PERCEPTRONS

One of the most exciting developments during the early days of neural networks was the perceptron. The perceptron which was introduced by Frank Rosenblatt (1,2) is based on a network of binary decision units (3) which model nerve cells in the human brain. The perceptron is used to classify or recognize patterns, that is, to perceive. In other words, the perceptron acts as a function from a set of patterns to a set of classes. Rosenblatt's perceptron convergence theorem provided an algorithm which enables the perceptron to learn every mapping it can represent (2,4,5,6). This learning ability of perceptrons gave rise to the hope that it would be possible to construct a model of the human brain in terms of a multiple-layer perceptron.

These high expectations were crushed in the eyes of many researchers by Minsky and Papert (4), who pointed out the limitations of single-layer perceptrons. Minsky and Papert's main observation was that some very simple pattern recognition problems, namely the linearly inseparable problems, cannot be solved by means of a single-layer perceptron. Their most famous counterexample is the XOR-problem which consists of associating the binary patterns (0, 0) and (1, 1) with one class, and associating the patterns (1, 0) and (0, 1) with another class. They also addressed the scaling problem, that is, the fact that training times increase very rapidly for certain problems as the number of input lines increases. Their criticism of neural networks is valid and mathematically accurate and it led to a highly pessimistic view of the future of neural networks at the time. Minsky and Papert did not take into account, however, that multilayer versions of the perceptron are capable of solving an arbitrary dichotomy.

The advent of backpropagation in the mid-1980s renewed major interest in neural networks since it provided for a practicable algorithm to train multilayer perceptrons (7). The simplicity of standard backpropagation is one of the reasons why multilayer perceptrons are still the most widely used kind of neural networks. Other factors include the adaptability, ease of implementation, and demonstrated utility to a variety of applications in pattern recognition, control, and prediction.

This article gives a brief review of the perceptron concept and attempts to point out some critical issues involved in the design and implementation of multilayer perceptrons. The organization of the article is as follows: First we introduce the reader to the neural network terminology as well as the concepts of single-layer and multilayer perceptrons. We discuss several training algorithms of multilayer perceptrons, deal with the neural network's ability to model the data, address VLSI implementations of multilayer perceptrons, and finally present a statistical perceptron model called stochastic perceptron.

GENERAL NEURAL NETWORK CONCEPTS

Since the early days of computer science it has become evident that conventional computers lack certain abilities that every human being possesses. In particular, these machines do not display a form of intelligent behavior. There have been two approaches geared at improving this situation. One is based on symbolism and the other one is based on connectionism. The former approach models intelligence in terms of computer programs which are able to manipulate symbols given a certain amount of "knowledge" and following a certain set of rules. The connectionist approach to introducing intelligence to computer systems relies on the hope that it is possible to model the structure of the biological neural systems such as the human brain. A biological nervous system consists of a network of neurons which continually receive and transmit signals. A simple model of a biological neuron consists of a processing element receiving several inputs.

In Fig. 1 the symbols $x_1, \ldots, x_n$ represent the strengths of the impulses. The *synaptic weights* or connection strengths—denoted by the symbols $w_1, \ldots, w_n$—interpret the role that the synapses play in the transmission of impulses. The output signal is represented by the symbol y. The dependence of the

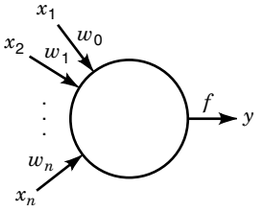

Figure 1. A simple model of a neuron. The strength of the outgoing impulse is modeled by $f([\sum_{i=1}^{n} w_i x_i] - \theta])$, where $\sum_{i=1}^{n} w_i x_i$ is a weighted sum of the incoming impulses $x_1, \ldots, x_n$. The symbol f denotes an activation function and the symbol θ denotes a threshold.

output y on the inputs $x_1, \ldots, x_n$ is given by the following rule:

$$y = f\left(\left[\sum_{i=1}^{n} w_i \cdot x_i\right] - \theta\right) \tag{1}$$

where θ is a *threshold value* or *bias* and f is the neuron's *activation function.* One of the most commonly used activation functions is the Heaviside step function given by

$$f : \mathbf{R} \to \mathbf{R}$$
$$x \to \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{else} \end{cases} \tag{2}$$

The neurons in an artificial neural network are sometimes also called *nodes* or *units.*

Neural Network Topologies

The topology of a neural network refers to its framework and its interconnection scheme. In many cases the framework of a neural network consists of several layers of nodes. The literature on neural networks distinguishes between the following types of layers:

- *Input Layer.* A layer of neurons which receive external input from outside the network
- *Output Layer.* The layer of neurons which produces the output of the network
- *Hidden Layer.* A layer composed of neurons whose interaction is restricted to other neurons in the network

A neural network is called a *single-layer neural network* if it has no hidden layers of nodes, or equivalently if it has just one layer of weights. A multilayer neural network is equipped with one or more hidden layer of nodes. A *feedforward neural network* refers to a neural network whose connections point in the direction of the output layer. A *recurrent neural network* has connections between nodes of the same layer and/or connections pointing in the direction of the input layer. A schematic representation of an exemplar feedforward neural network is given in Fig. 2.

Training and Learning

One of the principal components of intelligence is the ability to learn. Learning can be achieved in a neural network by adjusting the connection weights of the network. There are two basic forms of learning in a neural network: supervised learning and unsupervised learning. *Supervised learning* relies on the presentation of some input data and the corresponding target data. During the learning process a weight adjustment takes place which aims at minimizing the difference (error) between the target data and the output corresponding to the input data. In *unsupervised learning,* only input data are given to the network. In this setting, learning is based on grouping patterns into clusters. The weights are adjusted such that similar patterns produce the same output. *Training* refers to the actual presentation of input and possibly target data to the neural network. A neural network learns by being trained. (We have to mention that many authors prefer not to distinguish between learning and training.) The purpose of neural network training and learning is effective recall and generalization in the application phase. *Recall* consists of presenting and processing the same data which was used in the training and learning phase. Effective *generalization* is the ability of the network to perform well on new data and it is one of the main goals in the design of learning rules. The first learning rules emerged from the psychological studies of Donald Hebb and Frank Rosenblatt (8,1). Hebb's neurophysiological postulate stated that the synaptic connection strength between two neurons increases when one neuron repeatedly or persistently takes part in the activation of the other neuron or vice versa. Although the Hebbian learning rule represents a form of unsupervised learning, it can also be used in a supervised manner. Rosenblatt conceived a supervised learning rule for pattern recognition, where a teacher is necessary in order to indicate how to classify objects. The artificial neural network model he proposed in order to solve these problems was the perceptron.

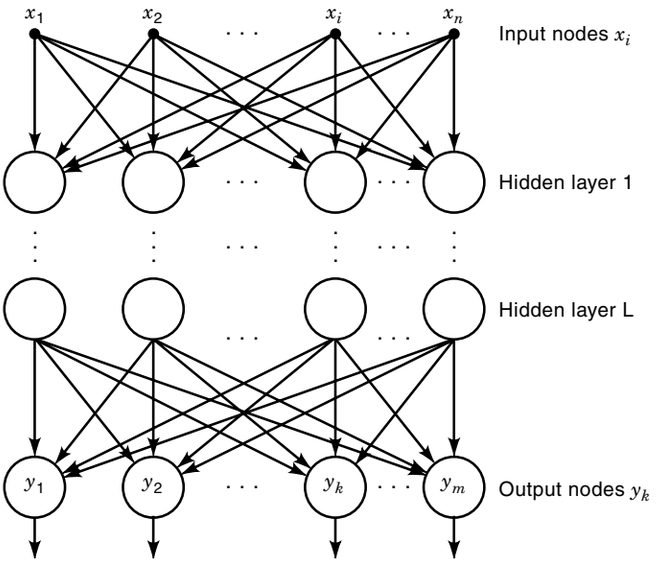

Figure 2. A multilayer feedforward neural network with L hidden layers. We speak of an $(L + 1)$-layer neural network since there are $L + 1$ layers of weights. At each node the weighted sum of the inputs is computed followed by an application of the activation function.

INTRODUCTION TO PERCEPTRONS

Single-Layer Perceptrons

The single-layer perceptron serves as a classifier. It associates input patterns with one of two classes, say class 0 and class 1. The single-layer perceptron merely consists of an input layer and one node in the output layer. An input pattern $\mathbf{x} = (x_1, \ldots, x_n)$ is classified as a class 1 pattern if

$$\sum_{i=1}^{n} w_i x_i \geq \theta$$

where $\mathbf{w} = (w_1, \ldots, w_n)$ denotes the vector of the synaptic weights and where θ denotes the threshold parameter. The

pattern $\mathbf{x}$ is classified as belonging to class 0 if

$$\sum_{i=1}^{n} w_i x_i < \theta$$

Figure 3 provides a schematic representation of a single-layer perceptron. The perceptron's activation function is the Heaviside step function of Eq. (2). As a matter of convenience we used w_0 to denote the bias $-\theta$. In this notation, the perceptron computes the output y as

$$f\left(w_0 + \sum_{i=1}^{n} w_i x_i\right)$$

and the bias can be treated as an additional weight if we extend the input pattern $\mathbf{x}$ as follows: $\mathbf{x} = (x_0, x_1, \ldots, x_n)$, where $x_0 = 1$.

The equation

$$\sum_{i=1}^{n} w_i x_i = \theta$$

determines a hyperplane which is called the perceptron's decision surface. In the case where $n = 2$, the decision surface is a line. Two classes of patterns are called linearly separable if the two classes can be separated by means of a perceptron decision surface. Clearly, patterns belonging to two different classes cannot always be divided by such a decision surface. The XOR-problem provides a simple example of a situation where two classes of patterns are not linearly separable. XOR is a binary operator on $\{0, 1\}^2$ such that for all $(a, b) \in \{0, 1\}^2$:

$$a \text{ XOR } b = \begin{cases} 0 & \text{if } a = b \\ 1 & \text{else} \end{cases} \tag{3}$$

Thus, the XOR-operator divides the pattern space $\{0, 1\}^2$ into two the subsets $C_0 = \{(0, 0), (1, 1)\}$ and $C_1 = \{(0, 1), (1, 0)\}$. The points in the domain of the problem are plotted in Fig. 4. Open dots represent points in C_0. Solid dots represent points in C_1.

Single-Layer Perceptron Learning

In 1962 Rosenblatt presented the perceptron convergence theorem which induces a supervised learning algorithm for solving arbitrary classification problems into two classes (2). The algorithm modifies the weights at time $k + 1$ in the direction of the current error $E(k)$ which is defined as the difference of the target output and the actual output at time k.

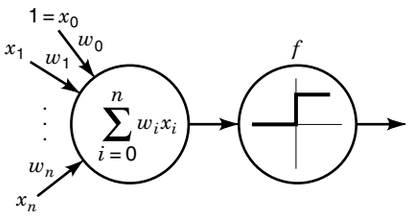

Figure 3. Functionality of a single-layer perceptron. The threshold θ is incorporated into this figure in terms of an additional weight or bias w_0. This figure expresses the fact that a single-layer perceptron computes $f(w_0 + \sum_{i=1}^{n} w_i x_i)$ for inputs $x_1, \ldots, x_n$, where f is the Heaviside step function drawn inside the circle on the right side.

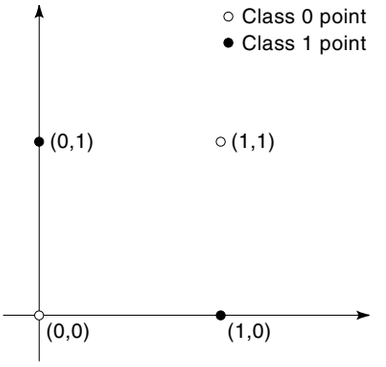

Figure 4. Representation of domain for XOR. The XOR-problem provides a simple example which illustrates the deficiencies of a single-layer perceptron. The problem consists of dividing the four patterns plotted above into two classes. A single-layer perceptron cannot solve this simple classification problem since the decision boundary of a single-layer perceptron is a line in the two-dimensional case.

The algorithm can be described as follows. Suppose we are given a set of training patterns $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^P$. The order in which the patterns are processed does not matter. Initialize the step counter k to be 0 and the counter p indicating the pattern number to be 1. Let $\mathbf{w}(0) = (w_1(0), \ldots, w_n(0))$ denote the initial vector of the weights.

1. Set $\mathbf{x} = \mathbf{x}^p$ and compute the activation $y(k)$ for input pattern $\mathbf{x}$.
2. Compute the current output error $E(k)$ as follows:

$$E(k) = t^p - y(k) \tag{4}$$

   where t^p is the target value for the pattern $\mathbf{x} = \mathbf{x}^p$ and $y(k)$ is the output value at time k.
3. Modify the vector $\mathbf{w}(k) = (w_1(k), \ldots, w_n(k))$ of the connection weights at time k by adding the factor $\eta \cdot E(k) \cdot \mathbf{x}$, that is:

$$\mathbf{w}(k+1) = \mathbf{w}(k) + \eta \cdot E(k) \cdot \mathbf{x} \tag{5}$$

   If the threshold activation function f is replaced by the identity function, this updating scheme is known as the delta rule (60).
4. Increment the step counter k. Update the counter p representing the pattern number by setting:

$$p := p(\text{mod } P) + 1 \tag{6}$$

Figure 5 illustrates an application of the perceptron learning algorithm. Class 1 points have been plotted with diamonds and Class 0 points have been plotted with crosses. The lines plotted in the figure represent decision surfaces after $k = 0$, 20, 40, and 80 training patterns have been presented to the single-layer perceptron.

This algorithm is guaranteed to find a weight adjustment which solves the classification problem in a finite number of

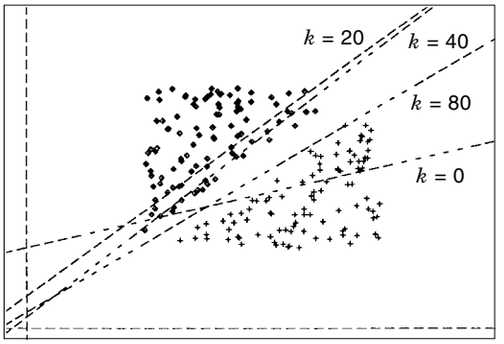

Figure 5. The perceptron's decision surface after step k of the learning algorithm. This figure illustrates an application of the perceptron learning algorithm. Class 1 points have been plotted with diamonds and Class 0 points have been plotted with crosses. The lines plotted in the figure represent decision surfaces after $k = 0$, 20, 40, and 80 training patterns have been presented to the single-layer perceptron.

steps if the given two classes are linearly separable. However, the algorithm does not converge at all when the classes are linearly inseparable and it is difficult to recognize this situation beforehand. Minsky and Papert recognized the heart of the problem: single-layer perceptrons only have one layer of adaptive weights (4). A suitable data representation may transform an originally linearly inseparable problem into a linearly separable one. However, once chosen, the data representation is fixed.

Multilayer Perceptrons

Multilayer perceptrons are feedforward neural networks with at least one hidden layer of nodes. Thus, they have at least two layers of adaptive weights. Figure 6 illustrates the framework and the connection scheme of a two-layer perceptron. The framework of a multilayer perceptron may include a bias parameter in every layer of nodes. As before, this situation can be modeled by extending the input vectors by an additional component of 1.

The activation functions of multilayer perceptrons are either threshold functions or belong to the family of sigmoidal functions whose graphs are characterized by a monotonically increasing s-shaped curve. A generic sigmoid activation function is given as follows:

$$f(x) = \frac{a}{1 + e^{-bx+c}} + d \tag{7}$$

The parameters a, b, c, and d control the height, the slope, and the horizontal and vertical justification of the curve. Figure 7 shows sigmoidal functions for different parameter values.

In the previous section, we noted that single layer perceptrons can separate patterns positioned on different sides of a hyperplane. A two-layer perceptron with threshold units can form a single convex region as a decision boundary. This property is due to the fact that the output unit can be used computing a multivariable logical AND of the hidden units by setting the bias to $-m$, where m is the number of hidden units. Setting the threshold parameter to -1 would generate a multivariable OR function. Thus, three-layer perceptrons with threshold activation functions can approximate arbitrary decision boundaries provided that the number of hidden units is variable. Formally, the approximation can be achieved in terms of a fine grid of hypercubes. Gibson & Cowan as well as Blum & Li have pointed out that two-layer perceptrons with threshold activation functions are incapable of approximating arbitrary decision regions (9,10). Of course, this statement does not preclude the fact that there exist examples of complex, nonconvex decision regions which can be generated by two-layer perceptrons with threshold units (11,12). Feedforward neural networks with two layers of weights and sigmoidal activation functions are able to approximate arbitrary decision regions to arbitrary accuracy. This theorem follows from a result stating that these perceptrons are able to approximate arbitrarily well any continuous mapping from $\mathbb{R}^n$ to $\mathbb{R}$. Feedforward neural networks with differentiable activation functions such as sigmoidal functions can be trained efficiently using the backpropagation algorithm.

TRAINING AND LEARNING IN MULTILAYER PERCEPTRONS

Backpropagation

Training in multilayer perceptrons is performed in a supervised form and aims at minimizing a previously defined error function. Rosenblatt's perceptron learning algorithm deter-

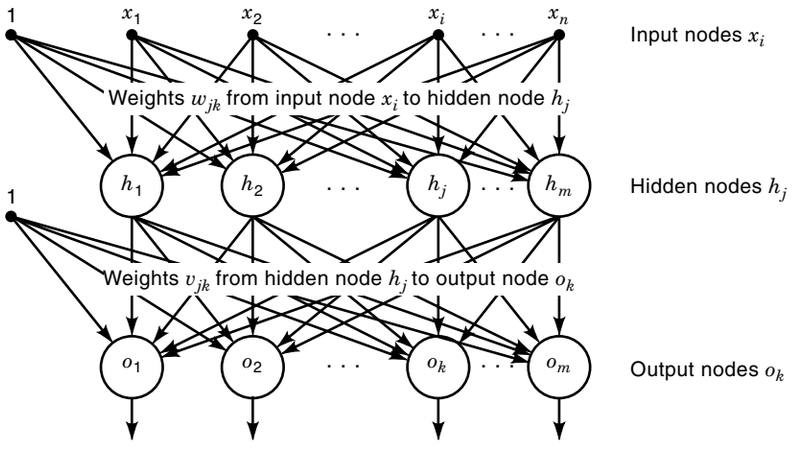

Figure 6. Two-layer perceptron. Note that this pictorial representation includes the biases, which are denoted by $w_{0,j}$ and $v_{0,k}$. Assuming a common activation function f for all hidden nodes and output nodes, the activations h_j and o_k are computed as follows: $h_j = f(\sum_{i=0}^{n} w_{ij}x_i)$ and $o_k f(\sum_{j=0}^{n} v_{jk}h_j)$, where $1 = x_0 = h_0$.

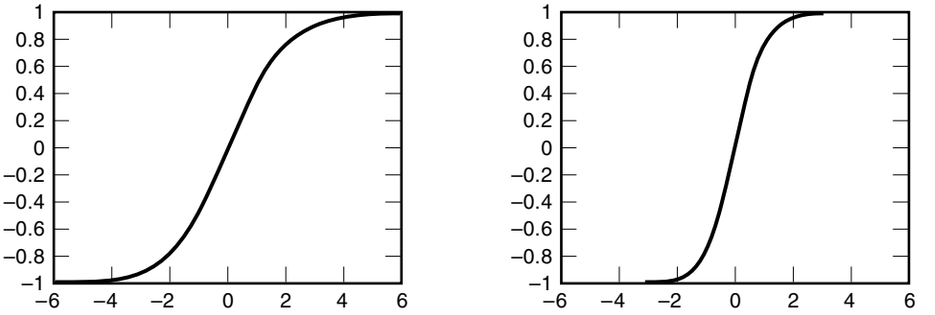

Figure 7. Sigmoidal functions with different parameter values. Sigmoidal functions are commonly used as activation functions in multilayer perceptrons. A bipolar logistic function with $a = 2$, $b = 1$, $c = 0$, and $d = -1$ is shown on the left and the hyperbolic tangent function with $a = 2$, $b = 2$, $c = 0$, and $d = -1$ is shown on the right.

mines a sequence of weight adjustments such that the error will vanish in a finite number of steps. The weights are modified according to their error contribution. Similar learning algorithms do not exist for feedforward neural networks with threshold activation functions and multiple layers of weights.

Fortunately, there are proven methods for the minimization of differentiable functions such as sigmoids which resemble threshold functions. Gradient descent, the simplest and most commonly used of these optimization methods, relies on the partial derivatives of the (error) function in order to determine a local minimum. Strictly speaking, backpropagation only refers to the calculation of the error function derivatives. The importance of backpropagation lies in the fact that the evaluation of the error function derivatives can be performed in $O(W)$ operations, where W is the number of weights and biases in the network, instead of $O(W^2)$ which are required to evaluate the partial derivatives directly. Most training algorithms for multilayer perceptrons consist of a backpropagation phase and a weight modification phase. Many authors refer to the entire training algorithm as backpropagation.

Suppose the training set consists of P patterns $\mathbf{x}^1, \ldots, \mathbf{x}^P$. Each pattern vector $\mathbf{x}^p$, where p ranges from 1 to P, produces an output vector $\mathbf{y}^p = (y_1^p, \ldots, y_m^p)$. The total error E is measured in terms of the errors E^p where E^p is the error generated by an individual pattern $\mathbf{x}^p$. In most cases, the error can be written as

$$E = \sum_{p=1}^{P} E^p \tag{8}$$

One of the most common choices for the error measure E^p is

$$E^p = \frac{1}{2} \sum_{l=1}^{m} \left(t_l^p - y_l^p\right) \tag{9}$$

where $t^p = (t_1^p, \ldots, t_m^p)$ is the target output for the pattern vector $\mathbf{x}^p$. The errors E and E^p can be viewed as functions of all the weights in the network. Due to the representation of E as a sum of the individual errors E^p, the problem of determining the derivatives of E^p with respect to the weights reduces to the problem of determining the derivatives of E^p with respect to the weights. Hecht-Nielsen employs

$$\lim_{P \to \infty} \frac{1}{P} \sum_{p=1}^{P} E^p$$

the expected value of the random variable E^p, as the error function in his description of back-propagation (53). Note that E is nothing but a finite approximation of

$$\lim_{P \to \infty} \sum_{p=1}^{P} E^p$$

The description of the algorithm for evaluating the derivatives of E^p with respect to the weights will reveal that these derivatives can be expressed as a product of the activation of a certain node and another parameter δ corresponding to another node. The algorithm performs the following basic steps:

1. Present the pattern $\mathbf{x}^p$ to the network and compute the activations of the nodes
2. Compute the δ-parameters for the output units [Eq. (15)]
3. Use the δ-parameters of the units in the layer $l + 1$ to compute the δ-parameters of the units in the lth layer [Eq. (17), backpropagation]
4. Evaluate the required derivatives by using the product representation of the derivatives mentioned above [Eq. (14)]

We now describe in detail the general method for evaluating the derivatives of the error function E^p in a multilayer feedforward neural network with differentiable activation functions. Suppose that the pattern $\mathbf{x}^p$ has been presented to the network. From now on its output is simply denoted by $\mathbf{y} = (y_1, \ldots, y_m)$ instead of $\mathbf{y}^p = (y_1^p, \ldots, y_m^p)$. Let z_i^l be the activation of the ith node in the lth layer of nodes. The weight connecting the ith unit of layer l to the jth unit of layer $l + 1$ is denoted by w_{ji}^l.

Each unit of a hidden layer or the output layer first computes a weighted sum of its inputs of the form

$$s_j^{l+1} = \sum_i w_{ji}^l \cdot z_i^l \tag{10}$$

The activation of the jth unit of layer $l + 1$ is obtained by applying a differentiable activation function g to the sum s_j^{l+1}:

$$z_j^{l+1} = g\left(s_j^{l+1}\right) \tag{11}$$

The activation functions may vary in different layers of nodes. However, we chose to ignore this distinction so as to avoid an unnecessary clutter of notation.

Since the weights w_{ji}^l only influence the error E^p via the summed input s_j^{l+1} to the jth node of layer $l + 1$, an applica-

tion of the chain rule gives:

$$\frac{\partial E^p}{\partial w_{ji}^l} = \frac{\partial E^p}{\partial s_j^{l+1}} \cdot \frac{\partial s_j^{l+1}}{\partial w_{ji}^l} \tag{12}$$

By Eq. (10)

$$\frac{\partial s_j^{l+1}}{\partial w_{ji}^l} = z_i^l \tag{13}$$

Denoting $\partial E^p/\partial s_j^{l+1}$ by δ_j^{l+1}, we can write

$$\frac{\partial E^p}{\partial w_{ji}^l} = \delta_j^{l+1} \cdot z_i^l \tag{14}$$

If L represents the number of layers of neurons, then the symbols $\delta_1^L, \ldots, \delta_m^L$ denote the δ-parameters of the output units. These parameters can be immediately computed as follows:

$$\delta_j^L = \frac{\partial E^p}{\partial s_j^L} = \frac{\partial E^p}{\partial y_j} \cdot g'\left(s_j^L\right) \tag{15}$$

Using the chain rule for partial derivatives again, we obtain the following formula for the δ's of the hidden units. These parameters are denoted by the symbol δ_j^l where l ranges from 2 to $L - 1$.

$$\delta_j^l = \frac{\partial E^p}{\partial s_j^l} = \sum_k \frac{\partial E^p}{\partial s_k^{l+1}} \cdot \frac{\partial s_k^{l+1}}{\partial s_j^l} = \sum_k \delta_k^{l+1} \cdot \frac{\partial s_k^{l+1}}{\partial s_j^l} \tag{16}$$

In view of Eq. (10), the partial derivative of s_k^{l+1} with respect to s_j^l is given by $w_{kj}^l \cdot g'(s_j^l)$. Note that pulling the factor $g'(s_j^l)$ out of the summation yields the following backpropagation formula:

$$\delta_j^l = g'\left(s_j^l\right) \cdot \sum_k w_{kj}^l \cdot \delta_k^{l+1} \tag{17}$$

The term on the right hand side is computed in Step 3 of the backpropagation algorithm in order to determine the δ's of layer l once the δ's of layer $l + 1$ are known.

Multilayer Perceptron Training

We now discuss some training algorithms for multilayer perceptrons which utilize error back-propagation. From now on we will simply enumerate the weights in the form $w_1, w_2, \ldots, w_W$, where W is the total number of weights. Thus the weights form a vector $\mathbf{w} = (w_1, w_2, \ldots, w_W$. The gradient ∇E of an error function E with respect to the weights consists of the partial derivatives $\partial E/\partial w_1, \partial E/\partial w_2, \ldots, \partial E/\partial w_W$.

Before training it is necessary to initialize the weights and biases. The vector of these initial weights is denoted by $\mathbf{w}(0) = (w_1(0), w_2(0), \ldots, w_W(0))$. Furthermore, a step size parameter η must be chosen. The training algorithms alternate between a backpropagation phase and a weight modification phase. The latter phase consist of adding a vector $\Delta\mathbf{w}(k)$ to the current weight vector $\mathbf{w}(k)$ at time k, where the modification $\Delta\mathbf{w}(k)$ depends on the step size parameter η. The simplest of these algorithms uses gradient descent for weight adjustment (generalized delta rule) and is described below:

Set $k = 0$ and execute Steps 1 and 2 until a stopping criterion is met.

1. Perform the backpropagation phase for all training patterns $\mathbf{x}^1, \ldots, \mathbf{x}^P$ which produces the gradients $\nabla E^1, \ldots, \nabla E^P$
2. Update the weights as follows:

$$\mathbf{w}(k+1) = \mathbf{w}(k) + \Delta\mathbf{w}(k)$$
$$\text{where } \Delta\mathbf{w}(k) = -\eta \sum_{p=1}^{P} \nabla E^p|_{\mathbf{w}(k)} \tag{18}$$

Increment the counter k.

Note that in the preceding training algorithm the weights are updated every time the whole set of training patterns has been presented to the network. The algorithm is said to operate in *batch, off-line,* or *deterministic* mode. If the training set is large, this technique leads to a slow learning process since it involves a sweep through the whole training set for each weight update. An alternative method is the *real-time, on-line,* or *stochastic* mode where the weights are adjusted after each pattern presentation as follows:

Set $k = 0$, $p = 1$, and execute Steps 1 and 2 until a stopping criterion is met.

1. Perform the backpropagation phase for the training pattern $\mathbf{x}^p$ yielding partial derivatives ∇E^p
2. Update the weights as follows:

$$\mathbf{w}(k+1) = \mathbf{w}(k) + \Delta\mathbf{w}(k)$$
$$\text{where } \Delta\mathbf{w}(k) = -\eta \nabla E^p|_{\mathbf{w}(k)} \tag{19}$$

Increment the counter k. The new value of p is given by $p(\text{mod } P) + 1$.

Since both versions of this algorithm are based on gradient descent, they only implement a search for a local minimum. The chances for attaining the global minimum of the error function can be increased by executing several independent training procedures with randomly initialized weights. Another possibility would be to choose a more complex architecture with a larger number of weights, since the local minima are usually lower in this case.

In many instances, multilayer perceptron learning requires a huge number of sweeps through the whole training set or epochs until the error function reaches an acceptably low value. The principal reason for the phenomenon is that the error surface often has narrow ravines, that is, regions whose curvature is very large in one direction and rather small in the orthogonal direction. In this situation, the choice of the learning parameter η is problematic. A large step size may cause divergent oscillations across the ravine. A small value for η will lead to a slow learning process since the weight vector will first slowly converge to the bottom of the ravine before it crawls along the bottom and finally reaches a local minimum. The technique presented in the next section constantly adapts the step size in order to improve the learning speed of the multilayer perceptron.

Adaptive Step Size Technique

In this technique each weight w_i, where $i = 1, \ldots, W$, has an individual step size parameter η_i which is changed at every iteration. The rate of change depends on the signs of successive gradient components. In real-time mode, we obtain the following equations:

$$\eta_i(k+1) = \begin{cases} \rho \cdot \eta_i(k) & \text{if } \dfrac{\partial E^p}{\partial w_i}\Big|_{\mathbf{w}(k+1)} \text{ and } \dfrac{\partial E^p}{\partial w_i}\Big|_{\mathbf{w}(k)} \text{ have the same sign} \\ \sigma \cdot \eta_i(k) & \text{else} \end{cases}$$
$$\text{where } \rho > 1 \text{ and } \sigma < 1 \tag{20}$$

By this simple strategy, an individual step size η_i will be increased if the current weight update is performed in the same direction as the previous one, that is, further weight updates in this direction are required. The step size parameter η_i is decreased if the current weight adjustment is performed in a different direction than the previous one, that is, the weight w_i was previously changed by a too large amount. The adaptive step size technique is able to deal particularly well with ravines which are more or less parallel to some axis corresponding to an individual weight w_{ji}. If the error surface forms a ravine that is oblique to all axes, Silva and Almeida suggest a combination of this technique with the momentum technique presented next (13,14).

Momentum Technique

In the momentum technique, an additional term $\alpha \cdot w_i(k)$ is added to each weight update term $\Delta w_i(k)$ (15). In batch mode, this procedure results in the following weight update equation:

$$\mathbf{w}(k+1) = \mathbf{w}(k) + \Delta\mathbf{w}(k)$$
$$\text{where } \Delta\mathbf{w}(k) = -\eta \sum_{p=1}^{P} \nabla E^p|_{\mathbf{w}(k)} + \alpha \cdot \mathbf{w}(k) \tag{21}$$
$$\text{and } 0 \le \alpha < 1$$

Clearly, $\Delta\mathbf{w}(k) = -\eta \cdot \nabla E^p|_{\mathbf{w}(k)} + \alpha \cdot \mathbf{w}(k)$ in real-time mode.

The term $\alpha \cdot w_i(k)$ is called the *momentum term*. This term has a cumulative effect if successive weight updates occur in similar direction. On the other hand, the contributions from successive momentum terms will tend to cancel out if the weight vector oscillates from one ravine wall to another ravine wall. The intended effect of the momentum technique is to lead the weight vector faster in the direction of the local minimum. The choice of the momentum parameter α is crucial to achieve this goal. A small parameter α will normally introduce little improvement compared to the regular gradient descent algorithm. A large choice of α may drive the weight vector up the ravine wall (and possibly out of the ravine) at the location of a bend in the ravine, particularly if a large amount of momentum has previously been acquired.

Enhanced Gradient Descent

As we have seen, simple gradient descent with momentum does not guarantee convergence—not even to a local minimum. Several methods exist to alleviate these convergence problems. One of the major problems concerning simple gradient descent with momentum is the fact that its effectiveness depends on an appropriate choice for the step size parameter η and the learning parameter α, both of which have to be chosen by trial and error. Instead of adopting this time-consuming random approach we might prefer to choose the parameters η and α automatically.

One of these automatic approaches is called *bold driver technique* (16,17). The first step is to check how the error function has changed after each step of the gradient descent.

Increase in Error. The weight vector is reset to its previous value, the step size parameter is multiplied by a number $\sigma < 1$ (typical choice: 0.5), and the momentum coefficient α is set to zero. [The local minimum must have been overshot. Therefore, a new attempt to reduce the error is made with a smaller step size and without momentum.]

Decrease in Error. The weight change is accepted and the step size parameter η is multiplied by a number $\rho > 1$ (typical choice: 1.1). [A decrease in error suggests that the algorithm is on its way toward a local minimum.]

Line Search

All the techniques for weight adjustment we have discussed so far proceeded in a certain direction with a certain step size given by the learning parameters. The procedure of line search is based on the following idea: Once the direction of the next step is fixed, the optimal reduction of an error function E can be achieved by minimizing $E(\mathbf{w}(k) + \lambda\mathbf{d}(k))$ with respect to $\lambda \in \mathbb{R}$.

Line Search can be employed when training multilayer perceptrons both in batch mode and in real-time mode. Choose an initial weight vector $\mathbf{w}(0)$ and set $k = 0$. Perform the following steps until a stopping criterion is met:

1. Determine a search direction $\mathbf{d}(k)$.
2. Minimize $E(\mathbf{w}(k) + \lambda\mathbf{d}(k))$ with respect to λ. Let λ_o be the variable where the minimum is adopted.
3. Update the weights by setting $\mathbf{w}(k+1) = \mathbf{w}(k) + \lambda_o\mathbf{d}(k)$ and increment the counter k.

Successive gradient vectors seem to provide the best choice for the sequence of search directions at first glance. However, practical examples show that successive steps in the opposite direction of the gradient will usually take many iterations to arrive at the minimum. The last sections of this article will deal with different training algorithms which are based on line search (18).

Conjugate Gradient (CG) Method

A better choice for the search directions $\mathbf{d}(k)$ is the so-called conjugate gradient direction (19). A version of the general line search algorithm outlined above is called *conjugate gradient algorithm* if $\mathbf{d}(1) = -\nabla E|\mathbf{w}(1)$ and $\mathbf{d}(k)$ is in the conjugate gradient direction for all $k > 1$. The conjugate gradient directions satisfy

$$\mathbf{d}(k+1)H\mathbf{d}(k) = 0 \tag{22}$$

where H denotes the Hessian matrix. An explicit evaluation of the Hessian matrix is unnecessary. The Hestenes–Stiefel formula, the Polak–Ribiere formula, or the Fletcher–Reeves

formula provide ways to compute the new conjugate gradient direction $\mathbf{d}(k+1)$ using only $\mathbf{d}(k)$ and gradient information (20). Backpropagation can be employed again for finding the gradients.

If the error function is a quadratic polynomial, this algorithm is guaranteed to find a minimum of a quadratic error function in W steps. In the case of a general nonquadratic error function the algorithm makes use of an approximation in terms of a quadratic error function in the neighborhood of a given point. These approximations are usually updated after a sequence of W iterations. Due to the difference between the actual error function and the quadratic approximation, the algorithm needs to be run for many iterations until a stopping criterion is reached.

Newton's Method

Newton's method selects $-(H^{-1} \cdot \nabla E)|_{\mathbf{w}}$, where H denotes the Hessian matrix, as a search direction. The vector $-(H^{-1} \cdot \nabla E)|_{\mathbf{w}}$, known as the *Newton direction* or the *Newton step,* points directly towards the minimum of the error surface if the error function is a quadratic polynomial. In the general case, a quadratic approximation of the error function is chosen and the Newton step, involving the evaluation of the Hessian, is applied iteratively. This approach involves several problems:

1. If the Hessian is not positive definite, the Newton step is not guaranteed to move toward a local minimum. It may move toward a local maximum or a saddle point instead. The model trust region approach resolves this problem by adding a suitably large multiple of the identity matrix to the Hessian, yielding a positive definite matrix as a result (18). A closer look reveals that hereby a compromise between Newton's method and the standard gradient descent method is formed.
2. The stability of Newton's method is affected if the step size, computed by a line search, takes the weight vector outside the validity of the quadratic approximation. This problem can be counteracted by forming a new quadratic approximation in the neighborhood of the current point.
3. The Hessian must be evaluated and inverted at each iteration of the algorithm. The evaluation of the Hessian costs $O(PW^2)$ steps and its inversion costs $O(W^3)$ steps in terms of the number of patterns P and the number of weights and biases W. In order to avoid the execution of these computationally expensive operations, one might simply choose to neglect all off-diagonal terms. This approximation of the Hessian reduces the computational cost significantly since the diagonal terms can easily be computed by means of backpropagation and the inversion of a diagonal matrix is trivial. However, this approach has turned out to be unsuccessful for many practical neural network applications where the Hessian is far from diagonal. Quasi-Newton (QN) methods represent a practical approach to circumvent the direct calculation of the Hessian matrix.

Quasi-Newton Methods

Quasi-Newton methods are derived from Newton's method and adopt $-(H^{-1} \cdot \nabla E)|_{\mathbf{w}}$ as a search direction as well. However, instead of directly calculating the Hessian matrix and computing its inverse, Quasi-Newton methods iteratively construct an approximation of H^{-1}, using only first-order information in the process. The current method of choice for this construction is the Broyden–Fletcher–Goldfarb–Shanno method (21).

Comparison of CG and QN Methods

QN methods are computationally more stable than CG methods. In contrast to CG methods, it is not necessary in these algorithms to perform the line searches with great accuracy in order to obtain a reduction of error. This property leads to a faster convergence of QN methods compared to CG methods (55).

On the other hand, the construction of the matrix approximating H^{-1} entails storage requirements of $O(W^2)$. Since CG methods only require $O(W)$ storage, they are preferred for large-scale problems involving a multitude of weights.

Recently a number of researchers have devised several low-storage QN methods which combine the speed advantages of QN methods with the linear storage requirements of CG methods (22,23,17).

GENERALIZATION

In the last section, we gave the impression that training only serves the purpose of effectively minimizing the error function, which measures the performance of the multilayer perceptron on some set of training data. However, the most important role of training is to condition the network such that it generalizes well and models all the data. As mentioned earlier, the ability to generalize represents the most important component of the network's learning ability. *Generalization* refers to the network's performance in the application phase. Since it is either impossible or computationally prohibitive to include all problem data in the training process, the network should aim at predicting the structure of the problem data by detecting some structure in the training data. There are several techniques for measuring and improving the network's generalization performance. Many of these methods are geared at optimizing the size of the network which is an influential factor in the generalization capabilities of the network. Therefore, we consider it appropriate to make a few remarks on this topic beforehand.

Network Size

Supervised training with training data is analogous to fitting a curve through a number of data points reminiscent of polynomial curve fitting. The function corresponding to this curve is of a form which is determined by the architecture of the network. A multilayer perceptron computes a function from $\mathbb{R}^n$ to $\mathbb{R}^m$ which is given by a concatenation of multiplications, additions, and sigmoidal or hardlimiting functions.

The function has a number of free parameters which correspond to the weights of the network. An insufficient number of free parameters leads to a poor fit through the given data points yielding poor recall. By increasing the number of free parameters the curve can better approximate the given data points. For example, a polynomial of degree n or higher can achieve a perfect fit to $n+1$ data points. However, by choos-

ing a function with many free parameters to represent the data one risks *overfitting the data,* that is, the curve will reveal large oscillations from one data point to another. Figure 8 illustrates this principle with a polynomial of degree 10 used for interpolation of 6 data points. A polynomial with smaller degree would model the data points reasonably well without exhibiting oscillations. Good generalization results can be achieved if the curve which is the outcome of training not only lies in the vicinity of the training data points but also in the vicinity of the problem data points. Since the problem data points are unknown, their location has to be predicted based on the location of the training data points. In most cases, a smoother function with a smaller amount of free parameters provides a better basis for predicting the location of new, unknown data points.

The preceding remarks indicate that a neural network with a sufficiently large number of weights can be trained to attain perfect recall of training data. The drawback is that a multitude of weights will lead to bad generalization behavior. Such a network will tend to detect non-existent regularities in the data. In many neural network applications, the training data is subject to some form of noise. Training a network with too many weights will have the undesired effect of modeling the noise instead of the structure of the problem data. The two basic alternatives to resolve this situation are:

- Reducing the size of the network
- Increasing the problem complexity

Network Pruning and Network Growing

Generally speaking, the optimal network topology is the smallest network that trains well. Of course, the simplest approach to finding the optimal network topology is to experiment with networks of different sizes. Although this approach is computationally very expensive it is still used in practice. The computational effort can be reduced by restricting the set of networks under consideration. For example, one might consider only two-layer perceptrons with sigmoidal activation functions in the training experiments since networks of this form have the capability to approximate an arbitrary decision region (51).

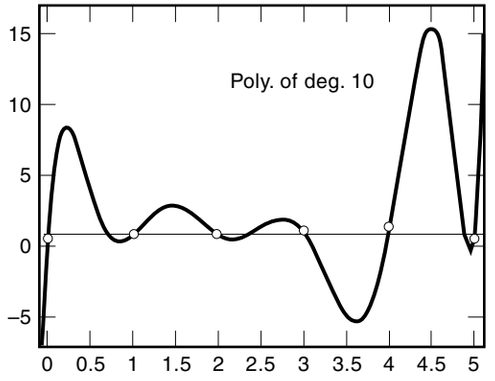

Figure 8. Polynomial approximation of data points. The polynomial of degree 10 whose graph is plotted in the figure intersects the six given data points but reveals large oscillations. The fact that the straight line approximates the data points reasonably well indicates that the location of unknown data points can be better predicted by a line. In the context of the analogy of polynomial curve fitting and perceptron training, a polynomial of small degree corresponds to a perceptron having a small number of weights whereas a polynomial of large degree corresponds to a perceptron having a large number of weights.

Network pruning and *network growing* algorithms are more sophisticated approaches for optimizing the size of a neural network. Pruning techniques start with a relatively large network which is iteratively reduced in size either by removing connections or complete units. The algorithms alternate between a training phase which consists of applying a standard training algorithm to the network and a (connection or node) removal phase. The removal phase involves the computation of the saliency, a measure of the importance of the weights, the nodes respectively. In each iteration some of the low-saliency objects are deleted. Network pruning techniques include optimal brain damage (24), optimal brain surgeon (25), as well as the skeletonizing algorithm of Mozer and Smolensky (26).

Network growing algorithms adopt a bottom-up approach: starting from a small network, nodes are added to the network until a sufficiently small training error is reached. The most famous of these techniques is called cascade correlation (27). The term cascade correlation is derived from the architecture of the network this algorithm constructs. The resulting networks have sigmoidal hidden units and both feedforward and recurrent connections.

Regularization

In the previous section we remarked that neural networks can be viewed as functions and neural network training can be viewed as function interpolation. Among two neural networks producing similar error for the same set of training data the neural network corresponding to the smoother function tends to generalize best. Regularization is a technique which enhances the smoothness of the interpolating function by the addition of a regularization term to the error function E:

$$\tilde{E} = E + \rho C \tag{23}$$

The function C is a penalty term whose influence on the total cost function $\tilde{E}$ is controlled by the parameter $\rho \geq 0$. Note that adding ρC to the original error function E increases the complexity of the function to be minimized. Consequently, the problem of minimizing $\tilde{E}$ is more difficult than the problem of minimizing E. The total error $\tilde{E}$ provides for a compromise between the fit of the training data and the smoothness of the function used for approximating the data. Small ρ's favor fitting the training data while large ρ's favor smoothing out the interpolating function.

Choosing a regularizer of the form

$$C = \frac{1}{2} \sum_{p=1}^{P} \sum_{i=1}^{n} \sum_{k=1}^{m} \left(\frac{\partial y_k}{\partial x_i^2} \right)^2 \Big|_{\mathbf{x}^p} \tag{24}$$

will directly penalize the curvature of the interpolating function, since curvature is measured in terms of second-order derivatives (28,29).

A more simple and more common regularization term, called *weight decay,* is given by half of the sum of all the

weights and biases:

$$C = \frac{1}{2}\sum_{i=1}^{W} w_i^2 \tag{25}$$

Note that this choice of a penalty term forces the weights to become small. Small weights will cause the weighted sums of the inputs at a certain node to be small as well. Thus, the sigmoid is predominantly applied in a neighborhood of the origin where its behavior is almost linear. Only larger weights would lead the sigmoid to a region of larger curvature. Therefore, the function represented by the n-layer perceptron resembles a polynomial of degree n. Since multilayer perceptrons typically have a small number of layers, the resulting function will be rather smooth.

The use of the term weight decay becomes clear when considering simple gradient descent for weight modification in the training algorithm. The weights are changed as follows:

$$\begin{aligned} &\mathbf{w}(k+1) = \mathbf{w}(k) + \Delta\mathbf{w}(k) \\ &\text{where } \Delta\mathbf{w}(k) = -\eta\nabla\tilde{E}|_{\mathbf{w}(k)} = -\eta(\nabla E|_{\mathbf{w}(k)} + \rho\mathbf{w}(k)) \end{aligned} \tag{26}$$

In the absence of ∇E we can write

$$\frac{\partial\mathbf{w}(k)}{\partial k} = -\eta\rho\mathbf{w}(k) \tag{27}$$

since $\Delta\mathbf{w}(k)$ is the discrete form of the derivative of $\mathbf{w}$ with respect to k. Eq. (27) has the unique solution

$$\mathbf{w}(k) = \mathbf{w}(0)\cdot e^{-\eta\rho\mathbf{w}(k)} \tag{28}$$

yielding that all the weights decay exponentially to zero.

Some regularizers, which are similar to weight decay, are capable of acting as weight pruners by pushing the subset of weights which is least important in the reduction of the original error E towards zero while leaving other weights large. This property leads to an algorithm which prunes all the weights at each iteration that fall below a certain threshold. Examples include weight elimination and linear decay (30,31).

Recently, some authors have proposed the choice of a penalty function C which is tailored to achieve robust classifications and good generalization performance (32,33). In this case, robustness refers to lack of sensitivity with respect to small perturbations in the input space, for example, due to noise. The robustness of the network mapping will also lead to smoothness of the interpolating function—the property which is responsible for generalization capabilities. The sensitivity of the multilayer perceptron is given by the derivatives of the output $\mathbf{y}$ with respect to the input $\mathbf{x}$. If $\tilde{\mathbf{y}}$ denotes the output corresponding to a specific input $\tilde{\mathbf{x}}$, we obtain the sensitivity component $\partial y_i/\partial x_k$ at location $\tilde{\mathbf{x}}$ as follows:

$$\frac{\partial y_i}{\partial x_k}|_{\tilde{\mathbf{x}}} = \sum_{j_1,\ldots,j_{L-1}} w^L_{ij_{L-1}} w^{L-1}_{j_{L-1}j_{L-2}} \cdots w^1_{j_1 k} f'(\tilde{y}_i) f'\left(\tilde{s}^{L-1}_{j_{L-1}}\right)\cdots f'\left(\tilde{s}^1_{j_1}\right) \tag{29}$$

where $\tilde{s}^l_j$ denotes the weighted sum computed at the jth node of lth hidden layer. Adding the sums of squares of all sensitivity components at all training patterns $\mathbf{x}^1, \ldots, \mathbf{x}^p$ to the original error function would encourage robust classification, but is computationally very expensive. Note that small sensitivity components can be obtained by producing either small weights like in weight decay or small derivatives of the hidden layer activations. Figure 9 indicates that both goals cannot be accomplished at the same time. (Also note that a combination of medium-sized weights and derivatives will lead to a relatively large product.)

Jeong and Lee choose to force the hidden layer activations into their saturation range by imposing a penalty in the form of the sums of all hidden layer activations. The learning process reveals some features of Hebbian learning when using a standard gradient descent method with error backpropagation. Initializing the weights with very small values provides a successful learning process in simulation experiments.

Drucker and Le Cun take a direct path to converting the original error function E into a robust error function. The new error function $\tilde{E}$ consists of the sum of E and a regularizer given by a multiple of the following term at a particular location $\tilde{\mathbf{x}}$:

$$C = \frac{1}{2}\left(\frac{\partial E}{\partial x_1}\right)^2 + \frac{1}{2}\left(\frac{\partial E}{\partial x_2}\right)^2 + \cdots + \frac{1}{2}\left(\frac{\partial E}{\partial x_n}\right)^2 \tag{30}$$

Drucker and Le Cun's experiments yield an improved generalization performance over standard gradient descent with backpropagation, but also an increased computational effort due to the fact that calculating the appropriate derivatives requires two backpropagation phases.

Validation and Testing

Validation methods have been designed in order to select a network model with an optimal generalization performance. The choice of the neural network model may for example be between networks differing in the number of hidden units or between neural networks having different regularization parameters ρ. Validation methods require a set of training data and an independent set of data called validation data. The

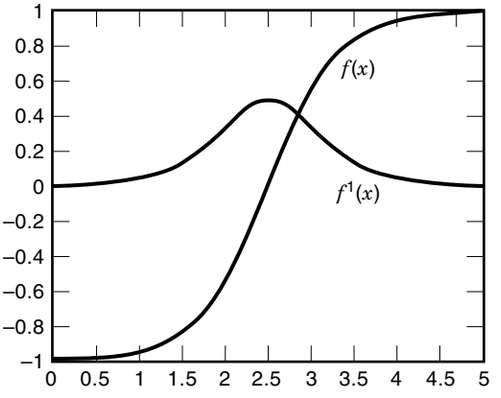

Figure 9. Bipolar logistic function and its derivative. The generalization performance of a multilayer perceptron can be enhanced by reducing (in absolute value) the sum of products of all weights and derivatives of node activations. The figure shows that small weights and small derivatives cannot be achieved at the same time, since the derivative assumes larger values in the region around the origin.

following steps are executed for all neural network models under consideration:

1. Train the neural net with the set of training data. The set of weights which minimizes the error function is fixed.
2. Check the generalization performance of the current model by evaluating the error function using the validation data as inputs.

The neural network model having the smallest error with respect to the validation data is selected.

Often the results of these approaches are confirmed by presenting yet another set of data called *test data* to the network. Use of this technique is meant to safeguard against overfitting to the validation data.

Stopped training is a validation method in which the quality of the current network is tested at each iteration by means of validation data. The goal is to select the network which performs best on the validation data. After the goal is met with some certainty, the training is halted. This strategy which is illustrated in Fig. 10 avoids an overly tight fit to the training data. Stopped training can be successfully applied to networks whose number of weights far exceeds the number of training patterns (58).

In practice, an independent set which can be designated to be a validation set is often not available. The method of *cross-validation* partitions a single data set into distinct subsets which serve as training data or validation data in different iterations of the general validation method already described. If the original data set is denoted by S, we have

$$S = S_1 \cup \cdots \cup S_n \quad \text{and } S_i \cap S_j = \varnothing \; \forall i = j \tag{31}$$

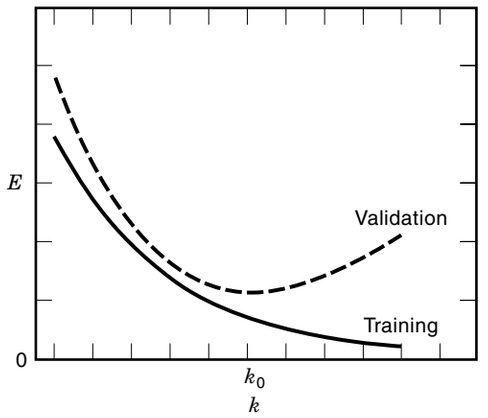

Figure 10. Early stopping of the training process. The original data are divided into training data and validation data, which are both used to periodically evaluate the error function. The figure shows the error E at iteration k with respect to the training data and the validation data in a typical training session. While the error with respect to the training data generally decreases with each iteration, the error with respect to the validation data decreases at first, but increases later. At this point training is stopped and the network which has the minimal error with respect to the validation data (the one found at iteration k_0) is selected.

The validation method is executed n times. In iteration i, the set difference $S - S_i$ acts as the training data set and the set S_i acts as the validation set. If $|S_i| = 1$ for all $i = 1, \ldots, n$, we speak of the *leave-one-out* method.

Bootstrapping and Jackknifing

Bootstrapping uses resamples of the original training set in order to estimate the generalization performance (51). Resamples are subsamples of size n which are taken with replacement from the training set $x_1, \ldots, x_n$. In its simplest form, the bootstrap algorithm determines a set of weights for each bootstrap sample and then estimates the standard error of the outputs depending on the calculated sets of weights by using a Monte Carlo method (59). The technique of jackknifing is based on equally sized subsamples without replacement from the training set (56). These subsamples are used to estimate the bias, the variance, and the distribution of a statistic. In this computationally intensive fashion, a jackknife estimate of the generalization error can be obtained (57).

Vapnik–Chervonenkis-Dimension

In this section, we restrict our attention to multilayer perceptrons with hard-limiting activation functions and binary inputs and outputs. Vapnik and Chervonenkis developed the concept of Vapnik–Chervonenkis-dimension (VC-dimension) which provides an estimate of the generalization performance of a neural network in the worst-case scenario (34). They express the network's generalization performance, denoted by g, in terms of the probability that an arbitrary pattern of the same distribution as the training patterns is classified correctly.

Vapnik and Chervonenkis provided an upper bound for the probability that the network's generalization performance differs by more than ϵ from the fraction of patterns in the training set which are classified correctly. Note that for a perfect fit of the training patterns, we obtain an upper bound for the probability that $g < 1 - \epsilon$, or equivalently a lower bound for the probability that $g \geq 1 - \epsilon$.

The upper bound mentioned can be expressed in terms of the network's VC-dimension, which is denoted by $\dim_{\mathrm{VC}}$. The quantity $\dim_{\mathrm{VC}}$ is the largest number of patterns P such that the neural network can solve every binary classification problem of P patterns.

Let U be the total number of units in a multilayer perceptron with threshold activation functions and let W be the total number of weights and biases. Baum and Haussler (35) showed that

$$\dim_{\mathrm{VC}} \leq 2W \log_2(eU) \tag{32}$$

From this estimate they derived the following statement for $0 < \epsilon \leq \frac{1}{8}$. Let g_T denote the fraction of training patterns which is classified correctly. If the network has been trained with at least $W/2 \log_2 (U/\epsilon)$ patterns such that $g_T \geq 1 - (\epsilon/2)$ then the network will correctly classify a fraction $1 - \epsilon$ of future patterns with high probability.

They also proposed the estimate $P_{\min} \simeq W/\epsilon$ for the minimal number of training patterns required to correctly classify at least a fraction of $1 - \epsilon$ patterns by means of a two-layer perceptron with threshold units. Thus, the number of training

patterns needed in the case $\epsilon = \frac{1}{10}$ amounts to $10W$. In practice we hope to encounter more favorable ratios than in this worst-case estimate, particularly after applying the techniques for improving the generalization performance we discussed in this chapter.

HARDWARE IMPLEMENTATIONS IN VLSI

The massively parallel structure of neural networks, in particular multilayer perceptrons, cannot be exploited by means of software running on serial machines. Therefore, software implementations on conventional computers lack the speed requirements for many real-time applications such as high energy physics. General purpose parallel machines certainly provide the necessary speed and parallelism, but have a high price tag. More cost-effective alternatives are analog and digital VLSI implementations. We briefly review these methods with a special emphasis on multilayer perceptron implementations. We have to mention that the range of neural network hardware is changing very rapidly over time. Thus, the information provided in this chapter will soon be outdated. More up-to-date information on VLSI hardware including manufacturers can be found in (50).

Analog VLSI Implementations

In the opinion of Carver Mead, who is virtually the inventor of digital VLSI technology, simulating a neural network on a digital computer strips away from the real-time nature of biological neural systems. Therefore, Carver Mead is using analog VLSI technology to build visual and auditory systems that work in real time (54).

In analog implementations, signals are modeled by physical variables such as a voltage, a current charge, a frequency, or a time duration. This analog representation of neural network (NN) parameters has various advantages and drawbacks:

On the one hand, analog NN hardware obtains high processing speeds and high densities of components by exploiting the physical properties of analog signals to perform neural network operations. On the other hand, this representation is characterized by very poor absolute precision, since it is very susceptible to outside influences such as variations in temperature, power supply, components, and so on. Thus, analog chip design is a very difficult task, which is further complicated by problems of weight storage and the need for a multiplier which behaves linearly over a wide range. Synthesis tools such as computer-aided design (CAD) do not exist for analog hardware design.

Due to these problems, working analog neural network implementations are still limited. They mostly serve in elementary applications, for example, as the front ends of perception systems.

Digital Integrated Circuit Implementations

Digital VLSI is a proven and mature technology which has been used for many years in conventional computers. In contrast to analog NN chips, digital neurocomputers are sold by a large number of manufacturers for a reasonable price. Moreover, digital neural network implementations tend to be able to solve a larger variety of tasks than analog implementations. An algorithm can easily be mapped onto a digital system in a top-down approach. Multilayer feedforward neural network is the prevalent neural network design implementation. A number of CAD systems are available to support the designer's work.

In digital VLSI technology, the weights can be simply stored in random-access memory (RAM). The accuracy of digital VLSI hardware is given by the number of bits of the operands and accumulators. However, digital VLSI hardware is subject to serious constraints in chip area. A large number of neurons, high numerical precision, and high speed elements are very area consuming. Thus a compromise has to be found between accuracy, processing speed, and the number of neurons on the chip. Typically, digital VLSI chips have a higher precision, but lower speed and density than analog chips.

A digital neural network implementation can either consist of a single VLSI chip or multiple chips can be composed to form a neural network architecture. Multiple chip architectures include slice architectures and radial basis function networks. SIMD and systolic arrays are built using multiprocessor chips. Arrays of SIMD chips are particularly suited for the implementation of multilayer feedforward neural networks since all processors on one particular chip execute the same instruction in parallel but on different data. Common control and data buses can combine multiple chips. For example, the adaptive solutions CNAPS system forms a SIMD array using Inova N6400 chips. Systolic arrays are based on the concept of pipe-lining: After performing a single calculation a processor passes the result on to the next processor. Siemens MA-16 chips can be employed to build systolic arrays.

Hybrid VLSI Implementations

Hybrid implementations try to form a compromise between digital and analog VLSI technologies by taking the best of both worlds. Usually some or all of the internal processing is performed in analog fashion while the communication with the outside environment is digital to facilitate the incorporation into digital systems. For example, the AT&T ANNA artificial neural network ALU (arithmetic/logic unit) operates internally with capacitor charge to store the weights, but has digital inputs and outputs. The Neuroclassifier chip of the University of Twente is a two-layer, fully interconnected network with 70 analog inputs, six hidden-layer neurons and one to six analog outputs, whose five-bit digital weights are stored on on-chip static random-access memory (SRAM). It has been successfully applied to the classification of high energy physics particles and to real-time image processing.

Training Modes for Neural Network Hardware

We distinguish between different training modes in hardware depending on the location where all or parts of the training phase is realized. As we will point out this issue is closely related to the precision of the weight representation which is required to establish successful learning. A categorization of training modes for multilayer perceptrons using error backpropagation can be given as follows:

Off-Chip Learning. The whole training process takes place on a separate computer with high precision. The results are quantized and loaded onto the chip. Only recall is performed on-chip. Practical experiments have revealed that low on-chip

accuracy suffices to achieve successful learning. For example, the ANNA chip which does not have any on-chip learning capabilities has been successfully used for high-speed character recognition although it only uses a six-bit weight resolution and a three-bit resolution for inputs and outputs (36).

Chip-On-The-Loop Learning. In this approach, the forward propagation part of the training process is realized on-chip while the error backpropagation and the weight updates are performed off-chip on a high-precision computer. The resulting floating point representations of the weights are discretized using a staircase-shaped multiple-threshold function and then the forward propagation pass of the training phase is repeated.

On-Chip Learning. In the event that the complete training process is executed on-chip, we speak of on-chip learning. Consequently, only limited accuracy is available for weight training. Several simulations indicate that weight training with standard backpropagation only leads to successful learning if the weights have a precision of at least 16 bits (37,38). This requirement is due to the fact that the weight quantization step often exceeds the weight updates which prevents the weights from changing. A number of weight discretization algorithms and hardware friendly training algorithms such as weight propagation are capable of alleviating this problem (39,40,41,42).

Performance Evaluation of VLSI Implementations

Ideally, a neural network hardware implementation should incorporate the basic principles in the design of powerful biological neural nets while being adapted to perform biologically inspired as well as other applications. The most important of these principles are:

- *A large number of neurons:* The human brain has about 10^{12} neurons.
- *A large number of interconnections:* There are about 1000 synapses per neuron in the brain.
- *Learning capability:* This requires changeable weights.
- *High processing speed*

The speed of implementations of multilayer perceptrons is typically rated in connections per second (CPS) and connection updates per second (CUPS). The CPS value measures the rate of multiplications and accumulate operations in the recall phase. The CUPS value provides the rate of weight updates in the training phase. This value usually refers to weight training of multilayer perceptrons using error backpropagation, but it can be given for other algorithms and other neural networks as well.

We now provide a comparison of several VLSI chips used for multilayer neural network implementations with respect to the total number of neurons and synapses, learning capability, and accuracy (43).

The precision of node activations and weights is measured in bits. In Table 1 [adapted from (43)], backpropagation is abbreviated as BP and processing element is abbreviated as PE.

STOCHASTIC PERCEPTRONS

Stochastic Perceptrons and Probabilistic Concepts

The belief that biological neurons are probabilistic devices has motivated an extension of the perceptron concept. The stochastic perceptron is a classifier like the conventional perceptron. The functionality of the stochastic perceptron is similar to the functionality of the perceptron as illustrated in Fig. 3, although the activation function f is not necessarily a threshold function but an arbitrary function into the interval [0, 1]. Furthermore, the stochastic perceptron does not produce a deterministic decision which associates a pattern $\mathbf{x}$ with class 0 or with class 1. Instead, it assigns class membership with probability given by the weighted sum of its inputs. If y denotes an output value, the probability that the stochastic perceptron assigns an input pattern $\mathbf{x}$ to class 1 is given by

$$P(y = 1|\mathbf{x}) = f\left(\sum_{i=1}^{n} w_i x_i\right) \tag{33}$$

Note that a threshold parameter θ does not need to occur in this formulation since it can be incorporated in the definition of the function f. In the following discussion we restrict ourselves to monotonically increasing activation functions f. Thus, our discussion includes the sigmoidal activation functions used in multilayer perceptrons. The input patterns only adopt values in the Boolean domain $\mathcal{I}^n = \{+1, -1\}^n$. The input space has an unknown underlying distribution denoted by D. The notation $p_D(\mathbf{x})$ is used for the probability of observing vector value $\mathbf{x}$ under the distribution D.

The class of stochastic perceptrons can be embedded into the class of probabilistic concepts (p-concepts) (44). A p-concept consists of a function $c : \mathcal{I}^n \to [0, 1]$ and probabilistic device which generates an output of $y = 1$ with probability $c(\mathbf{x})$ for input $\mathbf{x}$.

PAC Learning Criterion

For each classification of an input space with underlying distribution D there exists a p-concept called target p-concept

Table 1. [adapted from (52)]

Type	Name	Learning	Precision	Neurons	Speed
Analog	Intel ETANN	—	6 b × 6 b	64	2 GCPS
Digital	Philips L-Neuro 2.3	—	16 b − 32 b	12 PE	720 MCPS
	MCE MT19003	—	13 b	8	32 MCPS
	Hitachi WSI	BP	9 b × 8 b	576	250 MCPS, 64 MCUPS
Hybrid	AT&T ANNA	—	3 b × 6 b	16 − 256	2.1 GCPS
	Neuroclassifier	—	6 b × 5 b	6	21 GCPS
	Ricoh RN-200	BP	na	16	3.0 GCPS

which provides an exact model. A learning algorithm for stochastic perceptrons must be geared at finding a good approximation of the target p-concept in terms of a stochastic perceptron. Note that the adaptive parameters of a stochastic perceptron not only include the weights w_i but also the activation function f. Thus, given a set of training patterns a learning algorithm determines a set of w_i and an activation function f yielding a stochastic perceptron approximating the target p-concept. Following general statistical nomenclature, this stochastic perceptron is called the hypothesis and is denoted by h.

The success of a learning algorithm can be expressed in terms of a version of the Probably Approximately Correct (PAC) learning criterion (45). This formulation depends on a error measure E which is defined as follows:

$$E(h, c) = \sum_{\mathbf{x}} p_D(\mathbf{x}) |h(\mathbf{x}) - c(\mathbf{x})| \tag{34}$$

where h denotes the hypothesis and c denotes the target p-concept. The error measure E is called *variation distance.*

Marchand and Hadjifaradji presented a learning algorithm which PAC learns the class of stochastic perceptrons under a certain class of distributions. The expression "PAC learns" means the following: If the target p-concept is a stochastic perceptron and the underlying distribution is k-blocking, the algorithm then the algorithm will find for any $0 < \epsilon, \delta < 1$ a hypothesis h such that $E(h, c) < \epsilon$ with confidence $1 - \delta$.

k-Blocking Distributions

The PAC learning algorithm is based on the fact that a weight w_i of the target stochastic perceptron can be detected by changing the variable x_i while assigning a fixed value to a certain set of other variables. This set is called the blocking set and is denoted by B. Formally, we have:

$$p_D(\mathbf{x}_U | \mathbf{x}_B = \mathbf{b}, x_i = +1) = p_D(\mathbf{x}_U | \mathbf{x}_B = \mathbf{b}, x_i = -1) \quad \forall \mathbf{b}, \forall \mathbf{x}_U \tag{35}$$

Here U denotes the complement of $B \cup \{x_i\}$ in $\{x_1, \ldots, x_n\}$. The symbols $\mathbf{x}_U$ and $\mathbf{x}_B$ stand for the restriction of $\mathbf{x}$ on U and B, respectively. The symbol $\mathbf{b}$ denotes an assignment for B. We say that B is a minimal blocking set if there is no subset of B which is a blocking set.

If all the variables are statistically independent from each other the empty set forms a blocking set for every variable x_i. In this case, the influence of w_i on the probability that $y = 1$ can be estimated by fixing x_i at value $+1$ or at value -1 (46). The algorithm of Marchand and Hadjifaradji satisfies the PAC learning criterion for the more general case of k-blocking distributions which are defined as follows.

A distribution D is called k-blocking if $|B_i| \leq k \ \forall \ i = 1, 2, \ldots, n$ whenever B_i is a minimal blocking set for variable x_i. A standard calculation shows that all Markov distributions of kth order belong to the class of $2k$-blocking distributions. Thus, the k-blocking family comprises many distributions found in practice, for example, the distribution of standard row scans of thresholded images (48).

Learning Stochastic Perceptrons

As noted before, the weight w_i of a hypothesis stochastic perceptron can be derived by fixing a blocking set of a variable x_i at a certain value. This idea gives rise the definition of the *blocked influence* of x_i:

$$\begin{aligned} \text{Binf}(x_i|\mathbf{b}_i) = {} & P(y = 1 | \mathbf{x}_{B_i} = b_i, x_i = 1) \\ & - P(y = 1 | \mathbf{x}_{B_i} = b_i, x_i = -1) \end{aligned} \tag{36}$$

where B_i is a blocking set for variable x_i and $\mathbf{b}_i$ is an assignment for $\mathbf{x}_{B_i}$. Note that $\text{Binf}(x_i|\mathbf{b}_i)$ not only depends on x_i but also on the choice of the blocking set B_i and the vector $\mathbf{b}_i$. The main importance of $\text{Binf}(x_i|\mathbf{b}_i)$ lies in the fact that, regardless of the choice of B_i and $\mathbf{b}_i$, we have the following relations whenever the target p-concept is a stochastic perceptron.

$$\text{Binf}(x_i|\mathbf{b}_i) \begin{cases} \geq 0 & if\ w_i = +1 \\ = 0 & if\ w_i = 0 \\ \leq 0 & if\ w_i = -1 \end{cases} \tag{37}$$

This relationship gives rise to a simple rule for finding the weights w_i of the target stochastic perceptron provided a blocked influence $\text{Binf}(x_i|\mathbf{b}_i)$ can be determined.

The search for a blocking set may potentially be too expensive, even under the assumption that the distribution D is k-blocking. In most real-world applications, we can restrict ourselves to searching for a blocking of size k in a neighborhood of x_i.

Once B_i is found and set to an arbitrary value $\mathbf{b}_i$, an empirical estimate of $\text{Binf}(x_i|\mathbf{b}_i)$, denoted by $\widehat{\text{Binf}}(x_i|\mathbf{b}_i)$, can be calculated based on the training set. Hoeffding's inequality yields a number of training patterns which suffices to guarantee a good estimate (47). If $\text{Binf}(x_i|\mathbf{b}_i)$ is very small, this number is prohibitively large. A lemma shows that the variables x_i whose blocked influence $\text{Binf}(x_i|\mathbf{b}_i)$ is very small for all $\mathbf{b}_i$ can be ignored. The corresponding weights w_i can be set to zero without losing much accuracy in the approximation of the target stochastic perceptron c. For all other x_i, the weight w_i is set to $+1$ if

$$\max_{\mathbf{b}_i} \{\text{Binf}(x_i|\mathbf{b}_i)\}$$

is positive and the weight w_i is set to -1 if

$$\max_{\mathbf{b}_i} \{\text{Binf}(x_i|\mathbf{b}_i)\}$$

is negative. If s denotes the weighted sum of the components of a vector $\mathbf{x}$ we know with large confidence that the following equation holds for the target c:

$$c(\mathbf{x}) = P\left(y = 1 | \sum_{i=1}^{n} w_i x_i = s\right) \tag{38}$$

The number of training patterns needs to be large enough for yet another application of Hoeffding's inequality which ensures with large confidence that, disregarding insignificant

vector values $\mathbf{x}$, a good approximation of $c(\mathbf{x})$ is obtained by

$$h(\mathbf{x}) = \hat{P}\left(y = 1 | \sum_{i=1}^{n} w_i x_i = s\right) \tag{39}$$

CONCLUSION

This article offers an introduction to the concept of perceptrons, and indicates that the perceptron continues to be a hot research topic in many respects. The performance of the perceptron has been immensely improved since the days of Frank Rosenblatt through advances in the underlying mathematics, in hardware, and in software. Different types of perceptron concepts are being introduced. Perceptrons are finding applications in various areas. The most widely known and successful applications of perceptrons are in pattern recognition, control, and prediction. Examples include recognition of handwritten digits, speech recognition, face recognition, automatic steering of vehicles, and time series prediction (49). Other important topics we failed to discuss include data representation, comparison of error functions, perceptron software, and optical implementations.

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