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Book review

Jure Zupan and Johann Gasteiger: *Neural Networks for Chemists. An Introduction.* Verlag Chemie, Weinheim 1993, ISBN 3-527-28603-9, ISBN 1-56081-793-3

Recently, neural networks have opened up unexpected new possibilities for chemistry from the point of view of how to correlate structure-property or structure-activity relationships. Examples of these applications are very diverse, from standard applications like QSAR to prediction of molecular structure by molecular spectra. Neural networks represent a considerable generalization of the well-known pattern-recognition approach based on the simple perceptron idea; since the 1960s this approach has been widely applied in chemistry as a very useful classification tool (see K. Varmuza, Pattern Recognition in Chemistry, Lecture Notes in Chemistry, Vol. 21, Springer Verlag, Berlin 1980). Neural networks will also be (or already are) widely used in chemistry as a classification and prediction tool. In the chemical community the neural networks are often still presented as something very obscure invented by computer scientists to simulate the human mind. On a very general level, this might be correct, but if we remove this common belief, neural networks may be abstracted to simple mathematical structures with features very similar to a nonlinear regression and/or cluster analysis.

The textbook by Zupan and Gasteiger is dedicated to neural networks and their application in chemistry. This book can be used as the first introductory text for chemists who are interested in completely understanding all aspects of neural networks as classification and prediction tools. The first part of the book describes the basic types of neural networks and, as such, can also be used as a textbook for non-chemists. All concepts are illustrated by simple examples and discussed in detail. Consequently, a careful reader endowed with basic skills in mathematics and programing will be able to code and actively apply any type of neural networks presented in the textbook.

The second part of the textbook is devoted to numerous applications of neural networks in chemistry and chemical technology. Attention is mainly focused on structure-property and structure-activity relationships. Examples of these applications cover all fields of chemical research from standard applications like QSAR to prediction of chemical reactivity, molecular structure, and nonlinear projection of molecular electrostatic potentials by Kohonen feature mapping.

An excerpt from this textbook has recently been published in *Angewandte Chemie* (see J. Gasteiger and J. Zupan, Angew. Chem. Int. Ed. Engl. 32 (1993), 503–527). I casually compared the chapter on ABAM (Adaptive Bidirectional Associative Memory) in this paper with its counterpart in the textbook. Each of these works presents different results for the active process of ABAM illustrated by five simple two-dimensional 5×5 binary patterns. Which results are correct?

This textbook is an excellent introduction to the theory and practice of neural networks for all computationally oriented chemists who are interesting in their chemical applications. It is also suitable for last year undergraduates in chemistry.

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