# 22 Prospects of Neural Networks for Chemical Applications

A review of neural network applications in chemistry appeared a few years ago in the journal *Analytica Chimica Acta* (**248** (1991), 1 – 30); it was titled "Neural Networks: A New Tool for Solving Chemical Problems, or Just a Passing Phase?". Today, the question in the title can be answered quite clearly. The very fact that we have written an introduction on it shows that we are convinced that there is a bright future for the application of neural networks in chemistry. In the last few years, neural networks have become an established tool in applied and theoretical chemistry. Their versatility and ease of use have inspired numerous applications, new ideas and new perspectives in the field itself, as well as in the handling of chemical data.

Now, with the publication of the second edition of this book, all this can only be emphasized. The very fact that a second edition is asked for underlines the important role neural networks have gained in chemistry and will continue to do so. We have passed through the initial hype of using neural networks in chemistry, have seen some disillusions and skepticism, and see now a steady and well-established use of these tools in analyzing chemical information.

One of the most valuable and interesting consequences of chemical applications of neural networks is that it forces us to reconsider the representation and interpretation of our data.

The representation of data is very important for the extraction of vital or interesting information from experimental data. However, the directness of the neural network approach has brought this fact to new prominence; whether in Kohonen learning or in the back-propagation of errors, the representation of data is crucial. Furthermore, the representation of outputs, or targets associated with outputs, is critical as well, because the target information needed to train, adapt, or label the networks plays a central role in changing the weights, the most important parameters in any neural network.

Transforming a variable into a new one, changing the scale, or normalizing a variable's values can completely change the properties of the network. The correction of weights, in spite of all the well-defined equations, has become an "art" with the introduction of arbitrary parameters like "learning rate" and "momentum". Variable learning rate constants are not the exclusive attribute of back-propagation learning procedures only: they are encountered in ABAM, Kohonen, and counter-propagation learning algorithm as well.

Controlling the learning rate means controlling the amount of information necessary to push the network towards a proper solution. This sensitive procedure is already rather well developed and will become more and more important in the future.

While neural networks have enormous potential for making multicategory decisions on one level, there is at present an increasing tendency to solve complex problems in parts, and then put the partial solutions together; it is as if the authors are afraid of using large multicategory decision networks. While this does minimize training time, pasting together a decision hierarchy from smaller partial solutions is a very serious distortion of the nature of the problem. Apparently, because global-solution methods are not yet fully developed or tested, some authors trust the partial solutions more than general ones. This might become a trend in neural network research: global vs. local models. In our opinion, the only real generalization of solutions is possible by cyclic or stepwise use of both unsupervised and supervised learning methods, and by exchanging the results and adapting the representations to actual local needs.

Another rapidly growing trend from the neural network research is the appearance of small special-application networks built into user-friendly shells (black boxes). Just as ordinary people are content to use the telephone without knowing how it works, end users of artificial intelligence systems are happy to get predictions, as long as they turn out to be beneficial.

There is a trend of patenting such dedicated solutions, an increasing number of which include the neural network applications. If this trend continues, soon less and less information will be coming from the industrial laboratories about what is happening in this field. Therefore, it is even more important for the universities, government and nonprofit institutions to support research in neural networks.

In the last few years it has been confirmed by many applications that artificial neural networks are an important tool for chemists to handle various types of problems. However, no matter how enthusiastic one might be about the new method, it should never be forgotten that neural networks are only mathematical tools which should carefully be designed, trained, and above all, verified. The reader should never skip or neglect the verification of the obtained artificial neural networks. Careful selection of the test set, various cross-validations either by 'leave-one' or 'leave-more-than-one-out', the comparison of results obtained by neural networks with results obtained by other methods, or any other standard validation technique should always be applied before the final judgment on the success or failure of neural networks is proclaimed.

One thing has to be mentioned at the end. As in all other data handling applications, neural networks are not exempt from sensitivity to badly chosen initial data. Never forget the golden rule: "garbage in – garbage out". If you extract only one thing from this book, let it be the importance of proper selection of data.