The Generalized Delta Rule

The learning procedure we propose involves the presentation of a set of pairs of input and output patterns. The system first uses the input vector to produce its own output vector and then compares this with the desired output, or target vector. If there is no difference, no learning takes place. Otherwise the weights are changed to reduce the difference. In this case, with no hidden units, this generates the standard delta rule as described in Chapters 2 and 11. The rule for changing weights following presentation of input/output pair p is given by

$$\Delta_p w_{ji} = \eta(t_{pj} - o_{pj})i_{pi} = \eta\delta_{pj}i_{pi}$$ (1)

where t_{pj} is the target input for jth component of the output pattern for pattern p, o_{pj} is the jth element of the actual output pattern produced by the presentation of input pattern p, i_{pi} is the value of the ith element of the input pattern, $\delta_{pj} = t_{pj} - o_{pj}$, and $\Delta_p w_{ji}$ is the change to be made to the weight from the ith to the jth unit following presentation of pattern p.

The delta rule and gradient descent There are many ways of deriving this rule. For present purposes, it is useful to see that for linear units it minimizes the squares of the differences between the actual and the desired output values summed over the output units and all pairs of input/output vectors. One way to show this is to show that the derivative of the error measure with respect to each weight is proportional to the weight change dictated by the delta rule, with negative constant of proportionality. This corresponds to performing steepest descent on a surface in weight space whose height at any point in weight space is equal to the error measure. (Note that some of the following sections are written in italics. These sections constitute informal derivations of the claims made in the surrounding text and can be omitted by the reader who finds such derivations tedious.)

To be more specific, then, let

$$E_p = \frac{1}{2}\sum_j(t_{pj} - o_{pj})^2$$ (2)

be our measure of the error on input/output pattern p and let $E = \sum E_p$ be our overall measure of the error. We wish to show that the delta rule implements a gradient descent in E when the units are linear. We will proceed by simply showing that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj}i_{pi},$$

which is proportional to $\Delta_p w_{ji}$ as prescribed by the delta rule.

When there are no hidden units it is straightforward to compute the relevant derivative. For this purpose we use the chain rule to write the derivative as the product of two parts: the derivative of the error with respect to the output of the unit times the derivative of the output with respect to the weight.

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}}\frac{\partial o_{pj}}{\partial w_{ji}}.$$ (3)

The first part tells how the error changes with the output of the jth unit and the second part tells how much changing w_{ji} changes that output. Now, the derivatives are easy to compute. First, from Equation 2

$$\frac{\partial E_p}{\partial o_{pj}} = -(t_{pj} - o_{pj}) = -\delta_{pj}.$$ (4)

Not surprisingly, the contribution of unit u_j to the error is simply proportional to δ_{pj}. Moreover, since we have linear units,

$$o_{pj} = \sum_i w_{ji}i_{pi},$$ (5)

from which we conclude that

$$\frac{\partial o_{pj}}{\partial w_{ji}} = i_{pi}.$$

Thus, substituting back into Equation 3, we see that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj}i_{pi}$$ (6)

as desired. Now, combining this with the observation that

$$\frac{\partial E}{\partial w_{ji}} = \sum_p \frac{\partial E_p}{\partial w_{ji}}$$

should lead us to conclude that the net change in w_{ji} after one complete cycle of pattern presentations is proportional to this derivative and hence that the delta rule implements a gradient descent in E. In fact, this is strictly true only if the values of the weights are not changed during this cycle. By changing the weights after each pattern is presented we depart to some extent from a true gradient descent in E. Nevertheless, provided the learning rate (i.e., the constant of proportionality) is sufficiently small, this departure will be negligible and the delta rule will implement a very close approximation to gradient descent in sum-squared error. In particular, with small enough learning rate, the delta rule will find a set of weights minimizing this error function.

The delta rule for semilinear activation functions in feedforward neworks We have shown how the standard delta rule essentially implements gradient descent in sum-squared error for linear activation functions. In this case, without hidden units, the error surface is shaped like a bowl with only one minimum, so gradient descent is guaranteed to find the best set of weights. With hidden units, however, it is not so obvious how to compute the derivatives, and the error surface is not

concave upwards, so there is the danger of getting stuck in local minima. The main theoretical contribution of this chapter is to show that there is an efficient way of computing the derivatives. The main empirical contribution is to show that the apparently fatal problem of local minima is irrelevant in a wide variety of learning tasks.

At the end of the chapter we show how the generalized delta rule can be applied to arbitrary networks, but, to begin with, we confine ourselves to *layered feedforward* networks. In these networks, the input units are the bottom layer and the output units are the top layer. There can be many layers of hidden units in between, but every unit must send its output to higher layers than its own and must receive its input from lower layers than its own. Given an input vector, the output vector is computed by a forward pass which computes the activity levels of each layer in turn using the already computed activity levels in the earlier layers.

Since we are primarily interested in extending this result to the case with hidden units and since, for reasons outlined in Chapter 2, hidden units with linear activation functions provide no advantage, we begin by generalizing our analysis to the set of nonlinear activation functions which we call *semilinear* (see Chapter 2). A semilinear activation function is one in which the output of a unit is a nondecreasing and differentiable function of the net total output,

$$net_{pj} = \sum_i w_{ji} o_{pi}, \tag{7}$$

where $o_i = i_i$ if unit i is an input unit. Thus, a semilinear activation function is one in which

$$o_{pj} = f_j(net_{pj}) \tag{8}$$

and f is differentiable and nondecreasing. The generalized delta rule works if the network consists of units having semilinear activation functions. Notice that linear threshold units do not satisfy the requirement because their derivative is infinite at the threshold and zero elsewhere.

To get the correct generalization of the delta rule, we must set

$$\Delta_p w_{ji} \propto -\frac{\partial E_p}{\partial w_{ji}},$$

where E is the same sum-squared error function defined earlier. As in the standard delta rule it is again useful to see this derivative as resulting from the product of two parts: one part reflecting the change in error as a function of the change in the net input to the unit and one part representing the effect of changing a particular weight on the net input. Thus we can write

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial net_{pj}} \frac{\partial net_{pj}}{\partial w_{ji}}. \tag{9}$$

By Equation 7 we see that the second factor is

$$\frac{\partial net_{pj}}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_k w_{jk} o_{pk} = o_{pi}. \tag{10}$$

Now let us define

$$\delta_{pj} = -\frac{\partial E_p}{\partial net_{pj}}.$$

(By comparing this to Equation 4, note that this is consistent with the definition of δ_{pj} used in the original delta rule for linear units since $o_{pj} = net_{pj}$ when unit u_j is linear.) Equation 9 thus has the equivalent form

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} o_{pi}.$$

This says that to implement gradient descent in E we should make our weight changes according to

$$\Delta_p w_{ji} = \eta \delta_{pj} o_{pi}, \tag{11}$$

just as in the standard delta rule. The trick is to figure out what δ_{pj} should be for each unit u_j in the network. The interesting result, which we now derive, is that there is a simple recursive computation of these δ's which can be implemented by propagating error signals backward through the network.

To compute $\delta_{pj} = -\partial E_p/\partial net_{pj}$, we apply the chain rule to write this partial derivative as the product of two factors, one factor reflecting the change in error as a function of the output of the unit and one reflecting the change in the output as a function of changes in the input. Thus, we have

$$\delta_{pj} = -\frac{\partial E_p}{\partial net_{pj}} = -\frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial net_{pj}}. \tag{12}$$

Let us compute the second factor. By Equation 8 we see that

$$\frac{\partial o_{pj}}{\partial net_{pj}} = f'_j(net_{pj}),$$

which is simply the derivative of the squashing function f_j for the jth unit, evaluated at the net input net_{pj} to that unit. To compute the first factor, we consider two cases. First, assume that unit u_j is an output unit of the network. In this case, it follows from the definition of E_p that

$$\frac{\partial E_p}{\partial o_{pj}} = -(t_{pj} - o_{pj}),$$

which is the same result as we obtained with the standard delta rule. Substituting for the two factors in Equation 12, we get

$$\delta_{pj} = (t_{pj} - o_{pj}) f'_j(net_{pj}) \tag{13}$$

for any output unit u_j. If u_j is not an output unit we use the chain rule to write

$$\sum_k \frac{\partial E_p}{\partial net_{pk}} \frac{\partial net_{pk}}{\partial o_{pj}} = \sum_k \frac{\partial E_p}{\partial net_{pk}} \frac{\partial}{\partial o_{pj}} \sum_i w_{ki} o_{pi}$$

$$= \sum_k \frac{\partial E_p}{\partial net_{pk}} w_{kj} = -\sum_k \delta_{pk} w_{kj}.$$

In this case, substituting for the two factors in Equation 12 yields

$$\delta_{pj} = f'_j(net_{pj}) \sum_k \delta_{pk} w_{kj} \qquad (14)$$

whenever u_j is not an output unit. Equations 13 and 14 give a recursive procedure for computing the δ's for all units in the network, which are then used to compute the weight changes in the network according to Equation 11. This procedure constitutes the generalized delta rule for a feedforward network of semilinear units.

These results can be summarized in three equations. First, the generalized delta rule has exactly the same form as the standard delta rule of Equation 1. The weight on each line should be changed by an amount proportional to the product of an error signal, δ, available to the unit receiving input along that line and the output of the unit sending activation along that line. In symbols,

$$\Delta_p w_{ji} = \eta \delta_{pj} o_{pi}.$$

The other two equations specify the error signal. Essentially, the determination of the error signal is a recursive process which starts with the output units. If a unit is an output unit, its error signal is very similar to the standard delta rule. It is given by

$$\delta_{pj} = (t_{pj} - o_{pj}) f'_j(net_{pj})$$

where $f'_j(net_{pj})$ is the derivative of the semilinear activation function which maps the total input to the unit to an output value. Finally, the error signal for hidden units for which there is no specified target is determined recursively in terms of the error signals of the units to which it directly connects and the weights of those connections. That is,

$$\delta_{pj} = f'_j(net_{pj}) \sum_k \delta_{pk} w_{kj}$$

whenever the unit is not an output unit.

The application of the generalized delta rule, thus, involves two phases: During the first phase the input is presented and propagated forward through the network to compute the output value o_{pj} for each unit. This output is then compared with the targets, resulting in an error signal δ_{pj} for each output unit. The second phase involves a backward pass through the network (analogous to the initial forward pass) during which the error signal is passed to each unit in the network and the appropriate weight changes are made.

This second, backward pass allows the recursive computation of δ as indicated above. The first step is to compute δ for each of the output units. This is simply the difference between the actual and desired output values times the derivative of the squashing function. We can then compute weight changes for all connections that feed into the final layer. After this is done, then compute δ's for all units in the penultimate layer. This propagates the errors back one layer, and the same process can be repeated for every layer. The backward pass has the same computational complexity as the forward pass, and so it is not unduly expensive.

We have now generated a gradient descent method for finding weights in any feedforward network with semilinear units. Before reporting our results with these networks, it is useful to note some further observations. It is interesting that not all weights need be variable. Any number of weights in the network can be fixed. In this case, error is still propagated as before; the fixed weights are simply not modified. It should also be noted that there is no reason why some output units might not receive inputs from other output units in earlier layers. In this case, those units receive two different kinds of error: that from the direct comparison with the target and that passed through the other output units whose activation it affects. In this case, the correct procedure is to simply add the weight changes dictated by the direct comparison to that propagated back from the other output units.

Simulation Results

We now have a learning procedure which could, in principle, evolve a set of weights to produce an arbitrary mapping from input to output. However, the procedure we have produced is a gradient descent procedure and, as such, is bound by all of the problems of any hill climbing procedure—namely, the problem of local maxima or (in our case) minima. Moreover, there is a question of how long it might take a system to learn. Even if we could guarantee that it would eventually find a solution, there is the question of whether our procedure could learn in a reasonable period of time. It is interesting to ask what hidden units the system actually develops in the solution of particular problems. This is the question of what kinds of internal representations the system actually creates. We do not yet have definitive answers to these questions. However, we have carried out many simulations which lead us to be optimistic about the local minima and time questions and to be surprised by the kinds of representations our learning mechanism discovers. Before pro-

Table 1

Input patterns		Output patterns
00	→	0
01	→	1
10	→	1
11	→	0

Table 2

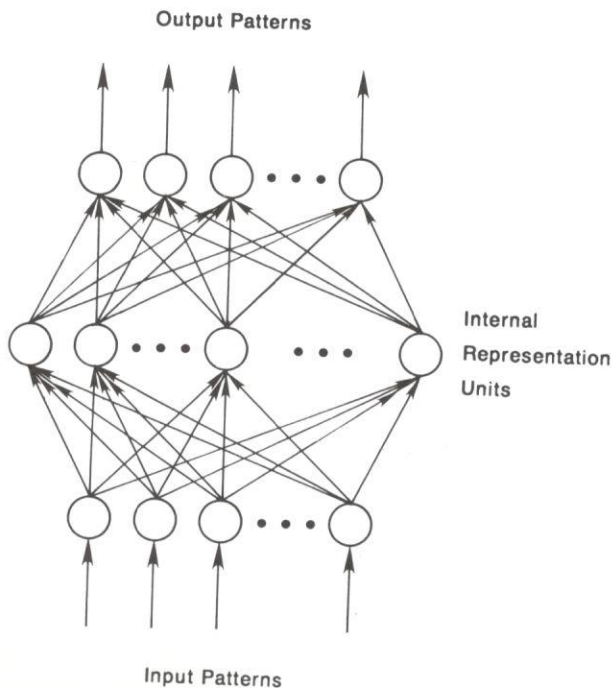| Input patterns		Output patterns
000	→	0
010	→	1
100	→	1
111	→	0

Output Patterns

Figure 1 A multilayer network. In this case the information coming to the input units is *recoded* into an internal representation and the outputs are generated by the internal representation rather than by the original pattern. Input patterns can always be encoded, if there are enough hidden units, in a form so that the appropriate output pattern can be generated from any input pattern.
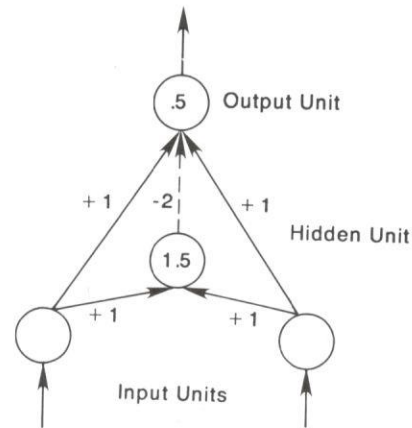

Figure 2 A simple XOR network with one hidden unit. See text for explanation.

basic responses to this lack. One response is represented by competitive learning (Chapter 5) in which simple *unsupervised* learning rules are employed so that useful hidden units develop. Although these approaches are promising, there is no external force to *insure* that hidden units appropriate for the required mapping are developed. The second response is to simply *assume* an internal representation that, on some a priori grounds, seems reasonable. This is the tack taken in the chapter on verb learning (Chapter 18) and in the interactive activation model of word perception (McClelland & Rumelhart, 1981; Rumelhart & McClelland, 1982). The third approach is to attempt to *develop* a learning procedure capable of learning an internal representation adequate for performing the task at hand. One such development is presented in the discussion of Boltzmann machines in Chapter 7. As we have seen, this procedure involves the use of stochastic units, requires the network to reach equilibrium in two different phases, and is limited to symmetric networks. Another recent approach, also employing stochastic units, has been developed by Barto (1985) and various of his colleagues (cf. Barto & Anandan, 1985). In this chapter we present another alternative that works with deterministic units, that involves only local computations, and that is a clear generalization of the delta rule. We call this the *generalized delta rule*. From other considerations, Parker (1985) has independently derived a similar generalization, which he calls *learning-logic*. Le Cun (1985) has also studied a roughly similar learning scheme. In the remainder of this chapter we first derive the generalized delta rule, then we illustrate its use by providing some results of our simulations, and finally we indicate some further generalizations of the basic idea.

The Problem

We now have a rather good understanding of simple two-layer associative networks in which a set of input patterns arriving at an input layer are mapped directly to a set of output patterns at an output layer. Such networks have no *hidden* units. They involve only *input* and *output* units. In these cases there is no *internal representation*. The coding provided by the external world must suffice. These networks have proved useful in a wide variety of applications (cf. Chapters 2, 17, and 18). Perhaps the essential character of such networks is that they map similar input patterns to similar output patterns. This is what allows these networks to make reasonable generalizations and perform reasonably on patterns that have never before been presented. The similarity of patterns in a PDP system is determined by their overlap. The overlap in such networks is determined outside the learning system itself—by whatever produces the patterns.

The constraint that similar input patterns lead to similar outputs can lead to an inability of the system to learn certain mappings from input to output. Whenever the representation provided by the outside world is such that the similarity structure of the input and output patterns are very different, a network without internal representations (i.e., a network without hidden units) will be unable to perform the necessary mappings. A classic example of this case is the *exclusive-or* (XOR) problem illustrated in Table 1. Here we see that those patterns which overlap least are supposed to generate identical output values. This problem and many others like it cannot be performed by networks without hidden units with which to create their own internal representations of the input patterns. It is interesting to note that had the input patterns contained a third input taking the value 1 whenever the first two have value 1 as shown in Table 2, a two-layer system would be able to solve the problem.

Minsky and Papert (1969) have provided a very careful analysis of conditions under which such systems are capable of carrying out the required mappings. They show that in a large number of interesting cases, networks of this kind are incapable of solving the problems. On the other hand, as Minsky and Papert also pointed out, if there is a layer of simple perceptron-like hidden units, as shown in Figure 1, with which the original input pattern can be augmented, there is always a recoding (i.e., an internal representation) of the input patterns in the hidden units in which the similarity of the patterns among the hidden units can support any required mapping from the input to the output units. Thus, if we have the right connections from the input units to a large enough set of hidden units, we can always find a representation that will perform any mapping from input to output through these hidden units. In the case of the XOR problem, the addition of a feature that detects the conjunction of the input units changes the similarity structure of the patterns sufficiently to allow the solution to be learned. As illustrated in Figure 2, this can be done with a single hidden unit. The numbers on the arrows represent the strengths of the connections among the units. The numbers written in the circles represent the thresholds of the units. The value of $+1.5$ for the threshold of the hidden unit insures that it will be turned on only when both input units are on. The value 0.5 for the output unit insures that it will turn on only when it receives a net positive input greater than 0.5. The weight of -2 from the hidden unit to the output unit insures that the output unit will not come on when both input units are on. Note that from the point of view of the output unit, the hidden unit is treated as simply another input unit. It is as if the input patterns consisted of three rather than two units.

The existence of networks such as this illustrates the potential power of hidden units and internal representations. The problem, as noted by Minsky and Papert, is that whereas there is a very simple guaranteed learning rule for all problems that can be solved without hidden units, namely, the perceptron convergence procedure (or the variation due originally to Widrow and Hoff, 1960, which we call the delta rule; see Chapter 11), there is no equally powerful rule for learning in networks with hidden units. There have been three