ARTIFICIAL NEURAL NETWORKS AND THEIR APPLICATION IN THE DIAGNOSTICS OF AQUEOUS MEDIA*

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Artificial neural networks (ANN) are a subset of a wide family of machine learning algorithms which are often called data-driven, due to their capability of learning by example, requiring no physically grounded analytical or computational model or *a priori* knowledge of the studied object. The scope of problems that are solved by such methods includes those of prediction, evaluation, classification, clusterization, inverse problems, and other data analysis problems.

As other physical methods based on indirect measurements, laser spectroscopy implies solution of inverse problems (IP) – determination of the values of the sought-for parameters by the shape of measured spectra. It should be noted that spectra of aqueous media are especially difficult to model, due to possible presence of multiple dissolved components, and their interaction among each other and with hydrogen bonds of water molecules. That is why ANN as a data-driven method of solving IP are demanded and can be efficiently used in laser spectroscopy of water media.

In the lecture, methodological aspects of using ANN are discussed. From the point of view of data processing methods, any IP can have various formulations: as a regression, classification (for discrete-valued IP) or optimization problem. The key differences of ANN as a method of solving IP from alternative methods are discussed.

When solving IP, ANN can be used within one of several methodological approaches: “model-based”, “experiment-based”, and “quasi-model”. The difference among these approaches, their properties and areas of application are described.

A separate question arises if the IP being solved is a multi-parameter one. The possible approaches to the order of determination of parameters are autonomous determination, simultaneous determination of all parameters, group determination (with joining of parameters into groups with simultaneous determination within each group), and stepwise determination (when some of the parameters already determined are used as additional inputs for determination of some other parameters).

The material is illustrated at the example especially interesting for the specialists in ecology and optics of coastal zones. The discussed IP is that of identification and determination of concentrations of inorganic ions in multi-component aqueous solutions. The process of IP solution is discussed step by step, from problem statement through selection of the methodological approach, to additional methods such as group determination and cluster-based approach.

The general purpose of the lecture is to attract attention of a wide audience of spectroscopists working with aqueous media to the great opportunities opened by use of ANN and of the latest methodologic achievement in IP solution by ANN.

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