Basic Chemometrics

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This 1h30min course will discuss the nature of spectral data and the statistical methods necessary for their analysis. In this three-part training, the fundamentals of principal component analysis will be described as a basis for data exploration, regression and classification. Building on these learnings, latent variable based methods (Principal component regression, Partial Least-Squares regression) will be described through the use of examples from various fields of NIR spectroscopy.

At the end of the course, participants are expected to be able to describe how a Principal Component Analysis works, how its outputs can be used for spectral data analysis (regression and classification). They will also understand the difference between Principal component regression and Partial Least-Squares regression based model. Finally, they should be able to deploy classification of spectral data based on latent variables.