we may think of the interactive mechanism characterizing a Hebbian synapse in statistical terms. In particular, the correlation over time between presynaptic and postsynaptic signals is viewed as being responsible for a synaptic change. Accordingly, a Hebbian synapse is also referred to as a *correlational synapse.* Correlation is indeed the basis of learning (Eggermont, 1990).

Synaptic Enhancement and Depression

The definition of a Hebbian synapse presented here does not include additional processes that may result in weakening of a synapse connecting a pair of neurons. Indeed, we may generalize the concept of a Hebbian modification by recognizing that positively correlated activity produces synaptic strengthening, and that either uncorrelated or negatively correlated activity produces synaptic weakening (Stent, 1973). Synaptic depression may also be of a noninteractive type. Specifically, the interactive condition for synaptic weakening may simply be noncoincident presynaptic or postsynaptic activity.

We may go one step further by classifying synaptic modifications as *Hebbian, anti-Hebbian, and non-Hebbian* (Palm, 1982). According to this scheme, a Hebbian synapse increases its strength with positively correlated presynaptic and postsynaptic signals, and decreases its strength when these signals are either uncorrelated or negatively correlated. Conversely, an anti-Hebbian synapse weakens positively correlated presynaptic and postsynaptic signals, and strengthens negatively correlated signals. In both Hebbian and anti-Hebbian synapses, however, the modification of synaptic efficiency relies on a mechanism that is time-dependent, highly local, and strongly interactive in nature. In that sense, an anti-Hebbian synapse is still Hebbian in nature, though not in function. A non-Hebbian synapse, on the other hand, does not involve a Hebbian mechanism of either kind.

Mathematical Models of Hebbian Modifications

To formulate Hebbian learning in mathematical terms, consider a synaptic weight w_{kj} of neuron k with presynaptic and postsynaptic signals denoted by x_j and y_k, respectively. The adjustment applied to the synaptic weight w_{kj} at time step n is expressed in the general form

$$\Delta w_{kj}(n) = F(y_k(n), x_j(n)) \tag{2.8}$$

where $F(\cdot,\cdot)$ is a function of both postsynaptic and presynaptic signals. The signals $x_j(n)$ and $y_k(n)$ are often treated as dimensionless. The formula of Eq. (2.8) admits many forms, all of which qualify as Hebbian. In what follows, we consider two such forms.

Hebb's hypothesis. The simplest form of Hebbian learning is described by

$$\Delta w_{kj}(n) = \eta y_k(n) x_j(n) \tag{2.9}$$

where η is a positive constant that determines the *rate of learning*. Equation (2.9) clearly emphasizes the correlational nature of a Hebbian synapse. It is sometimes referred to as the *activity product rule*. The top curve of Fig. 2.3 shows a graphical representation of Eq. (2.9) with the change Δw_{kj} plotted versus the output signal (postsynaptic activity) y_k. From this representation we see that the repeated application of the input signal (presynaptic activity) x_j leads to an increase in y_k and therefore *exponential growth* that finally drives the synaptic connection into saturation. At that point no information will be stored in the synapse and selectivity is lost.

Covariance hypothesis. One way of overcoming the limitation of Hebb's hypothesis is to use the *covariance hypothesis* introduced in Sejnowski (1977a, b). In this hypothesis, the presynaptic and postsynaptic signals in Eq. (2.9) are replaced by the departure of presynaptic and postsynaptic signals from their respective average values over a certain time interval. Let $\bar{x}$ and $\bar{y}$ denote the *time-averaged values* of the presynaptic signal x_j and postsynaptic signal y_k, respectively. According to the covariance hypothesis, the adjustment applied to the synaptic weight w_{kj} is defined by

$$\Delta w_{kj} = \eta(x_j - \bar{x})(y_k - \bar{y}) \tag{2.10}$$

where η is the learning-rate parameter. The average values x and y constitute presynaptic and postsynaptic thresholds, which determine the sign of synaptic modification. In particular, the covariance hypothesis allows for the following:

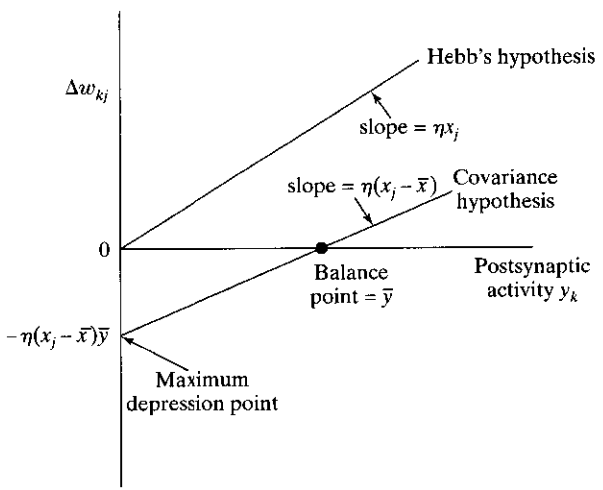


FIGURE 2.3 Illustration of Hebb's hypothesis and the covariance hypothesis.

- Convergence to a nontrivial state, which is reached when $x_k = \bar{x}$ or $y_j = \bar{y}$.
- Prediction of both synaptic *potentiation* (i.e., increase in synaptic strength) and synaptic *depression* (i.e., decrease in synaptic strength).

Figure 2.3 illustrates the difference between Hebb's hypothesis and the covariance hypothesis. In both cases the dependence of Δw_{kj} on y_k is linear; however, the intercept with the y_k-axis in Hebb's hypothesis is at the origin, whereas in the covariance hypothesis it is at $y_k = \bar{y}$.

We make the following important observations from Eq. (2.10):

1. Synaptic weight w_{kj} is enhanced if there are sufficient levels of presynaptic and postsynaptic activities, that is, the conditions $x_j > \bar{x}$ and $y_k > \bar{y}$ are both satisfied.
2. Synaptic weight w_{kj} is depressed if there is either
   - a presynaptic activation (i.e., $x_j > \bar{x}$) in the absence of sufficient postsynaptic activation (i.e., $y_k < \bar{y}$), or
   - a postsynaptic activation (i.e., $y_k > \bar{y}$) in the absence of sufficient presynaptic activation (i.e., $x_j < \bar{x}$).

This behavior may be regarded as a form of temporal competition between the incoming patterns.

There is strong physiological evidence[4] for Hebbian learning in the area of the brain called the *hippocampus*. The hippocampus plays an important role in certain aspects of learning or memory. This physiological evidence makes Hebbian learning all the more appealing.

2.5 COMPETITIVE LEARNING

In *competitive learning*,[5] as the name implies, the output neurons of a neural network compete among themselves to become active (fired). Whereas in a neural network based on Hebbian learning several output neurons may be active simultaneously, in competitive learning only a single output neuron is active at any one time. It is this feature that makes competitive learning highly suited to discover statistically salient features that may be used to classify a set of input patterns.

There are three basic elements to a competitive learning rule (Rumelhart and Zipser, 1985):

- A set of neurons that are all the same except for some randomly distributed synaptic weights, and which therefore *respond differently* to a given set of input patterns.
- A *limit* imposed on the "strength" of each neuron.
- A mechanism that permits the neurons to *compete* for the right to respond to a given subset of inputs, such that only *one* output neuron, or only one neuron per group, is active (i.e., "on") at a time. The neuron that wins the competition is called a *winner-takes-all neuron*.

Accordingly the individual neurons of the network learn to specialize on ensembles of similar patterns; in so doing they become *feature detectors* for different classes of input patterns.

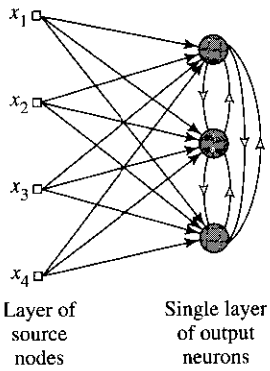


FIGURE 2.4 Architectural graph of a simple competitive learning network with feedforward (excitatory) connections from the source nodes to the neurons, and lateral (inhibitory) connections among the neurons; the lateral connections are signified by open arrows.

In the simplest form of competitive learning, the neural network has a single layer of output neurons, each of which is fully connected to the input nodes. The network may include feedback connections among the neurons, as indicated in Fig. 2.4. In the network architecture described herein, the feedback connections perform *lateral inhibition*,[6] with each neuron tending to inhibit the neuron to which it is laterally connected. In contrast, the feedforward synaptic connections in the network of Fig. 2.4 are all *excitatory*.

For a neuron k to be the winning neuron, its induced local field v_k for a specified input pattern $\mathbf{x}$ must be the largest among all the neurons in the network. The output signal y_k of winning neuron k is set equal to one; the output signals of all the neurons that lose the competition are set equal to zero. We thus write

$$y_k = \begin{cases} 1 & \text{if } v_k > v_j \text{ for all } j, j \neq k \\ 0 & \text{otherwise} \end{cases} \tag{2.11}$$

where the induced local field v_k represents the combined action of all the forward and feedback inputs to neuron k.

Let w_{kj} denote the synaptic weight connecting input node j to neuron k. Suppose that each neuron is allotted a *fixed* amount of synaptic weight (i.e., all synaptic weights are positive), which is distributed among its input nodes; that is,

$$\sum_j w_{kj} = 1 \qquad \text{for all } k \tag{2.12}$$

A neuron then learns by shifting synaptic weights from its inactive to active input nodes. If a neuron does not respond to a particular input pattern, no learning takes place in that neuron. If a particular neuron wins the competition, each input node of that neuron relinquishes some proportion of its synaptic weight, and the weight relinquished is then distributed equally among the active input nodes. According to the standard *competitive learning rule*, the change Δw_{kj} applied to synaptic weight w_{kj} is defined by

$$\Delta w_{kj} = \begin{cases} \eta(x_j - w_{kj}) & \text{if neuron } k \text{ wins the competition} \\ 0 & \text{if neuron } k \text{ loses the competition} \end{cases} \tag{2.13}$$

where η is the learning-rate parameter. This rule has the overall effect of moving the synaptic weight vector $\mathbf{w}_k$ of winning neuron k toward the input pattern $\mathbf{x}$.

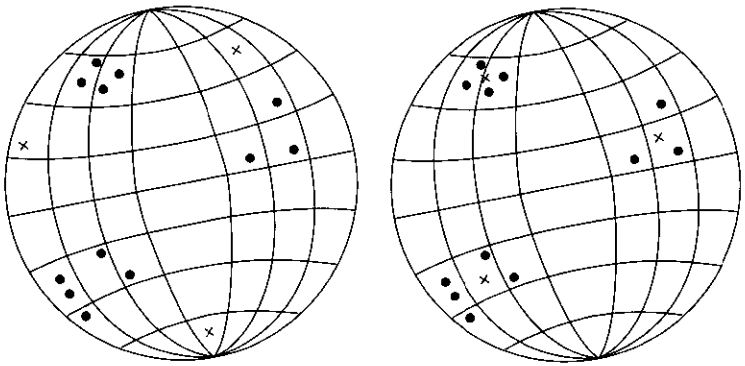


FIGURE 2.5 Geometric interpretation of the competitive learning process. The dots represent the input vectors, and the crosses represent the synaptic weight vectors of three output neurons. (a) Initial state of the network. (b) Final state of the network.

We may use the geometric analogy depicted in Fig. 2.5 to illustrate the essence of competitive learning (Rumelhart and Zipser, 1985). It is assumed that each input pattern (vector) $\mathbf{x}$ has some constant Euclidean length so that we may view it as a point on an N-dimensional unit sphere where N is the number of input nodes. N also represents the dimension of each synaptic weight vector $\mathbf{w}_k$. It is further assumed that all neurons in the network are constrained to have the same Euclidean length (norm), as shown by

$$\sum_j w_{kj}^2 = 1 \qquad \text{for all } k \tag{2.14}$$

When the synaptic weights are properly scaled they form a set of vectors that fall on the same N-dimensional unit sphere. In Fig. 2.5a we show three natural groupings (clusters) of the stimulus patterns represented by dots. This figure also includes a possible initial state of the network (represented by crosses) that may exist before learning. Figure 2.5b shows a typical final state of the network that results from the use of competitive learning. In particular, each output neuron has discovered a cluster of input patterns by moving its synaptic weight vector to the center of gravity of the discovered cluster (Rumelhart and Zipser, 1985; Hertz et al., 1991). This figure illustrates the ability of a neural network to perform *clustering* through competitive learning. However, for this function to be performed in a "stable" fashion the input patterns must fall into sufficiently distinct groupings to begin with. Otherwise the network may be unstable because it will no longer respond to a given input pattern with the same output neuron.

2.6 BOLTZMANN LEARNING

The Boltzmann learning rule, named in honor of Ludwig Boltzmann, is a stochastic learning algorithm derived from ideas rooted in statistical mechanics.[7] A neural net-

work designed on the basis of the Boltzmann learning rule is called a *Boltzmann machine* (Ackley et al., 1985; Hinton and Sejnowski, 1986).

In a Boltzmann machine the neurons constitute a recurrent structure, and they operate in a binary manner since, for example, they are either in an "on" state denoted by +1 or in an "off" state denoted by −1. The machine is characterized by an *energy function, E*, the value of which is determined by the particular states occupied by the individual neurons of the machine, as shown by

$$E = -\frac{1}{2}\sum_{j}\sum_{\substack{k \\ j \neq k}} w_{kj} x_k x_j \tag{2.15}$$

where x_j is the state of neuron j, and w_{kj} is the synaptic weight connecting neuron j to neuron k. The fact that $j \neq k$ means simply that none of the neurons in the machine has self-feedback. The machine operates by choosing a neuron at random—for example, neuron k—at some step of the learning process, then flipping the state of neuron k from state x_k to state $-x_k$ at some temperature T with probability

$$P(x_k \rightarrow -x_k) = \frac{1}{1 + \exp(-\Delta E_k / T)} \tag{2.16}$$

where ΔE_k is the *energy change* (i.e., the change in the energy function of the machine) resulting from such a flip. Notice that T is not a physical temperature, but rather a *pseudotemperature,* as explained in Chapter 1. If this rule is applied repeatedly, the machine will reach *thermal equilibrium.*

The neurons of a Boltzmann machine partition into two functional groups: *visible* and *hidden.* The visible neurons provide an interface between the network and the environment in which it operates, whereas the hidden neurons always operate freely. There are two modes of operation to be considered:

- *Clamped condition,* in which the visible neurons are all clamped onto specific states determined by the environment.
- *Free-running condition,* in which all the neurons (visible and hidden) are allowed to operate freely.

Let ρ_{kj}^{+} denote the *correlation* between the states of neurons j and k, with the network in its clamped condition. Let ρ_{kj}^{-} denote the *correlation* between the states of neurons j and k with the network in its free-running condition. Both correlations are averaged over all possible states of the machine when it is in thermal equilibrium. Then, according to the *Boltzmann learning rule,* the change Δw_{kj} applied to the synaptic weight w_{kj} from neuron j to neuron k is defined by (Hinton and Sejnowski, 1986)

$$\Delta w_{kj} = \eta(\rho_{kj}^{+} - \rho_{kj}^{-}), \qquad j \neq k \tag{2.17}$$

where η is a learning-rate parameter. Note that both ρ_{kj}^{+} and ρ_{kj}^{-} range in value from −1 to +1.

A brief review of statistical mechanics is presented in Chapter 11; in that chapter we also present a detailed treatment of the Boltzmann machine and other stochastic machines.

2.7 CREDIT-ASSIGNMENT PROBLEM

When studying learning algorithms for distributed systems, it is useful to consider the notion of *credit assignment* (Minsky, 1961). Basically, the credit-assignment problem is the problem of assigning *credit* or *blame* for overall outcomes to each of the internal decisions made by a learning machine and which contributed to those outcomes. (The credit assignment problem is also referred to as the *loading problem*, the problem of "loading" a given set of training data into the free parameters of the network.)

In many cases the dependence of outcomes on internal decisions is mediated by a sequence of actions taken by the learning machine. In other words, internal decisions affect which particular actions are taken, and then the actions, not the internal decisions, directly influence overall outcomes. In these situations, we may decompose the credit-assignment problem into two subproblems (Sutton, 1984):

1. The assignment of credit for outcomes to actions. This is called the *temporal credit-assignment problem* in that it involves the instants of time *when* the actions that deserve credit were actually taken.
2. The assignment of credit for actions to internal decisions. This is called the *structural credit-assignment problem* in that it involves assigning credit to the *internal structures* of actions generated by the system.

The structural credit-assignment problem is relevant in the context of a multicomponent learning machine when we must determine precisely which particular component of the system should have its behavior altered and by how much in order to improve overall system performance. On the other hand, the temporal credit-assignment problem is relevant when there are many actions taken by a learning machine that result in certain outcomes, and we must determine which of these actions were responsible for the outcomes. The combined temporal and structural credit-assignment problem faces any distributed learning machine that attempts to improve its performance in situations involving temporally extended behavior (Williams, 1988).

The credit-assignment problem, for example, arises when error-correction learning is applied to a multilayer feedforward neural network. The operation of each hidden neuron, as well as that of each output neuron in such a network is important to its correct overall operation on a learning task of interest. That is, in order to solve the prescribed task the network must assign certain forms of behavior to all of its neurons through the specification of error-correction learning. With this background in mind, consider the situation described in Fig. 2.1a. Since the output neuron k is visible to the outside world, it is possible to supply a desired response to this neuron. As far as the output neuron is concerned, it is a straightforward matter to adjust the synaptic weights of the output neuron in accordance with error-correction learning, as outlined in Section 2.2. But how do we assign credit or blame for the action of the hidden neurons when the error-correction learning process is used to adjust the respective synaptic weights of these neurons? The answer to this fundamental question requires more detailed attention; it is presented in Chapter 4, where algorithmic details of the design of multilayer feedforward neural networks are described.

2.8 LEARNING WITH A TEACHER

We now turn our attention to learning paradigms. We begin by considering *learning with a teacher,* which is also referred to as *supervised learning*. Figure 2.6 shows a block diagram that illustrates this form of learning. In conceptual terms, we may think of the teacher as having knowledge of the environment, with that knowledge being represented by a set of *input–output examples*. The environment is, however, *unknown* to the neural network of interest. Suppose now that the teacher and the neural network are both exposed to a training vector (i.e., example) drawn from the environment. By virtue of built-in knowledge, the teacher is able to provide the neural network with a desired response for that training vector. Indeed, the desired response represents the optimum action to be performed by the neural network. The network parameters are adjusted under the combined influence of the training vector and the error signal. The *error signal* is defined as the difference between the desired response and the actual response of the network. This adjustment is carried out iteratively in a step-by-step fashion with the aim of eventually making the neural network *emulate* the teacher; the emulation is presumed to be optimum in some statistical sense. In this way knowledge of the environment available to the teacher is transferred to the neural network through training as fully as possible. When this condition is reached, we may then dispense with the teacher and let the neural network deal with the environment completely by itself.

The form of supervised learning we have just described is the error-correction learning discussed previously in Section 2.2. It is a closed-loop feedback system, but the unknown environment is not in the loop. As a performance measure for the system we may think in terms of the mean-square error or the sum of squared errors over the training sample, defined as a function of the free parameters of the system. This function may be visualized as a multidimensional *error-performance surface* or simply *error surface,* with the free parameters as coordinates. The true error surface is *averaged* over all possible input–output examples. Any given operation of the system under the

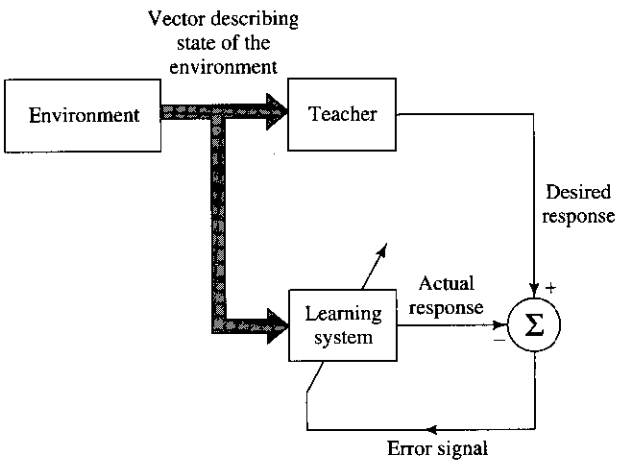


FIGURE 2.6 Block diagram of learning with a teacher.

teacher's supervision is represented as a point on the error surface. For the system to improve performance over time and therefore learn from the teacher, the operating point has to move down successively toward a minimum point of the error surface; the minimum point may be a local minimum or a global minimum. A supervised learning system is able to do this with the useful information it has about the *gradient* of the error surface corresponding to the current behavior of the system. The gradient of an error surface at any point is a vector that points in the direction of *steepest descent*. In fact, in the case of supervised learning from examples, the system may use an *instantaneous estimate* of the gradient vector, with the example indices presumed to be those of time. The use of such an estimate results in a motion of the operating point on the error surface that is typically in the form of a "random walk." Nevertheless, given an algorithm designed to minimize the cost function, an adequate set of input–output examples, and enough time permitted to do the training, a supervised learning system is usually able to perform such tasks as pattern classification and function approximation.

2.9 LEARNING WITHOUT A TEACHER

In supervised learning, the learning process takes place under the tutelage of a teacher. However, in the paradigm known as *learning without a teacher,* as the name implies, there is *no* teacher to oversee the learning process. That is to say, there are no labeled examples of the function to be learned by the network. Under this second paradigm, two subdivisions are identified:

1. Reinforcement learning/Neurodynamic programming

In *reinforcement learning,*[8] the learning of an input–output mapping is performed through continued interaction with the environment in order to minimize a scalar index of performance. Figure 2.7 shows the block diagram of one form of a reinforcement learning system built around a *critic* that converts a *primary reinforcement signal* received from the environment into a higher quality reinforcement signal called the *heuristic reinforcement signal,* both of which are scalar inputs (Barto et al., 1983). The

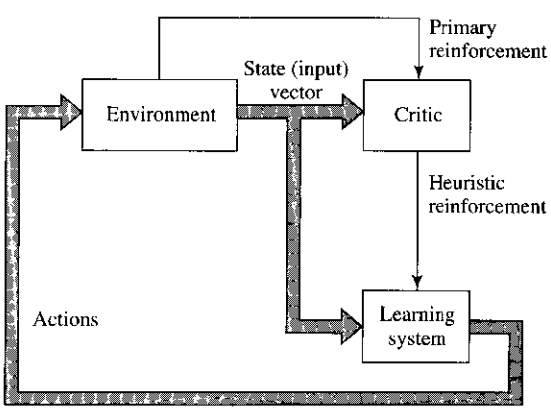


FIGURE 2.7 Block diagram of reinforcement learning.

system is designed to learn under *delayed reinforcement,* which means that the system observes a temporal sequence of stimuli (i.e., state vectors) also received from the environment, which eventually result in the generation of the heuristic reinforcement signal. The goal of learning is to minimize a *cost-to-go function,* defined as the expectation of the cumulative cost of *actions* taken over a sequence of steps instead of simply the immediate cost. It may turn out that certain actions taken earlier in that sequence of time steps are in fact the best determinants of overall system behavior. The function of the *learning machine,* which constitutes the second component of the system, is to *discover* these actions and to feed them back to the environment.

Delayed-reinforcement learning is difficult to perform for two basic reasons:

- There is no teacher to provide a desired response at each step of the learning process.
- The delay incurred in the generation of the primary reinforcement signal implies that the learning machine must solve a *temporal credit assignment problem.* By this we mean that the learning machine must be able to assign credit and blame individually to each action in the sequence of time steps that led to the final outcome, while the primary reinforcement may only evaluate the outcome.

Notwithstanding these difficulties, delayed-reinforcement learning is very appealing. It provides the basis for the system to interact with its environment, thereby developing the ability to learn to perform a prescribed task solely on the basis of the outcomes of its experience that result from the interaction.

Reinforcement learning is closely related to *dynamic programming,* which was developed by Bellman (1957) in the context of optimal control theory. Dynamic programming provides the mathematical formalism for sequential decision making. By casting reinforcement learning within the framework of dynamic programming, the subject matter becomes all the richer for it, as demonstrated in Bertsekas and Tsitsiklis (1996). An introductory treatment of dynamic programming and its relationship to reinforcement learning is presented in Chapter 12.

2. Unsupervised Learning

In *unsupervised* or *self-organized* learning there is no external teacher or critic to oversee the learning process, as indicated in Fig. 2.8. Rather, provision is made for a *task-independent measure* of the quality of representation that the network is required to learn, and the free parameters of the network are optimized with respect to that measure. Once the network has become tuned to the statistical regularities of the input data, it develops the ability to form internal representations for encoding features of the input and thereby to create new classes automatically (Becker, 1991).

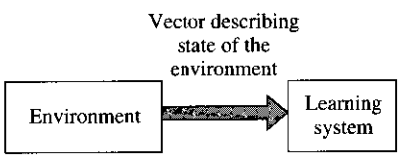


FIGURE 2.8 Block diagram of unsupervised learning.

To perform unsupervised learning we may use a competitive learning rule. For example, we may use a neural network that consists of two layers—an input layer and a competitive layer. The input layer receives the available data. The competitive layer consists of neurons that compete with each other (in accordance with a learning rule) for the "opportunity" to respond to features contained in the input data. In its simplest form, the network operates in accordance with a "winner-takes-all" strategy. As described in Section 2.5, in such a strategy the neuron with the greatest total input "wins" the competition and turns on; all the other neurons then switch off.

Different algorithms for unsupervised learning are described in Chapters 8 through 11.

2.10 LEARNING TASKS

In previous sections of this chapter we have discussed different learning algorithms and learning paradigms. In this section, we describe some basic learning tasks. The choice of a particular learning algorithm is influenced by the learning task that a neural network is required to perform. In this context we identify six learning tasks that apply to the use of neural networks in one form or another.

Pattern Association

An *associative memory* is a brainlike distributed memory that learns by *association*. Association has been known to be a prominent feature of human memory since Aristotle, and all models of cognition use association in one form or another as the basic operation (Anderson, 1995).

Association takes one of two forms: *autoassociation* or *heteroassociation*. In autoassociation, a neural network is required to *store* a set of patterns (vectors) by repeatedly presenting them to the network. The network is subsequently presented a partial description or distorted (noisy) version of an original pattern stored in it, and the task is to *retrieve* (*recall*) that particular pattern. Heteroassociation differs from autoassociation in that an arbitrary set of input patterns is *paired* with another arbitrary set of output patterns. Autoassociation involves the use of unsupervised learning, whereas the type of learning involved in heteroassociation is supervised.

Let $\mathbf{x}_k$ denote a *key pattern* (vector) applied to an associative memory and $\mathbf{y}_k$ denote a *memorized pattern* (vector). The pattern association performed by the network is described by

$$\mathbf{x}_k \rightarrow \mathbf{y}_k, \qquad k = 1, 2, \ldots, q \tag{2.18}$$

where q is the number of patterns stored in the network. The key pattern $\mathbf{x}_k$ acts as a stimulus that not only determines the storage location of memorized pattern $\mathbf{y}_k$, but also holds the key for its retrieval.

In an autoassociative memory, $\mathbf{y}_k = \mathbf{x}_k$, so the input and output (data) spaces of the network have the same dimensionality. In a heteroassociative memory, $\mathbf{y}_k \neq \mathbf{x}_k$; hence, the dimensionality of the output space in this second case may or may not equal the dimensionality of the input space.

There are two phases involved in the operation of an associative memory:

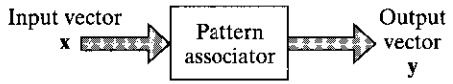


FIGURE 2.9 Input–output relation of pattern associator.

- *Storage phase,* which refers to the training of the network in accordance with Eq. (2.18).
- *Recall phase,* which involves the retrieval of a memorized pattern in response to the presentation of a noisy or distorted version of a key pattern to the network.

Let the stimulus (input) $\mathbf{x}$ represent a noisy or distorted version of a key pattern $\mathbf{x}_j$. This stimulus produces a response (output) $\mathbf{y}$, as indicated in Fig. 2.9. For perfect recall, we should find that $\mathbf{y} = \mathbf{y}_j$, where $\mathbf{y}_j$ is the memorized pattern associated with the key pattern $\mathbf{x}_j$. When $\mathbf{y} \neq \mathbf{y}_j$ for $\mathbf{x} = \mathbf{x}_j$, the associative memory is said to have made an *error* in recall.

The number q of patterns stored in an associative memory provides a direct measure of the *storage capacity* of the network. In designing an associative memory, the challenge is to make the storage capacity q (expressed as a percentage of the total number N of neurons used to construct the network) as large as possible and yet insist that a large fraction of the memorized patterns is recalled correctly.

Pattern Recognition

Humans are good at pattern recognition. We receive data from the world around us via our senses and are able to recognize the source of the data. We are often able to do so almost immediately and with practically no effort. For example, we can recognize the familiar face of a person even though that person has aged since our last encounter, identify a familiar person by his or her voice on the telephone despite a bad connection, and distinguish a boiled egg that is good from a bad one by smelling it. Humans perform pattern recognition through a learning process; so it is with neural networks.

Pattern recognition is formally defined as *the process whereby a received pattern/signal is assigned to one of a prescribed number of classes (categories).* A neural network performs pattern recognition by first undergoing a training session, during which the network is repeatedly presented a set of input patterns along with the category to which each particular pattern belongs. Later, a new pattern is presented to the network that has not been seen before, but which belongs to the same population of patterns used to train the network. The network is able to identify the class of that particular pattern because of the information it has extracted from the training data. Pattern recognition performed by a neural network is statistical in nature, with the patterns being represented by points in a multidimensional *decision space.* The decision space is divided into regions, each one of which is associated with a class. The decision boundaries are determined by the training process. The construction of these boundaries is made statistical by the inherent variability that exists within and between classes.

In generic terms, pattern-recognition machines using neural networks may take one of two forms:

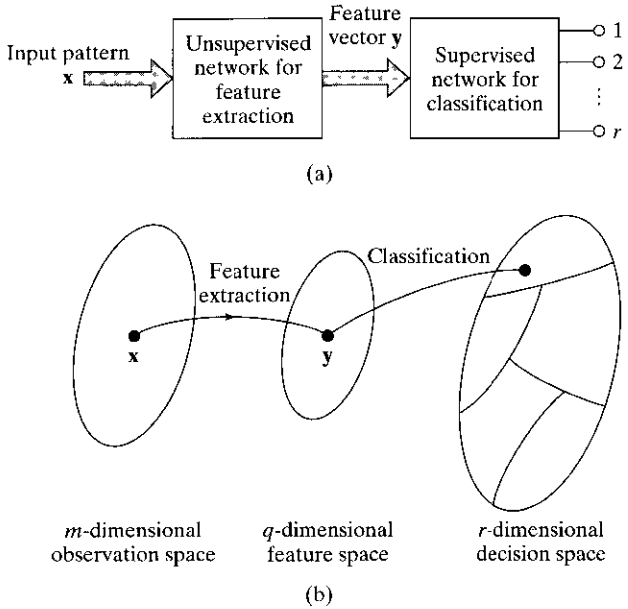


FIGURE 2.10 Illustration of the classical approach to pattern classification.

- The machine is split into two parts, an unsupervised network for *feature extraction* and a supervised network for *classification*, as shown in Fig. 2.10a. Such a method follows the traditional approach to statistical pattern recognition (Duda and Hart, 1973; Fukunaga, 1990). In conceptual terms, a pattern is represented by a set of m observables, which may be viewed as a point $\mathbf{x}$ in an m-dimensional *observation (data) space*. Feature extraction is described by a transformation that maps the point $\mathbf{x}$ into an intermediate point $\mathbf{y}$ in a q-dimensional *feature space* with $q < m$, as indicated in Fig. 2.10b. This transformation may be viewed as one of dimensionality reduction (i.e., data compression), the use of which is justified on the grounds that it simplifies the task of classification. The classification is itself described as a transformation that maps the intermediate point $\mathbf{y}$ into one of the classes in an r-dimensional decision space, where r is the number of classes to be distinguished.
- The machine is designed as a single multilayer feedforward network using a supervised learning algorithm. In this second approach, the task of feature extraction is performed by the computational units in the hidden layer(s) of the network.

Which of these two approaches is adopted in practice depends on the application of interest.

Function Approximation

The third learning task of interest is that of function approximation. Consider a nonlinear input–output mapping described by the functional relationship

$$\mathbf{d} = \mathbf{f}(\mathbf{x}) \tag{2.19}$$

where the vector $\mathbf{x}$ is the input and the vector $\mathbf{d}$ is the output. The vector-valued function $\mathbf{f}(\cdot)$ is assumed to be unknown. To make up for the lack of knowledge about the function $\mathbf{f}(\cdot)$, we are given the set of labeled examples:

$$\mathcal{T} = \{(\mathbf{x}_i, \mathbf{d}_i)\}_{i=1}^{N} \tag{2.20}$$

The requirement is to design a neural network that approximates the unknown function $\mathbf{f}(\cdot)$ such that the function $\mathbf{F}(\cdot)$ describing the input–output mapping actually realized by the network is close enough to $\mathbf{f}(\cdot)$ in a Euclidean sense over all inputs, as shown by

$$\|\mathbf{F}(\mathbf{x}) - \mathbf{f}(\mathbf{x})\| < \epsilon \qquad \text{for all } \mathbf{x} \tag{2.21}$$

where ϵ is a small positive number. Provided that the size N of the training set is large enough and the network is equipped with an adequate number of free parameters, then the approximation error ϵ can be made small enough for the task.

The approximation problem described here is a perfect candidate for supervised learning with $\mathbf{x}_i$ playing the role of input vector and $\mathbf{d}_i$ serving the role of desired response. We may turn this issue around and view supervised learning as an approximation problem.

The ability of a neural network to approximate an unknown input–output mapping may be exploited in two important ways:

- *System identification.* Let Eq. (2.19) describe the input–output relation of an unknown memoryless *multiple input-multiple output (MIMO) system*; by a "memoryless" system we mean a system that is time invariant. We may then use the set of labeled examples in Eq. (2.20) to train a neural network as a model of the system. Let $\mathbf{y}_i$ denote the output of the neural network produced in response to an input vector $\mathbf{x}_i$. The difference between $\mathbf{d}_i$ (associated with $\mathbf{x}_i$) and the network output $\mathbf{y}_i$ provides the error signal vector $\mathbf{e}_i$, as depicted in Fig. 2.11. This error signal is in turn used to adjust the free parameters of the network to minimize the squared difference between the outputs of the unknown system and the neural network in a statistical sense, and is computed over the entire training set.
- *Inverse system.* Suppose next we are given a known memoryless MIMO system whose input–output relation is described by Eq. (2.19). The requirement in this

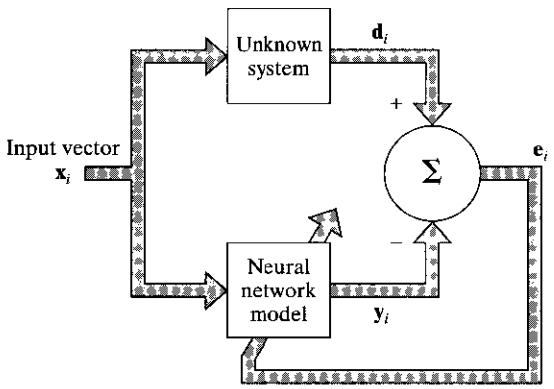


FIGURE 2.11 Block diagram of system identification.

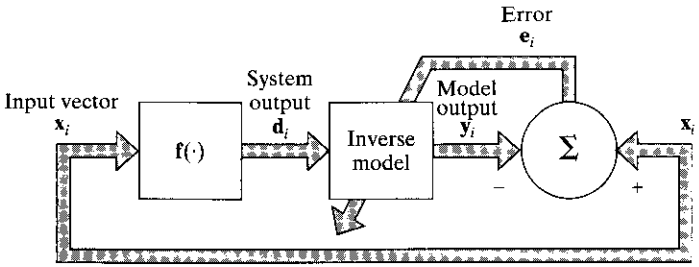


FIGURE 2.12 Block diagram of inverse system modeling.

case is to construct an *inverse system* that produces the vector $\mathbf{x}$ in response to the vector $\mathbf{d}$. The inverse system may thus be described by

$$\mathbf{x} = \mathbf{f}^{-1}(\mathbf{d}) \tag{2.22}$$

where the vector-valued function $\mathbf{f}^{-1}(\cdot)$ denotes the inverse of $\mathbf{f}(\cdot)$. Note, however, that $\mathbf{f}^{-1}(\cdot)$ is not the reciprocal of $\mathbf{f}(\cdot)$; rather, the use of superscript -1 is merely a flag to indicate an inverse. In many situations encountered in practice, the vector-valued function $\mathbf{f}(\cdot)$ is much too complex, and inhibits a straightforward formulation of the inverse function $\mathbf{f}^{-1}(\cdot)$. Given the set of labeled examples in Eq. (2.20), we may construct a neural network approximation of $\mathbf{f}^{-1}(\cdot)$ by using the scheme shown in Fig. 2.12. In the situation described here, the roles of $\mathbf{x}_i$ and $\mathbf{d}_i$ are interchanged: the vector $\mathbf{d}_i$ is used as the input and $\mathbf{x}_i$ is treated as the desired response. Let the error signal vector $\mathbf{e}_i$ denote the difference between $\mathbf{x}_i$ and the actual output $\mathbf{y}_i$ of the neural network produced in response to $\mathbf{d}_i$. As with the system identification problem, this error signal vector is used to adjust the free parameters of the neural network to minimize the squared difference between the outputs of the unknown inverse system and the neural network in a statistical sense, and is computed over the complete training set.

Control

The control of a *plant* is another learning task that can be done by a neural network; by a "plant" we mean a process or critical part of a system that is to be maintained in a controlled condition. The relevance of learning to control should not be surprising because, after all, the human brain is a computer (i.e., information processor), the outputs of which as a whole system are *actions*. In the context of control, the brain is living proof that it is possible to build a generalized controller that takes full advantage of parallel distributed hardware, can control many thousands of actuators (muscle fibers) in parallel, can handle nonlinearity and noise, and can optimize over a long-range planning horizon (Werbos, 1992).

Consider the *feedback control system* shown in Fig. 2.13. The system involves the use of unity feedback around a plant to be controlled; that is, the plant output is fed back directly to the input.[9] Thus, the plant output $\mathbf{y}$ is subtracted from a *reference signal* $\mathbf{d}$ supplied from an external source. The error signal $\mathbf{e}$ so produced is applied to a neural

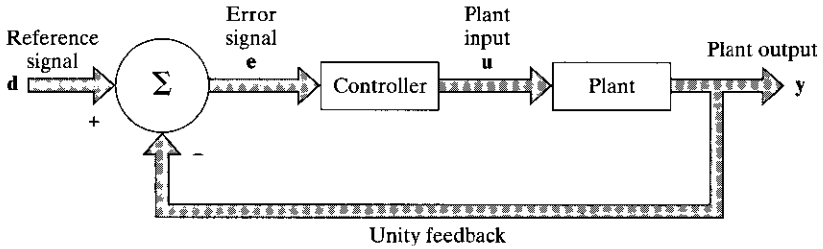


FIGURE 2.13 Block diagram of feedback control system.

controller for the purpose of adjusting its free parameters. The primary objective of the controller is to supply appropriate inputs to the plant to make its output **y** track the reference signal **d**. In other words, the controller has to invert the plant's input–output behavior.

We note that in Fig. 2.13 the error signal **e** has to propagate through the neural controller before reaching the plant. Consequently, to perform adjustments on the free parameters of the plant in accordance with an error-correction learning algorithm we need to know the Jacobian matrix

$$\mathbf{J} = \left\{ \frac{\partial y_k}{\partial u_j} \right\} \tag{2.23}$$

where y_k is an element of the plant output **y** and u_j is an element of the plant input **u**. Unfortunately, the partial derivatives $\partial y_k / \partial u_j$ for various k and j depend on the operating point of the plant and are therefore not known. We may use one of two approaches to account for them:

- *Indirect learning.* Using actual input–output measurements on the plant, a neural network model is first constructed to produce a copy of it. This model is in turn used to provide an estimate of the Jacobian matrix **J**. The partial derivatives constituting this Jacobian matrix are subsequently used in the error-correction learning algorithm for computing the adjustments to the free parameters of the neural controller (Nguyen and Widrow, 1989; Suykens et al., 1996; Widrow and Walach, 1996).
- *Direct learning.* The signs of the partial derivatives $\partial y_k / \partial u_j$ are generally known and usually remain constant over the dynamic range of the plant. This suggests that we may approximate these partial derivatives by their individual signs. Their absolute values are given a distributed representation in the free parameters of the neural controller (Saerens and Soquet, 1991; Schiffman and Geffers, 1993). The neural controller is thereby enabled to learn the adjustments to its free parameters directly from the plant.

Filtering

The term *filter* often refers to a device or algorithm used to extract information about a prescribed quantity of interest from a set of noisy data. The noise may arise from a variety of sources. For example, the data may have been measured by means of noisy

sensors or may represent an information-bearing signal that has been corrupted by transmission through a communication channel. Another example is that of a useful signal component corrupted by an interfering signal picked up from the surrounding environment. We may use a filter to perform three basic information processing tasks:

1. *Filtering.* This task refers to the extraction of information about a quantity of interest at discrete time n by using data measured up to and including time n.
2. *Smoothing.* This second task differs from filtering in that information about the quantity of interest need not be available at time n, and data measured later than time n can be used in obtaining this information. This means that in smoothing there is a *delay* in producing the result of interest. Since, in the smoothing process, we are able to use data obtained not only up to time n but also after time n, we expect smoothing to be more accurate than filtering in some statistical sense.
3. *Prediction.* This task is the forecasting side of information processing. The aim here is to derive information about what the quantity of interest will be like at some time $n + n_0$ in the future, for some $n_0 > 0$, by using data measured up to and including time n.

A filtering problem humans are familiar with is the *cocktail party problem.*[10] We have a remarkable ability to focus on a speaker in the noisy environment of a cocktail party, despite the fact that the speech signal originating from that speaker is buried in an undifferentiated noise background due to other interfering conversations in the room. It is thought that some form of preattentive, preconscious analysis must be involved in resolving the cocktail party problem (Velmans, 1995). In the context of (artificial) neural networks, a similar filtering problem arises under the umbrella of *blind signal separation* (Comon, 1994; Bell and Sejnowski, 1995; Amari et al., 1996). To formulate the blind signal separation problem, consider a set of unknown source signals $\{s_i(n)\}_{i=1}^{m}$ that are mutually independent of each other. These signals are linearly mixed by an unknown sensor to produce the m-by-1 observation vector (see Fig. 2.14)

$$\mathbf{x}(n) = \mathbf{A}\,\mathbf{u}(n) \tag{2.24}$$

where

$$\mathbf{u}(n) = [u_1(n), u_2(n), \ldots, u_m(n)]^T \tag{2.25}$$

$$\mathbf{x}(n) = [x_1(n), x_2(n), \ldots, x_m(n)]^T \tag{2.26}$$

and $\mathbf{A}$ is an unknown nonsingular *mixing matrix* of dimensions m-by-m. Given the observation vector $\mathbf{x}(n)$, the requirement is to recover the original signals $u_1(n)$, $u_2(n), \ldots, u_m(n)$ in an unsupervised manner.

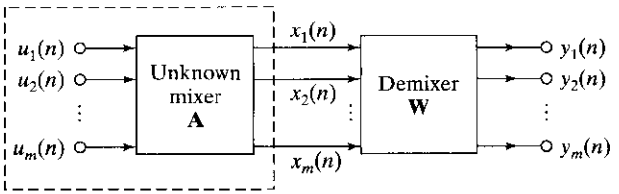


FIGURE 2.14 Block diagram of blind source separation.

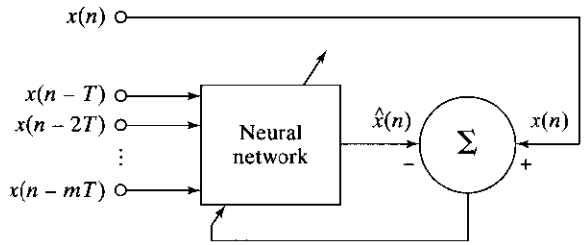


FIGURE 2.15 Block diagram of nonlinear prediction.

Turning now to the prediction problem, the requirement is to predict the present value $x(n)$ of a process, given past values of the process that are uniformly spaced in time as shown by $x(n - T), x(n - 2T), \ldots, x(n - mT)$, where T is the sampling period and m is the prediction order. Prediction may be solved by using error-correction learning in an unsupervised manner since the training examples are drawn directly from the process itself, as depicted in Fig. 2.15, where $x(n)$ serves the purpose of desired response. Let $\hat{x}(n)$ denote the one-step prediction produced by the neural network at time n. The error signal $e(n)$ is defined as the difference between $x(n)$ and $\hat{x}(n)$, which is used to adjust the free parameters of the neural network. On this basis, prediction may be viewed as a form of *model building* in the sense that the smaller we make the prediction error in a statistical sense, the better the network serves as a model of the underlying physical process responsible for generating the data. When this process is *nonlinear,* the use of a neural network provides a powerful method for solving the prediction problem because of the nonlinear processing units that could be built into its construction. The only possible exception to the use of nonlinear processing units, however, is the output unit of the network: If the dynamic range of the time series $\{x(n)\}$ is unknown, the use of a linear output unit is the most reasonable choice.

Beamforming

Beamforming is a *spatial* form of filtering and is used to distinguish between the spatial properties of a target signal and background noise. The device used to do the beamforming is called a *beamformer.*

The task of beamforming is compatible with the use of a neural network, for which we have relevant cues from psychoacoustic studies of human auditory responses (Bregman, 1990) and studies of feature mapping in the cortical layers of auditory systems of echo-locating bats (Suga, 1990a; Simmons and Sailant, 1992). The echo-locating bat illuminates the surrounding environment by broadcasting short-duration frequency-modulated (FM) sonar signals, and then uses its auditory system (including a pair of ears) to focus attention on its prey (e.g., flying insect). The ears provide the bat with some form of spatial filtering (interferometry to be precise), which is then exploited by the auditory system to produce *attentional selectivity.*

Beamforming is commonly used in radar and sonar systems where the primary task is to detect and track a target of interest in the combined presence of receiver noise and interfering signals (e.g., jammers). This task is complicated by two factors.

- The target signal originates from an unknown direction.
- There is no *a priori* information available on the interfering signals.

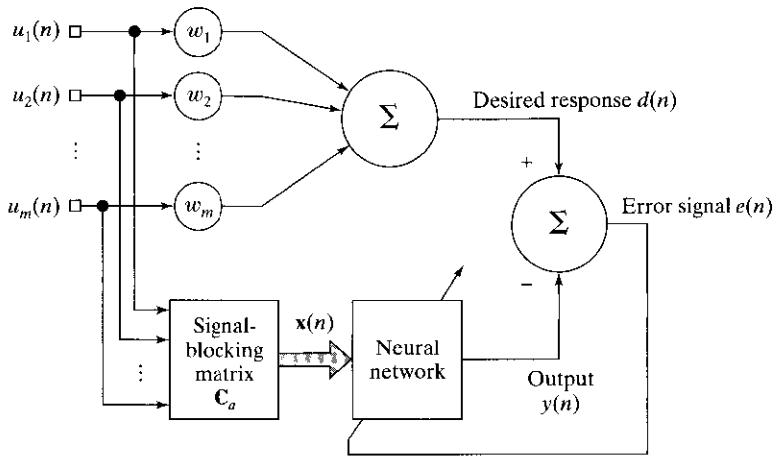


FIGURE 2.16 Block diagram of generalized sidelobe canceller.

One way of coping with situations of this kind is to use a *generalized sidelobe canceller* (GSLC), the block diagram of which is shown in Fig. 2.16. The system consists of the following components (Griffiths and Jim, 1982; Van Veen, 1992; Haykin, 1996):

- An *array of antenna elements*, which provides a means of sampling the observed signal at discrete points in space.
- A *linear combiner* defined by a set of fixed weights $\{w_i\}_{i=1}^{m}$, the output of which is a desired response. This linear combiner acts like a "spatial filter," characterized by a radiation pattern (i.e., a polar plot of the amplitude of the antenna output versus the incidence angle of an incoming signal). The mainlobe of this radiation pattern is pointed along a prescribed direction, for which the GSLC is *constrained* to produce a distortionless response. The output of the linear combiner, denoted by $d(n)$, provides a desired response for the beamformer.
- A *signal-blocking matrix* $\mathbf{C}_a$, the function of which is to cancel interference that leaks through the sidelobes of the radiation pattern of the spatial filter representing the linear combiner.
- A *neural network* with adjustable parameters, which is designed to accommodate statistical variations in the interfering signals.

The adjustments to the free parameters of the neural network are performed by an error-correcting learning algorithm that operates on the error signal $e(n)$, defined as the difference between the linear combiner output $d(n)$ and the actual output $y(n)$ of the neural network. Thus the GSLC operates under the supervision of the linear combiner that assumes the role of a "teacher." As with ordinary supervised learning, notice that the linear combiner is outside the feedback loop acting on the neural network. A beamformer that uses a neural network for learning is called a *neural beamformer* or *neuro-beamformer*. This class of learning machines comes under the general heading of *attentional neurocomputers* (Hecht-Nielsen, 1990).

The diversity of the six learning tasks discussed here is testimony to the *universality* of neural networks as information-processing systems. In a fundamental sense,

these learning tasks are all problems of learning a *mapping* from (possibly noisy) examples of the mapping. Without the imposition of prior knowledge, each of the tasks is in fact *ill posed* in the sense of nonuniqueness of possible solution mappings. One method of making the solution well posed is to use the theory of regularization as described in Chapter 5.

2.11 MEMORY

Discussion of learning tasks, particularly the task of pattern association, leads us naturally to think about *memory*. In a neurobiological context, memory refers to the relatively enduring neural alterations induced by the interaction of an organism with its environment (Teyler, 1986). Without such a change there can be no memory. Furthermore, for the memory to be useful it must be accessible to the nervous system in order to influence future behavior. However, an activity pattern must initially be stored in memory through a *learning process*. Memory and learning are intricately connected. When a particular activity pattern is learned, it is stored in the brain where it can be recalled later when required. Memory may be divided into "short-term" and "long-term" memory, depending on the retention time (Arbib, 1989). *Short-term memory* refers to a compilation of knowledge representing the "current" state of the environment. Any discrepancies between knowledge stored in short-term memory and a "new" state are used to update the short-term memory. *Long-term memory,* on the other hand, refers to knowledge stored for a long time or permanently.

In this section we study an associative memory that offers the following characteristics:

- The memory is distributed.
- Both the stimulus (key) pattern and the response (stored) pattern of an associative memory consist of data vectors.
- Information is stored in memory by setting up a spatial pattern of neural activities across a large number of neurons.
- Information contained in a stimulus not only determines its storage location in memory but also an address for its retrieval.
- Although neurons do not represent reliable and low-noise computing cells, the memory exhibits a high degree of resistance to noise and damage of a diffusive kind.
- There may be interactions between individual patterns stored in memory. (Otherwise the memory would have to be exceptionally large for it to accommodate the storage of a large number of patterns in perfect isolation from each other.) There is therefore the distinct possibility for the memory to make *errors* during the recall process.

In a *distributed memory,* the basic issue of interest is the simultaneous or near-simultaneous activities of many different neurons, which are the result of external or internal stimuli. The neural activities form a spatial pattern inside the memory that contains information about the stimuli. The memory is therefore said to perform a distributed mapping that transforms an activity pattern in the input space into another activity pattern in the output space. We may illustrate some important properties of a

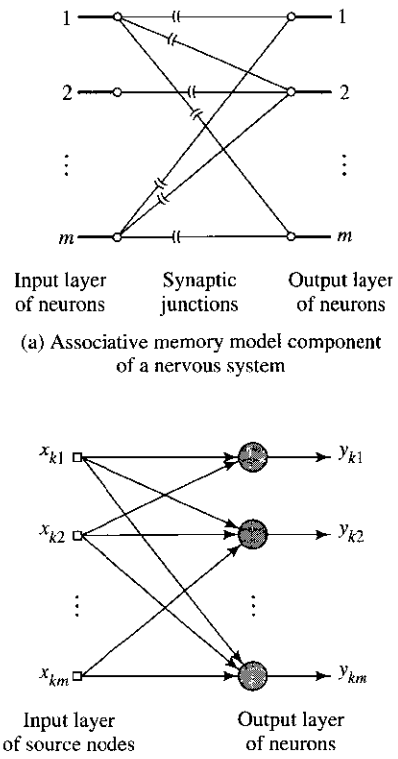


FIGURE 2.17 Associative memory models.

distributed memory mapping by considering an idealized neural network that consists of two layers of neurons. Figure 2.17a illustrates a network that may be regarded as a *model component of a nervous system* (Cooper, 1973; Scofield and Cooper, 1985). Each neuron in the input layer is connected to every one of the neurons in the output layer. The actual synaptic connections between the neurons are complex and redundant. In the model of Fig. 2.17a, a single ideal junction is used to represent the integrated effect of all the synaptic contacts between the dendrites of a neuron in the input layer and the axon branches of a neuron in the output layer. The level of activity of a neuron in the input layer may affect the level of activity of every other neuron in the output layer.

The corresponding situation for an artificial neural network is depicted in Fig. 2.17b. Here we have an input layer of source nodes and an output layer of neurons acting as computation nodes. In this case, the synaptic weights of the network are included as integral parts of the neurons in the output layer. The connecting links between the two layers of the network are simply wires.

In the following mathematical analysis, the neural networks in Figs. 2.17a and 2.17b are both assumed to be *linear*. The implication of this assumption is that each neuron acts as a linear combiner, as depicted in the signal-flow graph of Fig. 2.18. To proceed with the analysis, suppose that an activity pattern $\mathbf{x}_k$ occurs in the input layer of the network and that an activity pattern $\mathbf{y}_k$ occurs simultaneously in the output layer. The issue we wish to consider here is that of learning from the association

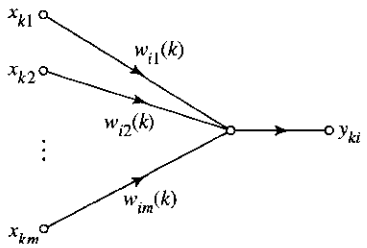


FIGURE 2.18 Signal-flow graph model of a linear neuron labeled i.

between the patterns $\mathbf{x}_k$ and $\mathbf{y}_k$. The patterns $\mathbf{x}_k$ and $\mathbf{y}_k$ are represented by vectors, written in their expanded forms as:

$$\mathbf{x}_k = [x_{k1}, x_{k2}, \ldots, x_{km}]^T$$

and

$$\mathbf{y}_k = [y_{k1}, y_{k2}, \ldots, y_{km}]^T$$

For convenience of presentation we have assumed that the input space dimensionality (i.e., the dimension of vector $\mathbf{x}_k$) and the output space dimensionality (i.e., the dimension of vector $\mathbf{y}_k$) are the same, equal to m. From here on we refer to m as *network dimensionality* or simply *dimensionality*. Note that m equals the number of source nodes in the input layer or neurons in the output layer. For a neural network with a large number of neurons, which is typically the case, the dimensionality m can be large.

The elements of both $\mathbf{x}_k$ and $\mathbf{y}_k$ can assume positive and negative values. This is a valid proposition in an artificial neural network. It may also occur in a nervous system by considering the relevant physiological variable to be the difference between an actual activity level (e.g., firing rate of a neuron) and a nonzero spontaneous activity level.

With the networks of Fig. 2.17 assumed to be linear, the association of key vector $\mathbf{x}_k$ with memorized vector $\mathbf{y}_k$ may be described in matrix form as:

$$\mathbf{y}_k = \mathbf{W}(k)\mathbf{x}_k, \qquad k = 1, 2, \ldots, q \tag{2.27}$$

where $\mathbf{W}(k)$ is a weight matrix determined solely by the input–output pair $(\mathbf{x}_k, \mathbf{y}_k)$.

To develop a detailed description of the weight matrix $\mathbf{W}(k)$, consider Fig. 2.18 that shows a detailed arrangement of neuron i in the output layer. The output y_{ki} of neuron i due to the combined action of the elements of the key pattern $\mathbf{x}_k$ applied as stimulus to the input layer is given by

$$y_{ki} = \sum_{j=1}^{m} w_{ij}(k)x_{kj}, \qquad i = 1, 2, \ldots, m \tag{2.28}$$

where the $w_{ij}(k), j = 1, 2, \ldots, m$, are the synaptic weights of neuron i corresponding to the kth pair of associated patterns. Using matrix notation, we may express y_{ki} in the equivalent form

$$y_{ki} = [w_{i1}(k), w_{i2}(k), \ldots, w_{im}(k)] \begin{bmatrix} x_{k1} \\ x_{k2} \\ \vdots \\ x_{km} \end{bmatrix}, \qquad i = 1, 2, \ldots, m \tag{2.29}$$

The column vector on the right-hand side of Eq. (2.29) is recognized as the key vector $\mathbf{x}_k$. By substituting Eq. (2.29) in the definition of the m-by-1 stored vector $\mathbf{y}_k$, we get

$$\begin{bmatrix} y_{k1} \\ y_{k2} \\ \vdots \\ y_{km} \end{bmatrix} = \begin{bmatrix} w_{11}(k) & w_{12}(k) & \dots & w_{1m}(k) \\ w_{21}(k) & w_{22}(k) & \dots & w_{2m}(k) \\ \vdots & \vdots & \vdots & \vdots \\ w_{m1}(k) & w_{m2}(k) & \dots & w_{mm}(k) \end{bmatrix} \begin{bmatrix} x_{k1} \\ x_{k2} \\ \vdots \\ x_{km} \end{bmatrix} \tag{2.30}$$

Equation (2.30) is the expanded form of the matrix transformation or mapping described in Eq. (2.27). In particular, the m-by-m weight matrix $\mathbf{W}(k)$ is defined by

$$\mathbf{W}(k) = \begin{bmatrix} w_{11}(k) & w_{12}(k) & \dots & w_{1m}(k) \\ w_{21}(k) & w_{22}(k) & \dots & w_{2m}(k) \\ \vdots & \vdots & \vdots & \vdots \\ w_{m1}(k) & w_{m2}(k) & \dots & w_{mm}(k) \end{bmatrix} \tag{2.31}$$

The individual presentations of the q pairs of associated patterns $\mathbf{x}_k \rightarrow \mathbf{y}_k$, $k = 1, 2, \dots, q$, produce corresponding values of the individual matrix, namely, $\mathbf{W}(1), \mathbf{W}(2), \dots, \mathbf{W}(q)$. Recognizing that this pattern association is represented by the weight matrix $\mathbf{W}(k)$, we may define an *m–by–m memory matrix* that describes the summation of the weight matrices for the entire set of pattern associations as follows:

$$\mathbf{M} = \sum_{k=1}^{q} \mathbf{W}(k) \tag{2.32}$$

The memory matrix $\mathbf{M}$ defines the overall connectivity between the input and output layers of the associative memory. In effect, it represents the *total experience* gained by the memory as a result of the presentations of q input–output patterns. Stated in another way, the memory matrix $\mathbf{M}$ contains a piece of every input–output pair of activity patterns presented to the memory.

The definition of the memory matrix given in Eq. (2.32) may be restructured in the form of a recursion as shown by

$$\mathbf{M}_k = \mathbf{M}_{k-1} + \mathbf{W}(k), \qquad k = 1, 2, \dots, q \tag{2.33}$$

where the initial value $\mathbf{M}_0$ is zero (i.e., the synaptic weights in the memory are all initially zero), and the final value $\mathbf{M}_q$ is identically equal to $\mathbf{M}$ as defined in Eq. (2.32). According to the recursive formula of Eq. (2.33), the term $\mathbf{M}_{k-1}$ is the old value of the memory matrix resulting from $(k - 1)$ pattern associations, and $\mathbf{M}_k$ is the updated value in light of the increment $\mathbf{W}(k)$ produced by the kth association. Note, however, that when $\mathbf{W}(k)$ is added to $\mathbf{M}_{k-1}$, the increment $\mathbf{W}(k)$ loses its distinct identity among the mixture of contributions that form $\mathbf{M}_k$. In spite of the synaptic mixing of different associations, information about the stimuli may not have been lost, as demonstrated in the sequel. Notice also that as the number q of stored patterns increases, the influence of a new pattern on the memory as a whole is progressively reduced.

Correlation Matrix Memory

Suppose that the associative memory of Fig. 2.17b has learned the memory matrix $\mathbf{M}$ through the associations of key and memorized patterns described by $\mathbf{x}_k \rightarrow \mathbf{y}_k$, where $k = 1, 2, \ldots, q$. We may postulate $\hat{\mathbf{M}}$, denoting an *estimate* of the memory matrix $\mathbf{M}$ in terms of these patterns as (Anderson, 1972, 1983; Cooper, 1973):

$$\hat{\mathbf{M}} = \sum_{k=1}^{q} \mathbf{y}_k \mathbf{x}_k^T \tag{2.34}$$

The term $\mathbf{y}_k \mathbf{x}_k^T$ represents the *outer product* of the key pattern $\mathbf{x}_k$ and the memorized pattern $\mathbf{y}_k$. This outer product is an "estimate" of the weight matrix $\mathbf{W}(k)$ that maps the output pattern $\mathbf{y}_k$ onto the input pattern $\mathbf{x}_k$. Since the pattern $\mathbf{x}_k$ and $\mathbf{y}_k$ are both m-by-1 vectors by assumption, it follows that their output product $\mathbf{y}_k \mathbf{x}_k^T$, and therefore the estimate $\hat{\mathbf{M}}$, is an m-by-m matrix. This dimensionality is in perfect agreement with that of the memory matrix $\mathbf{M}$ defined in Eq. (2.32). The format of the summation of the estimate $\hat{\mathbf{M}}$ bears a direct relation to that of the memory matrix defined in that equation.

A typical term of the outer product $\mathbf{y}_k \mathbf{x}_k^T$ is written as $y_{ki} x_{kj}$, where x_{kj} is the output of source node j in the input layer, and y_{ki} is the output of neuron i in the output layer. In the context of synaptic weight $w_{ij}(k)$ for the kth association, source node j acts as a presynaptic node and neuron i in the output layer acts as a postsynaptic node. Hence, the "local" learning process described in Eq. (2.34) may be viewed as a *generalization of Hebb's postulate of learning.* It is also referred to as the *outer product rule* in recognition of the matrix operation used to construct the memory matrix $\hat{\mathbf{M}}$. Correspondingly, an associative memory so designed is called a *correlation matrix memory*. Correlation, in one form or another, is indeed the basis of learning, association, pattern recognition, and memory recall in the human nervous system (Eggermont, 1990.)

Equation (2.34) may be reformulated in the equivalent form

$$\begin{aligned} \hat{\mathbf{M}} &= [\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_q] \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_q^T \end{bmatrix} \\ &= \mathbf{Y}\mathbf{X}^T \end{aligned} \tag{2.35}$$

where

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_q] \tag{2.36}$$

and

$$\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_q] \tag{2.37}$$

The matrix $\mathbf{X}$ is an m-by-q matrix composed of the entire set of key patterns used in the learning process; it is called the *key matrix.* The matrix $\mathbf{Y}$ is an m–by–q matrix composed of the corresponding set of memorized patterns; it is called the *memorized matrix.*

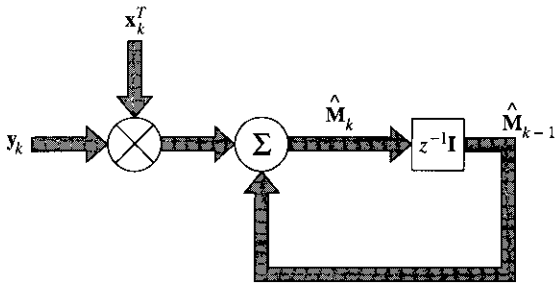


FIGURE 2.19 Signal-flow graph representation of Eq. (2.38).

Equation (2.35) may also be restructured in the form of a recursion as follows:

$$\hat{\mathbf{M}}_k = \hat{\mathbf{M}}_{k-1} + \mathbf{y}_k\mathbf{x}_k^T, \qquad k = 1, 2, \ldots, q \tag{2.38}$$

A signal-flow graph representation of this recursion is depicted in Fig. 2.19. According to this signal-flow graph and the recursive formula of Eq. (2.38), the matrix $\hat{\mathbf{M}}_{k-1}$ represents an old estimate of the memory matrix; and $\hat{\mathbf{M}}_k$ represents its updated value in the light of a new association performed by the memory on the patterns $\mathbf{x}_k$ and $\mathbf{y}_k$. Comparing the recursion of Eq. (2.38) with that of Eq. (2.33), we see that the outer product $\mathbf{y}_k\mathbf{x}_k^T$ represents an estimate of the weight matrix $\mathbf{W}(k)$ corresponding to the kth association of key and memorized patterns, $\mathbf{x}_k$ and $\mathbf{y}_k$.

Recall

The fundamental problem posed by the use of an associative memory is the address and recall of patterns stored in memory. To explain one aspect of this problem, let $\hat{\mathbf{M}}$ denote the memory matrix of an associative memory, which has been completely learned through its exposure to q pattern associations in accordance with Eq. (2.34). Let a key pattern $\mathbf{x}_j$ be picked at random and reapplied as *stimulus* to the memory, yielding the *response*

$$\mathbf{y} = \hat{\mathbf{M}}\mathbf{x}_j \tag{2.39}$$

Substituting Eq. (2.34) in (2.39), we get

$$\begin{aligned} \mathbf{y} &= \sum_{k=1}^{m} \mathbf{y}_k\mathbf{x}_k^T\mathbf{x}_j \\ &= \sum_{k=1}^{m} (\mathbf{x}_k^T\mathbf{x}_j)\mathbf{y}_k \end{aligned} \tag{2.40}$$

where, in the second line, it is recognized that $\mathbf{x}_k^T\mathbf{x}_j$ is a scalar equal to the *inner product* of the key vectors $\mathbf{x}_k$ and $\mathbf{x}_j$. We may rewrite Eq. (2.40) as

$$\mathbf{y} = (\mathbf{x}_j^T\mathbf{x}_j)\mathbf{y}_j + \sum_{\substack{k=1 \\ k \neq j}}^{m} (\mathbf{x}_k^T\mathbf{x}_j)\mathbf{y}_k \tag{2.41}$$

Let each of the key patterns $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_q$ be normalized to have unit energy; that is,

$$\begin{aligned} E_k &= \sum_{l=1}^{m} x_{kl}^2 \\ &= \mathbf{x}_k^T \mathbf{x}_k \\ &= 1, \qquad k = 1, 2, \ldots, q \end{aligned} \tag{2.42}$$

Accordingly, we may simplify the response of the memory to the stimulus (key pattern) $\mathbf{x}_j$ as

$$\mathbf{y} = \mathbf{y}_j + \mathbf{v}_j \tag{2.43}$$

where

$$\mathbf{v}_j = \sum_{\substack{k=1 \\ k \neq j}}^{m} (\mathbf{x}_k^T \mathbf{x}_j) \mathbf{y}_k \tag{2.44}$$

The first term on the right-hand side of Eq. (2.43) represents the "desired" response $\mathbf{y}_j$; it may therefore be viewed as the "signal" component of the actual response $\mathbf{y}$. The second term $\mathbf{v}_j$ is a "noise vector" that arises because of the *crosstalk* between the key vector $\mathbf{x}_j$ and all the other key vectors stored in memory. The noise vector $\mathbf{v}_j$ is responsible for making errors on recall.

In the context of a linear signal space, we may define the *cosine of the angle* between a pair of vectors $\mathbf{x}_j$ and $\mathbf{x}_k$ as the inner product of $\mathbf{x}_j$ and $\mathbf{x}_k$ divided by the product of their individual Euclidean *norms* or *lengths* as shown by

$$\cos(\mathbf{x}_k, \mathbf{x}_j) = \frac{\mathbf{x}_k^T \mathbf{x}_j}{\|\mathbf{x}_k\| \|\mathbf{x}_j\|} \tag{2.45}$$

The symbol $\|\mathbf{x}_k\|$ signifies the Euclidean norm of vector $\mathbf{x}_k$, defined as the square root of the energy of $\mathbf{x}_k$:

$$\begin{aligned} \|\mathbf{x}_k\| &= (\mathbf{x}_k^T \mathbf{x}_k)^{1/2} \\ &= E_k^{1/2} \end{aligned} \tag{2.46}$$

Returning to the situation, note that the key vectors are normalized to have unit energy in accordance with Eq. (2.42). We may therefore reduce the definition of Eq. (2.45) to

$$\cos(\mathbf{x}_k, \mathbf{x}_j) = \mathbf{x}_k^T \mathbf{x}_j \tag{2.47}$$

We may then redefine the noise vector of Eq. (2.44) as

$$\mathbf{v}_j = \sum_{\substack{k=1 \\ k \neq j}}^{m} \cos(\mathbf{x}_k, \mathbf{x}_j) \mathbf{y}_k \tag{2.48}$$

We now see that if the key vectors are *orthogonal* (i.e., perpendicular to each other in a Euclidean sense), then

$$\cos(\mathbf{x}_k, \mathbf{x}_j) = 0, \qquad k \neq j \tag{2.49}$$

and therefore the noise vector $\mathbf{v}_j$ is identically zero. In such a case, the response $\mathbf{y}$ equals $\mathbf{y}_j$. The *memory associates perfectly* if the key vectors from an *orthonormal set;* that is, if they satisfy the following pair of conditions:

$$\mathbf{x}_k^T \mathbf{x}_j = \begin{cases} 1, & k = j \\ 0, & k \neq j \end{cases} \tag{2.50}$$

Suppose now that the key vectors do form an orthonormal set, as prescribed in Eq. (2.50). What is then the limit on the *storage capacity* of the associative memory? Stated in another way, what is the largest number of patterns that can be reliably stored? The answer to this fundamental question lies in the rank of the memory matrix $\hat{\mathbf{M}}$. The *rank* of a matrix is defined as the number of independent columns (rows) of the matrix. That is, if r is the rank of such a rectangular matrix of dimensions l-by-m, we then have $r \leq \min(l, m)$. In the case of a correlation memory, the memory matrix $\hat{\mathbf{M}}$ is an m-by-m matrix, where m is the dimensionality of the input space. Hence the rank of the memory matrix $\mathbf{M}$ is limited by the dimensionality m. We may thus formally state that the number of patterns that can be reliably stored in a correlation matrix memory can never exceed the input space dimensionality.

In real-life situations, we often find that the key patterns presented to an associative memory are neither orthogonal nor highly separated from each other. Consequently, a correlation matrix memory characterized by the memory matrix of Eq. (2.34) may sometimes get confused and make *errors.* That is, the memory occasionally recognizes and associates patterns never seen or associated before. To illustrate this property of an associative memory, consider a set of key patterns.

$$\{\mathbf{x}_{\text{key}}\}: \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_q$$

and a corresponding set of memorized patterns,

$$\{\mathbf{y}_{\text{mem}}\}: \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_q$$

To express the closeness of the key patterns in a linear signal space, we introduce the concept of *community.* We define the community of the set of patterns $\{\mathbf{x}_{\text{key}}\}$ as the lower bound on the inner products $\mathbf{x}_k^T \mathbf{x}_j$ of any two patterns $\mathbf{x}_j$ and $\mathbf{x}_k$ in the set. Let $\hat{\mathbf{M}}$ denote the memory matrix resulting from the training of the associative memory on a set of key patterns represented by $\{\mathbf{x}_{\text{key}}\}$ and a corresponding set of memorized patterns $\{\mathbf{y}_{\text{mem}}\}$ in accordance with Eq. (2.34). The response of the memory, $\mathbf{y}$, to a stimulus $\mathbf{x}_j$ selected from the set $\{\mathbf{x}_{\text{key}}\}$ is given by Eq. (2.39), where it is assumed that each pattern in the set $\{\mathbf{x}_{\text{key}}\}$ is a unit vector (i.e., a vector with unit energy). Let it be further assumed that

$$\mathbf{x}_k^T \mathbf{x}_j \geq \gamma \qquad \text{for } k \neq j \tag{2.51}$$

If the lower bound γ is large enough, the memory may fail to distinguish the response $\mathbf{y}$ from that of any other key pattern contained in the set $\{\mathbf{x}_{\text{key}}\}$. If the key patterns in this set have the form

$$\mathbf{x}_j = \mathbf{x}_0 + \mathbf{v} \tag{2.52}$$

where $\mathbf{v}$ is a stochastic vector, it is likely that the memory will recognize $\mathbf{x}_0$ and associate with it a vector $\mathbf{y}_0$ rather than any of the actual pattern pairs used to train it in the

first place; $\mathbf{x}_0$ and $\mathbf{y}_0$ denote a pair of patterns never seen before. This phenomenon may be termed *animal logic,* which is not logic at all (Cooper, 1973).

2.12 ADAPTATION

In performing a task of interest, we often find that *space* is one fundamental dimension of the learning process; *time* is the other. The *spatiotemporal* nature of learning is exemplified by many of the learning tasks (e.g., control, beamforming) discussed in Section 2.10. Species ranging from insects to humans have an inherent capacity to represent the temporal structure of experience. Such a representation makes it possible for an animal to *adapt* its behavior to the temporal structure of an event in its behavioral space (Gallistel, 1990).

When a neural network operates in a *stationary* environment (i.e., an environment whose statistical characteristics do not change with time), the essential statistics of the environment can, in theory, be *learned* by the network under the supervision of a teacher. In particular, the synaptic weights of the network can be computed by having the network undergo a training session with a set of data that is representative of the environment. Once the training process has completed, the synaptic weights of the network should capture the underlying statistical structure of the environment, which would justify "freezing" their values thereafter. Thus a learning system relies on *memory,* in one form or another, to recall and exploit past experiences.

Frequently, however, the environment of interest is *nonstationary,* which means that the statistical parameters of the information-bearing signals generated by the environment vary with time. In situations of this kind, the traditional methods of supervised learning may prove to be inadequate because the network is not equipped with the necessary means to *track* the statistical variations of the environment in which it operates. To overcome this shortcoming, it is desirable for a neural network to continually *adapt* its free parameters to variations in the incoming signals in a *real-time* fashion. Thus an *adaptive system* responds to every distinct input as a novel one. In other words the learning process encountered in an adaptive system never stops, with learning going on while signal processing is being performed by the system. This form of learning is called *continuous learning* or *learning-on-the-fly.*

Linear adaptive filters, built around a linear combiner (i.e., a single neuron operating in its linear mode), are designed to perform continuous learning. Despite their simple structure (and perhaps because of it), they are widely used in such diverse applications as radar, sonar, communications, seismology, and biomedical signal processing. The theory of linear adaptive filters has reached a highly mature stage of development (Haykin, 1996; Widrow and Stearns, 1985). However, the same cannot be said about nonlinear adaptive filters.[11]

With continuous learning as the property of interest and a neural network as the vehicle for its implementation, the question we need to address is: How can a neural network adapt its behavior to the varying temporal structure of the incoming signals in its behavioral space? One way of addressing this fundamental issue is to recognize that statistical characteristics of a nonstationary process usually change slowly enough for the process to be considered *pseudostationary* over a window of short enough duration. Examples include:

- The mechanism responsible for the production of a speech signal may be considered essentially stationary over a period of 10 to 30 milliseconds.
- Radar returns from an ocean surface remain essentially stationary over a period of several seconds.
- With long-range weather forecasting in mind, weather related data may be viewed as essentially stationary over a period of minutes.
- In the context of long-range trends extending into months and years, stock market data may be considered as essentially stationary over a period of days.

We may thus exploit the pseudostationary property of a stochastic process to extend the utility of a neural network by *retraining* it at some regular intervals to account for statistical fluctuations of the incoming data. Such an approach may, for example, be suitable for processing stock market data.

For a more refined *dynamic* approach to learning, we may proceed as follows:

- Select a window short enough for the input data to be considered pseudostationary, and use the data to train the network.
- When a new data sample is received, update the window by dropping the oldest data sample and shifting the remaining data samples back by one time unit to make room for the new sample.
- Use the updated data window to retrain the network.
- Repeat the procedure on a continuing basis.

We may thus build temporal structure into the design of a neural network by having the network undergo *continual training* with *time-ordered examples*. According to this dynamic approach, a neural network is viewed as a *nonlinear adaptive filter* that represents a generalization of linear adaptive filters. However, for this dynamic approach to nonlinear adaptive filters to be feasible, the resources available must be *fast* enough to complete all the described computations in one sampling period. Only then can the filter keep up with changes in the input.

2.13 STATISTICAL NATURE OF THE LEARNING PROCESS

The last part of the chapter deals with statistical aspects of learning. In this context we are not interested in the evolution of the weight vector $\mathbf{w}$ as a neural network is cycled through a learning algorithm. We instead focus on the deviation between a "target" function $f(\mathbf{x})$ and the "actual" function $F(\mathbf{x}, \mathbf{w})$ realized by the neural network where the vector $\mathbf{x}$ denotes the input signal. The deviation is expressed in statistical terms.

A neural network is merely one form in which *empirical knowledge* about a physical phenomenon or environment of interest may be encoded through training. By "empirical" knowledge we mean a set of measurements that characterizes the phenomenon. To be more specific, consider the example of a stochastic phenomenon described by a random vector $\mathbf{X}$ consisting of a set of *independent variables*, and a random scalar D representing a *dependent variable*. The elements of the random vector $\mathbf{X}$ may have different physical meanings of their own. The assumption that the dependent variable D is a scalar has been made merely to simplify the exposition without any loss of generality. Suppose also that we have N realizations of the random vector $\mathbf{X}$ denoted by

$\{\mathbf{x}_i\}_{i=1}^N$, and a corresponding set of realizations of the random scalar D denoted by $\{d_i\}_{i=1}^N$. These realizations (measurements) constitute the training sample denoted by

$$\mathcal{T} = \{(\mathbf{x}_i, d_i)\}_{i=1}^N \tag{2.53}$$

Ordinarily we do *not* have knowledge of the exact functional relationship between $\mathbf{X}$ and D, so we proceed by proposing the model (White, 1989a)

$$D = f(\mathbf{X}) + \epsilon \tag{2.54}$$

where $f(\cdot)$ is a *deterministic* function of its argument vector, and ϵ is a random *expectational error* that represents our "ignorance" about the dependence of D and $\mathbf{X}$. The statistical model described by Eq. (2.54) is called a *regressive model*; it is depicted in Fig. 2.20a. The expectational error ϵ is, in general, a random variable with zero mean and positive probability of occurrence. On this basis, the regressive model of Fig. 2.20a has two useful properties:

1. *The mean value of the expectational error ϵ, given any realization $\mathbf{x}$, is zero*; that is,

$$E[\epsilon|\mathbf{x}] = 0 \tag{2.55}$$

where E is the statistical expectation operator. As a corollary to this property, we may state that the *regression function $f(\mathbf{x})$ is the conditional mean of the model output D, given that the input $\mathbf{X} = \mathbf{x}$*, as shown by

$$f(\mathbf{x}) = E[D|\mathbf{x}] \tag{2.56}$$

This property follows directly from Eq. (2.54) in light of Eq. (2.55).

2. *The expectational error ϵ is uncorrelated with the regression function $f(\mathbf{X})$*; that is

$$E[\epsilon f(\mathbf{X})] = 0 \tag{2.57}$$

This property is the well-known *principle* of *orthogonality*, which states that all the information about D available to us through the input $\mathbf{X}$ has been encoded

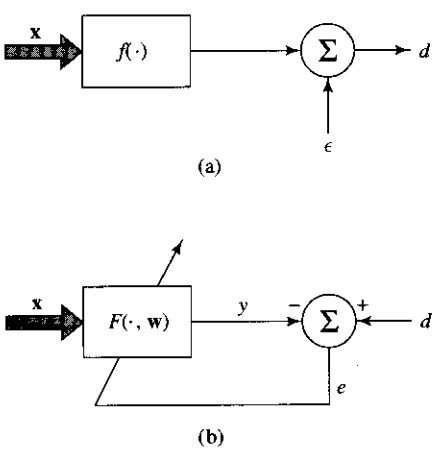


FIGURE 2.20 (a) Regressive model (mathematical). (b) Neural network model (physical).

into the regression function $f(\mathbf{X})$. Equation (2.57) is readily demonstrated by writing:

$$\begin{aligned} E[\epsilon f(\mathbf{X})] &= E[E[\epsilon f(\mathbf{X})|\mathbf{x}]] \\ &= E[f(\mathbf{X})E[\epsilon|\mathbf{x}]] \\ &= E[f(\mathbf{X}) \cdot 0] \\ &= 0 \end{aligned}$$

The regressive model of Fig. 2.20a is a "mathematical" description of a stochastic environment. Its purpose is to use the vector $\mathbf{X}$ to explain or predict the dependent variable D. Figure 2.20b is the corresponding "physical" model of the environment. The purpose of this second model, based on a neural network, is to encode the empirical knowledge represented by the training sample $\mathcal{T}$ into a corresponding set of synaptic weight vectors, $\mathbf{w}$, as shown by

$$\mathcal{T} \rightarrow \mathbf{w} \tag{2.58}$$

In effect, the neural network provides an "approximation" to the regressive model of Fig. 2.20a. Let the actual response of the neural network, produced in response to the input vector $\mathbf{x}$, be denoted by the random variable

$$Y = F(\mathbf{X}, \mathbf{w}) \tag{2.59}$$

where $F(\cdot, \mathbf{w})$ is the input–output function realized by the neural network. Given the training data $\mathcal{T}$ of Eq. (2.53), the weight vector $\mathbf{w}$ is obtained by minimizing the cost function

$$\mathscr{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(d_i - F(\mathbf{x}_i, \mathbf{w}))^2 \tag{2.60}$$

where the factor $1/2$ has been used to be consistent with earlier notations and those used in subsequent chapters. Except for the scaling factor $1/2$, the cost function $\mathscr{E}(\mathbf{w})$ is the squared difference between the desired response d and the actual response y of the neural network, averaged over the entire training data set $\mathcal{T}$. The use of Eq. (2.60) as the cost function implies the use of "batch" training, by which we mean that the adjustments to the synaptic weights of the network are performed over the entire set of training examples rather than on an example-by-example basis.

Let the symbol $E_{\mathcal{T}}$ denote the *average operator* taken over the entire training sample $\mathcal{T}$. The variables or their functions that come under the average operator $E_{\mathcal{T}}$ are denoted by $\mathbf{x}$ and d; the pair $(\mathbf{x}, d)$ represents an example in the training sample $\mathcal{T}$. In contrast, the statistical expectation operator E acts on the whole ensemble of random variables $\mathbf{X}$ and D, which includes $\mathcal{T}$ as a subset. The difference between the operators E and $E_{\mathcal{T}}$ should be carefully identified in what follows.

In light of the transformation described in Eq. (2.58), we may interchangably use $F(\mathbf{x}, \mathbf{w})$ and $F(\mathbf{x}, \mathcal{T})$ and therefore rewrite Eq. (2.60) in the equivalent form

$$\mathscr{E}(\mathbf{w}) = \frac{1}{2}E_{\mathcal{T}}[(d - F(\mathbf{x},\mathcal{T}))^2] \tag{2.61}$$

By adding and subtracting $f(\mathbf{x})$ to the argument $(d - F(\mathbf{x}, \mathcal{T}))$ and then using Eq. (2.54), we may write

$$\begin{aligned} d - F(\mathbf{x}, \mathcal{T}) &= (d - f(\mathbf{x})) + (f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T})) \\ &= \epsilon + (f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T})) \end{aligned}$$

By substituting this expression in Eq. (2.61) and then expanding terms, we may recast the cost function $\mathscr{E}(\mathbf{w})$ in the equivalent form

$$\mathscr{E}(\mathbf{w}) = \frac{1}{2}E_{\mathcal{T}}[\epsilon^2] + \frac{1}{2}E_{\mathcal{T}}[f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T}))^2] + E_{\mathcal{T}}[\epsilon(f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T}))] \tag{2.62}$$

However, the last expectation term on the right-hand side of Eq. (2.62) is zero for two reasons:

- The expectational error ϵ is uncorrelated with the regression function $f(\mathbf{x})$ by virtue of Eq. (2.57), interpreted in terms of the operator $E_{\mathcal{T}}$.
- The expectational error ϵ pertains to the regressive model of Fig. 2.20a, whereas the approximating function $F(\mathbf{x}, \mathbf{w})$ pertains to the neural network model of Fig. 2.20b.

Accordingly, Eq. (2.62) reduces to

$$\mathscr{E}(\mathbf{w}) = \frac{1}{2}E_{\mathcal{T}}[\epsilon^2] + \frac{1}{2}E_{\mathcal{T}}[(f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T}))^2] \tag{2.63}$$

The first term on the right-hand side of Eq. (2.63) is the variance of the expectational (regressive modeling) error ϵ, evaluated over the training sample $\mathcal{T}$. This term represents the *intrinsic error* because it is independent of the weight vector $\mathbf{w}$. It may be ignored as far as the minimization of the cost function $\mathscr{E}(\mathbf{w})$ with respect to $\mathbf{w}$ is concerned. Hence, the particular value of the weight vector $\mathbf{w}^*$ that minimizes the cost function $\mathscr{E}(\mathbf{w})$ will also minimize the ensemble average of the squared distance between the regression function $f(\mathbf{x})$ and the approximating function $F(\mathbf{x}, \mathbf{w})$. In other words, the *natural measure* of the effectiveness of $F(\mathbf{x}, \mathbf{w})$ as a predictor of the desired response d is defined by

$$L_{\text{av}}(f(\mathbf{x}), F(\mathbf{x}, \mathbf{w})) = E_{\mathcal{T}}[f(\mathbf{x}) - F(\mathbf{x}, \mathcal{T}))^2] \tag{2.64}$$

This result is fundamentally important because it provides the mathematical basis for the tradeoff between the bias and variance resulting from the use of $F(\mathbf{x}, \mathbf{w})$ as the approximation to $f(\mathbf{x})$ (Geman et al., 1992).

Bias/Variance Dilemma

Invoking the use of Eq. (2.56), we may redefine the squared distance between $f(\mathbf{x})$ and $F(\mathbf{x}, \mathbf{w})$ as:

$$L_{\text{av}}(f(\mathbf{x}), F(\mathbf{x}, \mathbf{w})) = E_{\mathcal{T}}[(E[D|\mathbf{X} = \mathbf{x}] - F(\mathbf{x}, \mathcal{T}))^2] \tag{2.65}$$

This expression may also be viewed as the average value of the *estimation error* between the regression function $f(\mathbf{x}) = E[D|\mathbf{X} = \mathbf{x}]$ and the approximating function $F(\mathbf{x}, \mathbf{w})$, evaluated over the entire training sample $\mathcal{T}$. Notice that the conditional mean

$E[D|\mathbf{X} = \mathbf{x}]$ has a constant expectation with respect to the training data sample $\mathcal{T}$. Next we find that

$$E[D|\mathbf{X} = \mathbf{x}] - F(\mathbf{x}, \mathcal{T}) = (E[D|\mathbf{X} = \mathbf{x}] - E_{\mathcal{T}}[F(\mathbf{x}, \mathcal{T})]) + (E_{\mathcal{T}}[F(\mathbf{x}, \mathcal{T})] - F(\mathbf{x}, \mathcal{T}))$$

where we have simply added and subtracted the average $E_{\mathcal{T}}[F(\mathbf{x}, \mathcal{T})]$. By proceeding in a manner similar to that described for deriving Eq. (2.62) from (2.61), we may reformulate Eq. (2.65) as the sum of two terms (see Problem 2.22):

$$L_{\text{av}}(f(\mathbf{x}), F(\mathbf{x}, \mathcal{T})) = B^2(\mathbf{w}) + V(\mathbf{w}) \tag{2.66}$$

where $B(\mathbf{w})$ and $V(\mathbf{w})$ are themselves defined by

$$B(\mathbf{w}) = E_{\mathcal{T}}[F(\mathbf{x}, \mathcal{T})] - E[D|\mathbf{X} = \mathbf{x}] \tag{2.67}$$

and

$$V(\mathbf{w}) = E_{\mathcal{T}}[(F(\mathbf{x}, \mathcal{T}) - E_{\mathcal{T}}[F(\mathbf{x}, \mathcal{T})])^2] \tag{2.68}$$

We now make two important observations:

1. The term $B(\mathbf{w})$ is the *bias* of the average value of the approximating function $F(\mathbf{x}, \mathcal{T})$, measured with respect to the regression function $f(\mathbf{x}) = E[D|\mathbf{X} = \mathbf{x}]$. This term represents the inability of the neural network defined by the function $F(\mathbf{x}, \mathbf{w})$ to accurately approximate the regression function $f(\mathbf{x}) = E[D|\mathbf{X} = \mathbf{x}]$. We may therefore view the bias $B(\mathbf{w})$ as an *approximation error*.
2. The term $V(\mathbf{w})$ is the *variance* of the approximating function $F(\mathbf{x}, \mathbf{w})$, measured over the entire training sample $\mathcal{T}$. This second term represents the inadequacy of the information contained in the training sample $\mathcal{T}$ about the regression function $f(\mathbf{x})$. We may therefore view the variance $V(\mathbf{w})$ as the manifestation of an *estimation error*.

Figure 2.21 illustrates the relations between the target and approximating functions, and shows how the estimation errors, namely bias and variance, accumulate. To

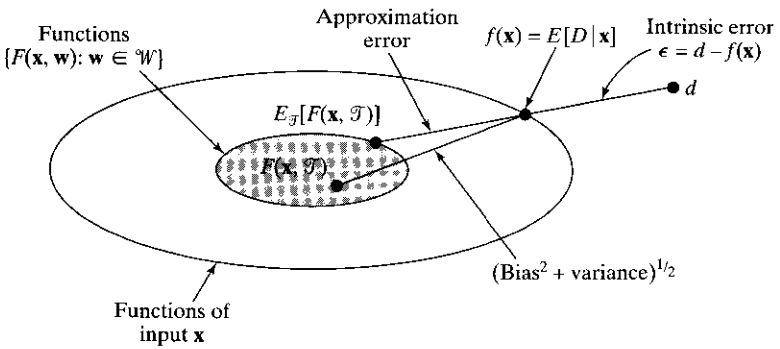


FIGURE 2.21 Illustration of the various sources of error in solving the regression problem.

achieve good overall performance, the bias $B(\mathbf{w})$ and the variance $V(\mathbf{w})$ of the approximating function $F(\mathbf{x}, \mathbf{w}) = F(\mathbf{x}, \mathcal{T})$ would both have to be small.

Unfortunately, we find that in a neural network that learns by example and does so with a training sample of fixed size, the price for achieving a small bias is a large variance. For a single neural network, it is only when the size of the training sample becomes infinitely large that we can hope to eliminate both bias and variance at the same time. We then have a *bias/variance dilemma*, and the consequence is prohibitively slow convergence (Geman et al., 1992). The bias/variance dilemma may be circumvented if we are willing to *purposely* introduce bias, which then makes it possible to eliminate the variance or to reduce it significantly. Needless to say, we must be sure that the bias built into the network design is harmless. In the context of pattern classification, for example, the bias is said to be "harmless" in the sense that it will contribute significantly to mean-square error only if we try to infer regressions that are not in the anticipated class. In general, bias must be *designed* for each specific application of interest. A practical way of achieving such an objective is to use a *constrained* network architecture, which usually performs better than a general-purpose architecture. For example, the constraints and therefore the bias may take the form of prior knowledge built into the network design using (1) *weight-sharing* where several synapses of the network are controlled by a single weight, and/or (2) *local receptive fields* assigned to individual neurons in the network, as demonstrated in the application of a multilayer perceptron to the optical character recognition problem (LeCun et al., 1990a). These network design issues were briefly discussed in Section 1.7.

2.14 STATISTICAL LEARNING THEORY

In this section we continue the statistical characterization of neural networks by describing a *learning theory* that addresses the fundamental issue of how to control the generalization ability of a neural network in mathematical terms. The discussion is presented in the context of supervised learning.

A model of supervised learning consists of three interrelated components, illustrated in Fig. 2.22 and abstracted in mathematical terms as follows (Vapnik, 1992, 1998):

1. *Environment.* The environment is stationary, supplying a vector $\mathbf{x}$ with a fixed but unknown cumulative (probability) distribution function $F_{\mathbf{X}}(\mathbf{x})$.
2. *Teacher.* The teacher provides a desired response d for every input vector $\mathbf{x}$ received from the environment, in accordance with a conditional cumulative distribution function $F_{\mathbf{X}}(\mathbf{x}|d)$ that is also fixed but unknown. The desired response d and input vector $\mathbf{x}$ are related by

$$d = f(\mathbf{x}, v) \tag{2.69}$$

   where v is a noise term, permitting the teacher to be "noisy."
3. *Learning machine (algorithm).* The learning machine (neural network) is capable of implementing a set of input–output mapping functions described by

$$y = F(\mathbf{x}, \mathbf{w}) \tag{2.70}$$

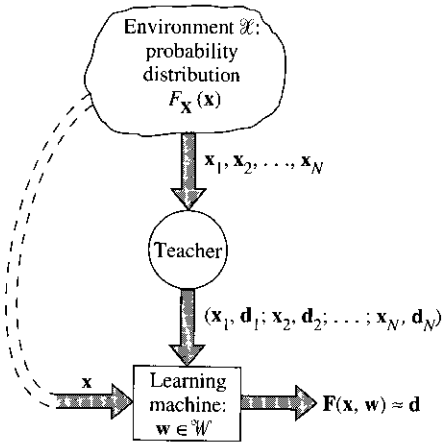


FIGURE 2.22 Model of the supervised learning process.

where y is the actual response produced by the learning machine in response to the input $\mathbf{x}$, and $\mathbf{w}$ is a set of free parameters (synaptic weights) selected from the parameter (weight) space $\mathcal{W}$.

Equations (2.69) and (2.70) are written in terms of the examples used to perform the training.

The supervised learning problem is that of selecting the particular function $F(\mathbf{x}, \mathbf{w})$ that approximates the desired response d in an optimum fashion, with "optimum" being defined in some statistical sense. The selection itself is based on the set of N *independent, identically distributed (iid)* training examples described in Eq. (2.53) and reproduced here for convenience of presentation:

$$\mathcal{T} = \{(\mathbf{x}_i, d_i)\}_{i=1}^{N}$$

Each example pair is drawn by the learning machine from $\mathcal{T}$ with a joint cumulative (probability) distribution function $F_{\mathbf{X},D}(\mathbf{x}, d)$, which, like the other distribution functions, is also fixed but unknown. The feasibility of supervised learning depends on this question: Do the training examples $\{(\mathbf{x}_i, d_i)\}$ contain sufficient information to construct a learning machine capable of good generalization performance? An answer to this fundamental question lies in the use of tools pioneered by Vapnik and Chervonenkis (1971). Specifically, we proceed by viewing the supervised learning problem as an *approximation problem,* which involves finding the function $F(\mathbf{x}, \mathbf{w})$ that is the best possible approximation to the desired function $f(\mathbf{x})$.

Let $L(d, F(\mathbf{x}, \mathbf{w}))$ denote a measure of the *loss* or *discrepancy* between the desired response d corresponding to an input vector $\mathbf{x}$ and the actual response $F(\mathbf{x}, \mathbf{w})$ produced by the learning machine. A popular definition for the loss $L(d, F(\mathbf{x}, \mathbf{w}))$ is the *quadratic loss function* defined as the squared distance between $d = f(\mathbf{x})$ and the approximation $F(\mathbf{x}, \mathbf{w})$ as shown by[12]

$$L(d, F(\mathbf{x}, \mathbf{w})) = (d - F(\mathbf{x}, \mathbf{w}))^2 \tag{2.71}$$

The squared distance of Eq. (2.64) is the ensemble-averaged extension of $L(d, F(\mathbf{x}, \mathbf{w}))$, with the averaging being performed over all the example pairs $(\mathbf{x}, d)$.

Most of the literature on statistical learning theory deals with a specific loss. The strong point of the statistical learning theory presented here is that it does *not* depend critically on the form of the loss function $L(d, F(\mathbf{x}, \mathbf{w}))$. Later in the section we do restrict the discussion to a specific loss function.

The expected value of the loss is defined by the *risk functional*

$$R(\mathbf{w}) = \int L(d, F(\mathbf{x}, \mathbf{w}))dF_{\mathbf{X},D}(\mathbf{x}, d) \tag{2.72}$$

where the integral is a multi-fold integral taken over all possible values of the example pair $(\mathbf{x}, d)$. The goal of supervised learning is to minimize the risk functional $R(\mathbf{w})$ over the class of approximating functions $\{F(\mathbf{x}, \mathbf{w}), \mathbf{w} \in \mathcal{W}\}$. However, evaluation of the risk functional $R(\mathbf{w})$ is complicated because the joint cumulative distribution function $F_{\mathbf{X},D}(\mathbf{x}, d)$ is usually unknown. In supervised learning, the only information available is contained in the training data set $\mathcal{T}$. To overcome this mathematical difficulty, we use the inductive principle of empirical risk minimization (Vapnik, 1982). This principle relies entirely on availability of the training data set $\mathcal{T}$, which makes it perfectly suited to the design philosophy of neural networks.

Some Basic Definitions

Before proceeding further, we digress briefly to introduce some basic definitions that we use in the material to follow.

Convergence in probability. Consider a sequence of random variables $a_1, a_2, \ldots, a_N$. This sequence of random variables is said to *converge in probability* to a random variable a_0 if for any $\delta > 0$, the probabilistic relation

$$P(|a_N - a_0| > \delta) \xrightarrow{P} 0 \qquad \text{as } N \to \infty \tag{2.73}$$

holds.

Supremum and infimum. The supremum of a nonempty set $\mathcal{A}$ of scalars, denoted by $\sup \mathcal{A}$, is defined as the smallest scalar x such that $x \geq y$ for all $y \in \mathcal{A}$. If no such scalar exists, we say that the supremum of the nonempty set $\mathcal{A}$ is ∞. Similarly, the infimum of set $\mathcal{A}$, denoted by $\inf \mathcal{A}$, is defined as the largest scalar x such that $x \leq y$ for all $y \in \mathcal{A}$. If no such scalar exists, we say that the infimum of the nonempty set $\mathcal{A}$ is ∞.

Empirical risk functional. Given the training sample $\mathcal{T} = \{(\mathbf{x}_i, d_i)\}_{i=1}^N$, the empirical risk functional is defined in terms of the loss function $L(d_i, F(\mathbf{x}_i, \mathbf{w}))$ as

$$R_{\text{emp}}(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N} L(d_i, F(\mathbf{x}_i, \mathbf{w})) \tag{2.74}$$

Strict Consistency. Consider the set $\mathcal{W}$ of functions $L(d, F(\mathbf{x}, \mathbf{w}))$ whose underlying distribution is defined by the joint cumulative distribution function $F_{\mathbf{X},D}(\mathbf{x}, d)$. Let $\mathcal{W}(c)$ be any nonempty subset of this set of functions, such that

$$\mathcal{W}(c) = \left\{ \mathbf{w}: \int L(d, F(\mathbf{x}, \mathbf{w})) \geq c \right\} \tag{2.75}$$

where $c \in (-\infty, \infty)$. The empirical risk functional is said to be *strictly (nontrivially) consistent* if for any subset $\mathcal{W}(c)$ the following convergence in probability

$$\inf_{\mathbf{w} \in \mathcal{W}(c)} R_{\text{emp}}(\mathbf{w}) \xrightarrow{P} \inf_{\mathbf{w} \in \mathcal{W}(c)} R(\mathbf{w}) \qquad \text{as } N \to \infty \tag{2.76}$$

holds.

With these definitions we may resume the discussion of Vapnik's statistical learning theory.

Principle of Empirical Risk Minimization

The basic idea of the principle of *empirical risk minimization* is to work with the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ defined in Eq. (2.74). This new functional differs from the risk functional $R(\mathbf{w})$ of Eq. (2.72) in two desirable ways:

1. It does *not* depend on the unknown distribution function $F_{\mathbf{X},D}(\mathbf{x}, d)$ in an explicit sense.
2. In theory it can be minimized with respect to the weight vector $\mathbf{w}$.

Let $\mathbf{w}_{\text{emp}}$ and $F(\mathbf{x}, \mathbf{w}_{\text{emp}})$ denote the weight vector and the corresponding mapping that minimize the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ in Eq. (2.74). Similarly, let $\mathbf{w}_o$ and $\mathbf{F}(\mathbf{x}, \mathbf{w}_o)$ denote the weight vector and the corresponding mapping that minimize the actual risk functional $R(\mathbf{w})$ in Eq. (2.72). Both $\mathbf{w}_{\text{emp}}$ and $\mathbf{w}_o$ belong to the weight space $\mathcal{W}$. The problem we must now consider is the conditions under which the approximate mapping $F(\mathbf{x}, \mathbf{w}_{\text{emp}})$ is "close" to the desired mapping $F(\mathbf{x}, \mathbf{w}_o)$ as measured by the mismatch between $R(\mathbf{w}_{\text{emp}})$ and $R(\mathbf{w}_o)$.

For some fixed $\mathbf{w} = \mathbf{w}^*$, the risk functional $R(\mathbf{w}^*)$ determines the *mathematical expectation* of a random variable defined by

$$Z_{\mathbf{w}^*} = L(d, F(\mathbf{x}, \mathbf{w}^*)) \tag{2.77}$$

In contrast, the empirical risk functional $R_{\text{emp}}(\mathbf{w}^*)$ is the *empirical (arithmetic) mean* of the random variable $Z_{\mathbf{w}^*}$. According to the *law of large numbers,* which constitutes one of the main theorems of probability theory, in general cases we find that as the size N of the training sample $\mathcal{T}$ is made infinitely large, the empirical mean of the random variable $Z_{\mathbf{w}^*}$ converges to its expected value. This observation provides theoretical justification for the use of the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ in place of the risk functional $R(\mathbf{w})$. However, just because the empirical mean of $Z_{\mathbf{w}^*}$ converges to its expected value, there is no reason to expect that the weight vector $\mathbf{w}_{\text{emp}}$ that minimizes the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ will also minimize the risk functional $R(\mathbf{w})$.

We may satisfy this requirement in an approximate fashion by proceeding as follows. If the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ approximates the original risk functional

$R(\mathbf{w})$ *uniformly* in $\mathbf{w}$ with some *precision* ϵ, then the minimum of $R_{emp}(\mathbf{w})$ deviates from the minimum of $R(\mathbf{w})$ by an amount not exceeding 2ϵ. Formally, this means that we must impose a stringent condition, such that for any $\mathbf{w} \in \mathcal{W}$ and $\epsilon > 0$, the probabilistic relation

$$P\left(\sup_{\mathbf{w}} |R(\mathbf{w}) - R_{emp}(\mathbf{w})| > \epsilon\right) \to 0 \qquad \text{as } N \to \infty \tag{2.78}$$

holds (Vapnik, 1982). When Eq. (2.78) is satisfied, we say that a *uniform convergence in the weight vector* $\mathbf{w}$ *of the empirical mean risk to its expected value occurs.* Equivalently, provided that for any prescribed precision ϵ we can assert the inequality

$$P\left(\sup_{\mathbf{w}} |R(\mathbf{w}) - R_{emp}(\mathbf{w})| > \epsilon\right) < \alpha \tag{2.79}$$

for some $\alpha > 0$, then as a consequence the following inequality also holds:

$$P(R(\mathbf{w}_{emp}) - R(\mathbf{w}_o) > 2\epsilon) < \alpha \tag{2.80}$$

In other words, if the condition (2.79) holds, then with probability at least $(1 - \alpha)$, the solution $F(\mathbf{x}, \mathbf{w}_{emp})$ that minimizes the empirical risk functional $R_{emp}(\mathbf{w})$ will give an actual risk $R(\mathbf{w}_{emp})$ that deviates from the true minimum possible actual risk $R(\mathbf{w}_o)$ by an amount not exceeding 2ϵ. Indeed, the condition (2.79) implies that with probability $(1 - \alpha)$ the following two inequalities are satisfied simultaneously (Vapnik, 1982):

$$R(\mathbf{w}_{emp}) - R_{emp}(\mathbf{w}_{emp}) < \epsilon \tag{2.81}$$

$$R_{emp}(\mathbf{w}_o) - R(\mathbf{w}_o) < \epsilon \tag{2.82}$$

These two equations define the differences between the true risk and empirical risk functionals at $\mathbf{w} = \mathbf{w}_{emp}$ and $\mathbf{w} = \mathbf{w}_o$, respectively. Furthermore, since $\mathbf{w}_{emp}$ and $\mathbf{w}_o$ are the minimum points of $R_{emp}(\mathbf{w})$ and $R(\mathbf{w})$, respectively, it follows that

$$R_{emp}(\mathbf{w}_{emp}) \leq R_{emp}(\mathbf{w}_o) \tag{2.83}$$

By adding the inequalities (2.81) and (2.82), and then using (2.83), we may write the following inequality

$$R(\mathbf{w}_{emp}) - R(\mathbf{w}_o) < 2\epsilon \tag{2.84}$$

Also, since the inequalities (2.81) and (2.82) are both satisfied simultaneously with probability $(1 - \alpha)$, so is the inequality (2.84). We may also state that with probability α the inequality

$$R(\mathbf{w}_{emp}) - R(\mathbf{w}_o) > 2\epsilon$$

holds, which is a restatement of (2.80).

We are now ready to make a formal statement of the *principle of empirical risk minimization* in three interrelated parts (Vapnik, 1982, 1998):

1. In place of the risk functional $R(\mathbf{w})$, construct the empirical risk functional

$$R_{emp}(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N} L(d_i, F(\mathbf{x}_i, \mathbf{w}))$$

on the basis of the training set of i.i.d. examples

$$(\mathbf{x}_i, d_i), \qquad i = 1, 2, \ldots, N$$

2. Let $\mathbf{w}_{emp}$ denote the weight vector that minimizes the empirical risk functional $R_{emp}(\mathbf{w})$ over the weight space $\mathcal{W}$. Then $R(\mathbf{w}_{emp})$ converges in probability to the minimum possible values of the actual risk $R(\mathbf{w})$, $\mathbf{w} \in \mathcal{W}$, as the size N of the training sample is made infinitely large, provided that the empirical risk functional $R_{emp}(\mathbf{w})$ converges uniformly to the actual risk functional $R(\mathbf{w})$.
3. Uniform convergence as defined by

$$P\left(\sup_{\mathbf{w}\in\mathcal{W}} |R(\mathbf{w}) - R_{emp}(\mathbf{w})| > \epsilon\right) \to 0 \qquad \text{as } N \to \infty$$

is a necessary and sufficient condition for the consistency of the principle of empirical risk minimization.

For a physical interpretation of this important principle, we offer the following observation. Prior to the training of a learning machine, all approximating functions are equally likely. As the training of the learning machine progresses, the likelihood of those approximating functions $F(\mathbf{x}_i, \mathbf{w})$ that are consistent with the training data set $\{\mathbf{x}_i, d_i)\}_{i=1}^N$ is increased. As the size N of the training data set grows, and the input space is thereby "densely" populated, the minimum point of the empirical risk functional $R_{emp}(\mathbf{w})$ converges in probability to the minimum point of the true risk functional $R(\mathbf{w})$.

VC Dimension

The theory of uniform convergence of the empirical risk functional $R_{emp}(\mathbf{w})$ to the actual risk functional $R(\mathbf{w})$ includes bounds on the rate of convergence, which are based on an important parameter called the *Vapnik–Chervonenkis dimension,* or simply the *VC dimension,* named in honor of its originators, Vapnik and Chervonenkis (1971). The VC dimension is a measure of the *capacity* or *expressive power* of the family of classification functions realized by the learning machine.

To describe the concept of VC dimension in a manner suitable for our purposes, consider a binary pattern classification problem, for which the desired response is written as $d \in \{0, 1\}$. We use the term *dichotomy* to refer to a binary classification function or decision rule. Let $\mathcal{F}$ denote the ensemble of dichotomies implemented by a learning machine, that is,

$$\mathcal{F} = \{F(\mathbf{x}, \mathbf{w}): \mathbf{w} \in \mathcal{W}, F: \mathbb{R}^m\mathcal{W} \to \{0, 1\}\} \tag{2.85}$$

Let $\mathcal{L}$ denote the set of N points in the m-dimensional space $\mathcal{X}$ of input vectors, that is,

$$\mathcal{L} = \{\mathbf{x}_i \in \mathcal{X}; i = 1, 2, \ldots, N\} \tag{2.86}$$

A dichotomy implemented by the learning machine partitions $\mathcal{L}$ into two disjoint subsets $\mathcal{L}_0$ and $\mathcal{L}_1$, such that we may write

$$F(\mathbf{x},\mathbf{w}) = \begin{cases} 0 & \text{for } \mathbf{x} \in \mathcal{L}_0 \\ 1 & \text{for } \mathbf{x} \in \mathcal{L}_1 \end{cases} \tag{2.87}$$

Let $\Delta_{\mathcal{F}}(\mathcal{L})$ denote the number of distinct dichotomies implemented by the learning machine, and $\Delta_{\mathcal{F}}(l)$ denote the maximum of $\Delta_{\mathcal{F}}(\mathcal{L})$ over all $\mathcal{L}$ with $|\mathcal{L}| = l$, where $|\mathcal{L}|$ is the number of elements of $\mathcal{L}$. We say that $\mathcal{L}$ is *shattered* by $\mathcal{F}$ if $\Delta_{\mathcal{F}}(\mathcal{L}) = 2^{|\mathcal{L}|}$, that is, if all possible dichotomies of $\mathcal{L}$ can be induced by functions in $\mathcal{F}$. We refer to $\Delta_{\mathcal{F}}(l)$ as the *growth function.*

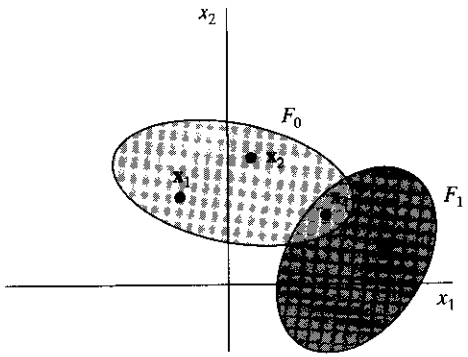


FIGURE 2.23 Diagram for Example 2.1

Example 2.1

Figure 2.23 illustrates a two-dimensional input space $\mathcal{X}$ consisting of four points $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, and $\mathbf{x}_4$. The decision boundaries of functions F_0 and F_1, indicated in the figure, correspond to the classes (hypotheses) 0 and 1 being true, respectively. From Fig. 2.23 we see that the function F_0 induces the dichotomy

$$\mathcal{D}_0 = \{\mathcal{S}_0 = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_4\}, \mathcal{S}_1 = \{\mathbf{x}_3\}\}$$

On the other hand, the function F_1 induces the dichotomy

$$\mathcal{D}_1 = \{\mathcal{S}_0 = \{\mathbf{x}_1, \mathbf{x}_2\}, \mathcal{S}_1 = \{\mathbf{x}_3, \mathbf{x}_4\}\}$$

With the set $\mathcal{S}$ consisting of four points, the cardinality $|\mathcal{S}| = 4$. Hence,

$$\Delta_{\mathcal{F}}(\mathcal{S}) = 2^4 = 16$$

■

Returning to the general discussion delineated by the ensemble $\mathcal{F}$ of dichotomies in Eq. (2.85) and the corresponding set of points $\mathcal{L}$ in Eq. (2.86), we may now formally define the VC dimension as (Vapnik and Chervonenkis, 1971; Kearns and Vazirani, 1994; Vidyasagar, 1997; Vapnik, 1998):

> The VC dimension of an ensemble of dichotomies $\mathcal{F}$ is the cardinality of the largest set $\mathcal{L}$ that is shattered by $\mathcal{F}$.

In other words, the VC dimension of $\mathcal{F}$, written as VCdim($\mathcal{F}$), is the largest N such that $\Delta_{\mathcal{F}}(N) = 2^N$. Stated in more familiar terms, the VC dimension of the set of classification functions $\{F(\mathbf{x}, \mathbf{w})\colon \mathbf{w} \in \mathcal{W}\}$ is the maximum number of training examples that can be learned by the machine without error for all possible binary labelings of the classification functions.

Example 2.2

Consider a simple decision rule in an m-dimensional space $\mathcal{X}$ of input vectors, which is described by

$$\mathcal{F}\colon y = \varphi(\mathbf{w}^T\mathbf{x} + b) \tag{2.88}$$

where $\mathbf{x}$ is an m-dimensional weight vector and b is a bias. The activation function φ is a threshold function; that is,

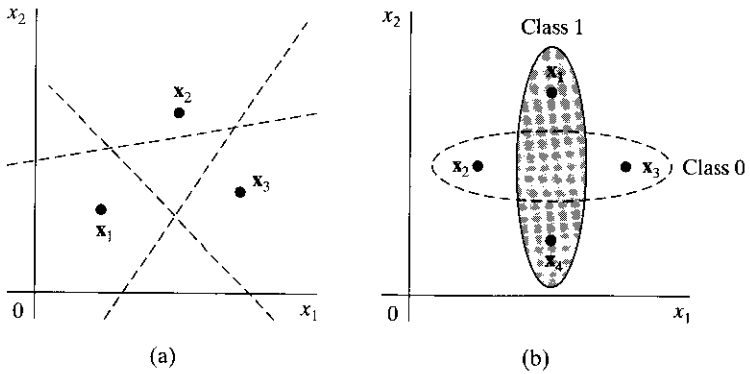


FIGURE 2.24 A pair of two-dimensional data distributions for Example 2.2.

$$\varphi(v) = \begin{cases} 1, & v \geq 0 \\ 0, & v < 0 \end{cases}$$

The VC dimension of the decision rule in Eq. (2.88) is given by

$$\text{VC dim}(\mathcal{F}) = m + 1 \tag{2.89}$$

To demonstrate this result, consider the situations described in Fig. 2.24 pertaining to a two-dimensional input space (i.e., $m = 2$). In Fig. 2.24a, we have three points $\mathbf{x}_1$, $\mathbf{x}_2$, and $\mathbf{x}_3$. Three different possible labelings of these points are included in Fig. 2.24a, from which we readily see that a maximum of three lines can shatter these points. In Fig. 2.24b we have points $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, and $\mathbf{x}_4$, with points $\mathbf{x}_2$ and $\mathbf{x}_3$ labeled as 0 and points $\mathbf{x}_1$ and $\mathbf{x}_4$ labeled as 1. This time, however, we see that points $\mathbf{x}_1$ and $\mathbf{x}_4$ cannot be shattered from $\mathbf{x}_2$ and $\mathbf{x}_3$ by a line. The VC dimension of the decision rule described in Eq. (2.88) with $m = 2$ is therefore 3, which is in accord with the formula of Eq. (2.89).

■

Example 2.3

With the VC dimension providing a measure of the capacity of a set of classification (indicator) functions, we may be led to expect that a learning machine with many free parameters would have a high VC dimension, whereas a learning machine with few free parameters would have a low VC dimension. We now present a counterexample[13] to this statement.

Consider the one parameter family of indicator functions, defined by

$$f(x, a) = \text{sgn}(\sin(ax)), \qquad a \in \mathbb{R}$$

where $\text{sgn}(\cdot)$ is the signum function. Suppose we choose any number N and the requirement is to find N points that can be shattered. This requirement is satisfied by the set of functions $f(x, a)$ by choosing

$$x_i = 10^{-i}, \qquad i = 1, 2, \ldots, N$$

To separate these data points into two classes determined by the sequence

$$d_1, d_2, \ldots, d_N, \qquad d_i \in \{-1, 1\}$$

it is sufficient that we choose the parameter a according to the formula:

$$a = \pi\left(1 + \sum_{i=1}^{N} \frac{(1 - d_i)10^i}{2}\right)$$

We thus conclude that the VC dimension of the family of indicator functions $f(x, a)$ with a single free paramenter a is infinite.

■

Importance of the VC dimension and its Estimation

The VC dimension is a purely *combinatorial concept* that has no connection with the geometric notion of dimension. It plays a central role in statistical learning theory as will be shown in the material presented in the next two subsections. The VC dimension is also important from a design point of view. Roughly speaking, the number of examples needed to learn a class of interest reliably is proportional to the VC dimension of that class. Therefore, an estimate of the VC dimension is of primary concern.

In some cases the VC dimension is determined by the free parameters of a neural network. In most practical cases, however, it is difficult to evaluate the VC dimension by analytic means. Nevertheless, *bounds* on the VC dimension of neural networks are often *tractable*. In this context, the following two results are of special interest:[14]

1. *Let $\mathcal{N}$ denote an arbitrary feedforward network built up from neurons with a threshold (Heaviside) activation function:*

$$\varphi(v) = \begin{cases} 1 & \text{for } v \geq 0 \\ 0 & \text{for } v < 0 \end{cases}$$

The VC dimension of $\mathcal{N}$ is $O(W \log W)$ where W is the total number of free parameters in the network.

This first result is due to Cover (1968) and Baum and Haussler (1989).

2. *Let $\mathcal{N}$ denote a multilayer feedforward network whose neurons use a sigmoid activation function*

$$\varphi(v) = \frac{1}{1 + \exp(-v)}$$

The VC dimension of $\mathcal{N}$ is $O(W^2)$, where W is the total number of free parameters in the network.

This second result is due to Koiran and Sontag (1996). They arrived at this result by first showing that networks consisting of two types of neurons, one linear and the other using a threshold activation function, already have a VC dimension proportional to W^2. This is a rather surprising result, since a purely linear network has a VC dimension proportional to W as shown in Example 2.2, while a purely threshold neural network has a VC dimension proportional to $W \log W$ by virtue of result 1. The desired result pertaining to a sigmoid neural network is then obtained by invoking two approximations. First, neurons with threshold activation functions are approximated by sigmoidal ones with large synaptic weights. Second, linear neurons are approximated by sigmoidal neurons with small synaptic weights.

The important point to note here is that multilayer feedforward networks have a *finite* VC dimension.

Constructive Distribution-free Bounds on the Generalization Ability of Learning Machines

At this point in the discussion we find it instructive to consider the specific case of binary pattern classification, for which the desired response is defined by $d \in \{0, 1\}$. In a corresponding way the loss function has only two possible values as shown by

$$L(d, F(\mathbf{x}, \mathbf{w})) = \begin{cases} 0 & \text{if } F(\mathbf{x}, \mathbf{w}) = d \\ 1 & \text{otherwise} \end{cases} \tag{2.90}$$

Under these conditions the risk functional $R(\mathbf{w})$ and the empirical risk functional $R_{\text{emp}}(\mathbf{w})$ defined in Eqs. (2.72) and (2.74) respectively, assume the following interpretations:

- The risk functional $R(\mathbf{w})$ is the *probability of classification error* (i.e., error rate), denoted by $P(\mathbf{w})$.
- The empirical risk functional $R_{\text{emp}}(\mathbf{w})$ is the *training error* (i.e., frequency of errors made during the training session), denoted by $\nu(\mathbf{w})$.

Now, according to the *law of large numbers* (Gray and Davisson, 1986), the empirical frequency of occurrence of an event converges almost surely to the actual probability of that event as the number of trials (assumed to be independent and identically distributed) is made infinitely large. In the context of the discussion presented here, this result means that for any weight vector $\mathbf{w}$, which does not depend on the training set, and for any precision $\epsilon > 0$, the following condition holds (Vapnik, 1982):

$$P\big(|P(\mathbf{w}) - \nu(\mathbf{w})| > \epsilon\big) \to 0 \qquad \text{as } N \to \infty \tag{2.91}$$

where N is the size of the training set. Note, however, that the condition (2.91) does not imply that the classification rule (i.e., a particular weight vector $\mathbf{w}$) that minimizes the training error $\nu(\mathbf{w})$ will also minimize the probability of classification error $P(\mathbf{w})$. For a training set of sufficiently large size N, the proximity between $\nu(\mathbf{w})$ and $P(\mathbf{w})$ follows from a stronger condition, which stipulates that the following condition holds for any $\epsilon > 0$ (Vapnik, 1982):

$$P(\sup_{\mathbf{w}} |P(\mathbf{w}) - \nu(\mathbf{w})| > \epsilon) \to 0 \qquad \text{as } N \to \infty \tag{2.92}$$

In such a case, we speak of *the uniform convergence of the frequency of training errors to the probability* that $\nu(\mathbf{w}) = P(\mathbf{w})$.

The notion of VC dimension provides a bound on the rate of uniform convergence. Specifically, for the set of classification functions with VC dimension h, the following inequality holds (Vapnik, 1982, 1998):

$$P\big(\sup_{\mathbf{w}} |P(\mathbf{w}) - \nu(\mathbf{w})| > \epsilon\big) < \left(\frac{2eN}{h}\right)^h \exp(-\epsilon^2 N) \tag{2.93}$$

where N is the size of the training sample and e is the base of the natural logarithm. We want to make the right-hand side of the inequality (2.93) small for large N in order to achieve uniform convergence. The factor $\exp(-\epsilon^2 N)$ is helpful in this regard, since it decays exponentially with increasing N. The remaining factor $(2eN/h)^h$ represents a *bound* on the growth function $\Delta_{\mathcal{F}}(l)$ for the family of functions $\mathcal{F} = \{F(\mathbf{x}, \mathbf{w}); \mathbf{w} \in \mathcal{W}\}$ for $l \geq h \geq 1$ as obtained by *Sauer's lemma*.[15] Provided that this function does *not* grow too fast, the right-hand side will go to zero as N goes to infinity; this requirement is satisfied if the VC dimension h is finite. In other words, a finite VC dimension is a necessary and sufficient condition for uniform convergence of the principle of empirical risk minimization. If the input space $\mathcal{X}$ has finite cardinality, any family of dichotomies $\mathcal{F}$ will have finite VC dimension with respect to $\mathcal{X}$, although the reverse is not necessarily true.

Let α denote the probability of occurrence of the event

$$\sup_{\mathbf{w}} |P(\mathbf{w}) - \nu(\mathbf{w})| \geq \epsilon$$

Then, with probability $1 - \alpha$, we may state that for all weight vectors $\mathbf{w} \in \mathcal{W}$ the following inequality holds:

$$P(\mathbf{w}) < \nu(\mathbf{w}) + \epsilon \tag{2.94}$$

Using the bound described in Eq. (2.93) and the definition for the probability α, we may thus set

$$\alpha = \left(\frac{2eN}{h}\right)^h \exp(-\epsilon^2 N) \tag{2.95}$$

Let $\epsilon_0(N, h, \alpha)$ denote the special value of ϵ that satisfies Eq. (2.95). Hence, we readily obtain the following important result (Vapnik, 1992):

$$\epsilon_0(N, h, \alpha) = \sqrt{\frac{h}{N}\left[\log\left(\frac{2N}{h}\right) + 1\right] - \frac{1}{N}\log\alpha} \tag{2.96}$$

We refer to $\epsilon_0(N, h, \alpha)$ as a *confidence interval,* the value of which depends on the size N of the training sample, the VC dimension h, and the probability α.

The bound described in (2.93) with $\epsilon = \epsilon_0(N, h, \alpha)$ is achieved for the worst case $P(\mathbf{w}) = \frac{1}{2}$, but not, unfortunately, for small $P(\mathbf{w})$, which is the case of interest in practice. For small $P(\mathbf{w})$, a more useful bound is obtained by considering a modification of the inequality (2.93) as follows (Vapnik, 1982, 1998):

$$P\left(\sup_{\mathbf{w}} \frac{|P(\mathbf{w}) - \nu(\mathbf{w})|}{\sqrt{P(\mathbf{w})}} > \epsilon\right) < \left(\frac{2eN}{h}\right)^h \exp\left(-\frac{\epsilon^2 N}{4}\right) \tag{2.97}$$

In the literature, different results are reported for the bound in (2.97), depending on which particular form of inequality is used for its derivation. Nevertheless, they all have a similar form. From (2.97) it follows that with probability $1 - \alpha$, and simultaneously for all $\mathbf{w} \in \mathcal{W}$ (Vapnik, 1992, 1998),

$$P(\mathbf{w}) \leq \nu(\mathbf{w}) + \epsilon_1(N, h, \alpha, \nu) \tag{2.98}$$

where $\epsilon_1(N, h, \alpha, \nu)$ is a new confidence interval defined in terms of the former confidence interval $\epsilon_0(N, h, \alpha)$ as follows (see Problem 2.25):

$$\epsilon_1(N, h, \alpha, \nu) = 2\epsilon_0^2(N, h, \alpha)\left(1 + \sqrt{1 + \frac{\nu(\mathbf{w})}{\epsilon_0^2(N, h, \alpha)}}\right) \tag{2.99}$$

This second confidence interval depends on the training error $\nu(\mathbf{w})$. For $\nu(\mathbf{w}) = 0$ it reduces to the special form

$$\epsilon_1(N, h, \alpha, 0) = 4\epsilon_0^2(N, h, \alpha) \tag{2.100}$$

We may now summarize the two bounds we have derived for the rate of uniform convergence:

1. In general, we have the following bound on the rate of uniform convergence:

$$P(\mathbf{w}) \leq \nu(\mathbf{w}) + \epsilon_1(N, h, \alpha, \nu)$$

where $\epsilon_1(N, h, \alpha, \nu)$ is as defined in Eq. (2.99).

2. For a small training error $\nu(\mathbf{w})$ close to zero, we have

$$P(\mathbf{w}) \lesssim \nu(\mathbf{w}) + 4\epsilon_0^2(N, h, \alpha)$$

which provides a fairly precise bound for real-case learning.

3. For a large training error $\nu(\mathbf{w})$ close to unity, we have the bound

$$P(\mathbf{w}) \lesssim \nu(\mathbf{w}) + \epsilon_0(N, h, \alpha)$$

Structural Risk Minimization

The *training error* is the frequency of errors made by a learning machine of some weight vector $\mathbf{w}$ during the training session. Similarly, the *generalization error* is defined as the frequency of errors made by the machine when it is tested with examples not seen before. Here it is assumed that the test data are drawn from the same population as the training data. Let these two errors be denoted by $\nu_{\text{train}}(\mathbf{w})$ and $\nu_{\text{gene}}(\mathbf{w})$, respectively. Note that $\nu_{\text{train}}(\mathbf{w})$ is the *same* as the $\nu(\mathbf{w})$ used in the previous subsection; we used $\nu(\mathbf{w})$ there to simplify the notation. Let h be the VC dimension of a family of classification functions $\{F(\mathbf{x}, \mathbf{w}); \mathbf{w} \in \mathcal{W}\}$ with respect to the input space $\mathcal{X}$. Then, in light of the theory on the rate of uniform convergence, we may state that with probability $1 - \alpha$, for a number of training examples $N > h$, and simultaneously for all classification functions $F(\mathbf{x}, \mathbf{w})$, the generalization error $\nu_{\text{gene}}(\mathbf{w})$ is lower than a *guaranteed risk* defined by the sum of a pair of competing terms (Vapnik, 1992, 1998)

$$\nu_{\text{guarant}}(\mathbf{w}) = \nu_{\text{train}}(\mathbf{w}) + \epsilon_1(N, h, \alpha, \nu_{\text{train}}) \tag{2.101}$$

where the confidence interval $\epsilon_1(N, h, \alpha, \nu_{\text{train}})$ is itself defined by Eq. (2.99). For a fixed number of training examples N, the training error decreases monotonically as the capacity or VC dimension h is increased, whereas the confidence interval increases monotonically. Accordingly, both the guaranteed risk and the generalization error go through a minimum. These trends are illustrated in a generic way in Fig. 2.25. Before the minimum point is reached, the learning problem is *overdetermined* in the sense that the machine capacity h is too small for the amount of training detail. Beyond the mini-

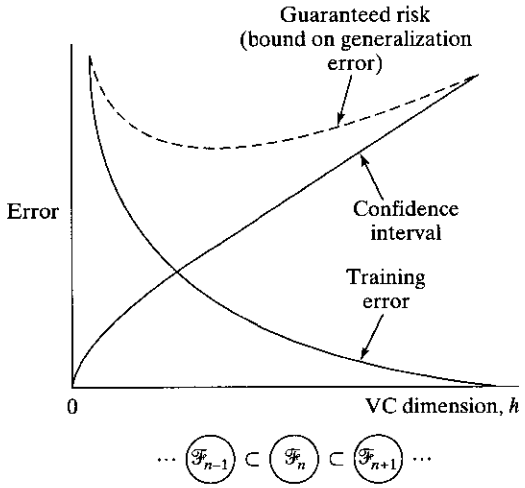


FIGURE 2.25 Illustration of the relationship between training error, confidence interval, and guaranteed risk.

mum point, the learning problem is *underdetermined* because the machine capacity is too large for the amount of training data.

The challenge in solving a supervised learning problem is therefore to realize the best generalization performance by matching the machine capacity to the available amount of training data for the problem at hand. The *method of structural risk minimization* provides an inductive procedure for achieving this goal by making the VC dimension of the learning machine a *control* variable (Vapnik, 1992, 1998). To be specific, consider an ensemble of pattern classifiers $\{F(\mathbf{x}, \mathbf{w}); \mathbf{w} \in \mathcal{W}\}$, and define a nested structure of n such machines

$$\mathcal{F}_k = \{F(\mathbf{x}, \mathbf{w}); \mathbf{w} \in \mathcal{W}_k\}, \qquad k = 1, 2, \ldots, n \tag{2.102}$$

such that we have (see Fig. 2.25)

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \cdots \subset \mathcal{F}_n \tag{2.103}$$

where the symbol $\subset$ signifies "is contained in." Correspondingly, the VC dimensions of the individual pattern classifiers satisfy the condition

$$h_1 \leq h_2 \leq \cdots \leq h_n \tag{2.104}$$

which implies that the VC dimension of each pattern classifier is finite. Then, the method of structural risk minimization may proceed as follows:

- The empirical risk (i.e., training error) for each pattern classifier is minimized.
- The pattern classifier $\mathcal{F}^*$ with the smallest guaranteed risk is identified; this particular machine provides the best compromise between the training error (i.e., quality of approximation of the training data) and the confidence interval, (i.e., complexity of the approximating function) which compete with each other.

Our goal is to find a network structure such that decreasing the VC dimension occurs at the expense of the smallest possible increase in training error.

The principle of structural risk minimization may be implemented in a variety of ways. For example, we may vary the VC dimension h by varying the number of hidden

neurons. Specifically, we evaluate an ensemble of fully connected multilayer feedforward networks, in which the number of neurons in one of the hidden layers is increased in a monotonic fashion. The principle of structural risk minimization states that the best network in this ensemble is the one for which the guaranteed risk is the minimum.

The VC dimension is not only central to the principle of structural risk minimization but also to an equally powerful learning model called probably approximately correct (PAC). This latter model, discussed in the next section, completes the last part of the chapter dealing with probabilistic and statistical aspects of learning.

2.15 PROBABLY APPROXIMATELY CORRECT MODEL OF LEARNING

The *probably approximately correct (PAC)* learning model is credited to Valiant (1984). As the name implies, the PAC model is a probabilistic framework for the study of learning and generalization in binary classification systems. It is closely related to supervised learning.

We begin with an environment $\mathcal{X}$. A set of $\mathcal{X}$ is called a *concept*, and a set of subsets of $\mathcal{X}$ is called a *concept class*. An *example* of a concept is an object in the domain of interest, together with a class label. If the example is a member of the concept, we refer to it as a *positive example*; if the object is *not* a member of the concept, we refer to it as a *negative example*. A concept for which examples are provided is called a *target concept*. We may acquire a sequence of training data of length N for a target concept c as shown by

$$\mathcal{T} = \{(\mathbf{x}_i, c(\mathbf{x}_i)\}_{i=1}^{N} \tag{2.105}$$

which may contain repeated examples. The examples $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ are drawn from the environment $\mathcal{X}$ at random, according to some fixed but unknown probability distribution. The following points are also noteworthy in Eq. (2.105):

- The target concept $c(\mathbf{x}_i)$ is treated as a function from $\mathcal{X}$ to $\{0, 1\}$. Moreover, $c(\mathbf{x}_i)$ is assumed to be unknown.
- The examples are usually assumed to be statistically independent, which means that the joint probability density function of any two examples, $\mathbf{x}_i$ and $\mathbf{x}_j$, say, is equal to the product of their individual probability density functions.

In the context of our previous terminology, the environment $\mathcal{X}$ may be identified with the input space of a neural network, and the target concept may be identified with the desired response for the network.

The set of concepts derived from the environment $\mathcal{X}$ is referred to as a *concept space* $\mathcal{C}$. For example, the concept space may contain "the letter A," "the letter B," and so on. Each of these concepts may be coded differently to generate a set of positive examples and a set of negative examples. In the framework of supervised learning, however, we have another set of concepts. A learning machine typically represents a set of functions, with each function corresponding to a specific state. For example, the machine may be designed to recognize "the letter A," "the letter B," and so on. The set of all functions (i.e., concepts) determined by the learning machine is referred to as a *hypothesis space* $\mathcal{H}$. The hypothesis space may or may not be equal to the concept

space. In a way the notions of concept space and hypothesis space are analogous to the function $f(\mathbf{x})$ and approximating function $F(\mathbf{x}, \mathbf{w})$, respectively, that were used in the previous section.

Suppose then we are given a target concept $c(\mathbf{x}) \in \mathscr{C}$, which takes only the value 0 or 1. We wish to learn this concept by means of a neural network by training it on the data set $\mathcal{T}$ defined in Eq. (2.105). Let $g(\mathbf{x}) \in \mathscr{G}$ denote the hypothesis corresponding to the input–output mapping that results from this training. One way of assessing the success of the learning process is to measure how close the hypothesis $g(\mathbf{x})$ is to the target concept $c(\mathbf{x})$. There will naturally be errors incurred, making $g(\mathbf{x}) \neq c(\mathbf{x})$. The reason errors are incurred is that we are trying to learn a function on the basis of limited information available about that function. The probability of training error is defined by

$$\nu_{\text{train}} = P(\mathbf{x} \in \mathscr{X} : g(\mathbf{x}) \neq c(\mathbf{x})) \tag{2.106}$$

The probability distribution in this equation must be the same as the one responsible for generating the examples. The goal of PAC learning is to ensure that ν_{train} is *usually small*. The domain that is available to the learning algorithm is controlled by the size N of the training sample $\mathcal{T}$. In addition, the learning algorithm is supplied with two control parameters:

- *Error parameter* $\epsilon \in (0, 1]$. This parameter specifies the error allowed in a good approximation of the target concept $c(\mathbf{x})$ by the hypothesis $g(\mathbf{x})$.
- *Confidence parameter* $\delta \in (0,1]$. This second parameter controls the likelihood of constructing a good approximation.

We may thus visualize the PAC learning model as depicted in Fig. 2.26.

With this background we may now formally state the PAC learning model (Valiant, 1984; Kearns and Vazirani, 1994; Vidyasagar, 1997):

> Let $\mathscr{C}$ be a concept class over the environment $\mathscr{X}$. The concept class $\mathscr{C}$ is said to be PAC learnable if there exists an algorithm $\mathscr{L}$ with the following property: For every target concept $c \in \mathscr{C}$, for every probability distribution on $\mathscr{X}$, and for all $0 < \epsilon < 1/2$ and $0 < \delta < 1/2$, if the learning algorithm $\mathscr{L}$ is supplied the set of training examples $\mathcal{T} = \{(\mathbf{x}_i, c(\mathbf{x}_i))\}_{i=1}^{N}$ and the parameters ϵ and δ, then with probability at least $1 - \delta$, the learning algorithm $\mathscr{L}$ outputs a hypothesis g with error $\nu_{\text{train}} \leq \epsilon$. This probability is taken over the random examples drawn from the set $\mathcal{T}$ and any internal randomization that may exist in the learning algorithm $\mathscr{L}$. The sample size N must be greater than a function of δ and ϵ.

In other words, provided that the size N of the training sample $\mathcal{T}$ is large enough, after the neural network has been trained on that data set it is "probably" the case that the

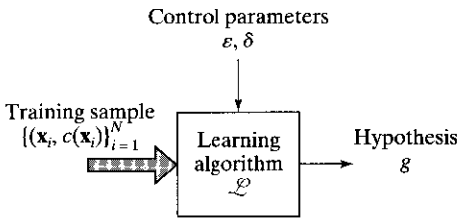


FIGURE 2.26 Block diagram illustrating the PAC learning model.

input–output mapping computed by the network is "approximately correct." Note that although there is a dependence on δ and ϵ, the number of examples, N, does not have to be dependent on the target concept c or the underlying probability distribution of $\mathcal{X}$.

Sample Complexity

In PAC learning theory, an issue of particular interest with practical implications is the issue of *sample complexity*. The focus in this issue is on how many random examples should be presented to the learning algorithm for it to acquire sufficient information to learn an unknown target concept c chosen from the concept class $\mathcal{C}$. Or, how large should the size N of the training set $\mathcal{T}$ be?

The issue of sample complexity is closely linked with the VC dimension. However, before proceeding further on this issue, we need to define the notion of a consistent concept. Let $\mathcal{T} = \{(\mathbf{x}_i, d_i)\}_{i=1}^{N}$ be any set of labeled examples, where each $\mathbf{x}_i \in \mathcal{X}$ and each $d_i \in (0,1)$. Let c be a target concept over the environment $\mathcal{X}$. Then, concept c is said to be *consistent* with the training set $\mathcal{T}$ (or, equivalently, $\mathcal{T}$ is consistent with c) if for all $1 \leq i \leq N$ we have $c(\mathbf{x}_i) = d_i$ (Kearns and Vazarini, 1994). Now, as far as PAC learning is concerned, it is *not* the size of the set of input–output functions computable by a neural network that is crucial, but rather it is the VC dimension of the network. More precisely, we have a key result presented in two parts (Blumer et al., 1989; Anthony and Biggs, 1992; Vidyasagar, 1997):

> Consider a neural network with a finite VC dimension $h \geq 1$.
>
> 1. Any consistent learning algorithm for that neural network is a PAC learning algorithm.
> 2. There is a constant K such that a sufficient size of training set $\mathcal{T}$ for any such algorithm is
>
> $$N = \frac{K}{\epsilon}\left(h \log\left(\frac{1}{\epsilon}\right) + \log\left(\frac{1}{\delta}\right)\right) \tag{2.107}$$
>
> where ϵ is the error parameter and δ is the confidence parameter.

The generality of this result is impressive: it is applicable to a supervised learning process regardless of the type of learning algorithm used, and the underlying probability distribution for generating the labeled examples. It is the broad generality of this result that has made it a subject of intensive research interest in neural network literature. Comparison of results predicted from bounds on measures based on the VC dimension with experimental results reveals a wide numerical discrepancy.[16] In a sense this should not be surprising because the discrepancy is merely a reflection of the *distribution-free, worst-case* nature of the theoretical measures, and on *average* we can always do better.

Computational Complexity

Another issue of primary concern in PAC learning is that of computational complexity. This issue concerns the computational effectiveness of a learning algorithm. More precisely, *computational complexity* deals with the worst-case "running time" needed to

train a neural network (learning machine), given a set of labeled examples of some finite size N.

In a practical situation, the running time of an algorithm naturally depends on the speed with which the underlying computations are performed. From a theoretical perspective, however, the intention is to have a definition of running time that is independent of the device used to do the computations. With this intention in mind, running time, and therefore computational complexity, is usually measured in terms of the number of operations (additions, multiplications, and storage) needed to perform the computation.

In assessing the computational complexity of a learning algorithm, we like to know how it varies with the example size m (i.e., size of the input layer of the neural network being trained). For the algorithm to be computationally *efficient* in this context, the running time should be $O(m^r)$ for some fixed integer $r \geq 1$. In such a case, the running time is said to increase polynomially with m, and the algorithm itself is said to be a *polynomial time algorithm*. Learning tasks performed by a polynomial time algorithm are usually regarded as "easy" (Anthony and Biggs, 1992).

The other parameter that requires attention is the error parameter ϵ. Whereas in the case of sample complexity the parameter ϵ is fixed but arbitrary, in assessing the computational complexity of a learning algorithm we like to know how it varies with ϵ. Intuitively, we expect that as ϵ is decreased, the learning task under study would become more difficult. It follows then that some condition would have to be imposed on the time taken for the algorithm to produce a probably approximately correct output. For efficient computation, the appropriate condition is to have the running time polynomial in $1/\epsilon$.

By putting these considerations together, we may make the following formal statement on computational complexity (Anthony and Biggs, 1992):

> A learning algorithm is computationally efficient with respect to error parameter ϵ, example size m, and size N of the training set if its running time is polynomial in N and if there is a value of $N_0(\delta,\epsilon)$ sufficient for PAC learning that is polynomial in both m and ϵ^{-1}.

2.16 SUMMARY AND DISCUSSION

In this chapter we discussed some important issues relating to the many facets of the learning process in the context of neural networks. In so doing we have laid down the foundations for much of the material in the rest of this book. The five learning rules, *error-correction learning, memory-based learning, Hebbian learning, competitive learning,* and *Boltzmann learning,* are basic to the design of neural networks. Some of these algorithms require the use of a teacher and some do not. The important point is that these rules enable us to go far beyond the reach of linear adaptive filters in both capability and universality.

In the study of supervised learning, a key provision is a "teacher" capable of supplying exact corrections to the network outputs when an error occurs as in error-correction learning; or "clamping" the free-running input and output units of the network to the environment as in Boltzmann learning. Neither of these models is possible in biological organisms, which have neither the exact reciprocal nervous connections needed for the back propagation of error corrections (in a multilayer feedforward

network) nor the nervous means for the imposition of behavior from outside. Nevertheless, supervised learning has established itself as a powerful paradigm for the design of artificial neural networks, as is demonstrated in Chapters 3 through 7.

In contrast, self-organized (unsupervised) learning rules such as Hebbian learning and competitive learning are motivated by neurobiological considerations. However, to improve our understanding of self-organized learning, we also need to look at Shannon's *information theory* for relevant ideas. Here we should mention the *maximum mutual information (Infomax) principle* due to Linsker (1988a, b), which provides the mathematical formalism for the processing of information in a self-organized neural network in a manner somewhat analogous to the transmission of information in a communication channel. The Infomax principle and its variants are discussed in Chapter 10.

A discussion of learning methods would be incomplete without mentioning the *Darwinian selective learning model* (Edelman, 1987; Reeke et al., 1990). *Selection* is a powerful biological principle with applications in both evolution and development. It is at the heart of the immune system (Edelman, 1973), the best understood biological recognition system. The Darwinian selective learning model is based on the theory of neural group selection. It presupposes that the nervous system operates by a form of selection akin to natural selection in evolution but takes place within the brain during the lifetime of each animal. According to this theory, the basic operational units of the nervous system are not single neurons but rather local groups of strongly interconnected cells. The membership of neurons in a group is changed by alterations in the neurons' synaptic weights. Local competition and cooperation among cells are clearly necessary to produce local order in the network. A collection of neuronal groups is referred to as a *repertoire*. Groups in a repertoire respond best to overlapping but similar input patterns due to the random nature of neural growth. One or more neuronal groups in a repertoire respond to every input pattern, thereby ensuring some response to unexpected input patterns that may be important. Darwinian selective learning is different from the learning algorithms commonly used in neural network design in that it assumes that there are many subnetworks by design, and that only those with the desired response are selected during the training process.

We complete this discussion with some concluding remarks on statistical and probabilistic aspects of learning. The VC dimension has established itself as a central parameter in statistical learning theory. It is basic to structural risk minimization and the probably approximately correct (PAC) model of learning. The VC dimension is an integral part of the underlying theory of so-called support vector machines, discussed in Chapter 6. In Chapter 7 we discuss a class of committee machines based on boosting, the theory of which is rooted in PAC learning.

As we progress through the rest of the book there will be many occasions and good reasons for revisiting the material presented in this chapter on the fundamentals of learning processes.

NOTES AND REFERENCES

1. The word "algorithm" is derived from the name of the Persian mathematician Mohammed al-Kowârisimi, who lived during the ninth century and who is credited with developing the step-by-step rules for the addition, subtraction, multiplication, and divi-

sion of ordinary decimal numbers. When his name was written in Latin it became Algorismus, from which *algorithm* is derived (Harel, 1987).

2. The nearest neighbor rule embodies a huge literature; see the collection of papers edited by Dasarathy (1991). This book includes the seminal work of Fix and Hodges (1951) and many other important papers on nearest neighbor pattern-classification techniques.
3. For a detailed review of Hebbian synapses, including a historical account, see Brown et al. (1990) and Frégnac and Schulz (1994). For additional review material, see Constantine-Paton et al. (1990).
4. **Long-Term Potentiation—Physiological Evidence for the Hebbian Synapse**
Hebb (1949) provided us with a way to think about synaptic memory mechanisms, but it was nearly a quarter of a century before experimental evidence was obtained in support of his proposals. In 1973, Bliss and Lomo published a paper describing a form of activation-induced synaptic modification in an area of the brain called the *hippocampus.* They applied pulses of electrical stimulation to the major pathway entering this structure while recording the synaptically evoked responses. When they were confident that they had characterized a stable baseline response morphology, they applied brief, high frequency trains of pulses to the same pathway. When they resumed application of the test pulses, they found the responses to be much larger in amplitude. Of most interest to memory researchers was the finding that this effect was very long lasting. They called the phenomenon *long-term potentiation* (LTP).

   There are now hundreds of papers published every year on the LTP phenomenon, and we know much about the underlying mechanisms. We know, for example, that the potentiation effects are restricted to the activated pathways. We also know that LTP shows a number of associative properties. What we mean by associative properties is that there are interaction effects between *co-active* pathways. In particular, if a weak input that would not normally induce an LTP effect is paired with a strong input, the weak input can be potentiated. This is called an *associative property* because it is similar to the associative properties of learning systems. In Pavlov's conditioning experiments, for example, a neutral (weak) auditory stimulus was paired with a strong (food) stimulus. The pairing resulted in the appearance of a *conditioned response,* salivation in response to the auditory stimulus.

   Much of the experimental work in this area has focused on the associative properties of LTP. Most of the synapses that have been shown to support LTP utilize glutamate as the neurotransmitter. It turns out, however, that there are a number of different receptors in the postsynaptic neuron that respond to glutamate. These receptors all have different properties, but we will consider just two of them. The main synaptic response is induced by activation of the AMPA receptor (these receptors are named according to the drugs to which they respond most strongly, but they are all glutamate receptors). When a response is recorded in an LTP experiment, it is primarily attributable to the activation of AMPA receptors. After synaptic activation the glutamate is released and binds with the receptors in the postsynaptic membrane. Ion channels that are part of the AMPA receptors open up, leading to the current flow that is the basis of the synaptic response.

   The second type of glutamate receptor, the NMDA receptor, has some interesting properties. Glutamate binding with the NMDA receptor is not enough to open the associated ion channel. That channel remains blocked until a sufficiently large voltage change has been produced by synaptic activity (involving the AMPA receptors). Consequently, while AMPA receptors are chemically dependent, the NMDA receptors are both chemically dependent and voltage dependent. We need one other piece of information to see the importance of this difference. The ion channel associated with the AMPA receptor is

linked to the movement of sodium ions (which produces the synaptic currents). The ion channel linked to the NMDA receptor allows calcium to move into the cell. While calcium movement also contributes to the membrane currents, its main role is as a signal that triggers a chain of events leading to a long-lasting increase in the strength of the response associated with the AMPA receptor.

We now have our mechanism for the Hebbian synapse. The NMDA receptor requires *both* presynaptic activity (glutamate release) *and* postsynaptic activity. How would that normally come about? By ensuring that there is a sufficiently strong input. Thus, when we pair a weak input with a strong input, the weak input releases its own glutamate, while the strong input ensures that there is a sufficiently strong voltage change to activate the NMDA receptors associated with the weak synapse.

Although Hebb's original proposal was for a unidirectional learning rule, neural networks are considerably more flexible if a *bidirectional* learning rule is used. It is an advantage to have synapses in which the synaptic weight can be decreased as well as increased. It is reassuring to know that there is also experimental evidence for a synaptic depression mechanism. If weak inputs are activated without the combined activation of strong inputs, the synaptic weight is often weakened. This is most typically seen in response to low-frequency activation of synaptic systems, and the phenomenon is called *long-term depression* (LTD). There is also some evidence for what is called a *heterosynaptic* depression effect. While LTD is a depression that is restricted to the activated input, heterosynaptic depression is restricted to the nonactivated input.

5. The idea of competitive learning may be traced back to the early works of von der Malsburg (1973) on the self-organization of orientation-sensitive nerve cells in the striate cortex, Fukushima (1975) on a self-organizing multilayer neural network known as the *neocognitron,* Willshaw and von der Malsburg (1976) on the formation of patterned neural connections by self-organization, and Grossberg (1972, 1976a,b) on adaptive pattern classification. Also, there is substantial evidence for competitive learning playing an important role in the formation of topographic maps in the brain (Durbin et al., 1989), and recent experimental work by Ambros-Ingerson et al. (1990) provides further physiological justification for competitive learning.
6. The use of lateral inhibition, as indicated in Fig. 2.4, is fashioned from neurobiological systems. Most sensory tissues, namely, retina of the eye, cochlea of the ear, and pressure-sensitive nerves of the skin, are organized in such a way that stimulation of any given location produces inhibition in the surrounding nerve cells (Arbib, 1989; Fischler and Firschein, 1987). In human perception, lateral inhibition manifests itself in a phenomenon called *Mach bands,* named after the physicist Ernest Mach (1865). For example, if we look at a sheet of paper half white and half black, we will see parallel to the boundary a "brighter than bright" band on the white side and a "darker than dark" band on the black side, even though in reality both of them have a uniform density. Mach bands are not physically present; rather, they are a visual illusion, representing "overshoots" and "undershoots" caused by the differentiating action of lateral inhibition.
7. The importance of statistical thermodynamics in the study of computing machinery was well recognized by John von Neumann. This is evidenced by the third of his five lectures on *Theory and Organization of Complicated Automata* at the University of Illinois in 1949. In his third lecture, on "Statistical Theories of Information," von Neumann said:

> Thermodynamical concepts will probably enter into this new theory of information. There are strong indications that information is similar to entropy and that degenerative processes of entropy are paralleled by degenerative processes in the processing of information. It is likely that you cannot define the function of an automaton, or its efficiency, without characterizing the milieu in which it works by

means of statistical traits like the ones used to characterize a milieu in thermodynamics. The statistical variables of the automaton's milieu will, of course, be somewhat more involved than the standard thermodynamic variable of temperature, but they will be similar in character.

8. It appears that the term "reinforcement learning" was coined by Minsky (1961) in his early studies of artificial intelligence, and then independently in control theory by Waltz and Fu (1965). However, the basic idea of "reinforcement" has its origins in experimental studies of animal learning in psychology (Hampson, 1990). In this context it is particularly illuminating to recall Thorndike's classical *law of effect* (Thorndike, 1911, p 244):

> Of several responses made to the same situation, those which are accompanied or closely followed by satisfaction to the animal will, other things being equal, be more firmly connected with the situation, so that, when it recurs, they will be more likely to recur; those which are accompanied or closely followed by discomfort to the animal will, other things being equal, have their connections with that situation weakened, so that, when it recurs, they will be less likely to occur. The greater the satisfaction or discomfort, the greater the strengthening or weakening of the bond.

Although it cannot be claimed that this principle provides a complete model of biological behavior, its simplicity and common sense approach have made it an influential learning rule in the classical approach to *reinforcement learning*.

9. The plant output is typically a physical variable. To control the plant, we clearly need to know the value of this variable; that is, we must measure the plant output. The system used for the measurement of a physical variable is called a *sensor*. To be precise therefore, the block diagram of Fig. 2.13 should include a sensor in its feedback path. We have omitted the sensor which, by implication, means that the transfer function of the sensor is assumed to be unity.

10. The "cocktail party phenomenon" refers to the remarkable human ability to selectively attend to and follow one source of auditory input in a noisy environment (Cherry, 1953; Cherry and Taylor, 1954). This ability manifests itself in a combination of three processes performed in the auditory system:

- *Segmentation*. The incoming auditory signal is segmented into individual channels, with each channel providing meaningful information about a listener's environment. Among the heuristics used by the listener to do this segmentation, *spatial location* is perhaps the most important (Moray, 1959).
- *Attention*. This pertains to the ability of the listener to focus attention on one channel while blocking attention to irrelevant channels (Cherry, 1953).
- *Switching*. This third process involves the ability to switch attention from one channel to another, which is probably mediated in a top-down manner by "gating" the incoming auditory signal (Wood and Cowan, 1995).

The conclusion to be drawn from these points is that the processing performed on the incoming auditory signal is indeed of a *spatiotemporal* kind.

11. The problem of designing an optimum linear filter that provides the theoretical framework for linear adaptive filters was first conceived by Kolmogorov (1942) and solved shortly afterward independently by Wiener (1949). On the other hand, a formal solution to the optimum nonlinear filtering problem is mathematically intractable. Nevertheless, in the 1950s a great deal of brilliant work was done by Zadeh (1953), Wiener and his collaborators (Wiener, 1958), and others that did much to clarify the nature of the problem.

Gabor was the first to conceive the idea of nonlinear adaptive filter in 1954, and went on to build such a filter with the aid of collaborators (Gabor et al., 1960). Basically, Gabor proposed a shortcut through the mathematical difficulties of nonlinear adaptive

filtering by constructing a filter that optimizes its response through learning. The output of the filter is expressed in the form

$$y(n) = \sum_{n=0}^{N} w_n x(n) + \sum_{n=0}^{N} \sum_{m=0}^{N} w_{n,m} x(n)x(m) + \cdots$$

where $x(0), x(1), \ldots, x(N)$ are samples of the filter input. (This polynomial is now referred to as the *Gabor–Kolmogorov polynomial* or *Volterra series.*) The first term of the polynomial represents a linear filter characterized by a set of coefficients $\{w_n\}$. The second term characterized by a set of dyadic coefficients $\{w_{n,m}\}$ is nonlinear; this term contains the products of two samples of the filter input, and so on for the higher-order terms. The coefficients of the filter are adjusted via gradient descent to minimize the mean-square value of the difference between a target (desired) response $d(N)$ and the actual filter output $y(N)$.

12. The cost function $L(d, F(\mathbf{x}, \mathbf{w}))$ defined in Eq. (2.71) applies to a scalar d. In the case of a vector $\mathbf{d}$ as the desired response, the approximating function takes the vector-valued form $\mathbf{F}(\mathbf{x}, \mathbf{w})$. In this case we use the squared Euclidean distance

$$L(\mathbf{d}, \mathbf{F}(\mathbf{x}, \mathbf{w})) = \|\mathbf{d} - \mathbf{F}(\mathbf{x}, \mathbf{w})\|^2$$

as the loss function. The function $\mathbf{F}(\cdot, \cdot)$ is a vector-valued function of its arguments.

13. According to Burges (1998), Example 2.3 that first appeared in Vapnik (1995) is due to E. Levin and J. S. Denker.

14. The upper bound of order $W \log W$ for the VC dimension of a feedforward neural network constructed from linear threshold units (perceptrons) was obtained by Baum and Haussler (1989). Subsequently, Maass (1993) showed that a lower bound also of order $W \log W$ holds for this class of networks.

The first upper bound on the VC dimension of a sigmoidal neural network was derived in Macintyre and Sontag (1993). Subsequently, Koiran and Sontag (1996) addressed an open question raised in Maass (1993):

> "Is the VC dimension of analog neural nets with the sigmoidal activation function $\sigma(y) = 1/1 + e^{-y}$ bounded by a polynomial in the number of programmable parameters?"

Koiran and Sontag answered this question in the affirmative in their 1996 paper, as described in the text.

This question has also been answered in the affirmative in Karpinski and Macintyre (1997). In this latter paper, a complicated method based on differential topology is used to show that the VC dimension of a sigmoidal neural network used as pattern classifier is bounded above by $O(W^4)$. There is a large gap between this upper bound and the lower bound derived in Koiran and Sontag (1996). In Karpinski and Macintyre (1997) it is conjectured that their upper bound could be lowered.

15. *Sauer's lemma* may be stated as (Sauer, 1972; Anthony and Biggs, 1992; Vidyasagar, 1997):

> Let $\mathcal{F}$ denote the ensemble of dichotomies implemented by a learning machine. If $\text{VCdim}(\mathcal{F}) = h$ with h finite, and $l \geq h \geq 1$, then the growth function $\Delta_{\mathcal{F}}(l)$ is bounded above by $(el/h)^h$ where e is the base of the natural logarithm.

16. In this note we present summaries of four important studies reported in the literature on sample complexity and the related issue of generalization.

First, Cohn and Tesauro (1992) present a detailed experimental study on the practical value of bounds on sample complexity based on the VC dimension as a design tool for pattern classifiers. In particular, the experiments were designed to test the relation-

ship between the generalization performance of a neural network and the *distribution-free, worst-case bound* derived from Vapnik's statistical learning theory. The bound considered therein is defined by Vapnik (1982)

$$v_{\text{gene}} \geq O\left(\frac{h}{N} \log\left(\frac{h}{N}\right)\right) \tag{1}$$

where v_{gene} is the generalization error, h is the VC dimension, and N is the size of the training set. The results presented by Cohn and Tesauro show that the average generalization performance is significantly better than that predicted from Eq. (1).

Second, Holden and Niranjan (1995) extend the earlier study of Cohn and Tesauro by addressing a similar question. However, there are three important differences that should be pointed out:

- All the experiments were performed on neural networks with known exact results or very good bounds on the VC dimension.
- Specific account of the learning algorithm was taken.
- The experiments were based on real-life data.

Although the results reported were found to provide sample complexity predictions of a significantly more practical value than those provided by earlier theories, there are still significant shortcomings in the theory that need to be overcome.

Third, Baum and Haussler (1989) report on the size N of the training sample needed to train a single-layer feedforward network of linear-threshold neurons for good generalization. It is assumed that the training examples are chosen from an arbitrary probability distribution, and that the test examples for evaluating the generalization performance are also drawn from the same distribution. Then, according to Baum and Haussler, the network will almost certainly provide generalization, provided two conditions are satisfied:

(1) The number of errors made on the training set is less than $\epsilon/2$.

(2) The number of examples, N, used in training is

$$N \geq O\left(\frac{W}{\epsilon} \log\left(\frac{W}{\epsilon}\right)\right) \tag{2}$$

where W is the number of synaptic weights in the network. Equation (2) provides a *distribution-free, worst-case bound* on the size N. Here again there can be a huge numerical gap between the actual size of the training sample needed and that calculated from the bound of Eq. (2).

Finally, Bartlett (1997) addresses the issue that in pattern-classification tasks using large neural networks we often find that a network is able to perform successfully with training samples that are considerably smaller in size than the number of weights in the network, as reported in Cohn and Tesauro (1992). In Bartlett's paper it is shown that for such tasks on which neural networks generalize well and if the synaptic weights are not too large, it is the size of the weights rather than the number of weights that determines the generalization performance of the network.

PROBLEMS

Learning Rules

2.1 The delta rule described in Eq. (2.3) and Hebb's rule described in Eq. (2.9) represent two different methods of learning. List the features that distinguish these two rules from each other.

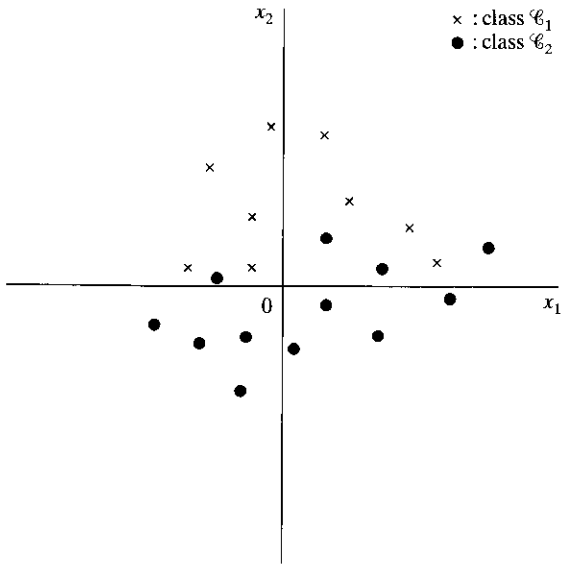


FIGURE P2.3

2.2 The error-correction learning rule may be implemented by using inhibition to subtract the desired response (target value) from the output, and then applying the anti-Hebbian rule (Mitchison, 1989). Discuss this interpretation of error-correction learning.

2.3 Figure P2.3 shows a two-dimensional set of data points. Part of the data points belongs to class $\mathscr{C}_1$ and the other part belongs to class $\mathscr{C}_2$. Construct the decision boundary produced by the nearest neighbor rule applied to this data sample.

2.4 Consider a group of people whose collective opinion on a topic of interest is defined as the weighted average of the individual opinions of its members. Suppose that if, over the course of time, the opinion of a member in the group tends to agree with the collective opinion of the group, the opinion of that member is given more weight. If, on the other hand, the particular member consistently disagrees with the collective opinion of the group, that member's opinion is given less weight. This form of weighting is equivalent to positive-feedback control, which has the effect of producing a consensus of opinion among the group (Linsker, 1988a).

Discuss the analogy between the situation described and Hebb's postulate of learning.

2.5 A generalized form of Hebb's rule is described by the relation

$$\Delta w_{kj}(n) = \alpha F(y_k(n))G(x_j(n)) - \beta w_{kj}(n)F(y_k(n))$$

where $x_j(n)$ and $y_k(n)$ are the presynaptic and postsynaptic signals, respectively; $F(\cdot)$ and $G(\cdot)$ are functions of their respective arguments; and $\Delta w_{kj}(n)$ is the change produced in the synaptic weight w_{kj} at time n in response to the signals $x_j(n)$ and $y_j(n)$. Find (a) the balance point and (b) the maximum depression that are defined by this rule.

2.6 An input signal of unit amplitude is applied repeatedly to a synaptic connection whose initial value is also unity. Calculate the variation in the synaptic weight with time using the following two rules:

(a) The simple form of Hebb's rule described in Eq. (2.9) assuming the learning-rate parameter $\eta = 0.1$.

(b) The covariance rule described in Eq. (2.10), assuming that the presynaptic activity $x = 0$ and the postsynaptic activity $\bar{y} = 1.0$.

2.7 The Hebbian synapse described in Eq. (2.9) involves the use of positive feedback. Justify the validity of this statement.

2.8 Consider the covariance hypothesis for self-organized learning described in Eq. (2.10). Assuming ergodicity (i.e., time averages can be substituted for ensemble averages), show that the expected value of Δw_{kj} in Eq. (2.10) may be expressed as

$$E[\Delta w_{kj}] = \eta(E[y_k x_j] - \bar{y}\,\bar{x})$$

How would you interpret this result?

2.9 According to Linsker (1986), Hebb's postulate of learning may be formulated as:

$$\Delta w_{ki} = \eta(y_k - y_o)(x_i - x_o) + a_1$$

where x_j and y_k are the presynaptic and postsynaptic signals, respectively and a_1, η, x_o, and y_o are all constants. Assume that neuron k is linear, as shown by

$$y_k = \sum_j w_{kj} x_j + a_2$$

where a_2 is another constant. Assume the same probability distribution for all the input signals, that is, $E[x_i] = E[x_j] = \mu$. Let the matrix $\mathbf{C}$ denote the covariance matrix of the input signals with its ij-th element defined by

$$c_{ij} = E[(x_i - \mu)(x_j - \mu)]$$

Determine Δw_{ki}.

2.10 Formulate the expression for the output y_j of neuron j in the network of Fig. 2.4. You may use the following:

$x_i = i$th input signal
w_{ji} = synaptic weight from input i to neuron j
c_{kj} = weight of lateral connection from neuron k to neuron j
v_j = induced local field of neuron j
$y_j = \varphi(v_j)$

What is the condition that would have to be satisfied for neuron j to be the winning neuron?

2.11 Repeat Problem 2.10, assuming that each output neuron includes self-feedback.

2.12 The connection pattern for lateral inhibition, namely "excitation close and inhibition further away," may be modeled as the difference between two Gaussian curves. The two curves have the same area, but the positive curve for excitation has a higher and narrower peak than the negative curve for inhibition. That is, we may express the connection pattern as

$$W(x) = \frac{1}{\sqrt{2\pi}\,\sigma_e} e^{-x^2/2\sigma_e^2} - \frac{1}{\sqrt{2\pi}\,\sigma_i} e^{-x^2/2\sigma_i^2}$$

where x is the distance from the neuron responsible for the lateral inhibition. The pattern $W(x)$ is used to scan a page, one half of which is white and the other half is black; the boundary between the two halves is perpendicular to the x-axis.

Plot the output that results from this scanning process with $\sigma_e = 1$ and $\sigma_i = 2$.

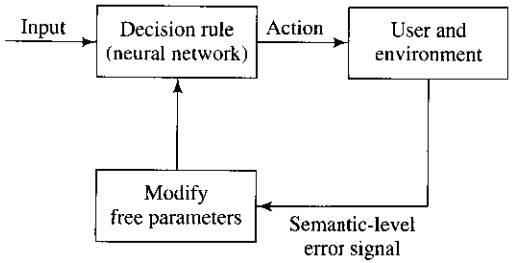


FIGURE P2.13

Learning Paradigms

2.13 Figure P2.13 shows the block diagram of an *adaptive language-acquisition system* (Gorin, 1992). The synaptic connections in the neural network part of the system are strengthened or weakened, depending on feedback as to the appropriateness of the machine's response to input stimuli. This system may be viewed as an example of reinforcement learning. Rationalize the validity of this statement.

2.14 To which of the two paradigms, learning with a teacher and learning without a teacher, do the following algorithms

(a) nearest neighbor rule
(b) k-nearest neighbor rule
(c) Hebbian learning
(d) Boltzmann learning rule

belong? Justify your answers.

2.15 Unsupervised learning can be implemented in an off-line or on-line fashion. Discuss the physical implications of these two possibilities.

2.16 Consider the difficulties that a learning machine faces in assigning credit for the outcome (win, loss, or draw) of a game of chess. Discuss the notions of temporal credit assignment and structural credit assignment in the context of this game.

2.17 A supervised learning task may be viewed as a reinforcement learning task by using as the reinforcement signal some measure of the closeness of the actual response of the system to the desired response. Discuss this relationship between supervised learning and reinforcement learning.

Memory

2.18 Consider the following orthonormal sets of key patterns, applied to a correlation matrix memory:

$$\mathbf{x}_1 = [1, 0, 0, 0]^T$$
$$\mathbf{x}_2 = [0, 1, 0, 0]^T$$
$$\mathbf{x}_3 = [0, 0, 1, 0]^T$$

The respective stored patterns are

$$\mathbf{y}_1 = [5, 1, 0]^T$$
$$\mathbf{y}_2 = [-2, 1, 6]^T$$
$$\mathbf{y}_3 = [-2, 4, 3]^T$$

(a) Calculate the memory matrix $\mathbf{M}$.

(b) Show that the memory associates perfectly.

2.19 Consider again the correlation matrix memory of Problem 2.18. The stimulus applied to the memory is a noisy version of the key pattern $\mathbf{x}_1$, as shown by

$$\mathbf{x} = [0.8, -0.15, 0.15, -0.20]^T$$

(a) Calculate the memory response $\mathbf{y}$.

(b) Show that the response $\mathbf{y}$ is closest to the stored pattern $\mathbf{y}_1$ in a Euclidean sense.

2.20 An autoassociative memory is trained on the following key vectors:

$$\mathbf{x}_1 = \tfrac{1}{4}[-2, -3, \sqrt{3}]^T$$
$$\mathbf{x}_2 = \tfrac{1}{4}[2, -2, -\sqrt{8}]^T$$
$$\mathbf{x}_3 = \tfrac{1}{4}[3, -1, \sqrt{6}]^T$$

(a) Calculate the angles between these vectors. How close are they to orthogonality with respect to each other?

(b) Using the generalization of Hebb's rule (i.e., the outer product rule), calculate the memory matrix of the network. Investigate how close to perfect the memory autoassociates.

(c) A masked version of the key vector $\mathbf{x}_1$, namely,

$$\mathbf{x} = [0, -3, \sqrt{3}]^T$$

is applied to the memory. Calculate the response of the memory, and compare your result with the desired response $\mathbf{x}_1$.

Adaptation

2.21 Figure P2.21 shows the block diagram of an adaptive system. The input signal to the *predictive model* is defined by past values of a process, as shown by

$$\mathbf{x}(n-1) = [x(n-1), x(n-2), \ldots, x(n-m)]$$

The model output, $\hat{x}(n)$, represents an *estimate* of the present value, $x(n)$, of the process. The *comparator* computes the error signal

$$e(n) = x(n) - \hat{x}(n)$$

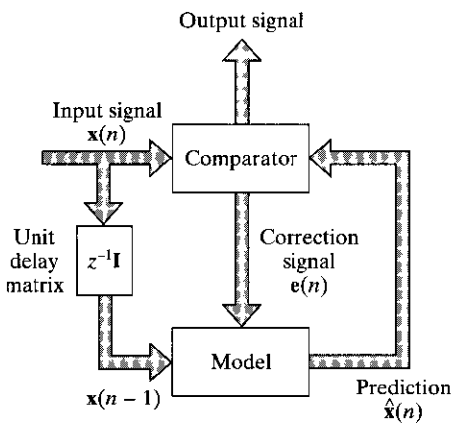


FIGURE P2.21

which in turn applies a correction to the adjustable parameters of the model. It also supplies an output signal for transfer to the next level of neural processing for interpretation. By repeating this operation on a level-by-level basis, the information processed by the system tends to be of progressively higher quality (Mead, 1990).

Fill in the details of the level of signal processing next to that described in Fig. P2.21.

Statistical learning theory

2.22 Following a procedure similar to that described for deriving Eq. (2.62) from (2.61), derive the formula for the ensemble-averaged function $L_{av}(f(\mathbf{x}), F(\mathbf{x}, \mathcal{T}))$ defined in Eq. (2.66).

2.23 In this problem we wish to calculate the VC dimension of a rectangular region aligned with one of the axes in a plane. Show that the VC dimension of this concept is four. You may do this by considering the following:

(a) Four points in a plane and a dichotomy realized by an axis-aligned rectangle.

(b) Four points in a plane, for which there is no realizable dichotomy by an axis-aligned rectangle.

(c) Five points in a plane, for which there is also no realizable dichotomy by an axis-aligned rectangle.

2.24 Consider a linear binary pattern classifier whose input vector $\mathbf{x}$ has dimension m. The first element of the vector $\mathbf{x}$ is constant and set to unity so that the corresponding weight of the classifier introduces a bias. What is the VC dimension of the classifier with respect to the input space?

2.25 The inequality (2.97) defines a bound on the rate of uniform convergence, which is basic to the principle of empirical risk minimization.

(a) Justify the validity of Eq. (2.98), assuming that the inequality (2.97) holds.

(b) Derive Eq. (2.99) that defines the confidence interval ϵ_1.

2.26 Continuing with Example 2.3, show that the four uniformly spaced points of Fig. P2.26 cannot be shattered by the one parameter family of indicator functions $f(x,a), a \in \mathbb{R}$.

2.27 Discuss the relationship between the bias-variance dilemma and structural risk minimization in the context of nonlinear regression.

2.28 **(a)** An algorithm used to train a multilayer feedforward network whose neurons use a sigmoid function is PAC learnable. Justify the validity of this statement.

(b) Can you make a similar statement for an arbitrary neural network whose neurons use a threshold activation function? Justify your answer.

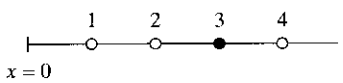


FIGURE P2.26