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ARTIFICIAL NEURAL NETWORKS IN SPECTROSCOPY. APPLICATIONS.

C.P. Suárez Araujo[a]; Radoslav Halko[b]; P. García Báez[c]; J.J. Santana Rodríguez[d]

[a] *Dept. of Computer Sciences and Systems, University of Las Palmas de G.C, Campus Universitario de Tafira, 35017, Las Palmas de G .C., Spain, e-mail: Hcpsuarez@dis.ulpgc.es.*

[b] *Dept. of Analytical Chemistry, Faculty of Natural Sciences, Comenius University; Mlynska dolina CH-2, 84215 Bratislava, Slovakia.*

[b] *Dept. of Analytical Chemistry, University of Comenius, Bratislava, Slovakia.*

[c] *Dept. of Statistics, Operating Research and Computation of La Laguna University; La Laguna, Spain*

[d] *Dept. of Chemistry, University of Las Palmas de G.C, Campus Universitario de Tafira, 35017, Las Palmas de G .C., Spain, e-mail: jsantana@dqui.ulpgc.es.*

Spectroscopy is a very important field which handles data, spectral type, related to compound structure. All spectroscopic techniques handle complex data, like multiparameter data set, working in non stationary environment and with non linear processes. An alternative and complementary approach to face these characteristics and problems is a computational model which has been biologically inspired, "the Artificial Neural Networks (ANNs)". The ANNs can be defined as a cognitive information processing structure (massively parallel dynamical system) based upon models of brain function. They are composed of highly interconnected computational elements with topology of graph, generating modular three-dimensional structures which are intended to interact with the environment. Its more appealing property is its learning capability. Its behaviour emerges from structural changes driven by local learning rules, having the capability of generalization. The ANNs capture high-dimensional inputs and generate relationships between the inputs and outputs from a training set. In addition, the encoded internal representation captures the similarity among input that results in generalisations. They can approximate any real valued function mapping and face tasks close to processes which are thought to occur in the brain.

The suitability of ANNs has been extensively demonstrated for its use in a wide variety of applications where real-time data analysis and information extraction are required in the field of chemistry.

This paper reviews the current use of ANNs in spectroscopy. These applications of ANNs are the most frequent and successful in the field of chemistry and they include various kinds of spectra: UV/VIS, NMR, MS, IR, gamma, fluorescence and so on.

In the spectroscopic applications, the most common approach to ANN is the one that combines the simple data reduction capability of conventional linear signal processing algorithms with the adaptive learning and recognition ability of multilayer non-linear neural network architecture. It enables to resolve different kinds of problems in the spectroscopy. ANNs are the most suitable for the specific tasks of the spectroscopic techniques, such as modelling, analysing of complex data like multidimensional spectra, identification, classification and recognition of spectral signals and for the calculation of quantitative and semi quantitative analysis of spectra. They aslo are well suited for the analysis of laboratory data that can be viewed as a pattern matching problem and for a large variety of other applications, that are referred to in the present paper.