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MEETING REPORT

TRICAP: Three-Way Methods in Chemistry and Psychology, Lake Chelan, WA, U.S.A., 4–9 May 1997

This meeting was a follow-up to the first 'TRIC' conference held in Epe (Netherlands) in August 1993.[1] That meeting was organized to bring together chemometricians and psychometricians who turned out to be involved in the use of very similar methods for the analysis of three-way data. The aim of that conference was to allow a high technical level and to evoke thorough discussions on possibly very technical issues related to these and other three-way methods. The conference succeeded very well in this and it was agreed that a follow-up should be organized some three years later, but now in America. The locale for this was found about two years ago, when Barry Wise volunteered to organize the next meeting in his beautiful home town—and he successfully did. The meeting was visited by 32 attendees of 14 different nationalities, from ten different countries. In total, 23 oral presentations (of 45 min each) were given and nine posters were presented.

The oral presentations were often interrupted for questions as well as discussions, thus ensuring very lively sessions. Questions were quite often related to terminology: an important benefit of a meeting like this one is that it clears up the confusion caused by different terminology in the two disciplines brought together; it was thus revealed that what is termed differently in the two disciplines may very well be equivalent or at least closely related. In the present meeting, interest was focused on more three-way methods than in the first TRIC meeting. There was considerable interest in the Tucker3 model and also in methods for somewhat special types of three-way data. An important point of interest of the present meeting was computational efficiency and also modeling particular data features (using constraints or penalties). These subjects seem to reflect the gradual maturation of three-way methods: for successful applications we need an efficient algorithm and we may want to incorporate data features into our analysis. Actually, several such successful applications were demonstrated at the meeting, all of them in chemistry, which may reflect that the most convincing applications of three-way methods can be found in this discipline. Since the first contributions on three-way methods emerged in psychometrics, one may nevertheless assume the existence of useful applications in psychology as well, which hopefully will be presented at the next TRICAP meeting, planned for the year 2000, in Denmark (for more information on this, refer to the authors of this report).

We will now continue with a brief overview of the meeting, not disregarding some of the most salient remarks by the speakers.

P. M. Kroonenberg and *W. J. Heiser* and later *R. Bro* and *R. A. Harshman* discussed the use of constraints in multiway analysis. Examples were orthogonality and non-negativity constraints and constraining components to be fixed in order to estimate lower-order interaction effects and main effects in ANOVA models. Kroonenberg's talk, by which the meeting was opened, also offered a very good introduction to three-way methods in general.

P. Paatero advocated a new algorithm called the multilinear engine for estimating large general multilinear models. In the multilinear engine the structural model and auxiliary constraints result in a very general, flexible and efficient algorithm amenable to largely any multilinear problem.

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D. Burdick discussed how the use of tensor algebra could be an advantage in multiway analysis. He advocated that from a tensor point of view both the three-way PARAFAC and Tucker3 models could be regarded as trilinear models and also showed that, using tensors, the appropriateness of different prepocessing steps (centering and scaling) could easily be verified.

P. Hopke, P. Paatero, H. Jia, R. T. Ross and *R. A. Harshman* had made an extensive investigation of the merits of different algorithms for estimating the trilinear model on four ill-conditioned data sets. The conclusion was that a simple ALS approach was the slowest, the direct trilinear decomposition the most unstable and the PMF3 algorithm the most efficient approach. The paper got the diversity award: its five authors are from five different disciplines. In our opinion, Hopke also deserved the patience award: he got so many interrupting questions and comments that during his presentation the audience talked more than he did himself.

A. de Juan, S. C. Rutan and *R. Tauler* showed by means of a simulation study the different merits of bilinear and trilinear models of three-way (chromatographic) data with possible retention time shifts. Guidelines were given on which approach to use in different situations, i.e. when to prefer two-way methods if the data could not be considered trilinear.

J. A. L. Kiers and later *C. A. Andersson* and *R. Henrion* gave an overview of different approaches to core rotation of Tucker3 cores, including a method called SIMPLIMAX for rotating to maximum number of zero elements of the core with or without prespecified structure. They showed core rotation to be useful for obtaining simplified structure. Kiers also discussed methods for speeding up ALS algorithms in general by means of regularized compression.

J. D. Carroll was awarded the best title award: 'Fitting general multilinear models to multiway data, with continuous, discrete, or mixed continuous and discrete parameters, via optimization of an OLS, WLS, weighted or unweighted least absolute deviations, or other Lp-norm based loss function'! As is clear from the title, he discussed a very general algorithm for handling various constraints in CANDECOMP/PARAFAC and INDSCAL, with particular attention to constraining parameter values to be binary.

S. Hong and *R. A. Harshman* gave a talk on a method for factor analysis where factors are differently shifted in time for different variables. Interestingly, even in the two-way case, solutions turned out to be unique, just as in PARAFAC.

K. Dahl, M. J. Piovoso and *K. A. Kosanovich* described a complicated batch process and showed how multiway data analysis (PARAFAC and GRAM) could be used as a supplement to the more traditional unfolding techniques used in MSPC. To some extent, depending on the data at hand, both methods aided in obtaining better product quality and reduced recycle time.

Y. Xie, P. K. Hopke and *P. Paatero* considered the analysis of environmental data with, as three modes, chemical constituents, weeks in a year and years. They compared this with a two-way analysis of these data where chemical constituents and (all) weeks formed the two modes. The author started his talk by demonstrating that Pieter Kroonenberg's screen-pointer, which was used and abused by every preceding speaker, had now finally broken.

R. Leardi and *C. Armaninos* talk was meant to demonstrate to 'normal people, not chemometricians' how useful and simple it is to fit the Tucker3 model. They showed how the three-way models of three-way data enabled proper conclusions to be drawn much more simply and faster than if the data were analyzed using traditional unfolding techniques.

E. M. Qannari, I. Wakeling, H. J. H. MacFie and *P. Courcoux* gave an elegant overview of methods for analyzing (three-way) sensory data. They showed that by hypothesizing on the quality of sensory data (in essence how well-trained the panel is), different models are appropriate ranging from unfold PCA over Procrustes analysis/STATIS to INDSCAL.

S. Winsberg and *G. de Soete* described a procedure for fitting the INDSCAL model when constraining the C-mode parameters—which in psychological applications usually refer to subjects

who judge similarities between certain objects—to be equal in certain optimal subsets. A mixture modeling approach was used for this, resulting in the only method presented here that was based on maximum likelihood fitting.

A. Louwerse, A. Smilde and *H. A. L. Kiers* developed a method for cross-validation of multiway models. They first came up with a correction for Eastment and Krzanowskis cross-validation for PCA. Next they demonstrated how this approach can be generalized to the Tucker3 method, especially for the purpose of finding the numbers of components to be used.

R. Ross, R. B. Abel and *S. Leurgans* discussed the use of experimental design in multiway analysis in the case where acquisition of three-way data is expensive. They argued critically for the use of D-optimal designs.

W. J. Dunn III, A. J. Hopfinger and *C. Duraiswami* and also *J. Nilsson* and *A. Smilde* discussed the use of unfold and multiway methods in QSARs. Both discussed the intrinsic problems in QSAR analysis. Dunn *et al*. compared direct trilinear decomposition with unfold PLS while Nilsson and Smilde showed that by the use of a pentalinear PLS model they were capable of increasing the predictive ability as well as finding sensible subsets of variables for simplifying the calibration models.

W. Windig and *A. Antalek* gave interesting applications of GRAM in magnetic resonance analysis, where the special characteristics of exponential decays coupled with extremely precise data make it possible to resolve the pure spectra using only a single sample. Owing to the precision of the data, there was no gain in using PARAFAC except for much longer computation times, and 'Why use a simple and direct method, when we have an indirect method that requires very many iterations'.

A. Smilde and *H. A. L. Kiers* introduced a new concept for defining multiway regression models based on principal covariate regression. By the use of a tuning parameter the focus on fitting the dependent or independent variables respectively is controlled; the independent variables can be described by any multiway model. *P. Geladi* talked about using multiway models for stabilizing solutions and enhancing the interpretability with respect to the reality being modeled. He did not hide his distrust in cross-validation: one sheet in large capitals told the audience 'Cross-validation sucks'.

R. Harshman introduced a new approach called morphing. With this approach it is possible to gradually change from e.g. a Tucker3 model to a PARAFAC model, or from a PARAFAC model to a two-way PCA model, by means of a penalty approach. It was outlined how the method could help in avoiding degeneracy yet still retain the uniqueness in some situations.

Finally, we just mention the titles of the nine posters presented: 'Exploring fluorescence intensity measurements with PCA in 4 dimensions', *C. A. Andersson* and *R. Henrion*; 'The application of positive matrix factorization to identification of sources of atmospheric aerosol over Alaska', *P. K. Hopke, A. V. Polissar, P. Paatero, W. C. Malm* and *J. F. Sisler;* 'Decomposition of multi-way fluorescence spectral data', *P. Courcoux, M. F. DeVaux, E. Vigneau* and *B. Novales*; 'Constrained PARAFAC and PARATUCK3 models for genetic study of multivariate data from fraternal vs. identical twins', *R. Harshman*; 'An "extended PARAFAC model" incorporating singly-subscripted constants: theory and application', *R. Harshman* and *M. Lundy*; 'The noise addition method for determining the number of significant factors with TLD and PARAFAC decompositions', *K. S. Booksh;* 'Two-way/three-way PMF analysis of Arctic particle composition data', *P. Paatero, Y. Xie* and *P. Hopke*; 'Synthetic degenerate PARAFAC models: construction, properties, connections with centering', *P. Paatero, R. Harshman* and *M. Lundy;* 'Evaluation of NIR-spectra from pharmaceutical tablets using PARAFAC constrained for positive solutions', *M. Andersson, M. Josefson* and *K.-G. Wahlund.*

One of the posters by Richard Harshman was awarded at the end of the meeting. It got the 'best placement award': it could never be missed, being posted on the refrigerator containing the entire beer stock for the conference attendees.

We conclude that the organizers, Barry Wise and Neal Gallagher, did a great job in organizing this conference (as well as a wonderful boat trip, all the way up Lake Chelan, making us enjoy the beautiful weather and acquiring a sun tan with which we hardly dared show up at our home institutes. . .). The aim of the conference was attained completely and we both concluded, independently, that this was the best conference we had ever attended. The organizers of TRICAP-2000 will have a difficult job.

REFERENCES

1. P. Geladi, *J. Chemometrics*, **8**, 97–98 (1994).

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