# Part I

# Basic Concepts

# 1 Defining the Area

**learning objectives**

- what a neural network is
- approaches to problem solving
- nomenclature

## 1.1 Learning from Information

The availability of information is increasingly important in our society. In fact, it has been suggested that we are becoming an information society. Information will become one of the most valuable assets in many of our activities, from business administration to science. However, it can already be observed that we are in danger of being swamped in a profusion of individual data, finding it more and more difficult to obtain the right information for a specific problem.

It is therefore of vital interest to analyze data, to extract knowledge from individual data, and to generalize from single observations to the underlying principles and the structure of the information. We must **learn** from individual observations.

Data analysis is nothing new; it has been performed for many years, mostly by statistical and pattern recognition methods. However, it has been clear for a long time that the human brain analyzes data and information quite differently from such methods, that it processes the flood of data and learns from them along quite different lines. Knowledge acquisition by the human brain is not performed by statistical methods!

Recognition of the inherent limitations of statistical and pattern recognition methods has led to the development of expert systems. In an expert system the knowledge specific to a certain domain of problems is kept apart from the inference mechanisms that draw conclusions from the knowledge (and thus make decisions). However, the mechanisms for acquiring knowledge for expert systems are still far from perfect. The method of a knowledge engineer interviewing experts to build a knowledge base has many drawbacks, including scientific, technical and psychological aspects. In any case, it is not the way the brain acquires knowledge.

Advances in neurophysiology and new experimental techniques such as electroencephalography (EEG), computer-assisted tomography (CAT), magnetic resonance imaging (MRI), positron emission tomography (PET), the superconducting quantum interference device (SQID), and single-photon emission computerized tomography (SPECT) have greatly enhanced our understanding of the anatomy of the human brain and the physical and chemical processes occurring within it. Furthermore, mathematical models and algorithms have been designed to mimic the information processing and knowledge acquisition methods of the human brain. These models are called *neural networks*.

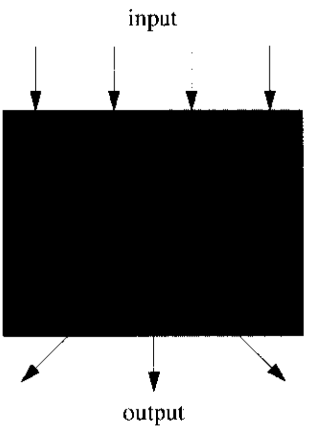


Figure 1-1: The black box.

The purpose of this textbook is twofold:

- First, to develop the **basic principles** and the scope and limitations of the more important neural network models.
- Second, and even more importantly, to understand how **to use** these neural networks for processing information, and thus learn relationships by means of which we can acquire knowledge.

## 1.2 General Objectives and Concepts

We will first consider a neural network as a black box that can accept a series of input data and produce from these one or more outputs (Figure 1-1).

The input values can be from the stock market and the output, a recommendation to buy or sell particular stocks. Or we can input medical data for a patient and obtain predictions of the kind of disease he/she has; or from a spectrum of a compound we can predict its structure; or input the movements of an object and output the reaction of the robot's arm in an automated laboratory.

For many users of neural networks it will not be necessary to know exactly what happens inside this black box; nevertheless they will be able to apply neural networks to their problems successfully. The purpose of this book is, however, to develop a gradual understanding of the operations inside this black box.

In the following chapter we will learn that there are basic operating units inside the box that are somehow connected (Figure 1-2). The inputs are passed along these connections, the lines of a *network*, and are distributed, transformed, and eventually reunited to produce outputs. The transformation of the data is performed in many basic processing *units*, called *artificial neurons* or simply *neurons*, which perform identical tasks.

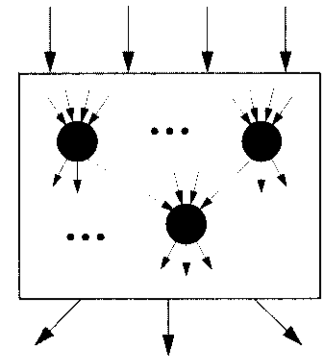
Figure 1-2: Basic units within the box.

Thus, as the name implies, neural networks consist of neurons connected into networks. We will first present the basic concept of a neuron and then look at the ways of connecting them.

## 1.3 What Neural Networks are Good for

The neural network, if considered as a black box, will transform an $m$-variable input into an $n$-variable output. The input or output variables can be:

- real numbers, preferably in the range from 0 to 1, or $-1$ to $+1$; if they are outside this range, the input data have to be preprocessed to bring them into it (some methods, however, can handle larger or smaller real values as well);
- binary numbers, i.e. 0 and 1; or
- bipolar numbers, i.e. $-1$ and $+1$.

The number of input and output variables is limited only by the available hardware and computation time. The number of output variables is usually smaller than that on the input side, but this is by no means mandatory.

The problems handled by neural networks can be quite varied. On the most general level they can be divided into four basic types:

- association (auto or hetero),
- classification,
- transformation (different representation),
- modeling.

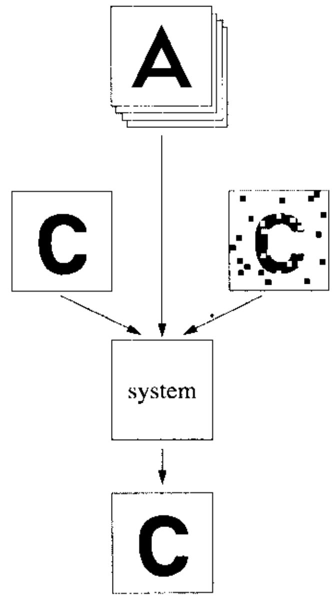

Figure 1-3: Auto-association. The original is reconstructed from an incomplete or corrupted input.

*Auto-association* means that the system is able to reconstruct the correct pattern if the pattern it learned is incomplete or corrupted. Figure 1-3 illustrates this, with the input consisting of the stack of 26 letters in the top of the figure. If the system is able to do an auto-association, then it is able to produce on output a perfect match of any of the learned capitals, even if the input letter was incomplete or corrupted.

On the other hand, *hetero-association* means that the system makes a one-to-one association between members of two sets of patterns. Figure 1-4 shows hetero-association of 26 capital letters with a set of 26 boxes, the filled one of which identifies the output letter. Thus, on input of a perfect or corrupted letter C, the system trained with 26 capital letters and able to do hetero-association will respond with a 26-box pattern having the third box occupied (letter C was defined as the third letter in the alphabet).

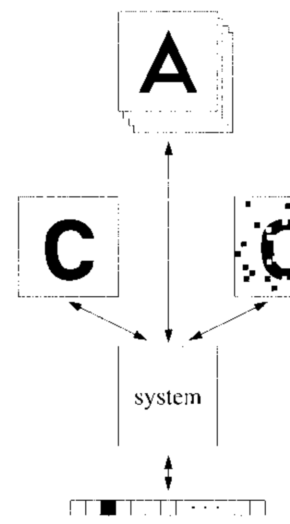


Figure 1-4: Hetero-association. The associated pattern is reconstructed from an ideal or corrupted input.

*Classification* is a more or less familiar concept. Its goal is to assign all given objects to appropriate classes (*clusters*) of objects, based on one or more properties that characterize a given class (Figure 1-5). Neural networks are mainly employed in one- or two-level clustering. The advantage of the neural network approach is that only a small proportion of multivariate objects is used for training, and afterwards the network is able to predict the class (cluster) to which an unknown object belongs. Some of these applications are very close to hetero-association applications.

The process of classification can be carried out in a *supervised* or in an *unsupervised manner*. During supervised learning the system is forced to assign each object to a specified class, while during unsupervised learning the clusters are formed naturally without any a priori given information.

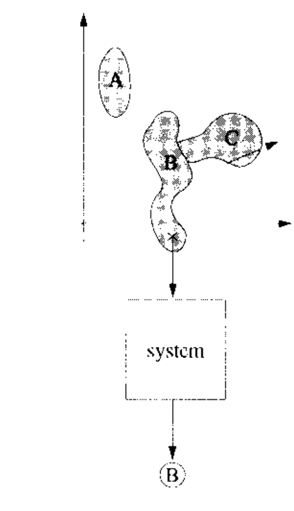


Figure 1-5: Classification of multivariate data.

*Transformation* or *mapping* of a multivariate space into another space of the same or lower dimensionality is a frequent application of neural networks. Many researchers consider that the essential process of thinking, learning and reasoning is the mapping of multivariate impulses coming from our sensory organs into a 2-dimensional plane of neurons in the brain. The mapping can be made from lower to higher dimensionality as well. However, this is less frequent; two-dimensional mapping is adequate for an easy, clear representation of multidimensional objects in many applications (Figure 1-6).

*Modeling*, one of the most frequently used mathematical applications in science, is the search for an analytical function or a procedure (model) that will give a specified $n$-variable output for any $m$-variable input. It is useful in many areas, from process control to expert system design. Standard modeling techniques require the mathematical function to be known in advance. During a "fitting" procedure (Figure 1-7), the parameters of this function are determined on the basis of the best agreement between the experimental (input) and calculated (output) data. The predictions are best if the experimental data covers the variable space evenly and with adequate density over the entire region. The advantage of the neural network model is that it does not require a knowledge of the mathematical function: the nonlinearity of a single unit transformation and a sufficiently large number of variable parameters (weights) ensure enough "freedom" to adapt the neural network to any relation between input and output data.

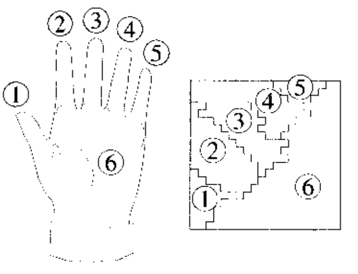


Figure 1-6: Mapping a three-dimensional surface (hand) into a rectangular plane of neurons.

## 1.4 Notation, Conventions and Abbreviations

The literature on neural networks contains a profusion of notations that makes it difficult for the beginner to compare one method with another. Throughout this textbook we will use a consistent nomenclature and notation.

Names of *scalar* (single-valued) values are printed with small italic letters:

$$a$$

The only **exception** is *Net* which starts with a capital letter so as not to confuse it with the terms "network", or "net".

Names of *vectors* and *matrices* are in bold italics, with initial caps:

$$\boldsymbol{A}$$

The individual values of an *input vector* (***Inp*** or ***X***) are given by lower case $x$, indexed with a subscript $i$ and of dimension $m$:

$$inp_i, x_i \qquad (i = 1, 2, ..., m)$$

The individual values of the *output vector* (***Out*** or ***Y***) of a collection of neurons are indexed with a subscript $j$ and are of dimension $n$:

$$out_j, y_j \qquad (j = 1, 2, ..., n)$$

The *weight matrix* of a layer of neurons, ***W***, thus has individual values $w_{ji}$, the first index referring to the neuron being considered, the second index specifying the input unit (the preceding neuron that transmits the signal):

$$w_{ji}$$

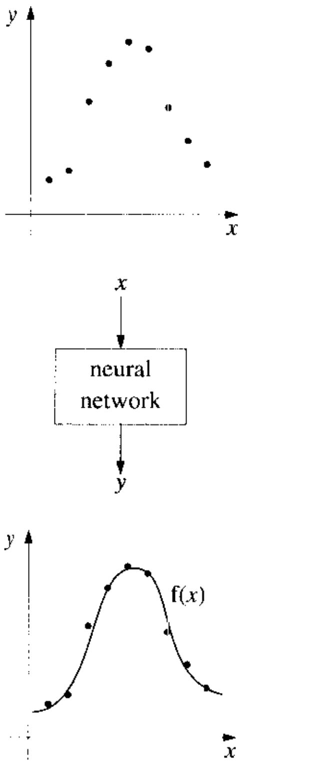


Figure 1-7: Modeling of experimental data with a neural network.

When the weight matrices of different levels are compared with each other, the first weight matrix of level $l$, $\boldsymbol{W}^l$, has as usual the indices $i$ and $j$, whereas the one of the next level $\boldsymbol{W}^{l+1}$ has the indices $j$ and $k$, with $k$ running from 1 to $r$:

$$w_{kj}$$

If there are several *input objects*, they are identified by a subscript $s$ having a maximum value of $p$. Thus, the input object is identified by $\boldsymbol{X}_s$, the individual components (signals) by:

$$x_{si}$$

In a multilayer network, the various *layers* are identified by a superscript $l$. Thus, the output vector of a layer $l$ is $\boldsymbol{Out}^l$, and its individual values are $out_j^l$.

$$\boldsymbol{Out}^l,\ out_j^l$$

*Iterations* through a neural network are characterized by a superscript $t$ in parentheses, $(t)$. Thus, the initial value of a weight matrix is $\boldsymbol{W}^{(0)}$; it will be changed in the next iteration to $\boldsymbol{W}^{(1)}$. The successive steps in changing values are indicated by superscripts "*old*" and "*new*":

$$\boldsymbol{W}^{(old)},\ \boldsymbol{W}^{(new)}$$

At the beginning of each chapter, we present the major topics and *objectives* that are to be learned. Some important remarks are highlighted in the text by framing. At the end of the chapter, the *essential equations* and formulas are collected. After each chapter a selection of relevant literature is given for *further reading*.

Important new concepts are highlighted in the text by writing them in *italics*. Words to be emphasized are printed in **boldface**.

## 1.5 Beyond a Printed Edition

A printed edition can only give a static view of a scientific field. However, neural networks in general, and their application to chemical problems in particular, is a rapidly expanding area. In order to account for this, we have installed a website at

*http://www2.ccc.uni-erlangen.de/ANN-book/*

to provide a forum for continuously updating information on the use of neural networks in chemistry. This also gives us the opportunity to provide electronic material such as presentation materials and access to programs and data sets to the readers.