Chemometrics in Food Chemistry: Chapter 12. Interval-Based Chemometric Methods in NMR Foodomics (Data Handling in Science and Technology)

Francesco Savorani, Morten Arendt Rasmussen, Åsmund Rinnan, Søren Balling Engelsen

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In classical empirical research a model requires that the number of variables must be less than the number of observations, but developments in chemometrics and modern analytical platforms have pushed people beyond the classical model. Typical “omics” data sets will include 100–1000 samples and often more than 10,000 variables and the advantage of using chemometrics to large data structures is the ability to efficiently deal with collinear data sets with many more variables than samples. However, the trend with ever more variables also pushes the chemometric tools to the limit as they will also increase the extent of spurious correlations and interferences. This chapter advocates for a systematic breakdown of the variable space in intervals in order to improve the interpretability and performance of chemometric methods. The term “i-chemometrics” is here introduced to encompass the whole class of interval-based chemometric methods. This chapter will describe the advantages of using the generic i-chemometric methods for data preprocessing, data exploration, regression, and sample classification/discrimination using examples from NMR foodomics. The main advantages are more parsimonious models, improved interpretability and, in many cases, improved performance.

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