



ANN Optimization in Chromatographic Analysis

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The optimization of a given chromatographic separation, by definition, aims at obtaining well-resolved peaks within a reasonable run time that could be determined quantitatively. This is often hindered by difficulties in establishing a proper procedure for simultaneous determination a large number of compounds.

Because of a number of variables involved in the chromatographic procedure, the univariate optimization procedure is too tedious, while multivariate methodologies allow testing numerous factors simultaneously and avoid using a large number of independent runs used in a traditional step-by-step approach. This is extremely important with complex mixtures. Additional benefits are decreasing times of analysis and less solvent consumption, because tedious experimental optimization trials can be avoided.

Retention mapping methods are useful optimization tools because the global optimum can be found. The retention mapping is designed to completely describe or 'map' the chromatographic behavior of solutes in the design space by response surface, which shows the relationship between the response such as the capacity factor of a solute or the separation factor between two solutes and several input variables such as the components of the mobile phase, in case of HPLC analysis. The response factor of every solute in the sample can be predicted, rather than performing many separations and simple choosing the best one obtained. One of the most interesting tools in optimization is artificial neural network (ANN).

Artificial neural networks have displayed promising performance and flexibility in different areas of life. The use of artificial intelligence and artificial neural networks (ANNs) is a very rapidly developing field in many areas of science and technology. ANN is a computer algorithm whose structure and function came from the structure and learning behavior of biological neurons. Certain algorithm is typically employed to classify a set of patterns into one of several classes. The classification rules are learned by the network from examples, of which the most common is the "supervised", learning where sample input-output pairs

are presented. The most common is that the network is trained using the back propagation learning algorithm. In back propagation, the network is first presented with an input and activation is propagated forward through the network to determine the network's response. The network's response is then compared with the known correct response. If the network's actual response does not match the correct response, the weights between connections in the network are modified slightly to produce a response more closely matching the correct response.

Since ANNs are learning to associate the inputs with outputs, evaluating the performance of the network from the training data may not produce the best results. If a network is left to train for too long, it will over-train and will lose the ability to generalize. Thus test data, rather than training data, are used to measure the performance of a trained model. Thus, three types of data set are used: training data (to train the network), test data (to monitor the neural network performance during training) and validation data (to measure the performance of a trained application), each with a corresponding error.

Capillary electrophoresis (CE) has been widely used as one of the most important separation techniques in modern analysis. The high efficiency of capillary columns, used in CE, results in good separations with very short run times and this is the main advantage of capillary electrophoresis. When compared to HPLC, CE produces narrower peaks and better resolution with greater peak capacity. In addition, CE is characterized by using small sample volumes (pico- to nanoliters) and low consumption of organic solvents.

Thus the introduction of ANN optimization in CE analysis is increasingly important.

The aim of this study was to apply the ANN with back propagation learning algorithm to optimize the electrophoretic behavior of several drug mixtures.

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