USE OF ENSEMBLE APPROACH IN NEURAL NETWORK SOLUTION OF THE INVERSE PROBLEM OF DIAGNOSTICS OF MULTI-COMPONENT SOLUTIONS OF INORGANIC SALTS BY RAMAN SPECTRA

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Diagnostics of the component composition of water solutions is a very topical task for a large scope of applications in ecology and industry. One of the very important requirements for such diagnostics is that the method should be express and non-contact. This requirement is met by the methods of laser spectroscopy, including Raman spectroscopy (1,2). Raman spectra of solutions of inorganic salts are sensitive both to the presence of specific components and to their concentrations. However, the dependence of Raman spectra on concentrations of specific salts is non-linear due to interactions among salts present in the solution. That is why the inverse problem of determination of concentrations of salts present in the solution is a very complex and incorrect one, especially if several (or many) salts are present in the solution, which is the case for nature waters.

One of the efficient modern methods to solve multi-parameter inverse problems is use of artificial neural networks (ANN). Due to their unique properties (learning by example, resistivity to noise and to contradictory data, universal approximation capability), ANN are successfully used as data processing method in spectroscopy.

The subject of this study[*] is the determination of concentrations of components in water solutions containing up to 5 salts from the following list: NaCl, NH_4Br, Li_2SO_4, KNO_3, CsI, by Raman spectra using perceptron type ANN (3). While all the salts in the solutions are fully dissociated, we can still speak of concentrations of salts (rather than ions), as all the 10 ions in the list are different, so the concentration of any cation is tied to the concentration of the corresponding anion. The experimental data array consisted of 9144 Raman spectra in the range of total salt concentrations from 0 to 2.5 M (within the limit of solubility for each specific salt combination). After initial selection of informative ranges, each spectrum contained 766 channels in the range 281-1831 cm^{-1} and 769 channels in the range 2700-3900 cm^{-1} (total 1535 input features).

Eight various architectures of multi-layer perceptron, having from one to three hidden layers, have been tested to determine the optimal ANN architecture. For each architecture, 5 identical ANN were trained differing only by weights initialization; the results were averaged. As it can be seen from Figure 1, the best results on the out-of-sample data set were obtained with the architecture having two hidden layers with 80 and 40 neurons. Smaller or larger ANN performed worse (4).

One of the methods to improve the quality of solutions obtained by adaptive algorithms like ANN is use of the so-called ensemble approach, when the answer of the simplest ensemble (like in this case) is the average value among the answers of all the networks. As various networks may make errors of different sign and on different samples, such an ensemble may give better results than any of the separate networks. The rightmost column in Figure 1 demonstrates the results obtained with the ensemble of ANN with the best architecture determined above. It can be seen that use of the ensemble approach gives additional error reduction on the average for more than 11%.

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Future studies should include search for the optimal ensemble composed of neural networks with various architectures.

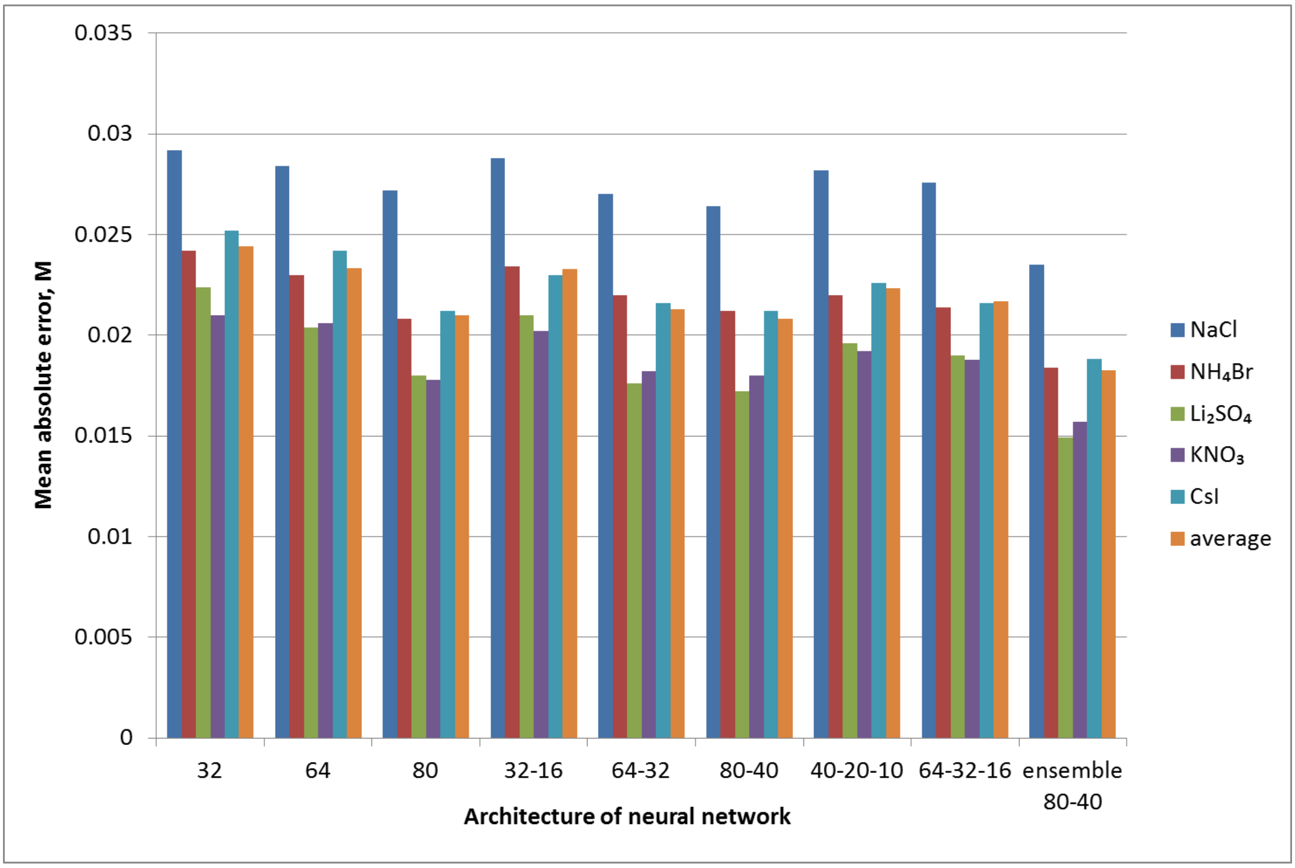

Figure 1: Mean absolute error of determination of salts concentrations by multi-layer perceptrons, average value over the results of 5 identical networks with the specified architectures, and the result provided by the ensemble with the specified architecture (rightmost group). Various colours denote the values for various salts and the values averaged over all salts.

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