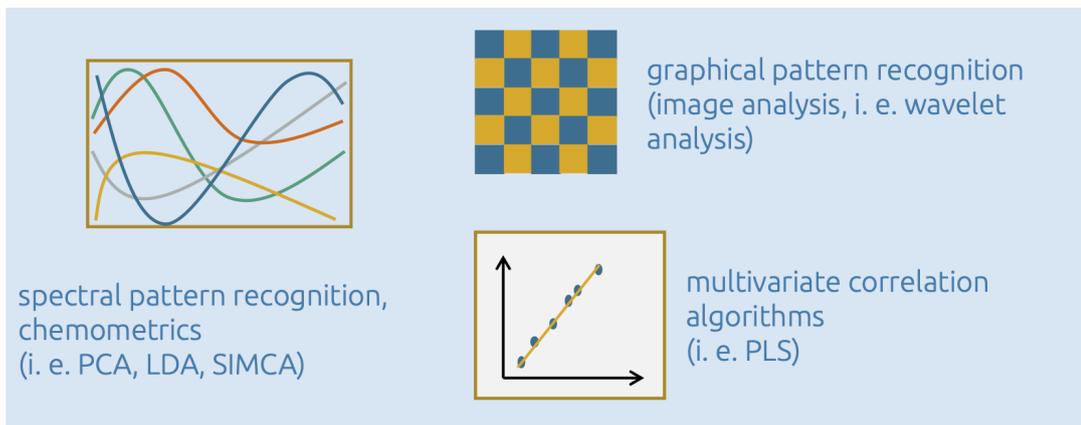


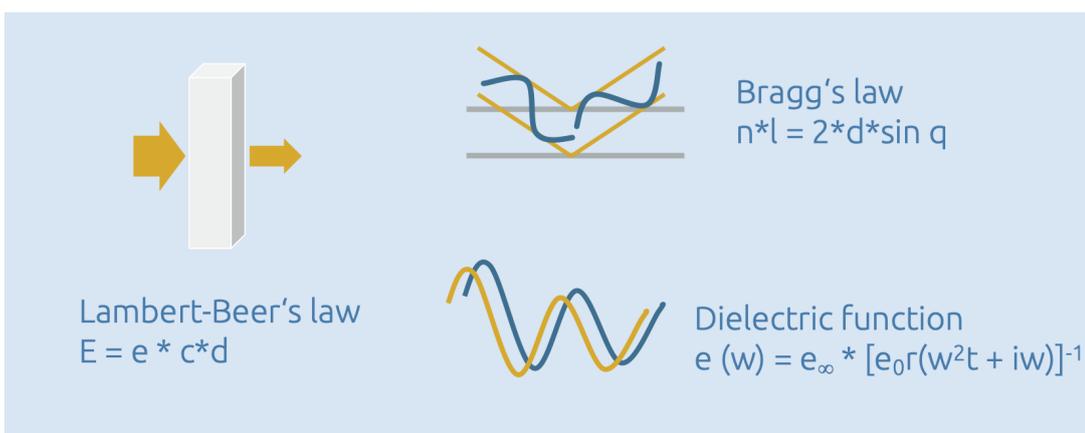
# Soft modeling vs. hard modeling

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.



This block illustrates four examples of soft modeling algorithms. It features four distinct visual elements: a box with multiple overlapping colored curves representing spectral patterns; a 4x4 grid of alternating blue and yellow squares representing graphical pattern recognition; a scatter plot with a linear regression line representing multivariate correlation algorithms; and a box with the text 'spectral pattern recognition, chemometrics (i. e. PCA, LDA, SIMCA)'. The text 'graphical pattern recognition (image analysis, i. e. wavelet analysis)' is positioned to the right of the grid, and 'multivariate correlation algorithms (i. e. PLS)' is positioned to the right of the scatter plot.

Examples for soft modeling algorithms



This block illustrates three examples of hard modeling algorithms. It features three distinct visual elements: a diagram of a light beam passing through a rectangular block with arrows indicating direction; a diagram of light rays reflecting off two parallel surfaces, illustrating Bragg's law; and a diagram of two overlapping sine waves representing a dielectric function. The text 'Lambert-Beer's law  $E = e * c * d$ ' is positioned below the block diagram. The text 'Bragg's law  $n * l = 2 * d * \sin \alpha$ ' is positioned to the right of the reflection diagram. The text 'Dielectric function  $\epsilon(\omega) = \epsilon_{\infty} * [\epsilon_0 r(\omega^2 t + i\omega)]^{-1}$ ' is positioned to the right of the sine wave diagram.

Examples for hard modeling algorithms

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