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Multivariate integration and visualization of multiblock data in chemical and biological applications

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Abstract

Thanks to improvements in technology more data than ever before is generated in almost all fields of science and industry.

The data is analyzed to hopefully provide valuable information and knowledge about a product or process, such as how to improve the quality of a manufactured product.

Analysis of collected data is often performed on a single dataset or data source at a time. In this thesis, I have focused on multiblock analysis, a concept that includes multiple sources or data blocks. Analogous to how the human senses combine to let us experience the world around us, multiblock analysis integrates multiple data sources, providing a fuller examination of the product or process under study.

My thesis introduces Joint and Unique Multiblock Analysis, JUMBA, a complete analysis workflow for data integration. I describe each step of JUMBA, including data pre-treatment, model building and validation as well as model interpretation. Special focus is put on several newly developed visualizations for model validation and interpretation to make it as easy as possible to draw conclusions from the analysis.

By reading my thesis, the reader will gain a working understanding of the process of performing multiblock analysis, including solutions to common problems that are often encountered.

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Multivariate analysis, PCA, PLS, OnPLS, JUMBA, Multiblock, calibration transfer

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