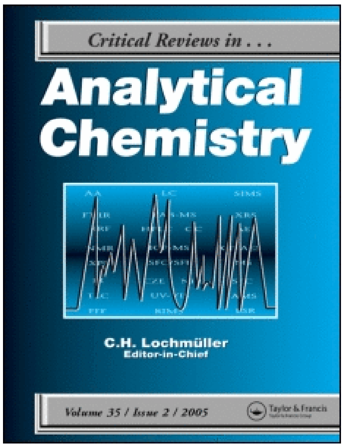

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Review on Multiway Analysis in Chemistry—2000-2005

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Review on Multiway Analysis in Chemistry—2000–2005

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This review describes advances in multiway analysis during the period 2000–2005. Multiway analysis started to take off in chemistry in the 1980s, but only in recent years has it been broadly applied to many diverse kinds of data. This review reflects how the field has matured and how the methods have been applied to more and more difficult types of data in new research areas. Multiway analysis is described in terms of different types of data, different areas of applications as well as more fundamental and theoretical results throughout the period. It is evident from this review that multiway analysis is presently a generally accepted and used tool whose full potential is far from reached.

Keywords PARAFAC, tucker, tensor, three-way

INTRODUCTION

Multiway analysis is concerned with the analysis of higher order data as defined, e.g., by Henk Kiers (1). Higher-order data is data that can be arranged in boxes as opposed to two-way data, matrices, that can be arranged in tables. Interestingly, the paper by Kiers, describes the first suggestion for a standardized notation for multiway analysis not only applicable in chemistry, but in data analysis in general. It is advised to use these suggestions for notation in order to make communication across and within different disciplines more straightforward.

Multiway data occurs frequently due to modern instrumental developments, so it is quite typical that multiway data analysis in recent years has been applied to new advanced instrumental data. But the maturing of the area has also led to a situation where multiway tools are more frequently used for other types of data such as process data, sensory data, etc. In certain situations, multiway data are rearranged into matrices and analyzed using ordinary multivariate data analysis, two-way analysis. This review does not go into such extensions of two-way analysis, but focuses on the tools that work directly on the three-way data or in general multiway data. Multiway analysis started in psychometrics in the 1960s and 1970s (2–5) partly based on problems in factor analysis dating back to the 1940s (6). Since then there has been an increasing collaboration between psychometricians and chemometricians on both fundamental and applied issues. In later years, multiway analysis has started to be used in signal processing and mathematics, but most results from these areas will not be covered in this review as they are of little relevance to chemical applications.

As an indication of the growth in multiway analysis, the period that this a review deals with has also witnessed a whole special issue of the Journal of Chemometrics devoted to multiway analysis (7) as well as the first book on multiway analysis (8) in chemistry. A review covering the 10-year period 1985 to 1995 contained 126 references (9) whereas this 5-year review contains more than 300 papers.

In the following the literature on multiway analysis is described in terms of three different types of areas. The first part of the review describes applications in terms types of data, while the second part describes multiway analysis in terms of different areas of application, and finally more theoretical aspects of multiway analysis are described.

DATA TYPES

Fluorescence Spectroscopy

Fluorescence spectroscopy is by far the most abundant type of data used for multiway analysis (10). This is undoubtedly due to the close relationship between the unique PARAFAC model and the fundamental structure of common fluorescence spectroscopic data. Andersen and Bro (11) gave an overview of the use of fluorescence excitation-emission spectroscopy and how to perform valid multiway analysis of such data. One of the most interesting aspects of using the PARAFAC model is that it enables the so-called second order advantage (12). That is, the possibility of doing quantitative chemical analytes even in the presence of uncalibrated interferents. A number of papers have dealt with this issue for different types of applications. Moberg et al. (13, 14) used PARAFAC to quantitate different chlorophylls and derived analytes. The PARAFAC based calibration method was shown to be superior to two-way techniques such as classical least squares. PARAFAC was used to perform quantitative

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analysis of pesticides using a fluorescent dye, with detection down to parts-per-trillion (15, 16). Fluorescence and second-order calibration was used to predict sulfathiazole in honey (17) and to quantify catecholamines (less successful) (18, 19). Using the kinetic development of fluorescence it was possible to quantitate methotrexate and leucovorin in human urine using four-way PARAFAC modeling (20). There are numerous other examples on the use of fluorescence data and second order calibration: carbendazim, fuberidazole and thiabendazole (21), naphthalenesulfonates using non fully resolved chromatographic analysis (22), doxorubicin (23), ciprofloxacin (24, 25), flumequine and oxolinic acid (26), enrofloxacine (27), verapamil (28), carbendazim, fuberidazole, and thiabendazole (29). An LED-based fluorescence instrument was developed and tested for calibration in the parts-per-billion to parts-per-trillion range for compounds such as 9,10-bis(phenylethynyl)- anthracene and rhodamine B using PARAFAC (30). PARAFAC was used to resolve drug mixtures of propranolol, dipyridamole and amiloride in aqueous solution (31), carbamazepine in serum (32), norfloxacin, enoxacin, and ofloxacin (33, 34), and different drugs in plasma (35).

In some applications, the second-order advantage is not a crucial aspect for solving the calibration problem; It should be “may be because the data is not possible to describe, in a chemically meaningful way, with PARAFAC” or because the components are only indirectly related to the dependent variable. The PARAFAC model may still be used similarly to how the principal component analysis can be used in principal component regression, but it is also possible to use alternative multiway methods. Pedersen et al. (36) showed that they got chemically meaningful PARAFAC models from fluorescence data of fish oil, and that they could use the resulting models for predicting the dioxin content.

Besides the use of fluorescence data for calibration purposes, it is also often used for qualitative analysis, classification, exploratory analysis etc. A fair part of these applications deal with food analysis and environmental analysis. Guimet and coworkers have performed a number of experiments on olive oils characterizing these using fluorescence spectroscopy as well as PARAFAC modeling for verifying possible adulteration (37–39). The multiway N-PLS regression approach was used to predict quality parameters such as peroxide values. Baunsgaard and coworkers on the other hand have published a number of papers on the use of fluorescence for understanding the quality of sugar as well as its intermediate products (40–42) showing how the chemical insight gained from PARAFAC models enabled a deeper understanding of e.g., the formation of colorants. Fluorescence was also used to monitor the quality of dry-cured Parma ham (43) and in yogurt (44) providing chemically meaningful information on major chemical/physical changes during processing. Fluorescence has also been used together with PARAFAC modeling for monitoring light-induced oxidation and changes in cheese with storage (45, 46). PARAFAC models were used to characterize the interaction of chlorpromazine hydrochloride and Neutral Red with DNA (47) and for single-cell temporal analysis of intracellular Ca^{2+} concentration and pH (48).

PARAFAC in combination with fluorescence spectroscopy has also proven useful for various types of applications within environmental analysis such as characterizing oil spills (49) based on fingerprinting polycyclic aromatic compounds (50, 51); characterizing stress by measuring hormones in urine (18); and resolving polycyclic aromatic hydrocarbons (52, 53). Also in environmental analysis, a new approach for chemical identification of dissolved organic matter for tracing pollution has been suggested, based on the use of fluorescence in combination with PARAFAC modeling (54). Finally Haack et al. (55) used PARAFAC and two- and three-way PLS to describe the chemistry and quality of cultivations with *Saccharomyces cerevisiae*.

Although, some view fluorescence excitation-emission data as the ideal type of data for, PARAFAC modeling, for example, there are in fact, a number of problems with typical fluorescence data that complicates practical application of PARAFAC. Most notably, different kinds of scattering signals pose a problem as the scattering signals do not follow the PARAFAC as well as not containing any chemical information. Several approaches have been tested to remedy the bad influence of scattering by downweighting the scatter, setting it to zero or modeling it (11, 56–61).

CHROMATOGRAPHY

Another area where multiway analysis has been extensively used is in chromatography. Ideally, a chromatographic experiment leads to perfect separation of chemical analytes and the resulting chromatograms can be directly converted to e.g., areas or concentrations and used for further analysis. Sometimes, though, it is not possible to achieve perfect separation, either because of the complexity of the samples or because faster chromatographic runs are preferred. In such situations, overlapping peaks result and data analysis can be used for further achieving selectivity by mathematical means or simply for fingerprinting the elution profiles (62). In gas chromatography (GC) multiway analysis has been used for a number of purposes. It has been shown that careful implementation of GC×GC provides data that can be subsequently analyzed by multiway methods enabling high-speed GC systems for complex process or food analysis (63–66). Quantitative and qualitative analysis of naphtha samples were demonstrated using comprehensive high-speed two-dimensional gas chromatography analyzed using N-PLS to predict the aromatic and naphthene (cycloalkanes) content of naphtha samples (67). Tucker and PARAFAC models were used to analyze GC data from Maillard reactions experiments (68). Gas chromatography-mass spectrometry (GCMS) was used for analyzing data from fuels that have undergone various levels of thermally induced oxidation. Regions of the GC-MS data were modeled with PARAFAC providing the mass spectra of individual fuel constituents (69). Also the eigenvalue based algorithm GRAM was used for analyzing GC × GC data of jet fuels (70, 71). Sinha et al. has shown how GC × GC coupled to time-of-flight mass spectrometry (GC × GC-TOFMS) and combined with PARAFAC provides a powerful analytical methodology where partially resolved components in complex mixtures can be identified directly. It was found that deconvolution results were best with selectivities above 0.18 (72, 73). Garcia et al. (74) compared traditional analytical quantification with the use of PARAFAC, PARAFAC2, Tucker and N-PLS on GCMS data for determining Clenbuterol bovine hair and urine. Five hormonal growth promoters (diethylstilbestrol, hexestrol, dienestrol, 17-beta-estradiol and 17-alpha-ethynylestradiol) were similarly analyzed and in addition the use of PARAFAC2 was tested for handling variations in elution time across chromatographic runs (75). For quantification using GC × GC, the use of GRAM is compared to two traditional peak integration methods providing substantial improvements in quantification precision, accuracy, and limit of detection (76).

As for GC, LC systems also provide data where multiway methods can be helpful. HPLC with infrared spectroscopic detection can be hampered by strong absorption bands of the eluent. It was shown that a modified PARAFAC or PARAFAC2 model that specifically models the eluent could alleviate the problem (77). An iterative approach to resolving overlapping peaks was suggested by Wang et al. (78) and an approach for extraction and quantification of sulfamethoxypyridazine, sulfamethoxazole and sulfadimethoxine in porcine kidney by HPLC-DAD was developed using PARAFAC to resolve overlapping peaks (79). PARAFAC was shown to be able to resolve partly separated peaks into their pure chromatographic, spectral and concentration profiles, even with severely overlapping spectra using a system of lidocaine and prilocaine analyzed by LC-DAD (80) and overlapping LC × LC data were resolved by Fraga and Corley (81).

FLOW INJECTION

In flow injection, threeway data often occur (82–84) and there are often problems with so-called rank overlap because of the lack of separation in the time mode. Least squares-based and eigenvalue-based algorithms were tested for calibration in FIA systems with a pH profile induced and with rank overlap (85). Benzoic and sorbic acids were determined in commercial orange juices using a flow injection system with pH gradient generation, diode array spectrophotometric detection, and PARAFAC as well as multivariate curve resolution (86). Levodopa and benserazide were quantified in pharmaceutical formulations based on the N-PLS modeling of kinetic-spectrophotometric data from a spectrally detected stopped-flow injection method where the analytes reacted with periodate (87).

MAGNETIC RESONANCE

Both low-field and high-field NMR is gaining momentum in new types of applications. And while the data structures are quite different, multiway analysis has been extensively used for both types of data. In low-field NMR, the use of multiway analysis arises from the often multi-exponential nature of the data. As shown initially by Antalek and Windig (88–90) such data can be modeled by rearranging the data appropriately (slicing) and then fit a PARAFAC model to the rearranged data. The resulting models provide direct access to the quantitative and qualitative information of the underlying exponentials. Often, the use of least squares fitting through alternating least squares is replaced by faster approximate methods based on eigenvalue decompositions (GRAM, TLD etc.). These methods are particularly useful for low-field NMR because the signal-to-noise ratio is high and the model error low leading to excellent performance of these methods. A refined algorithm for fitting low-field NMR called PowerSlicing was proposed by Engelsen and Bro (91–93). The method was used to determine fat content in minced meat as well as characterizing preslaughter stress in processed meat (94), predicting sensory attributes of potato samples (95) and for exploring properties of cod muscle (96). Nordon et al. (97) showed the superiority of the multiway approach both with respect to accuracy and possible automation in analysis of a glycerol-based polyether polyol (98). Multiway analysis has been used in a number of different types of high-field NMR applications. A PARAFAC-based method called MUNIN has been applied to deal with huge-size multidimensional NMR data (99–102). Three- and four-way PARAFAC models were used to model fMRI data from multiple runs of a bilateral finger-tapping paradigm (103). Independent component analysis and PARAFAC was used to model multisubject FMRI analysis (104). Dyrby et al. (91, 105–107) used PARAFAC for curve-resolution, Tucker models for exploratory studies and N-PLS for quantitative models of various metabonomic data.

EEG

EEG data was acquired during the testing phase of a new drug expected to have effect on the brain activity. The implemented test program (several patients followed in time, different doses, conditions, etc.) led to a six-way data set and Tucker modeling was shown to provide detailed information on the underlying phenomena (108). Multiway partial least squares regression was used to model EEG and fMRI data uniquely as a sum of "atoms" (109, 110) and PARAFAC was used to find the underlying structure of multichannel EEG recordings (111, 112).

Other

Geladi et al. has shown how NIR batch data can be modeled using multiway analysis (113, 114). Nielsen et al. (115) used an approach called COMDIM to characterize relations between NIR spectra, particle size distributions and chemical parameters of wheat flours. PARAFAC was used to model UV/Vis kinetic spectra studying amino acid transport through liquid membranes (116). Rank annihilation factor analysis (RAFA) was used for UV/Vis spectrophotometric studies of complex formation (117). Mixtures of acetylsalicylic acid and ascorbic acid were studied by UV/Vis spectra using a pH range and estimating spectra and pK_a values. N-PLS regression was performed to predict the content of the analytes in pharmaceutical samples (118). UV/Vis spectra were acquired as a function of time of an alkaline hydrolysis reaction of the antihypertensor Nifedipine. PARAFAC and PARAFAC2 methods were used for building calibration models (119).

Microsynchrotron radiation X-ray fluorescence were modeled with PARAFAC (120). Data from electronic nose data was modeled using PARAFAC2 for handling shifted time-profiles. The resulting data were used to classify samples of licorice (121). N-PLS was used to classify electronic nose data of microorganisms relevant for diagnosis of pneumonia (122). Water samples containing varying mixtures of toluene, ethyl benzene, and cumene were analyzed by purge-and-trap/direct sampling mass spectrometry. N-PLS and PARAFAC was employed for quantitative purposes and the PARAFAC models were shown to be able to predict samples that contained unmodeled, interfering compounds (123). PARAFAC was used to analyze both the time-dependent and polarization-angle-dependent IR spectra (124). PARAFAC has been used for modeling data from ICP-AES in order to gain better fundamental understanding of stability, robustness, etc. (125, 126). The use of voltabsorptometric determination of *o*-tolidine in presence of high concentration of ferrocyanide was as a model system for multiway calibration (127). PARAFAC of full skin impedance spectra was used to investigate human skin properties (128). The use of multi-way analysis for image analysis has also been discussed (129, 130).

APPLICATION AREAS

Calibration

Calibration is one of the major fields of application in chemometrics and also using multi-way methods (8, 131, 132). Several papers describe and compare different theoretical approaches to calibration (133–139) and a large number of applications especially within analytical chemistry has been published e.g., for determining creatinine in serum (140), flavilium cation, quinoidal basen, and E and Z ionized chalcones (141), dimethylphenol isomers (142), naphthalene, 1-naphthol and 2-naphthol (143), lorazepam (144), piroxicam (145), aromatic sulfonates (146), salicylate in plasma (147), verapamil (28), ciprofloxacin (25), trace levels of Cu, Zn, Co, Ni and Fe (148), pyridines (149), naproxen-salicylic acid-salicyluric acid mixtures (139). In QSAR there have been a number of approaches suggested often involving the use of N-PLS (150–156) and N-PLS was also used for predicting grain yield and protein content in wheat and barley (157). The method bilinear least-squares was used for quantifying various juice colorants from spectral-pH three-way arrays (158). Quantification of tetrachloro-dibenzoparadioxin was performed by solid-liquid extraction laser-excited time-resolved Shpol'skii spectroscopy using four-way PARAFAC (159).

MSPC

Multivariate statistical process control often involves multiway data and hence applications of multiway analysis have appeared especially in recent years (160–166). Experimental results from a pilot-scale paper mill filtration application was modeled using PARAFAC (167), PARAFAC2 was used for fault detection and diagnosis in a semiconductor etching (168), N-PLS was used to model the performance of an industrial fed-batch fermentation process (169), while a modified Tucker3 model was used for modeling first-order chemical batch reactions monitored by UV/Vis spectroscopy (170). PARAFAC and N-PLS was used to model dynamic behavior in an on-line batch process (171). Finally, PARAFAC was developed for on-line monitoring of batch processes (172). Other models based on multidimensional scaling have also been proprosed (173).

Metabonomics

Metabonomic data are often multiway of structure. Dyrby et al. (107) showed how a traditional dose-response experiment could be properly explored using Tucker3 models and PARAFAC was used for similar data (174). Idborg et al. (175) exemplified the use of PARAFAC and N-PLS in handling metabolite screening using liquid chromatography/electrospray ionization mass spectrometry. Lipoprotein characterization using 2D diffusion-edited NMR spectroscopy was analyzed with PARAFAC providing chemically meaningful spectra (106).

Environmental Analysis

Chemical analyses (dissolved oxygen, nitrates, etc.), physical data (turbidity, temperature, COND), and biological monitors (total and faecal coliforms, faecal streptococci) were monitored monthly during four years on freshwaters sampled at seven sites in northeastern Italy. Tucker models were used to explore patterns of information reflecting the environmental quality of the monitored freshwaters (176). A number of similar studies has shown and discussed the utility of particularly Tucker but also PARAFAC in environmental analysis (177–183). N-PLS was used for predicting average air temperature, dew temperature and precipitation (184) while PARAFAC was used to characterize polycyclic aromatic hydrocarbons (53). The availability and mobility of trace elements and heavy metals were analyzed using PARAFAC (185). Monitoring of photocatalytic degradation of phenol in aqueous suspensions of TiO_2 was based on fluorescence spectroscopy and PARAFAC (186). A multilinear model was developed for the analysis of the spatial patterns and possible sources affecting haze and its visual effects in the southwestern United States (187) and chemical composition data was analyzed using a mixed two-way/three-way model (188). There have been a number of projects related to characterizing dissolved organic matter from diverse aquatic environments with PARAFAC. The PARAFAC approach is used to replace more manual evaluations of the fluorescence measurements and a high number of papers are appearing on this (49, 54, 189–191). Modified versions of Tucker3 and PARAFAC have been developed for optimally handling interval-valued data and are used for analyzing air pollution data (192) and three-way environmental data are analyzed with STATIS, Tucker and PARAFAC2 (193).

Kinetics

Incorporation of kinetic constraints in PARAFAC-like models (194, 195) have been published as well as reports on the suitability of threeway methods for kinetic modeling (196, 197). Often times, direct application of multiway methods such as PARAFAC are hampered by the changes in actual shapes of kinetic profiles, yet there have been experiments where PARAFAC2 was used to overcome this problem (198). Kinetic-spectrophotometric analysis for quantification of nitrite in water and meat samples using PARAFAC (199) and simultaneous degradations of chlorophyll a and b was studied by fluorescence spectroscopy and resolved by PARAFAC (200). Kinetic calibration models were developed for carbaryl and while curveresolution and PARAFAC was able to predict new samples with unknown interferents, N-PLS was shown not to be able to as is expected from its regression properties. Bijlsma et al. have developed several models for describing various kinetic systems (201, 202) using combinations of hard and soft models (203). Rank annihilation was used for determining rate constants (204) and N-PLS used to predict levodopa and benserazide from kinetic-spectrophotometric data (87, 205). Time-dependent activity data of laccase enzyme was analyzed using Tucker3 (206, 207).

Sensory Analysis

Chewing sounds of different types of dry-crisp snacks were analysed by N-PLS, Tucker and PARAFAC in order to classify the samples (208). Time-intensity measurements of flavor release were modeled by a number of methods including PARAFAC2 (209). Scores from PARAFAC models were used as predictors to predict sensory qualities of different potatoes (95) as well as to predict sensory properties of hams (43). Tucker and PARAFAC was also used to model sensory profiling data (8, 68). Effects of oil type, lipid antioxidants on oxidative flavor stability of fish oil-enriched milk were evaluated using PARAFAC (210). GEMANOVA, a method for analyzing higher-order interactions in complex data was used for monitoring changes in fresh beef during storage (211).

Classification

Very little work has been done on dedicated multiway classification, although some new types of classification models have been suggested (212–214, 215). PARAFAC was used in trying to discriminate between phytoplankton classes using fluorescence spectra (216) and PARAFAC as well as N-PLS was used for distinguishing five species of *Penicillium* (217). Allosio et al. (218) used time-dependent NIR reflectance spectroscopy and PARAFAC to model a malting process. PARAFAC fluorescence analysis of olive oils was used to discriminate between non-adulterated and adulterated samples (38) while the chewing sound was used to detect differences in foods (208). Particle sizes were arranged as histograms for 21 size classes and analyzed with PARAFAC (219). Tucker3 modeling was used to study differences in patterns of nutritional content of foodstuffs (220).

THEORETICAL

In this last section, more theoretical papers on multiway analysis are described. There are a number of papers describing the general use and utility of multiway methods as well as proper notation (1, 8, 11, 131, 221–225). The use of Procrustes analysis for multiway analysis was described in an introductory tutorial (226) and robust versions of Tucker3 and PARAFAC have been developed (227, 228). Several methods have been proposed for second-order calibration (20, 229, 230). Generalized rank annihilation–GRAM–has been thoroughly described and used in recent years (231–236). Multiway multiblock component and covariates regression models are described by Smilde et al. (237) and new models have been developed for handling shifts in data (238–240). New methods for determining the optimal number of components in PARAFAC have been proposed (241–245).

The PARAFAC model has the very attractive uniqueness properties; a fact that has been one of the main reasons for its success. Yet, the identifiability conditions are still far from fully understood as explained recently (246, 247). Basic properties of multiway models are important also in practical applications. Many results arise from the tensor properties of multiway arrays (248–254). The rank of multiway arrays is not as simple a topic as for two-way matrices. New concepts arise and many aspects are not understood in detail (255–260). Plotting of parameters from multiway models was described in detail (261, 262). New notations and operations for multiway analysis have also been suggested (1, 224, 225).

In order to perform sensible analysis, preprocessing of the data is often mandatory. Preprocessing can range from simple centering and scaling to e.g., variable selection. The theory of centering and scaling was thoroughly addressed by Bro and Smilde (263) as well as tested in practical applications in multiway regression (156). Bylund et al. used warping for aligning chromatographic data prior to the application of PARAFAC (264) while Comas et al. performed a similar operation based on a time shifting operation (138). For reducing the amount of data without loosing essential information, it has been proposed to perform an initial variable selection based on genetic algorithms (265). With the increasing popularity of the PARAFAC model, a number of suggestions have been made for improved algorithms (266–275). Two papers have compared the many different existing algorithms (276, 277). New approaches to imposing smoothness constraints were suggested (278, 279) and dealing with missing values in PARAFAC was evaluated (280). A general algorithm for fitting different kinds of multiway models was developed based on the conjugate gradient method (281).

Several algorithms have been modified to enable a maximum likelihood fitting rather than the usual least squares fitting (53, 282–286). Jackknifing of PARAFAC was shown to be able to help identifying outliers as well as providing uncertainty estimates in PARAFAC (287) and bootstrapping was used for building confidence intervals (288, 289). Other papers have dealt with general statistical aspects of multiway models (234, 290, 291). Different approaches to getting sample-specific prediction errors have been developed for both PARAFAC and N-PLS (292–296). Various papers have dealt with figures of merit (297, 298).

Software

Several software packages are available for performing multiway analysis. The N-way toolbox ⟨www.models.kvl.dk⟩ is a free MATLAB toolbox that performs PARAFAC, Tucker, N-PLS, GRAM, TLD (299–301). Also at ⟨www.models.kvl.dk⟩, the following multiway methods and tools are available: PARAFAC2 (302, 303), PowerSlicing for low-field NMR data (92), Jackknifing of PARAFAC (287), alternative implementation of algorithms for PARAFAC (e.g., Levenberg Marquadt) in Matlab (276), PARAFAC for complex-valued arrays (304), MILES for maximum likelihood fitting of PARAFAC (286), GEMANOVA for multiplicative ANOVA models (211), and SENSABLE, a graphical user interface for analyzing data from electronic noses and tongues (121). At ⟨csmr.ca.sandia.gov/∼tgkolda/pubs⟩, a free MATLAB Tensor toolbox is available for performing basic mathematical operations on multiway arrays. There are several commercial programs with multiway methods included. At ⟨www.multid.se⟩, DATAN containing PARAFAC is available and at ⟨www.eigenvector.com⟩, PLS_Toolbox can be acquired giving access to PARAFAC, PARAFAC2, Tucker, N-PLS, GRAM, TLD as well as a number of additional multiway tools for preprocessing and handling. The Unscrambler available at ⟨www.camo.com⟩ contains N-PLS. At ⟨http://three-mode.leidenuniv.nl/⟩ an extensive list of available software is available.

REFERENCES

1. H. A. L. Kiers, Towards a standardized notation and terminology in multiway analysis. *Journal of Chemometrics* 14, 3 (2000):105–122.
2. L. R. Tucker, The extension of factor analysis to three-dimensional matrices, in *Contributions to Mathematical Psychology*, eds., N. Frederiksen and H. Gulliksen (New York: Holt, Rinehart & Winston, 1964):110–182.
3. L. R. Tucker, Some mathematical notes on three-mode factor analysis. *Psychometrika* 31 (1966):279–311.
4. R. A. Harshman, Foundations of the PARAFAC procedure: Models and conditions for an ‘explanatory’ multi-modal factor analysis. *UCLA Working Papers in Phonetics* 16 (1970):1–84.
5. J. D. Carroll and J. Chang, Analysis of individual differences in multidimensional scaling via an N-way generalization of ‘Eckart-Young’ decomposition. *Psychometrika* 35 (1970):283–319.
6. R. B. Cattell, Parallel proportional profiles and other principles for determining the choice of factors by rotation. *Psychometrika* 9 (1944):267–283.
7. C. A. Andersson and R. Bro, Special issue: Multiway analysis. *Journal of Chemometrics* 14, 3(2000):103.
8. A. K. Smilde, R. Bro, and P. Geladi, *Multi-way Analysis. Applications in the Chemical Sciences* (Chichester, Wiley, 2004).
9. R. Bro, J. Workman, Jr., P. Mobley, and B. R. Kowalski, Review of chemometrics applied to spectroscopy: 1985–1995, part III: Multi-way analysis. *Applied Spectroscopy Reviews* 32 (1997):237–261.
10. F. Vogt, B. Dable, J. Cramer, and K. Booksh, Recent advancements in chemometrics for smart sensors. *Analyst* 129, 6 (2004):492–502.
11. C. M. Andersen and R. Bro, Practical aspects of PARAFAC modelling of fluorescence excitation-emission data. *Journal of Chemometrics* 17 (2003):200–215.
12. E. Sanchez and B. R. Kowalski, Tensorial calibration: II. second-order calibration. *Journal of Chemometrics* 2 (1988):265–280.
13. L. Moberg, G. Robertsson, and B. Karlberg, 3d Spectrofluorimetric determination of chlorophylls and pheopigments using parallel factor analysis. *Talanta* 54, 1 (2001):161–170.
14. L. Moberg and B. Karlberg, Validation of a multivariate calibration method for the determination of chlorophyll a, b and c and their corresponding pheopigments. *Analytica Chimica Acta* 450, 1–2 (2001):143–153.
15. R. D. Jiji, G. G. Andersson, and K. S. Booksh, Application of PARAFAC for calibration with excitation-emission matrix fluorescence spectra of three classes of environmental pollutants. *Journal of Chemometrics* 14, 3 (2000):171–185.
16. M. L. Nahorniak, G. A. Cooper, Y. C. Kim, and K. S. Booksh, Three- and four-way parallel factor (PARAFAC) analysis of photochemically induced excitation-emission kinetic fluorescence spectra. *Analyst* 130, 1 (2005):85–93.
17. M. C. Mahedero, N. M. Diaz, A. M. de la Pena, A. E. Mansilla, D. G. Gomez, and D. B. Gil, Strategies for solving matrix effects in the analysis of sulfathiazole in honey samples using three-way photochemically induced fluorescence data. *Talanta* 65, 3 (2005):806–813.
18. R. P. Nikolajsen, A. M. Hansen, and R. Bro, Attempt to separate the fluorescence spectra of adrenaline and noradrenaline using chemometrics. *Luminescence* 16, 2 (March 2001):91–101.
19. R. P. H. Nikolajsen, K. S. Booksh, A. M. Hansen, and R. Bro, Quantifying catecholamines using multi-way kinetic modelling. *Analytica Chimica Acta* 475, 1–2(2003):137–150.
20. A. C. Olivieri, J. A. Arancibia, A. M. de la Pena, I. Duran-Meras, and A. E. Mansilla, Second-order advantage achieved with four-way fluorescence excitation-emission-kinetic data processed by parallel factor analysis and trilinear least-squares. Determination of methotrexate and leucovorin in human urine. *Analytical Chemistry* 76, 19 (2004):5657–5666.
21. M. J. Rodriguez-Cuesta, R. Boque, F. X. Rius, D. P. Zamora, M. M. Galera, and A. G. Frenich, Determination of carbendazim, fuberidazole and thiabendazole by three-dimensional excitation-emission matrix fluorescence and parallel factor analysis. *Analytica Chimica Acta* 491, 1 (2003):47–56.
22. R. A. Gimeno, J. L. Beltran, R. M. Marce, and F. Borrull, Determination of naphthalenesulfonates in water by on-line ion-pair solid-phase extraction and ion-pair liquid chromatography with fast- scanning fluorescence detection. *J. Chromatogr. A* 890, 2 (August 2000):289–294.
23. M. G. Trevisan and R. J. Poppi, Determination of doxorubicin in human plasma by excitation-emission matrix fluorescence and multi-way analysis. *Analytica Chimica Acta* 493, 1 (2003):69–81.
24. D. Gimenez, L. Sarabia, and M. C. Ortiz, The maintenance of a PARAFAC calibration and the second-order property:

Application to the determination of ciprofloxacin in presence of enrofloxacin by excitation-emission fluorescence. *Analytica Chimica Acta* 544, 1–2(2005):327–336.

25. P. C. Damiani, A. J. Nepote, M. Bearzotti, and A. C. Olivieri, A test field for the second-order advantage in bilinear least-squares and parallel factor analyses: Fluorescence determination of ciprofloxacin in human urine. *Analytical Chemistry* 76, 10 (2004):2798–2806.
26. J. A. Hernandez-Arteseros, J. L. Beltran, R. Compano, and M. D. Prat, Fast-scanning fluorescence spectroscopy as a detection system in liquid chromatography for confirmatory analysis of flumequine and oxolinic acid. *Journal of Chromatography A* 942, 1–2 (2002):275–281.
27. D. Gimenez, L. A. Sarabia, and M. C. Ortiz, Identification and quantification of enrofloxacine in poultry feeding water through excitation emission fluorescence and three-way PARAFAC calibration. *Analyst* 130, 12 (2005):1639–1647.
28. J. C. G. E. da Silva, J. M. M. Leitao, F. S. Costa, and J. L. A. Ribeiro, Detection of verapamil drug by fluorescence and trilinear decompositim techniques. *Analytica Chimica Acta* 453, 1 (2002):105–115.
29. A. G. Frenich, D. P. Zamora, M. M. Galera, and J. L. M. Vidal, Application of GRAM and TLD to the resolution and quantitation of real complex multicomponent mixtures by fluorescence spectroscopy. *Analytical and Bioanalytical Chemistry* 375, 7 (2003):974–980.
30. S. J. Hart and R. D. Jiji, Light emitting diode excitation emission matrix fluorescence spectroscopy. *Analyst* 127, 12 (2002):1693–1699.
31. Y. Z. Cao, C. Y. Mo, J. G. Long, H. Chen, H. L. Wu, and R. Q. Yu, Spectrofluorometric resolution of closely overlapping drug mixtures using chemometrics methods. *Analytical Sciences* 18, 3 (2002):333–336.
32. G. M. Escandar, D. G. Gomez, A. E. Mansilla, A. M. de la Pena, and H. C. Goicoechea, Determination of carbamazepine in serum and pharmaceutical preparations using immobilization on a nylon support and fluorescence detection. *Analytica Chimica Acta* 506, 2 (2004):161–170.
33. A. M. de la Pena, A. E. Mansilla, D. G. Gomez, A. C. Olivieri, and H. C. Goicoechea, Interference-free analysis using three-way fluorescence data and the parallel factor model. Determination of fluoroquinolone antibiotics in human serum. *Analytical Chemistry* 75, 11 (2003):2640–2646.
34. A. Espinosa-Mansilla, A. M. de la Pena, D. G. Gomez, and F. Salinas, Photoinduced spectrofluorimetric determination of fluoroquinolones in human urine by using three- and two-way spectroscopic data and multivariate calibration. *Analytica Chimica Acta* 531, 2 (2005):257–266.
35. M. M. Sena, M. G. Trevisan, and R. J. Poppi, PARAFAC: A chemometric tool for multi-dimensional data treatment. Applications in direct determination of drugs in human plasma by spectrofluorimetry. *Quimica Nova* 28, 5 (2005):910–920.
36. D. K. Pedersen, L. Munck, and S. B. Engelsen, Screening for dioxin contamination in fish oil by PARAFAC and N-PLSR analysis of fluorescence landscapes. *Journal of Chemometrics* 16, 8–10 (2002):451–460.
37. F. Guimet, J. Ferre, R. Boque, and F. X. Rius, Application of unfold principal component analysis and parallel factor analysis to the exploratory analysis of olive oils by means of excitation-emission matrix fluorescence spectroscopy. *Analytica Chimica Acta* 515, 1 (2004):75–85.
38. F. Guimet, J. Ferre, and R. Boque, Rapid detection of olive-pomace oil adulteration in extra virgin olive oils from the protected denomination of origin “Siurana” using excitation-emission fluorescence spectroscopy and three-way methods of analysis. *Analytica Chimica Acta* 544, 1–2 (2005):143–152.
39. F. Guimet, J. Ferre, R. Boque, M. Vidal, and J. Garcia, Excitation-emission fluorescence spectroscopy combined with three-way methods of analysis as a complementary technique for olive oil characterization. *Journal of Agricultural and Food Chemistry* 53, 24 (2005):9319–9328.
40. D. Baunsgaard, C. A. Andersson, A. Arndal, and L. Munck, Multi-way chemometrics for mathematical separation of fluorescent colorants and colour precursors from spectrofluorimetry of beet sugar and beet sugar thick juice as validated by HPLC analysis. *Food Chemistry* 70, 1 (2000):113–121.
41. D. Baunsgaard, L. Munck, and L. Nørgaard, Analysis of the effect of crystal size and color distribution on fluorescence measurements of solid sugar using chemometrics. *Applied Spectroscopy* 54, 11 (2000):1684–1689.
42. D. Baunsgaard, L. Nørgaard, and M. A. Godshall, Specific screening for color precursors and colorants in beet and cane sugar liquors in relation to model colorants using spectrofluorometry evaluated by hplc and multiway data analysis. *Journal of Agricultural and Food Chemistry* 49, 4 (April 2001):1687–1694.
43. J. K. S. Møller, G. Parolari, L. Gabba, J. Christensen, and L. H. Skibsted, Monitoring chemical changes of dry-cured parma ham during processing by surface autofluorescence spectroscopy. *Journal of Agricultural and Food Chemistry* 51, 5 (2003):1224–1230.
44. J. Christensen, E. M. Becker, and C. S. Frederiksen, Fluorescence spectroscopy and PARAFAC in the analysis of yogurt. *Chemometrics and Intelligent Laboratory Systems* 75, 2 (2005):201–208.
45. C. M. Andersen, M. Vishart, and V. K. Holm, Application of fluorescence spectroscopy in the evaluation of light-induced oxidation in cheese. *Journal of Agricultural and Food Chemistry* 53, 26 (2005):9985–9992.
46. J. Christensen, V. T. Povlsen, and J. Sørensen, Application of fluorescence spectroscopy and chemometrics in the evaluation of processed cheese during storage. *Journal Of Dairy Science* 86, 4 (2003):1101–1107.
47. Y. N. Ni, D. Q. Lin, and S. Kokot, Synchronous fluorescence and UV-vis spectrometric study of the competitive interaction of chlorpromazine hydrochloride and Neutral Red with DNA using chemometrics approaches. *Talanta* 65, 5 (2005):1295–1302.
48. H. Shirakawa and S. Miyazaki, Blind spectral decomposition of single-cell fluorescence by parallel factor analysis. *Biophysical Journal* 86, 3 (2004):1739–1752.
49. J. H. Christensen, A. B. Hansen, J. Mortensen, and O. Andersen, Characterization and matching of oil samples using fluorescence spectroscopy and parallel factor analysis. *Analytical Chemistry* 77, 7 (2005):2210–2217.
50. M. L. Nahorniak and K. S. Booksh, Optimizing the implementation of the PARAFAC method for near-real time calibration of excitation-emission fluorescence analysis. *Journal of Chemometrics* 17, 11 (2003):608–617.

51. S. J. Hart, G. J. Hall, and J. E. Kenny, A laser-induced fluorescence dual-fiber optic array detector applied to the rapid HPLC separation of polycyclic aromatic hydrocarbons. *Analytical and Bioanalytical Chemistry* 372, 1 (2002):205–215.
52. E. Selli, C. Zaccaria, F. Sena, G. Tomasi, and G. Bidoglio, Application of multi-way models to the time-resolved fluorescence of polycyclic aromatic hydrocarbons mixtures in water. *Water Research* 38, 9 (2004):2269–2276.
53. P. D. Wentzell, S. S. Nair, and R. D. Guy, Three-way analysis of fluorescence spectra of polycyclic aromatic hydrocarbons with quenching by nitromethane. *Analytical Chemistry* 73, 7 (2001):1408–1415.
54. C. A. Stedmon, S. Markager, and R. Bro, Tracing dissolved organic matter in aquatic environments using a new approach to fluorescence spectroscopy. *Marine Chemistry* 82, 3–4 (2003):239–254.
55. M. B. Haack, A. Eliasson, and L. Olsson, On-line cell mass monitoring of Saccharomyces cerevisiae cultivations by multi-wavelength fluorescence. *Journal of Biotechnology* 114, 1–2 (2004):199–208.
56. R. D. Jiji and K. S. Booksh, Mitigation of Rayleigh and Raman spectral interferences in multiway calibration of excitation-emission matrix fluorescence spectra. *Analytical Chemistry* 72, 4 (2000):718–725.
57. A. Rinnan and C. M. Andersen, Handling of first-order Rayleigh scatter in PARAFAC modelling of fluorescence excitation-emission data. *Chemometrics and Intelligent Laboratory Systems* 76, 1 (2005):91–99.
58. A. Rinnan, K. Booksh, and R. Bro, First order Rayleigh as a separate component in the decomposition of fluorescence landscapes. *Analytica Chimica Acta* 537 (2005):349–358.
59. L. G. Thygesen, Å. Rinnan, S. Barsberg, and J. K. S, Møller, Stabilizing the PARAFAC decomposition of fluorescence spectra by insertion of zeros outside the data area. *Chemometrics and Intelligent Laboratory Systems* 71, 2 (2004):97–106.
60. R. G. Zepp, W. M. Sheldon, and M. A. Moran, Dissolved organic fluorophores in southeastern US coastal waters: correction method for eliminating Rayleigh and Raman scattering peaks in excitation–emission matrices. *Marine Chemistry* 89 (2004):15–36.
61. Z. P. Chen and R. Q. Yu, Mitigating model deficiency in three-way data analysis by the combination of background constraining and iterative correcting techniques. *Analytica Chimica Acta* 487, 2 (2003):171–180.
62. E. R. Malinowski, *Factor Analysis in Chemistry* (John Wiley and Sons, New York, 2002).
63. K. J. Johnson, B. J. Prazen, R. K. Olund, and R. E. Synovec, GC × GC temperature programming requirements to produce bilinear data for chemometric analysis. *Journal of Separation Science* 25, 5–6 (2002):297–303.
64. R. E. Synovec, B. J. Prazen, K. J. Johnson, C. G. Fraga, and C. A. Bruckner, Chemometric analysis of comprehensive two-dimensional separations. *Advances in Chromatography*, 42 (2003):1–42.
65. V. G. van Mispelaar, A. C. Tas, A. K. Smilde, P. J. Schoenmakers, and A. C. van Asten, Quantitative analysis of target components by comprehensive two-dimensional gas chromatography. *Journal of Chromatography A* 1019, 1–2 (2003):15–29.
66. A. E. Sinha, C. G. Fraga, B. J. Prazen, and R. E. Synovec, Trilinear chemometric analysis of two-dimensional comprehensive gas chromatography-time-of-flight mass spectrometry data. *Journal of Chromatography A* 1027, 1–2 (2004):269–277.
67. B. J. Prazen, K. J. Johnson, A. Weber, and R. E. Synovec, Two-dimensional gas chromatography and trilinear partial least squares for the quantitative analysis of aromatic and naphthene content in naphtha. *Analytical Chemistry* 73, 23 (2001):5677–5682.
68. V. Pravdova, C. Boucon, S. de Jong, B. Walczak, and D. L. Massart, Three-way principal component analysis applied to food analysis: an example. *Analytica Chimica Acta* 462, 2 (2002):133–148.
69. K. J. Johnson, S. L. Rose-Pehrsson, and R. E. Morris, Monitoring diesel fuel degradation by gas chromatography-mass Spectroscopy and chemometric analysis. *Energy & Fuels* 18, 3 (2004):844–850.
70. C. G. Fraga, B. J. Prazen, and R. E. Synovec, Comprehensive two-dimensional gas chromatography and chemometrics for the high-speed quantitative analysis of aromatic isomers in a jet fuel using the standard addition method and an objective retention time alignment algorithm. *Analytical Chemistry* 72, 17 (September 2000):4154–4162.
71. C. G. Fraga, C. A. Bruckner, and R. E. Synovec, Increasing the number of analyzable peaks in comprehensive two dimensional separations through chemometrics. *Analytical Chemistry* 73, 3 (2001):675–683.
72. A. E. Sinha, J. L. Hope, B. J. Prazen, C. G. Fraga, E. J. Nilsson, and R. E. Synovec, Multivariate selectivity as a metric for evaluating comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry subjected to chemometric peak deconvolution. *Journal of Chromatography A* 1056, 1–2 (2004):145–154.
73. A. E. Sinha, J. L. Hope, B. J. Prazen, E. J. Nilsson, R. M. Jack, and R. E. Synovec, Algorithm for locating analytes of interest based on mass spectral similarity in GC × GC-TOF-MS data: analysis of metabolites in human infant urine. *Journal of Chromatography A* 1058, 1–2 (2004):209–215.
74. I. Garcia, L. Sarabia, M. C. Ortiz, and J. M. Aldama, Three-way models and detection capability of a gas chromatography-mass spectrometry method for the determination of clenbuterol in several biological matrices: the 2002/657/EC European Decision. *Analytica Chimica Acta* 515, 1 (2004):55–63.
75. I. Garcia, L. Sarabia, M. C. Ortiz, and J. M. Aldama, Building robust calibration models for the analysis of estrogens by gas chromatography with mass spectrometry detection. *Analytica Chimica Acta* 526, 2 (2004):139–146.
76. C. G. Fraga, B. J. Prazen, and R. E. Synovec, Enhancing the limit of detection for comprehensive two-dimensional gas chromatography (GC × GC) using bilinear chemometric analysis. *Journal of High Resolution Chromatography* 23, 3 (2000):215–224.
77. K. Istvan, R. Rajko, and G. Keresztury, Towards the solution of the eluent elimination problem in high-performance liquid chromatography-infrared spectroscopy measurements by chemometric methods. *Journal of Chromatography A* 1104, 1–2 (2006):154–163.
78. Z. G. Wang, J. H. Jiang, Y. J. Ding, H. L. Wu, and R. Q. Yu, Trilinear evolving factor analysis for the resolution of three-way multi-component chromatograms. *Analytica Chimica Acta* 558, 1–2 (2006):137–143.

79. I. Garcia, L. Sarabia, M. C. Ortiz, and J. M. Aldama, Robustness of the extraction step when parallel factor analysis (PARAFAC) is used to quantify sulfonamides in kidney by high performance liquid chromatography-diode array detection (HPLC-DAD). *Analyst* 129, 8 (2004):766–771.
80. K. Wiberg and S. P. Jacobsson, Parallel factor analysis of HPLC-DAD data for binary mixtures of lidocaine and prilocaine with different levels of chromatographic separation. *Analytica Chimica Acta* 514, 2 (2004):203–209.
81. C. G. Fraga and C. A. Corley, The chemometric resolution and quantification of overlapped peaks form comprehensive two-dimensional liquid chromatography. *Journal of Chromatography A* 1096, 1–2 (2005):40–49.
82. J. Saurina, S. Hernandez-Cassou, A. Izquierdo-Ridorsa, and R. Tauler, pH-Gradient spectrophotometric data files from flow-injection and continuous flow systems for two- and three-way data analysis. *Chemometrics and Intelligent Laboratory Systems* 50, 2 (2000):263–271.
83. J. Saurina and S. Hernandez-Cassou, Quantitative determinations in conventional flow injection analysis based on different chemometric calibration statregies: A review. *Analytica Chimica Acta* 438, 1–2 (2001):335–352.
84. B. Karlberg and R. Torgrip, Increasing the scope and power of flow-injection analysis through chemometric approaches. *Analytica Chimica Acta* 500, 1–2 (2003):299–306.
85. M. M. Reis, S. P. Gurden, A. K. Smilde, and M. M. C, Ferreira, Calibration and detailed analysis of second-order flow injection analysis data with rank overlap. *Analytica Chimica Acta* 422, 1 (2000):21–36.
86. N. R. Marsili, A. Lista, B. S. F. Band, H. C. Goicoechea, and A. C. Olivieri, New method for the determination of benzoic and sorbic acids in commercial orange juices based on second-order spectrophotometric data generated by a pH gradient flow injection technique. *Journal of Agricultural and Food Chemistry* 52, 9 (2004):2479–2484.
87. M. Pistonesi, M. E. Centurion, B. S. F. Band, P. C. Damiani, and A. C. Olivieri, Simultaneous determination of levodopa and benserazide by stopped-flow injection analysis and three-way multivariate calibration of kinetic-spectrophotometric data. *Journal of Pharmaceutical and Biomedical Analysis* 36, 3 (2004):541–547.
88. B. Antalek, J. M. Hewitt, W. Windig, P. D. Yacobucci, T. Mourey, and K. Le, The use of PGSE NMR and DECRA for determining polymer composition. *Magnetic Resonance in Chemistry* 40 (2002):S60-S71.
89. W. Windig and B. Antalek, Direct exponential curve resolution algorithm (DECRA): A novel application of the generalized rank annihilation method for a single spectral mixture data set with exponentially decaying contribution profiles. *Chemometrics and Intelligent Laboratory Systems* 37, 2 (1997):241–254.
90. W. Windig, B. Antalek, M. J. Robbins, N. Zumbulyadis, and C. E. Heckler, Applications of the direct exponential curve resolution algorithm (DECRA) to solid state nuclear magnetic resonance and mid-infrared spectra. *Journal of Chemometrics* 14, 3 (2000):213–227.
91. R. Bro, P. I. Hansen, N. Vierick, M. Dyrby, H. T. Pedersen, and S. B. Engelsen, A new principle for unique spectral decomposition of 2D NMR data, in *Magnetic Resonance in Food Science. The Multivariate Challenge*, eds. S. B. Engelsen, P. S. Belton, and H. J. Jakobsen, The Royal Society of Chemistry, 2005) 195–203.
92. S. B. Engelsen and R. Bro, PowerSlicing. *Journal of Magnetic Resonance* 163, 1 (2003):192–197.
93. H. T. Pedersen, R. Bro, and S. B. Engelsen, SLICING—in a novel approach for unique deconvolution of NMR relaxation decays, *Magnetic Resonance in Food Science: A View to the Future* Royal Society of Chemistry, Cambridge, 2001) 202–209.
94. H. T. Pedersen, R. Bro, and S. B. Engelsen, Towards rapid and unique curve resolution of low-field NMR relaxation data: Trilinear SLICING versus two-dimensional curve fitting. *Journal of Magnetic Resonance* 157 (2002):141–155.
95. V. T. Povlsen, Å. Rinnan, F. van den Berg, H. J. Andersen, and A. K. Thybo, Direct decomposition of NMR relaxation profiles and prediction of sensory attributes of potato samples. *Lebensmittel-Wissenschaft Und-Technologie-Food Science and Technology* 36, 4 (2003):423–432.
96. K. N. Jensen, H. S. Guldager, and B. M. Jørgensen, Three-way modelling of NMR relaxation profiles from thawed cod muscle. *Journal of Aquatic Food Product and Technology* 11 (2002):201–214.
97. A. Nordon, C. Meunier, R. H. Carr, P. J. Gemperline, and D. Littlejohn, Determination of the ethylene oxide content of polyether polyols by low-field H-1 nuclear magnetic resonance spectrometry. *Analytica Chimica Acta* 472, 1–2 (2002):133–140.
98. A. Nordon, P. J. Gemperline, C. A. McGill, and D. Littlejohn, Quantitative analysis of low-field NMR signals in the time domain. *Analytical Chemistry* 73, 17 (2001):4286–4294.
99. D. M. Korzhnev, I. V. Ibraghimov, M. Billeter, and V. Y. Orekhov, MUNIN: Application of three-way decomposition to the analysis of heteronuclear NMR relaxation data. *Journal of Biomolecular NMR* 21, 3 (2001):263–268.
100. V. Y. Orekhov, I. V. Ibraghimov, and M. Billeter, MUNIN: A new approach to multi-dimensional NMR spectra interpretation. *Journal of Biomolecular NMR* 20, 1 (2001):49–60.
101. V. Y. Orekhov, I. Ibraghimov, and M. Billeter, Optimizing resolution in multidimensional NMR by three-way decomposition. *Journal of Biomolecular NMR* 27, 2 (2003):165–173.
102. A. Gutmanas, P. Jarvoll, V. Y. Orekhov, and M. Billeter, Three-way decomposition of a complete 3D N-15-NOESY-HSQC. *Journal of Biomolecular NMR* 24, 3 (2002):191–201.
103. A. H. Andersen and W. S. Rayens, Structure-seeking multilinear methods for the analysis of MRI data. *Neuroimage* 22, 2 (2004):728–739.
104. C. F. Beckmann and S. M. Smith, Tensorial extensions of independent component analysis for multisubject FMRI analysis. *Neuroimage* 25, 1 (2005):294–311.
105. M. Dyrby, Multivariate analysis of highfield NMR data in food and medicine. PhD Dissertion, The Royal Veterinary & Agricultural University, Copenhagen, Denmark 2004.
106. M. Dyrby, M. Peteresen, A. D. Whittaker, L. Lambert, L. Nørgaard, R. Bro, and S. B. Engelsen, Analysis of lipoproteins using 2D diffusion-edited NMR spectroscopy and multi-way chemometrics. *Analytica Chimica Acta* 531 (2005):209–216.
107. M. Dyrby, D. Baunsgaard, R. Bro, and S. B. Engelsen, Multiway chemometric analysis of the metabolic response to toxins monitored by NMR. *Chemometrics and Intelligent Laboratory Systems* 76, 1 (2005):79–89.

108. F. Estienne, N. Matthijs, D. L. Massart, P. Ricoux, and D. Leibovici, Multi-way modelling of high-dimensionality electroencephalographic data. *Chemometrics and Intelligent Laboratory Systems* 58, 1 (2001):59–72.
109. E. Martinez-Montes, P. A. Valdes-Sosa, F. Miwakeichi, R. I. Goldman, and M. S. Cohen. Concurrent EEG/fMRI analysis by multiway partial least squares. *Neuroimage* 22, 3 (2004):1023–1034.
110. E. Martinez-Montes, P. A. Valdes-Sosa, F. Miwakeichi, R. I. Goldman, and M. S. Cohen. Concurrent EEG/fMRI analysis by multiway partial least squares (vol 22, pg 1023, 2004). *Neuroimage* 26, 3 (2005):973.
111. F. Miwakeichi, E. Martinez-Montes, P. A. Valdes-Sosa, N. Nishiyama, H. Mizuhara, and Y. Yamaguchia, Decomposing EEG data into space-time-frequency components using Parallel Factor Analysis. *Neuroimage* 22, 3 (2004):1035–1045.
112. M. Mørup, L. K. Hansen, C. S. Herrmann, J. Parnas, and S. M. Arnfred, Parallel Factor Analysis as an exploratory tool for wavelet transformed event-related EEG. *Neuroimage* 29, 3 (2006):938–947.
113. P. Geladi and P. Åberg, Three-way modelling of a batch organic synthesis process monitored by near infrared spectroscopy. *Journal of Near Infrared Spectroscopy* 9, 1 (2001):1–9.
114. P. Geladi and J. Forsström, Monitoring, of a batch organic synthesis by near-infrared spectroscopy: modeling and interpretation of three-way data. *Journal of Chemometrics* 16, 7 (2002):329–338.
115. J. P. Nielsen, D. Bertrand, E. Micklander, P. Courcoux, and L. Munck, Study of NIR spectra, particle size distributions and chemical parameters of wheat flours: A multi-way approach. *Journal of Near-Infrared Spectroscopy* 9 (2001):275–285.
116. A. M. Antunes, M. M. C. Ferreira, and P. L. O, Volpe, A chemometric study of amino acid transport through liquid membranes using UV-Vis spectroscopy. *Journal of Chemometrics* 16, 2 (2002):111–116.
117. H. Abdollahi and F. Nazari, Rank annihilation factor analysis for spectrophotometric study of complex formation equilibria. *Analytica Chimica Acta* 486, 1 (2003):109–123.
118. M. M. Sena, J. C. B. Fernandes, L. Rover, R. J. Poppi, and L. T. Kubota, Application of two- and three-way chemometric methods in the study of acetylsalicylic acid and ascorbic acid mixtures using ultraviolet spectrophotometry. *Analytica Chimica Acta* 409, 1–2 (2000):159–170.
119. J. M. M. Leitao and J. C. G, E. da Silva, PARAFAC and PARAFAC2 calibration models for antihypertensor Nifedipine quantification. *Analytica Chimica Acta* 559, 2 (2006):271–280.
120. E. R. Pereira, M. M. Sena, M. A. Z. Arruda, and R. J. Poppi, Exploratory analysis of L'vov platform surfaces for electrothermal atomic absorption spectrometry by using three-way chemometric tools. *Analytica Chimica Acta* 495, 1–2 (2003):177–193.
121. T. Skov and R. Bro, A new approach for modelling sensor based data. *Sensors and Actuators B* 106, 2 (2005):719–729.
122. S. Serneels, M. Moens, P. J. Van Espen, and F. Blockhuys, Identification of micro-organisms by dint of the electronic nose and trilinear partial least squares regression. *Analytica Chimica Acta* 516, 1–2 (2004):1–5.
123. W. P. Gardner, R. E. Shaffer, J. E. Girard, and J. H. Callahan, Application of quantitative chemometric analysis techniques to direct sampling mass spectrometry. *Analytical Chemistry* 73, 3 (2001):596–605.
124. Y. Q. Wu, B. Yuan, J. G. Zhao, and Y. Ozaki, Hybrid two-dimensional correlation and parallel factor studies on the switching dynamics of a surface-stabilized ferroelectric liquid crystal. *Journal Of Physical Chemistry B* 107, 31 (2003):7706–7715.
125. A. Marcos, M. Foulkes, and S. J. Hill, Application of a multi-way method to study long-term stability in ICP-AES. *Journal of Analytical Atomic Spectrometry* 16, 2 (2001):105–114.
126. A. Moreda-Pineiro, A. Marcos, A. Fisher, and S. J. Hill, Parallel factor analysis for the study of systematic error in inductively coupled plasma atomic emission spectrometry and mass spectrometry. *Journal of Analytical Atomic Spectrometry* 16, 4 (2001):360–369.
127. A. Herrero, S. Zamponi, R. Marassi, P. Conti, M. C. Ortiz, and L. A. Sarabia, Determination of the capability of detection of a hyphenated method: Application to spectroelectrochemistry. *Chemometrics and Intelligent Laboratory Systems* 61, 1–2 (2002):63–74.
128. P. Aberg, P. Geladi, I. Nicander, and S. Ollmar, Variation of skin properties within human forearms demonstrated by non-invasive detection and multi-way analysis. *Skin Research and Technology* 8, 3 (2002):194–201.
129. J. Huang, H. Wium, K. B. Qvist, and K. H. Esbensen, Multi-way methods in image analysis-relationships and applications. *Chemometrics and Intelligent Laboratory Systems* 66, 2 (2003):141–158.
130. M. A. O. Vasilescu and D. Terzopoulos, TensorTextures: Multilinear image-based rendering. *Acm Transactions on Graphics* 23, 3 (2004):336–342.
131. R. G. Brereton, Introduction to multivariate calibration in analytical chemistry. *Analyst* 125, 11 (2000):2125–2154.
132. R. Bro, Multivariate calibration—What is in chemometrics for the analytical chemist? *Analytica Chimica Acta* 500, 1–2 (2003):185–194.
133. R. Bro, A. K. Smilde, and S. de Jong, On the difference between low-rank and subspace approximation: Improved model for multilinear PLS regression. *Chemometrics and Intelligent Laboratory Systems* 58, 1 (2001):3–13.
134. I. Garcia, L. A. Sarabia, and M. C. Ortiz, Detection capability of tetracyclines analysed by a fluorescence technique: Comparison between bilinear and trilinear partial least squares models. *Analytica Chimica Acta* 501, 2 (2004):193–203.
135. A. Haimovich, R. Orselli, G. M. Escandar, and A. C. Olivieri, Spectroscopic bilinear least-squares methods exploiting the second-order advantage. Theoretical and experimental study concerning accuracy, sensitivity and prediction error. *Chemometrics and Intelligent Laboratory Systems* 80, 1 (2006):99–108.
136. Z. Zeng, Y. Y. Cheng, and G. F. Shen, A computational method for quantitative determining the active component of chinese medicine integrating PCA with GRAFA. *Acta Chimica Sinica* 61, 1 (2003):84–88.
137. H. L. Wu, R. Q. Yu, M. Shibukawa, and K. Oguma, Second-order standard addition method based on alternating trilinear decomposition. *Analytical Sciences* 16, 2 (2000):217–220.
138. E. Comas, R. A. Gimeno, J. Ferre, R. M. Marce, F. Borrull, and F. X. Rius, Time shift correction in second-order liquid

chromatographic data with iterative target transformation factor analysis. *Analytica Chimica Acta* 470, 2 (2002):163–173.

139. J. A. Arancibia, A. C. Olivieri, and G. M. Escandar, First- and second-order multivariate calibration applied to biological samples: determination of anti-inflammatories in serum and urine. *Analytical and Bioanalytical Chemistry* 374, 3 (2002):451–459.
140. M. V. Guterres, P. O. L. Volpe, and M. M. C., Ferreira, Multiway calibration for creatinine determination in human serum using the Jaffe reaction. *Applied Spectroscopy* 58, 1 (2004):54–60.
141. M. A. B. Levi, L. S. Scarminio, R. J. Poppi, and M. G. Trevisan, Three-way chemometric method study and UV-Vis absorbance for the study of simultaneous degradation of anthocyanins in flowers of the Hibiscus rosa-sinensys species. *Talanta* 62, 2 (2004):299–305.
142. J. Z. Lu, H. L. Wu, X. Y. Sun, H. Cui, J. Q. Sun, and R. Q. Yu, Simultaneous decomposition and determination of the complex dimethylphenol isomers by alternating trilinear decomposition algorithm combined with region selection. *Chinese Journal of Analytical Chemistry* 32, 10 (2004):1278–1282.
143. X. Ling, Y. Z. Cao, C. Y. Mo, and X. Y. Liu, Resolution of naphthalene, 1-naphthol and 2-naphthol using the parallel factor algorithm and three-way flourescence technique. *Chinese Journal of Analytical Chemistry* 29, 12 (2001):1412–1415.
144. J. Ghasemi and A. Niazi, Two- and three-way chemometrics methods applied for spectrophotometric determination of lorazepam in pharmaceutical formulations and biological fluids. *Analytica Chimica Acta* 533, 2 (2005):169–177.
145. J. A. Arancibia and G. M. Escandar, Two different strategies for the fluorimetric determination of piroxicam in serum. *Talanta* 60, 6 (2003):1113–1121.
146. E. Comas, R. A. Gimeno, J. Ferre, R. M. Marce, F. Borrull, and F. X. Rius, Using second-order calibration to identify and quantify aromatic sulfonates in water by high-performance liquid chromatography in the presence of coeluting interferences. *Journal of Chromatography A* 988, 2 (2003):277–284.
147. M. M. Sena, M. G. Trevisan, and R. J. Poppi, Combining standard addition method and second-order advantage for direct determination of salicylate in undiluted human plasma by spectrofluorimetry. *Talanta* 68, 5 (2006):1707–1712.
148. F. M. Fernandez, M. B. Tudino, and O. E. Troccoli, Multicomponent kinetic determination of Cu, Zn, Co, Ni and Fe at trace levels by first and second order multivariate calibration. *Analytica Chimica Acta* 433, 1 (2001):119–134.
149. C. G. Zampronio, S. P. Gurden, L. A. B. Moraes, M. N. Eberlin, A. K. Smilde, and R. J. Poppi, Direct sampling tandem mass spectrometry (MS/MS) and multiway calibration for isomer quantitation. *Analyst* 127, 8 (2002):1054–1060.
150. K. Hasegawa, M. Arakawa, and K. Funatsu, 3D-QSAR study of insecticidal neonicotinoid compounds based on 3-way partial least squares model. *Chemometrics and Intelligent Laboratory Systems* 47 (1999):33–40.
151. K. Hasegawa, M. Arakawa, and K. Funatsu, Rational choice of bioactive conformations through use of conformation analysis and 3-way partial least squares modeling. *Chemometrics and Intelligent Laboratory Systems* 50, 2 (2000):253–261.
152. K. Hasegawa, S. Matsuoka, M. Arakawa, and K. Funatsu, New molecular surface-based 3D-QSAR method using Kohonen neural network and 3-way PLS. *Computers and Chemistry* 26, 6 (2002):583–589.
153. K. Hasegawa, M. Arakawa, and K. Funatsu, Simultaneous determination of bioactive conformations and alignment rules by multi-way PLS modeling. *Computational Biology and Chemistry* 27, 3 (2003):211–216.
154. K. Hasegawa, S. Matsuoka, M. Arakawa, and K. Funatsu, Multiway PLS modeling of structure-activity data by incorporating electrostatic and lipophilic potentials on molecular surface. *Computational Biology and Chemistry* 27, 3 (2003):381–386.
155. M. M. C. Ferreira, Multivariate QSAR. *Journal of the Brazilian Chemical Society* 13, 6 (2002):742–753.
156. S. P. Gurden, J. A. Westerhuis, R. Bro, and A. K. Smilde, A comparison of multiway regression and scaling methods. *Chemometrics and Intelligent Laboratory Systems* 59, 1–2 (2001):121–136.
157. P. M. Hansen, J. R. Jorgensen, and A. Thomsen, Predicting grain yield and protein content in winter wheat and spring barley using repeated canopy reflectance measurements and partial least squares regression. *Journal of Agricultural Science* 139 (2002):307–318.
158. N. R. Marsili, A. Lista, B. S. F. Band, H. C. Goicoechea, and A. C. Olivieri, Evaluation of complex spectral-pH three-way arrays by modified bilinear least-squares: Determination of four different dyes in interfering systems. *Analyst* 130, 9 (2005):1291–1298.
159. H. C. Goicoechea, S. J. Yu, A. C. Olivieri, and A. D. Campiglia, Four-way data coupled to parallel factor model applied to environmental analysis: Determination of 2,3,7,8-tetrachloro-dibenzo-para-dioxin in highly contaminated waters by solid-liquid extraction laser-excited time-resolved Shpol'skii spectroscopy. *Analytical Chemistry* 77, 8 (2005):2608–2616.
160. A. K. Smilde, Comments on three-way analyses used for batch process data. *Journal of Chemometrics* 15, 1 (2001):19–27.
161. S. P. Gurden, J. A. Westerhuis, and A. K. Smilde, Monitoring of batch processes using spectroscopy. *AIChE Journal* 48, 10 (2002):2283–2297.
162. E. N. M. van Sprang, H. J. Ramaker, J. A. Westerhuis, S. P. Gurden, and A. K. Smilde, Critical evaluation of approaches for on-line batch process monitoring. *Chemical Engineering Science* 57 (2002):3979–3991.
163. E. N. M. van Sprang, H. J. Ramaker, J. A. Westerhuis, A. K. Smilde, S. P. Gurden, and D. Wienke, Near-infrared spectroscopic monitoring of a series of industrial batch processes using a bilinear grey model. *Applied Spectroscopy* 57, 8 (2003):1007–1019.
164. D. J. Louwerse and A. K. Smilde, Multivariate statistical process control of batch processes based on three-way models. *Chemical Engineering Science* 55, 7 (2000):1225–1235.
165. Z. I. Stefanov and K. A. Hoo, Hierarchical multivariate analysis of cockle phenomena. *Journal of Chemometrics* 17, 10 (2003):550–568.
166. Z. I. Stefanov, K. A. Hoo, W. McAdams, and M. Champagne, Cockle formation in coated magazine paper production. *IEEE Control Systems Magazine* 23, 6 (2003):59–68.
167. M. Kallioinen, S. P. Reinikainen, J. Nuortila-Jokinen, M. Manttari, T. Sutela, and P. Nurminen, Chemometrical approach in studies of membrane capacity in pulp and paper mill application. *Desalination* 175, 1 (2005):87–95.
168. B. M. Wise, N. B. Gallagher, and E. B. Martin, Application of PARAFAC2 to fault detection and diagnosis in semiconductor etch. *Journal of Chemometrics* 15, 4 (2001):285–298.

169. J. A. Lopes and J. C. Menezes, Industrial fermentation end-product modelling with multilinear PLS. *Chemometrics and Intelligent Laboratory Systems* 68, 1–2 (2003):75–81.
170. S. P. Gurden, J. A. Westerhuis, S. Bijlsma, and A. K. Smilde, Modelling of spectroscopic batch process data using grey models to incorporate external information. *Journal of Chemometrics* 15, 2 (2001):101–121.
171. J. H. Chen and J. H. Yen, Three-way data analysis with time lagged window for on-line batch process monitoring. *Korean Journal of Chemical Engineering* 20, 6 (2003):1000–1011.
172. X. Meng, A. J. Morris, and E. B. Martin, On-line monitoring of batch processes using a PARAFAC representation. *Journal of Chemometrics* 17, 1 (2003):65–81.
173. T. F. Cox, Multidimensional scaling used in multivariate statistical process control. *Journal of Applied Statistics* 28, 3–4 (2001):365–378.
174. S. C. Connor, W. Wu, B. C. Sweatman, J. Manini, J. N. Haselden, D. J. Crowther, and C. J. Waterfield, Effects of feeding and body weight loss on the H-1-NMR-based urine metabolic profiles of male Wistar–Han rats: Implications for biomarker discovery. *Biomarkers* 9, 2 (2004):156–179.
175. H. Idborg, P. O. Edlund, and S. P. Jacobsson, Multivariate approaches for efficient detection of potential metabolites from liquid chromatography/mass spectrometry data. *Rapid Communications In Mass Spectrometry* 18, 9 (2004):944–954.
176. P. Barbieri, G. Adami, S. Piselli, F. Gemiti, and E. Reisenhofer, A three-way principal factor analysis for assessing the time variability of freshwaters related to a municipal water supply. *Chemometrics and Intelligent Laboratory Systems* 62, 1 (2002):89–100.
177. R. Leardi, C. Armanino, S. Lanteri, and L. Alberotanza, Three-mode principal component analysis of monitoring data from Venice lagoon. *Journal of Chemometrics* 14, 3 (2000):187–195.
178. T. Miettinen, T. J. Hurse, M. A. Connor, S. P. Reinikainen, and P. Minkkinen, Multivariate monitoring of a biological wastewater treatment process: A case study at Melbourne Water's Western Treatment Plant. *Chemometrics and Intelligent Laboratory Systems* 73, 1 (2004):131–138.
179. J. C. Garcia-Diaz and J. M. Prats-Montalban. Characterization of soils irrigated with untreated urban wastewater using multiway techniques. *Chemometrics and Intelligent Laboratory Systems* 76, 1 (2005):15–24.
180. G. R. Flåten, B. Grung, and O. M. Kvalheim, Quantification of pollution levels by multiway modelling. *Journal of Chemometrics* 18, 3–4 (2004):173–182.
181. P. Paatero and S. Juntto, Determination of underlying components of a cyclical time series by means of two-way and three-way factor analytic techniques. *Journal of Chemometrics* 14, 3 (2000):241–259.
182. S. P. Reinikainen, P. Laine, P. Minkkinen, and P. Paatero, Factor analytical study on water quality in Lake Saimaa, Finland. *Fresenius Journal of Analytical Chemistry* 369, 7–8 (2001):727–732.
183. R. Tauler, S. Lacorte, M. Guillamon, R. Cespedes, P. Viana, and D. Barcelo, Chemometric modeling of main contamination sources in surface waters of Portugal. *Environmental Toxicology and Chemistry* 23, 3 (2004):565–575.
184. K. Bergant and L. Kajfez-Bogataj, N-PLS regression as empirical downscaling tool in climate change studies. *Theoretical and Applied Climatology* 81, 1–2 (2005):11–23.
185. R. Pardo, B. A. Helena, C. Cazurro, C. Guerra, L. Deban, C. M. Guerra, and M. Vega, Application of two- and three-way principal component analysis to the interpretation of chemical fractionation results obtained by the use of the BCR procedure. *Analytica Chimica Acta* 523, 1 (2004):125–132.
186. M. V. Bosco, M. Garrido, and M. S. Larrechi, Determination of phenol in the presence of its principal degradation products in water during a TiO_2-photocatalytic degradation process by three-dimensional excitation-emission matrix fluorescence and parallel factor analysis. *Analytica Chimica Acta* 559, 2 (2006):240–247.
187. W. Chueinta, P. K. Hopke, and P. Paatero, Multilinear model for spatial pattern analysis of the measurement of haze and visual effects project. *Environmental Science and Technology* 38, 2 (2004):544–554.
188. T. Yli-Tuomi, P. K. Hopke, P. Paatero, M. S. Basunia, S. Landsberger, Y. Viisanen, and J. Paatero, Atmospheric aerosol over Finnish Arctic: Source analysis by the multilinear engine and the potential source contribution function. *Atmospheric Environment* 37, 31 (2003):4381–4392.
189. R. M. Cory and D. M. McKnight, Fluorescence spectroscopy reveals ubiquitous presence of oxidized and reduced quinones in dissolved organic matter. *Environmental Science and Technology* 39, 21 (2005):8142–8149.
190. G. J. Hall, K. E. Clow, and J. E. Kenny, Estuarial fingerprinting through multidimensional fluorescence and multivariate analysis. *Environmental Science and Technology* 39, 19 (2005):7560–7567.
191. C. A. Stedmon and S. Markager, Tracing the production and degradation of autochthonous fractions of dissolved organic matter by fluorescence analysis. *Limnology and Oceanography* 50, 5 (2005):1415–1426.
192. P. Giordani and H. A. L, Kiers, Three-way component analysis of interval-valued data. *Journal of Chemometrics* 18, 5 (2004):253–264.
193. I. Stanimirova, B. Walczak, D. L. Massart, V. Simeonov, C. A. Saby, and E. Di Crescenzo, STATIS, a three-way method for data analysis. Application to environmental data. *Chemometrics and Intelligent Laboratory Systems* 73, 2 (2004):219–233.
194. E. Bezemer and S. C. Rutan, Three-way alternating least squares using three-dimensional tensors in MATLAB (R). *Chemometrics and Intelligent Laboratory Systems* 60, 1–2 (2002):239–251.
195. Y. M. Neuhold and M. Maeder, Hard-modelled trilinear decomposition (HTD) for an enhanced kinetic multicomponent analysis. *Journal of Chemometrics* 16, 5 (2002):218–227.
196. R. Dyson, M. Maeder, Y. M. Neuhold, and G. Puxty, Analyses of three-way data from equilibrium and kinetic investigations. *Analytica Chimica Acta* 490, 1–2 (2003):99–108.
197. S. R. Crouch, J. Coello, S. Maspoch, and M. Porcel, Evaluation of classical and three-way multivariate calibration procedures in kinetic-spectrophotometric analysis. *Analytica Chimica Acta* 424, 1 (2000):115–126.
198. J. M. D. Cueva, A. V. Rossi, and R. J. Poppi, Modeling kinetic spectrophotometric data of aminophenol isomers by PARAFAC2. *Chemometrics and Intelligent Laboratory Systems* 55, 1–2 (2001):125–132.
199. A. Niazi, J. Ghasemi, and A. Yazdanipour, PARAFAC decomposition of three-way kinetic-spectrophotometric spectral matrices based on phosphomolybdenum blue complex chemistry for nitrite

determination in water and meat samples. *Analytical Letters* 38, 14 (2005):2377–2392.

200. Y. X. Tan, J. H. Jiang, H. L. Wu, H. Cui, and R. Q. Yu, Resolution of kinetic system of simultaneous degradations of chlorophyll *a* and *b* by PARAFAC. *Analytica Chimica Acta* 412, 1–2 (2000):195–202.
201. S. Bijlsma, H. F. M. Boelens, H. C. J. Hoefsloot, and A. K. Smilde, Estimating reaction rate constants: comparison between traditional curve fitting and curve resolution. *Analytica Chimica Acta* 419 (2000):197–207.
202. S. Bijlsma and A. K. Smilde, Estimating reaction rate constants from a two-step reaction: a comparison between two-way and three-way methods. *Journal of Chemometrics* 14, 5–6 (2000):541–560.
203. A. de Juan, M. Maeder, M. Martinez, and R. Tauler, Combining hard- and soft-modelling to solve kinetic problems. *Chemometrics and Intelligent Laboratory Systems* 54, 2 (2000):123–141.
204. Z. L. Zhu, J. Xia, J. Zhang, and T. H. Li, Determination of rate constants from two-way kinetic-spectral data by using rank annihilation factor analysis. *Analytica Chimica Acta* 454, 1 (2002):21–30.
205. J. Coello, S. Maspoch, and N. Villegas, Simultaneous kinetic-spectrophotometric determination of levodopa and benserazide by bi- and three-way partial least squares calibration. *Talanta* 53, 3 (2000):627–637.
206. H. Morais, C. Ramos, E. Forgacs, T. Cserhati, J. Oliviera, and T. Illes, Three-dimensional principal component analysis employed for the study of the beta-glucosidase production of Lentinus edodes strains. *Chemometrics and Intelligent Laboratory Systems* 57, 1 (2001):57–64.
207. H. Morais, C. Ramos, E. Forgacs, A. Jakab, T. Cserhati, J. Oliviera, T. Illes, and Z. Illes, Comparison of principal analysis and the Tucker3 model—A case study. *Qsar and Combinatorial Science* 22, 4 (2003):449–455.
208. N. De Belie, M. Sivertsvik, and J. De Baerdemaeker, Differences in chewing sounds of dry-crisp snacks by multivariate data analysis. *Journal of Sound and Vibration* 266, 3 (2003):625–643.
209. I. Ovejero-Lopez, R. Bro, and W. L. P, Bredie, Univariate and multivariate modelling of flavour release in chewing gum using time-intensity: a comparison of data analytical methods. *Food Quality and Preference* 16, 4 (2005):327–343.
210. M. B. Let, C. Jacobsen, and A. S. Meyer, Effects of fish oil type, lipid antioxidants and presence of rapeseed oil on oxidative flavour stability of fish oil enriched milk. *European Journal of Lipid Science and Technology* 106, 3 (2004):170–182.
211. R. Bro and M. Jakobsen, Exploring complex interactions in designed data using GEMANOVA. Color changes in fresh beef during storage. *Journal of Chemometrics* 16, 6 (2002):294–304.
212. E. Ceulemans, I. Van Mechelen, and P. Kuppens, Adapting the formal to the substantive: Constrained Tucker3-HICLAS. *Journal of Classification* 21, 1 (2004):19–50.
213. E. Ceulemans and I. Van Mechelen, Hierarchical classes models for three-way three-mode binary data: Interrelations and model selection. *Psychometrika* 70, 3 (2005):461–480.
214. E. Ceulemans and I. Van Mechelen, Tucker2 hierarchical classes analysis. *Psychometrika* 69, 3 (2004):375–399.
215. R. S. K. Wong, Multidimensional association models—A multilinear approach. *Sociological Methods and Research* 30, 2 (2001):197–240.
216. Q. Q. Zhang, S. H. Lei, X. L. Wang, L. Wang, and C. J. Zhu, Discrimination of phytoplankton classes using characteristic spectra of 3D fluorescence spectra. *Spectrochimica Acta Part A—Molecular and Biomolecular Spectroscopy* 63, 2 (2006):361–369.
217. C. Wittrup, Comparison of chemometric methods for classification of fungal extracts based on rapid fluorescence spectroscopy. *Journal of Chemometrics* 14, 5–6 (2000):765–776.
218. N. Allosio, P. Boivin, D. Bertrand, and P. Courcoux, Characterisation of barley transformation into malt by three-way factor analysis of near infrared spectra. *Journal of Near Infrared Spectroscopy* 5 (1997):157–166.
219. P. Geladi, H. Bergner, and L. Ringqvist, From experimental design to images to particle size histograms to multiway analysis. An example of peat dewatering. *Journal of Chemometrics* 14, 3 (2000):197–211.
220. V. Pravdova, B. Walczak, D. L. Massart, H. Robberecht, R. Van Cauwenbergh, P. Hendrix, and H. Deelstra, Three-way principal component analysis for the visualization of trace elemental patterns in vegetables after different cooking procedures. *Journal of Food Composition and Analysis* 14, 2 (2001):207–225.
221. F. Estienne, Y. V. Heyden, and D. L. Massart, Chemometrics and modeling. *Chimia* 55, 1 (2001):70–80.
222. N. D. Sidiropoulos and R. Bro, PARAFAC Techniques for Signal separation, in *Signal Processing Advances in Communications*, eds, P. Stoica, G. B. Giannakis, Y. Hua, and L. Tong (Prentice-Hall, Englewood Cliffs, NJ, 2000).
223. R. Bro, F. van den Berg, A. K. Thybo, C. M. Andersen, B. M. Jørgensen, and H. andersen. Multivariate Data Analysis as a Tool in Advanced Quality Monitoring in the Food Production Chain. *Trends in Food Science and Technology* 13 (2002):235–244.
224. R. A. Harshman and S. J. Hong, 'Stretch' vs 'slice' methods for representing three-way structure via matrix notation. *Journal of Chemometrics* 16, 4 (2002):198–205.
225. R. A. Harshman, An index formalism that generalizes the capabilities of matrix notation and algebra to n-way arrays. *Journal of Chemometrics* 15, 9 (2001):689–714.
226. J. M. Andrade, M. P. Gomez-Carracedo, W. Krzanowski, and M. Kubista, Procrustes rotation in analytical chemistry, a tutorial. *Chemometrics and Intelligent Laboratory Systems* 72, 2 (2004):123–132.
227. V. Pravdova, F. Estienne, B. Walczak, and D. L. Massart, A robust version of the Tucker3 model. *Chemometrics and Intelligent Laboratory Systems* 59, 1–2 (2001):75–88.
228. S. A. Vorobyov, Y. Rong, N. D. Sidiropoulos, and A. B. Gershman, Robust iterative fitting of multilinear models. *IEEE Transactions on Signal Processing* 53, 8 (2005):2678–2689.
229. A. C. Olivieri, On a versatile second-order multivariate calibration method based on partial least-squares and residual bilinearization: Second-order advantage and precision properties. *Journal of Chemometrics* 19, 4 (2005):253–265.
230. J. A. Arancibia, A. C. Olivieri, D. B. Gil, A. E. Mansilla, B. Duran-Meras, and A. M. de la Pena, Trilinear least-squares and unfolded-PLS coupled to residual trilinearization: New chemometric tools for the analysis of four-way instrumental data. *Chemometrics and Intelligent Laboratory Systems* 80, 1 (2006):77–86.
231. N. M. Faber, J. Ferre, and R. Boque, Iteratively reweighted generalized rank annihilation method 1. Improved handling of

prediction bias. *Chemometrics and Intelligent Laboratory Systems* 55, 1–2 (2001):67–90.

232. N. M. Faber, R. Boque, and J. Ferre, Iteratively reweighted generalized rank annihilation method 2. Least squares property and variance expressions. *Chemometrics and Intelligent Laboratory Systems* 55, 1–2 (2001):91–100.
233. N. M. Faber, The price paid for the second-order advantage when using the generalized rank annihilation method (GRAM). *Journal of Chemometrics* 15, 9 (2001):743–748.
234. N. M. Faber, Quantifying the effect of measurement errors on the uncertainty in bilinear model predictions: A small simulation study. *Analytica Chimica Acta* 439, 2 (2001):193–201.
235. N. M. Faber, J. Ferre, R. Boque, and J. H. Kalivas, Second-order bilinear calibration: the effects of vectorising the data matrices of the calibration set. *Chemometrics and Intelligent Laboratory Systems* 63, 2 (2002):107–116.
236. N. M. Faber, Towards a rehabilitation of the generalized rank annihilation method (GRAM). *Analytical and Bioanalytical Chemistry* 372, 5–6 (2002):683–687.
237. A. K. Smilde, J. A. Westerhuis, and R. Boque, Multiway multiblock component and covariates regression models. *Journal of Chemometrics* 14, 3 (2000):301–331.
238. R. A. Harshman, S. J. Hong, and M. E. Lundy, Shifted factor analysis—Part I: Models and properties. *Journal of Chemometrics* 17, 7 (2003):363–378.
239. S. J. Hong and R. A. Harshman, Shifted factor analysis—Part II: Algorithms. *Journal of Chemometrics* 17, 7 (2003):379–388.
240. S. J. Hong and R. A. Harshman, Shifted factor analysis—Part III: N-way generalization and application. *Journal of Chemometrics* 17, 7 (2003):389–399.
241. R. Bro and H. A. L, Kiers, A new efficient method for determining the number of components in PARAFAC models. *Journal of Chemometrics* 17, 5 (2003):274–286.
242. Z. P. Chen, Z. Liu, Y. Z. Cao, and R. Q. Yu, Efficient way to estimate the optimum number of factors for trilinear decomposition. *Analytica Chimica Acta* 444, 2 (2001):295–307.
243. H. A. L. Kiers and A. D. Kinderen, A fast method for choosing the numbers of components in Tucker3 analysis. *British Journal of Mathematical and Statistical Psychology* 56 (2003):119–125.
244. H. P. Xie, J. H. Jiang, N. Long, G. L. Shen, H. L. Wu, and R. Q. Yu, Estimation of chemical rank of a three-way array using a two-mode subspace comparison approach. *Chemometrics and Intelligent Laboratory Systems* 66, 2 (2003):101–115.
245. H. P. Xie, J. H. Jiang, X. Chu, H. Cui, H. L. Wu, G. L. Shen, and R. Q. Yu, Competitive interaction of the antitumor drug daunorubicin and the fluorescence probe ethidium bromide with DNA as studied by resolving trilinear fluorescence data: the use of PARAFAC and its modification. *Analytical and Bioanalytical Chemistry* 373, 3 (2002):159–162.
246. J. M. F. ten Berge and N. D. Sidiropoulos, On uniqueness in Candecomp/Parafac. *Psychometrika* 67, 3 (2002):399–409.
247. J. M. F. Ten Berge and N. D. Sidiropoulos, Some new results on uniqueness in CANDECOMP/PARAFAC. *Psychometrika*, 67, (2002):399–409.
248. R. Henrion, On global, local and stationary solutions in three-way data analysis. *Journal of Chemometrics* 14, 3 (2000):261–274.
249. B. J. H. Zijlstra and H. A. L., Kiers, Degenerate solutions obtained from several variants of factor analysis. *Journal of Chemometrics* 16, 11 (2002):596–605.
250. S. Abrescia, A characterization of degenerate tridimensional tensors. *Journal of Pure and Applied Algebra* 187, 1–3 (2004):1–17.
251. L. De Lathauwer and J. Vandewalle, Dimensionality reduction in higher-order signal processing and rank- (R-1, R-2, . . . , R-N) reduction in multilinear algebra. *Linear Algebra and its Applications* 391 (2004):31–55.
252. L. De Lathauwer and J. Vandewalle, Dimensionality reduction in ICA and rank- (R-1, R-2, . . . , R-N) reduction in multilinear algebra. *Independent Component Analysis and Blind Signal Separation* 3195 (2004):295–302.
253. L. De Lathauwer, First-order perturbation analysis of the best rank- (R-1, R-2, R-3) approximation in multilinear algebra. *Journal of Chemometrics* 18, 1 (2004):2–11.
254. P. Paatero, Construction and analysis of degenerate PARAFAC models. *Journal of Chemometrics* 14, 3 (2000):285–299.
255. J. M. F. ten Berge and A. K. Smilde, Non-triviality and identification of a constrained Tucker3 analysis. *Journal of Chemometrics* 16, 12 (2002):609–612.
256. R. Rocci and J. M. F, ten Berge, Transforming three-way arrays to maximal simplicity. *Psychometrika* 67, 3 (2002):351–365.
257. J. M. F. ten Berge, H. A. L. Kiers, T. Murakami, and R. van der Heijden, Transforming three-way arrays to multiple orthonormality. *Journal of Chemometrics* 14, 3 (2000):275–284.
258. J. M. F. ten Berge, N. D. Sidiropoulos, and R. Rocci, Typical rank and indscal dimensionality for symmetric three-way arrays of order Ix2x2 or Ix3x3. *Linear Algebra and its Applications* 388 (2004):363–377.
259. J. M. F. ten Berge, The typical rank of tall three-way arrays. *Psychometrika* 65, 4 (2000):525–532.
260. H. A. L. Kiers, J. M. F. TenBerge, and R. Rocci, Uniqueness of three-mode factor models with sparse cores: The 3x3x3 case. *Psychometrika* 62 (1997):349–374.
261. H. A. L. Kiers, Some procedures for displaying results from three-way methods. *Journal of Chemometrics* 14, 3 (2000):151–170.
262. P. Geladi, M. Manley, and T. Lestander, Scatter plotting in multivariate data analysis. *Journal of Chemometrics* 17, 8–9 (2003):503–511.
263. R. Bro and A. K. Smilde, Centering and scaling in component analysis. *Journal of Chemometrics* 17, 1 (2003):16–33.
264. D. Bylund, R. Danielsson, G. Malmquist, and K. E. Markides, Chromatographic alignment by warping and dynamic programming as a pre-processing tool for PARAFAC modelling of liquid chromatography-mass spectrometry data. *Journal of Chromatography A* 961, 2 (2002):237–244.
265. W. Wu, Q. Guo, D. L. Massart, C. Boucon, and S. de Jong, Structure preserving feature selection in PARAFAC using a genetic algorithm and Procrustes analysis. *Chemometrics and Intelligent Laboratory Systems* 65, 1 (2003):83–95.
266. Y. Z. Cao, H. Chen, H. L. Wu, and R. Q. Yu, An algorithm for three-way data analysis that alternatively minimizes coupled vector (COV) resolution error and PARAFAC error. *Analytical Sciences* 19, 5 (2003):753–756.
267. Y. Z. Cao, Z. P. Chen, C. Y. Mo, H. L. Wu, and R. Q. Yu, A PARAFAC algorithm using penalty diagonalization error (PDE) for three-way data array resolution. *Analyst* 125, 12 (2000):2303–2310.
268. Z. P. Chen, H. L. Wu, Y. Li, and R. Q. Yu, Novel constrained PARAFAC algorithm for second-order linear calibration. *Analytica Chimica Acta* 423, 2 (2000):187–196.

269. Z. P. Chen, H. L. Wu, J. H. Jiang, Y. Li, and R. Q. Yu, A novel trilinear decomposition algorithm for second-order linear calibration. *Chemometrics and Intelligent Laboratory Systems* 52, 1 (2000):75–86.
270. Z. P. Chen, H. L. Wu, and R. Q. Yu, On the self-weighted alternating trilinear decomposition algorithm—the property of being insensitive to excess factors used in calculation. *Journal of Chemometrics* 15, 5 (2001):439–453.
271. Z. P. Chen, Y. Li, and R. Q. Yu, Pseudo alternating least squares algorithm for trilinear decomposition. *Journal of Chemometrics* 15, 3 (2001):149–167.
272. Y. Li, J. H. Jiang, H. L. Wu, Z. P. Chen, and R. Q. Yu, Alternating coupled matrices resolution method for three-way arrays analysis. *Chemometrics and Intelligent Laboratory Systems* 52, 1 (2000):33–43.
273. H. L. Jiang, H. L. Wu, Y. Li, and R. Yu, Alternating coupled vectors resolution (ACOVER) method for trilinear analysis of three-way data. *Journal of Chemometrics* 13, 6 (1999):557–578.
274. C. Y. Mo and Y. Z. Cao, An alternatively minimising covariant matrix error algorithm for three-way data resolution. *Chemia Analityczna* 50, 4 (2005):673–683.
275. J. Z. Lu, H. L. Wu, J. H. Jiang, N. Long, C. Y. Mo, and R. Q. Yu, An improved trilinear decomposition algorithm based on a Lagrange operator. *Analytical Sciences* 19, 7 (2003):1037–1043.
276. G. Tomasi and R. Bro, A comparison of algorithms for fitting the PARAFAC model. *Computational Statistics and Data Analysis* 50, 7 (2006):1700–1734.
277. N. M. Faber, R. Bro, and P. Hopke, Recent developments in CANDECOMP/ PARAFAC algorithms: A critical review. *Chemometrics and Intelligent Laboratory Systems* 65 (2003):119–137.
278. M. E. Timmerman and H. A. L, Kiers, Three-way component analysis with smoothness constraints. *Computational Statistics and Data Analysis* 40, 3 (2002):447–470.
279. M. M. Reis and M. M. C. Ferreira, PARAFAC with splines: A case study. *Journal of Chemometrics* 16, 8–10 (2002):444–450.
280. G. Tomasi and R. Bro, PARAFAC and missing values. *Chemometrics and Intelligent Laboratory Systems* 75 (2005):163–180.
281. J. H. Wang and P. K. Hopke, Equation-oriented system: an efficient programming approach to solve multilinear and polynomial equations by the conjugate gradient algorithm. *Chemometrics and Intelligent Laboratory Systems* 55, 1–2 (2001):13–22.
282. L. Vega-Montoto and P. D. Wentzell, Approaching the direct exponential curve resolution algorithm from a maximum likelihood perspective. *Analytica Chimica Acta* 556, 2 (2006):383–399.
283. L. Vega-Montoto and P. D. Wentzell, Mathematical improvements to maximum likelihood parallel factor analysis: experimental studies. *Journal of Chemometrics* 19, 4 (2005):236–252.
284. L. Vega-Montoto, H. Gu, and P. D. Wentzell, Mathematical improvements to maximum likelihood parallel factor analysis: theory and simulations. *Journal of Chemometrics* 19, 4 (2005):216–235.
285. L. Vega-Montoto and P. D. Wentzell, Maximum likelihood parallel factor analysis (MLPARAFAC). *Journal of Chemometrics* 17, 4 (2003):237–253.
286. R. Bro, N. D. Sidiropoulos, and A. K. Smilde, Maximum likelihood fitting using simple least squares algorithms. *Journal of Chemometrics* 16, 8–10 (2002):387–400.
287. J. Riu and R. Bro, Jack-knife technique for outlier detection and estimation of standard errors in PARAFAC models. *Chemometrics and Intelligent Laboratory Systems* 65, 1 (2003):35–49.
288. H. A. L. Kiers, Bootstrap confidence intervals for three-way methods. *Journal of Chemometrics* 18, 1 (2004):22–36.
289. S. Serneels and P. J. Van Espen, Bootstrap confidence intervals for trilinear partial least squares regression. *Analytica Chimica Acta* 544, 1–2 (2005):153–158.
290. X. Q. Liu and N. D. Sidiropoulos, Cramer-Rao lower bounds for low-rank decomposition of multidimensional arrays. *IEEE Transactions on Signal Processing* 49, 9 (2001):2074–2086.
291. N. M. Faber, Comment on a recently proposed resampling method. *Journal of Chemometrics* 15, 3 (2001):169–188.
292. A. C. Olivieri, Sample-specific standard prediction errors in three-way parallel factor analysis (PARAFAC) exploiting the second-order advantage. *Journal of Chemometrics* 18, 7–8 (2004):363–371.
293. R. Bro, A. Rinnan, and N. M. Faber, Standard error of prediction for multilinear PLS—2. Practical implementation in fluorescence spectroscopy. *Chemometrics and Intelligent Laboratory Systems* 75, 1 (2005):69–76.
294. N. M. Faber and R. Bro, Standard error of prediction for multiway PLS 1. Background and a simulation study. *Chemometrics and Intelligent Laboratory Systems* 61, 1–2 (2002):133–149.
295. S. Serneels, P. Lemberge, and P. J. Van Espen, Calculation of PLS prediction intervals using efficient recursive relations for the Jacobian matrix. *Journal of Chemometrics* 18, 2 (2004):76–80.
296. M. Linder and R. Sundberg, Precision of prediction in second-order calibration, with focus on bilinear regression methods. *Journal of Chemometrics* 16, 1 (2002):12–27.
297. A. C. Olivieri, Computing sensitivity and selectivity in parallel factor analysis and related multiway techniques: The need for further developments in net analyte signal theory. *Analytical Chemistry* 77, 15 (2005):4936–4946.
298. R. Boque, J. Ferre, N. M. Faber, and F. X. Rius, Limit of detection estimator for second-order bilinear calibration. *Analytica Chimica Acta* 451, 2 (2002):313–321.
299. C. A. Andersson and R. Bro, The N-way Toolbox for MATLAB. *Chemometrics and Intelligent Laboratory Systems*, 52, 1 (2000):1–4.
300. A. de Juan, N-way toolbox for MATLAB. *Journal of Chemometrics* 14, 4 (2000):379–380.
301. S. Gourvénec, G. Tomasi, C. Durville, E. Di Crescenzo, C. A. Saby, D. L. Massart, R. Bro, and G. Oppenheim, CuBatch, a MATLAB interface for n-mode data analysis. *Chemometrics and Intelligent Laboratory Systems* 77 (2005):122–130.
302. H. A. L. Kiers, J. M. F. ten Berge, and R. Bro, PARAFAC2—Part I. A direct fitting algorithm for the PARAFAC2 model. *Journal of Chemometrics* 13 (1999):275–294.
303. R. Bro, C. A. Andersson, and H. A. L. Kiers, PARAFAC2—Part II. Modeling chromatographic data with retention time shifts. *Journal of Chemometrics* 13 (1999):295–309.
304. R. Bro, N. D. Sidiropoulos, and G. B. Giannakis, A Fast Least Squares Algorithm for Separating Trilinear Mixtures. Proc. ICA99—Int. Workshop on Independent Component Analysis and Blind Signal Separation, Jan. 11–15, (Aussois, France, 1999), pp. 289–294.