

Meeting Report

TRICAP 2003: Three-way Methods in Chemistry and Psychology, University of Kentucky, Lexington, KY, USA, 22–27 June 2003

The fourth TRICAP meeting, organized by *Bill Rayens* in Lexington, June 2003, conveyed two main conclusions: TRICAP is by now an established conference series, and there is still plenty of unidentified territory for attractive and inspiring research in the multiway world [1–3]. Next to contributions from chemometrics and psychometrics, several appealing developments from the telecommunications/signal-processing research field were presented. A total of 28 participants contributed in 23 one-hour presentation and discussion sessions, together with nine posters presentations, forming the scientific heart of the conference.

Richard Harshman started off with the challenging concept of incorporating causal path structures into multilinear models. Theory and algorithms were presented that allowed for the direct incorporation of path networks on the manifest and/or latent variables. The uniqueness properties of CANDECOMP/PARAFAC (CP) models were addressed by *Tao Jiang* from a signal-processing perspective. Two new necessary and sufficient uniqueness conditions—motivated by Kruskal's permutation lemma—were presented. The presentation by *Rasmus Bro* had a strong user perspective, mainly focusing on the application of CP in analytical chemistry and food-related research. Aspects such as explaining the main ideas of three-way analysis to novice users, preprocessing of multiway fluorescence data, computation speed-up by parallelization and the potential of handling undesired signal shifts were covered from a practitioner point of view. Another study into the uniqueness conditions of CP decomposition was presented by *Lieven de Lathauwer*. Weak bounds for unique CP decomposition were determined as a function of simultaneous matrix diagonalization involving the inverse transformation. Constraining a large majority of Tucker3 core entries to zero was the topic of *Jos ten Berge's* paper. He showed that simplicity transformations and typical rank results can be used to determine whether certain constrained cores are trivial and whether a specific constrained Tucker3 solution is unique. A special introductory lecture on multilinear methods, open to local researchers and sponsored by the Kentucky NSF-EPSCoR Initiative in Functional Genomics, was given by *Pieter Kroonenberg*.

The paper by *Xiangqian Liu* handled the retrieval of constant-modulus multidimensional harmonic signals. An improved sufficient condition on almost sure identifiability was presented. Procrustes analysis for the alignment of molecular descriptors in a series of similar medicinal compounds was the topic of *Pieter Kroonenberg*. Using a modified algorithm to handle the variable number of atoms in different molecules, coalition of the backbone structures made

visual inspection of the different side-groups feasible. Two important issues that may hamper the CP modeling of fluorescence excitation–emission data—light scatter and missing values—were addressed by *Charlotte Andersen*. The two effects were illustrated and practical details were given on how one may preserve trilinear structure and enhance interpretation by means of correct preprocessing. *Weixiang Zhao* talked about environmental monitoring and source identification of volatile organic compounds. A combination of chemical/physical and constrained multiway factor models was able to identify sources together with meteorological and temporal effects. Relations among and selection of hierarchical classes models for three-way, three-mode binary data were the subject of *Eva Ceulemans*. The interrelations between the different types of hierarchical classes models were represented in a partially ordered hierarchy of the models, and a model selection strategy based on Akaike's information criterion was proposed and evaluated by means of a simulation study. CP analysis of data on self-rated emotions, which are traditionally analyzed by two-way PCA, was the theme of *David Stanley's* talk. The uniqueness property of CP enabled him to resolve a long-standing debate over the most appropriate position of the axes defining affective space. *Neal Gallagher* presented so-called purity-based starting positions for *N*-way alternating least squares algorithms. In the case of partial signal selectivity, such purity-based methods were shown to be simpler, faster and more versatile than e.g. direct trilinear decomposition.

Henk Kiers showed how the uncertainty of CP and Tucker3 parameters may be estimated by calculating confidence intervals from bootstrap results. Common bootstrapping matters such as how to obtain bootstrap samples, how to handle model non-uniqueness and computational workload were treated from a multi-way perspective. Analysis of variance and parameter probability values acquired by resampling methods for multiway, multiplicative models of experimental design data were the subject of *Frans van den Berg*. The potential of classical ANOVA-like results for multiway models was hinted at, but computational limits prevented hard conclusions. The issue of partial uniqueness of CP models in cases of perfect fit was addressed by *Jos ten Berge*. In the last session of the fourth meeting day, *Pentti Paatero* demonstrated his multilinear engine, a general solver for multiway models. Although its potential was clearly demonstrated in this workshop, the notational particularities of the solver were shown to limit its widespread application up till now.

Roma Tauler showed that the trilinear modeling approach is often inadequate for analyzing chemical data sets, as the

true experimental structure in such data often does not correspond to the trilinearity assumptions. He demonstrated that alternative methods performed better in several examples. *Philip Hopke's* paper studied the temporal and spatial structure of a large-scale environmental data set. Positive matrix factorization results allowed for the identification of concentration potential emission sources. A method termed warped factor analysis—a concept inspired by the data-preprocessing methods of dynamic time and correlation-optimized warping—was introduced by *Sungjin Hong*. This extension of shifted factor analysis is able to handle positional shifts and shape changes of sequential factors. Transforming CP or Tucker3 models so that the signal is concentrated in one part of the array was the subject of *Pentti Paatero*. Such transformations may yield—amongst other advantages—an important decrease in the computational workload. *Marieke Timmerman* presented a novel method for analyzing multisubject, multivariate time series called multi-level simultaneous component analysis. The technique provides a model of intra-individual variation as well as a model of inter-individual variation in level. The meeting's closing presentation by *Age Smilde* advocated the necessity for new methods to handle multiway data structures. Using examples from biology, he showed that contemporary research can be so information-rich, complex and structured that present-day three-way analysis might become insufficient in the near future.

The social and touristic needs were well covered by collective lunches and dinners, a visit to an authentic

Kentucky Bourbon distillery and a visit to Kentucky Horse Park, where the *local color* was nicely represented with bluegrass music, regional dishes and an interactive square dancing experience. We would like to congratulate *Bill Rayens* and the University of Kentucky on a successful conference, and we look forward to the next TRICAP to be organized by *Nikos Sidiropoulos* in Chania on the Greek island of Crete in 2006.

REFERENCES

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