Machine learning and AI

The multivariate methods of chemometrics - often also referred to as data mining, machine learning or deep learning/AI - offer the possibility of making superimposed and hidden information visible in the spectra. When using machine learning or AI methods, precise knowledge of the input data is a fundamental prerequisite. The methods of exploratory data analysis are suitable for structuring the input data (value range, distribution and characteristic values of features) and reducing the amount of data.
Machine learning methods make it possible to differentiate between spectra which, from a visual point of view, show almost no differences. With the help of algorithms and mathematical statistics, existing differences can be clarified and data that do not contribute to the distinction can be separated. What remains is the information with the maximum variance or distinction. The individual methods will be discussed elsewhere in this guide.

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