review of multivariate methods in applications. In *Statistics: An Appraisal* (H. A. David and H. T. David, eds.) 309-337. Iowa State Univ. Press.

HARSHMAN, R. A. (1970). Foundations of the PARAFAC procedure: Models and conditions for an "exploratory" multi-mode factor analysis. *UCLA Working Papers in Phonetics* **16** 1-84.

INGLE, JR., J. and CROUCH, S. R. (1988). *Spectrochemical Analysis.* Prentice Hall, Englewood Cliffs, NJ.

KAPTEYN, A., NEUDECKER, H. and WANSBEEK, T. (1986). An approach to *n*-mode components analysis. *Psychometrika* **51** 269-275.

KROONENBERG, P. M. (1983). Annotated bibliography of three-mode data by means of alternating least-squares algorithms. *British J. Math. Statist. Psych.* **36** 81-113.

KROONENBERG, P. M. (1991). The three-mode side of the three-way world. Technical report, Dept. Education, Leiden Univ.

KRUSKAL, J. B. (1977). Three-way arrays: Rank and uniqueness of trilinear decompositions with application to arithmetic complexity and statistics. *Linear Algebra Appl.* **18** 95-138.

LASTOVICKA, J. L. (1981). The extension of component analyses to 4-mode factor analysis. *Psychometrika* **46** 47-57.

LEE, C.-H. (1988). Multilinear analysis of fluorescence spectra of photosynthetic systems. Ph.D. dissertation, Ohio State Univ.

LEE, C.-H., KIM, K. and ROSS, R. T. (1991). Trilinear analysis for the resolution of overlapping fluorescence spectra. *Korean Biochemistry Journal* **24** 374-379.

LEURGANS, S. E. (1991). Multilinear models: Array formulas. Technical Report 473, Dept. Statistics, Ohio State Univ.

LEURGANS, S. E., ROSS, R. T. and ABEL, R. B. (1992). A decomposition for 3-way arrays. *SIAM J. Matrix. Anal. Appl.* To appear.

MALINOWSKI, E. R. and HOWERY, D. G. (1980). *Factor Analysis in Chemistry.* Wiley, New York.

NDOU, T. T. and WARNER, I. M. (1991). Applications of multidimensional absorption and luminescence spectroscopies in analytical chemistry. *Chemical Reviews* **91** 493-507.

PRINGLE, R. M. and RAYNER, A. A. (1971). *Generalized Inverse Matrices with Applications to Statistics.* Hafner, New York.

RAMOS, L. S., BEEBE, K. R., CAREY, W. P., SANCHEZ, E., ERICKSON, B. C., WILSON, B. E., WANGEN, L. E. and KOWALSKI, B. R. (1986). Chemometrics. *Analytical Chemistry* **58** 294R-315R.

ROSS, R. T., LEE, C.-H., DAVIS, C. M., FAYYAD, E. A. and LEURGANS, S. E. (1991). Resolution of fluorescence spectra of plant pigment-complexes using trilinear models. *Biochimica et Biophysica Acta* **1056** 317-320.

RUSSELL, M. D. and GOUTERMAN, M. (1988a). Excitation-emission-lifetime analysis of multicomponent systems—I. Principal component factor analysis. *Spectrochimica Acta* **44A** 857-861.

RUSSELL, M. D. and GOUTERMAN, M. (1988b). Excitation-emission-lifetime analysis of multicomponent systems—II. Synthetic model data. *Spectrochimica Acta* **44A** 863-872.

RUSSELL, M. D., GOUTERMAN, M. and VAN ZEE, J. A. (1988). Excitation-emission-lifetime analysis of multicomponent systems—III. Platinum, palladium and rhodium porphyrins. *Spectrochimica Acta* **44A** 873-882.

SANCHEZ, E. and KOWALSKI, B. R. (1988a). Tensorial calibration: I. First-order calculations. *Journal of Chemometrics* **2** 247-263.

SANCHEZ, E. and KOWALSKI, B. R. (1988b). Tensorial calibration: II. Second-order calibration. *Journal of Chemometrics* **2** 265-290.

SANCHEZ, E. J. and KOWALSKI, B. R. (1990). Tensorial resolution: A direct trilinear decomposition. *Journal of Chemometrics* **4** 29-45.

SANDS, R. and YOUNG, F. W. (1980). Component models for three-way data: An alternating least squares algorithm with optimal scaling features. *Psychometrika* **45** 39-67.

THAMPI, S. (1991). Resolution of intrinsic protein fluorescence using multilinear analysis. Master's thesis, Ohio State Univ.

TUCKER, L. R. (1963). Implications of factor analysis of three-way matrices for measurement of change. In *Problems in Measuring Change* (C. W. Harris, ed.) 122-137. Univ. Wisconsin Press.

Comment

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INTRODUCTION

Complicated multivariate models, and certainly the models used in multidimensional scaling, are most often used for exploratory purposes. The paper by Leurgans and Ross covers one of the fortunate, but rather exceptional, situations in which we can derive the form of the model from prior scientific knowledge. Another, similar, situation is the conformation of molecules using scaling techniques, and the seriation of artifacts in time or of genes along a chromosome. In this class of applications, the physical information we have tells us that a multilinear model is appropriate—only the coefficients (mixtures) and dimensionality (number of components) are unknown and must be estimated.

OTHER AREAS

Leurgans and Ross discuss the multilinear models pretty much in the context in which they use them. Thus, it looks a bit as if these models were created for spectroscopy. This is perfectly appropriate in a paper such as this, which concentrates on a particular field of application. But to give a somewhat wider perspective, I'll list a number of other areas, both mathematical and nonmathematical, in which multilinear models have been studied or applied.

1. *Efficient computation of matrix products and*

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other algebraic operations. After the famous result by Strassen (1968) was interpreted as saying that the rank of a particular $3 \times 3 \times 3$ array was always less than or equal to seven, this has remained a quite active field, with maybe 10–15 publications per year in journals such as *Linear Algebra and Its Applications.*

2. *General theory of arrays.* The multiplication operations discussed by Leurgans and Ross are of course familiar to any user of APL. In the seventies, when APL reached the peak of its popularity, this was developed into a theory of arrays by More (1973). Many of the operations on multiway arrays are defined formally in this theory.

3. Rank of multiway arrays. In the early days of matrix theory, there were quite a few people working on multidimensional extensions of matrices, tensors and polyadics. In particular, Rice and Hitchcock wrote a series of memoirs in the *Journal of Mathematics and Physics* around 1920, and Oldenburger followed this work up with papers in the *Transactions of the AMS* and the *Annals of Mathematics* in the thirties. As entries into this literature, we cite Hitchcock (1927) and Oldenburger (1934). In particular, they discussed various notions of rank for multiway arrays and the decomposition of a tensor into a sum of products (which is basically the INDSCAL-PARAFAC model). The mathematics never got very far, because really powerful results could not be obtained in the general case and because the notation ran away with the readability of the papers.

4. *Psychometrics.* Leurgans and Ross refer to the psychometric literature, but rather sparsely. For completeness, we give the two key references: the book by Kroonenberg (1983) and the edited volume by Law et al. (1984). The Kroonenberg book introduces the T2/T3 terminology, introduces alternating least squares algorithms and has many pages of applications. The Law et al. book has an excellent overview paper by Kruskal.

Multilinear models in psychometrics are mostly used in individual difference scaling, in which individuals weight the dimensions determining similarity differently. Actually, the INDSCAL-PARAFAC model was already proposed earlier by Bartlett, Rasch, Meredith and others in factor analysis, more specifically in the area of factorial invariance.

STATISTICS

There is very little stability analysis in the paper. And this is only natural, because so far very little has actually been done. For the T2 model, in which the elements of the slabs are covariances, the LISREL people have done some of the computations leading to standard errors. This is, of course, based on the asymptotic normality of the elements of the multi-way array. In general, however, we are much closer to a factorial ANOVA situation with one observation per cell. And then, of course, different types of asymptotics are possible, and nuisance parameters are rampant. The problem is far from solved in this case.

APPLICATIONS

The applications and the translation of spectroscopic facts into multilinear equations are the heart of the paper. I cannot comment on the importance of these models and algorithms to the field of chemometrics, because I know virtually nothing about that field. I do like these strong models, however, and I welcome applications of multivariate statistical techniques to the physical sciences.

In a sense, the applicability of these models justifies the attention they have gotten so far. But from the mathematical and the statistical point of view, the available results are still very primitive. We have an elaborate notation (actually, several elaborate notations), in many cases featuring specially defined operators, that make multiway arrays look like ordinary linear operators. As the efforts of Rice, Hitchcock and Oldenburger have shown, it is difficult to distill beautiful results out of this orgy of subscripts and ad hoc notation. Either there is not enough structure there, or we have not found the key yet. In the same way, we don't really know how to do statistical stability analysis yet. It should be possible, at least in principle, to generalize the results of Haberman for two-way matrices and simple exponential models. But that certainly will not be simple, and the relevance of this type of asymptotics has not even been demonstrated convincingly in these much simpler contexts. We also have plenty of algorithms, which exploit the partial linearity and which can be shown to converge. But to what? And how fast? Those questions can be answered completely only by proving something analogous to the singular value decomposition for three-way and multiway arrays. And such a result is not yet in sight.

Now, maybe it is the case that the error level is so low in spectroscopy and that the components are usually so well separated that stability analysis of any sort is not really necessary. This is the case in fitting the simple laws of physics, but from the examples it really does not look as if we are in that fortunate situation here.