


**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

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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
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 opera-
tions 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 de-
veloped 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 power-
ful 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 com-
pleteness, we give the two key references: the book by
Kroonenberg (1983) and the edited volume by Law et al.
terminology, introduces alternating least squares algo-
rithms 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 differ-
cently. 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 nota-
tions), in many cases featuring specially defined opera-
tors, that make multiway arrays look like ordinary
linear operators. As the efforts of Rice, Hitchcock and
Oldenburger have shown, it is difficult to distill beauti-
ful 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 cer-
tainly 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.