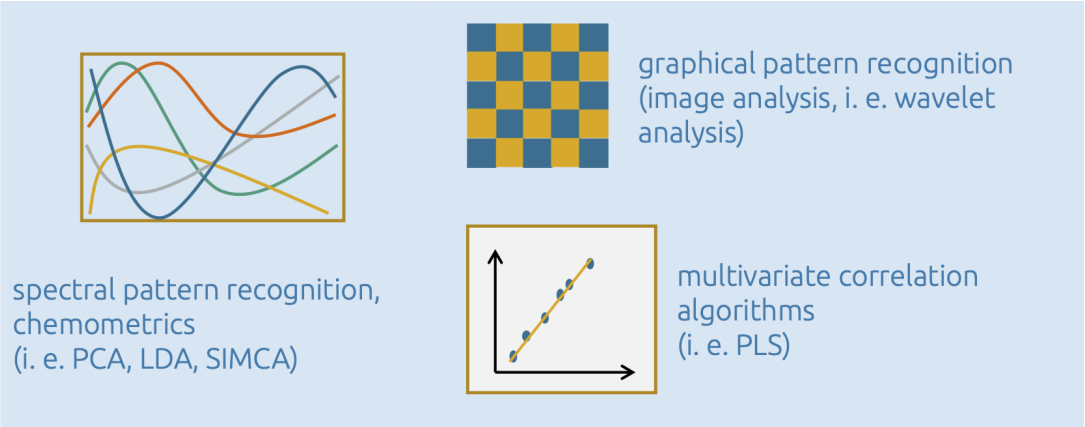
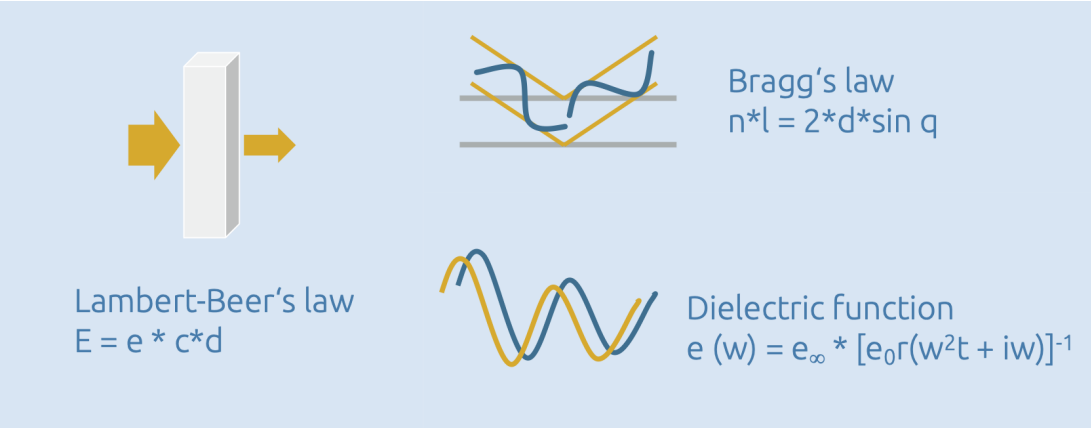
Soft modeling vs. hard modeling

In contrast to the machine learning methods of the 'soft modeling' approach, there is also the 'hard modeling' approach for evaluating the spectra. This refers to the physically exact description of the data. The simplest case is Lambert-Beer's law for describing the extinction. Other examples are the determination of optical properties (refractive index, absorption coefficient) and the sample structure (layer thicknesses) based on the description of the spectra using the laws of thin-film optics. The computing times required for hard modeling are significantly longer compared to the prediction in the soft modeling approach, but the results can also be used as a reference for classification or regression models.



Examples for soft modeling algorithms



Examples for hard modeling algorithms

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