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APPLICATION OF ARTIFICIAL NEURAL NETWORKS FOR SOLVING PHARMACEUTICAL ISSUES

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Summary. Nowadays, modern analytical instruments allow producing great amounts of information for a large number of samples (objects) that can be analyzed in relatively short time. This leads to the availability of multivariate data matrices that require the use of mathematical and statistical procedures, in order to efficiently extract the maximum useful information from data. When processing the data obtained as a result of the chromatographic analysis and various spectroscopic methods, as well as sensory systems, such as the electronic nose and electronic tongue, one cannot avoid applying modern chemometric methods, e.g., pattern recognition and classification algorithms, discriminative analysis, and artificial neural networks.

Keywords: artificial neural network, pharmaceutical production, pharmaceutical analysis, prediction, classification.

Artificial neural network (ANN) algorithms are modern mathematical models that are simulates human brain functioning. There exist numerous applications of ANNs in data analysis, adaptive control, prediction, classification, identification, etc. [1, 2].

Many different architectures and types of artificial neural networks are known. Artificial neural networks consist of neurons (artificial neurons). Other name of neurons is hidden units. Artificial neurons are connected with weights and form input, hidden and output layers. Neurons process information and these signals are transfer to the next layer by means of linear or non-linear activation functions [1-3].

One should choose the transfer or activation functions in each layer, the learning rule, and the number of neurons in each layer for constructing the architecture of an artificial neural network. The input signals multiplied by the weight parameters are summed and passed through a transfer function to produce the output for neurons [4, 5].

The radial basis function network is among the most commonly used types of ANNs. The radial basis function network is a supervised three-layered feed-forward

ANN that uses radial basis functions as activation functions. The radial basis function network was formulated initially by Broomhead and Lowe [2, 6].

The Elman network and dynamic neural network are the recurrent networks. The prominent feature of the recurrent network architecture is the presence of feedback or blocks of a dynamic delay. The Elman neural network is a two-layer network with the feedback from the output layer to the input of the hidden layer. Dynamic neural network is the feed-forward input-delay back propagation network [7, 8].

Probabilistic neural network is one of modifications of a radial basis function network. Usually, a spherical Gaussian basis function is used, although many other functions work equally well. Every hidden neuron is intended for single pattern storage of training set. The output layer of probabilistic neural network is the competitive layer which is used to determine the most likely class for a given input vector [8, 9].

Feed-forward neural network is the simplest and widely most useful type of the artificial neural networks. The signals moves from the input neurons, through the hidden neurons, and to the output neurons. This feature provided the name of this type of artificial neural network. In cascade neural network hidden neurons are added to the network once and keep unchanged in the afterwards [8, 10].

The Kohonen network is a simple two-layer unsupervised network. This type of ANN uses a competitive learning algorithm. During the training stage, the input vector is presented to the network and only one neuron (winning neuron) is activated. The winning neuron is selected as the neuron that has the smallest Euclidean distance to the input vector. Weight coefficients of the winning neuron are modified according to the learning rule. A comprehensive description of the competitive learning algorithm was published elsewhere. The Kohonen network is intended for the classification of input vectors into groups; the number of classes must be assigned a priori [11, 12].

Applications of artificial neural networks in the pharmaceutical industry have become increasingly important. Let present some examples of applying ANN techniques for solving pharmaceutical issues (Table 1).

Table 1

Examples of application of ANN algorithms in pharmacy

Application	Examples	Reference
Prediction of different types of activity	Prediction the antifungal properties of quaternary ammonium salts against Candida albicans.	[13]
	Prediction of the antimicrobial activity of quaternary ammonium salts against Staphylococcus aureus.	[14]
	Prediction of biological activity of compounds containing a 1, 3, 5-triazinyl sulfonamide.	[15]
Prediction of toxicity of compounds	Prediction of toxicity of phenols.	[3]
	Prediction of toxicity of hydrazine compounds.	[16]
	Prediction of toxicity of ionic liquids.	[17]
Control the process of the pharmaceutical production	Studying of controlled drug release.	[18]
	Prediction and optimization of estradiol release from ethylene–vinyl acetate membranes.	[19]
	pH-control system.	[20]

Table 1 continuation

pplication	Examples	Reference
Pharmaceutical analysis	Resolution of complex pharmaceutical formulations.	[21]
	Simultaneous spectrophotometric determination of diclofenac potassium and methocarbamol in binary mixture.	[22]
	Multivariate analysis of paracetamol, propiphenazone, caffeine and thiamine in quaternary mixtures.	[23]
Qualitative analyses (identification, classification)	Classification of pharmaceutical samples by electronic tongue.	[24]
	Classification of oligopeptides and amino acids by voltammetric electronic tongue.	[25]

The reviews [3, 26-29] are useful and interesting to study the application of artificial neural networks and other chemometric methods in the pharmaceutical industry.

Conclusion. Artificial neural networks have received much more attention recently. Thanks to their adaptive structure and learning capability, they are successfully used to solve pharmaceutical issues. Artificial neural networks are promising tool to reduce time and costs of pharmaceutical research.

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