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ABSTRACT

The most common analytical methods used today produce a vector of data for each sample measured. Measurements from multiple samples are logically arranged as 2-way matrices. The more sophisticated hyphenated techniques, such as chromatography followed by spectroscopy, produce a 2-way matrix for each sample. We refer to these analytical systems as "second order" because the data produced for each sample is a second order tensor. Multiple samples are logically arranged as a 3-way matrices where data from each sample is a "slice" of the data "cube." Methods for analyzing multi-way data are reviewed. This includes the factor analysis techniques Parallel Factor Analysis (PARAFAC) and Multivariate Curve Resolution (MCR) as well as the a number of multi-way regression techniques. In many instances multi-way analysis techniques coupled with second order analytical data offer distinct advantages over conventional methods because of their ability to quantitate in the face of previously unseen interferents and because of the uniqueness properties of the models which improves interpretability. These properties are especially important in environmental applications where the environment being sampled is uncontrolled.