SOME ADDITIONAL RESULTS ON PRINCIPAL COMPONENTS ANALYSIS
OF THREE-MODE DATA BY MEANS OF ALTERNATING
LEAST SQUARES ALGORITHMS

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Kroonenberg and de Leeuw (1980) have developed an alternating least-squares method
TUCKALS-3 as a solution for Tucker's three-way principal components model. The present
paper offers some additional features of their method. Starting from a reanalysis of Tucker's
problem in terms of a rank-constrained regression problem, it is shown that the fitted sum of
squares in TUCKALS-3 can be partitioned according to elements of each mode of the three-way
data matrix. An upper bound to the total fitted sum of squares is derived. Finally, a special case of
TUCKALS-3 is related to the Carroll/Harshman CANDECOMP/PARAFAC model.

Key words: partitioning of least-squares fit, rank-constrained regression, Candecomp, Parafac.

Introduction

Kroonenberg and de Leeuw (1980) have offered an alternating least-squares solution
(TUCKALS-3) for the three-mode principal component model developed by Tucker
(1963, 1964, 1966). Their solution is based on the observation that the optimal core matrix
can be expressed uniquely and explicitly in terms of the data and the component matrices
for the three modes. The latter component matrices are optimized by an alternating
least-squares algorithm.

The present paper is aimed at offering some results for TUCKALS-3 in addition to
those given by Kroonenberg and de Leeuw. First, it will be shown that the fitted sum of
squares in TUCKALS-3 can be partitioned according to elements of each mode. This
result is based on a rederivation of TUCKALS-3 in terms of a rank-constrained regres-
sion problem. Next, an upper bound to this fitted sum of squares will be derived. Finally,
a relationship between a special case of TUCKALS-3 and the Carroll/Harshman
CANDECOMP/PARAFAC model (see Harshman & Lundy, 1984a, 1984b and Carroll &
Pruzansky, 1984) will be demonstrated.

In the next section the main features of TUCKALS-3, as given by Kroonenberg and
de Leeuw (1980), will be revisited.

The Tucker-3 Model and the TUCKALS-3 Solution

Let Z be a three mode data matrix of order \( \ell \times m \times n \) with elements \( z_{ijk} \), \( i = 1, \ldots, \ell; j = 1, \ldots, m; k = 1, \ldots, n \). The least-squares fitting of the Tucker-3 model implies

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minimizing the residual sum of squares

\[ \sum_{i,j,k} (z_{ijk} - \hat{z}_{ijk})^2, \]  

where \( \hat{z}_{ijk} \) is a weighted sum of elements of an \( \ell \times s \) matrix \( G \), an \( m \times t \) matrix \( H \), an \( n \times u \) matrix \( E \), and an \( s \times t \times u \) core matrix \( C \) (Kroonenberg & de Leeuw, 1980, p. 70).

In TUCKALS-3 the matrices \( G, H \) and \( E \) are restricted to be column-wise orthonormal.

Let \( Z_e \) be the \( \ell \times mn \) matrix containing the \( m \) lateral \( \ell \times n \) planes of \( Z \), then the associated fitted parts of \( Z \) can be collected in the \( \ell \times mn \) matrix

\[ \hat{Z}_e = GC_e(H' \otimes E') \]  

where \( C_e \) is the \( s \times tu \) matrix containing the \( t \) lateral \( s \times u \) planes of \( C \), and \( \otimes \) is the Kronecker product. Clearly, minimizing (1) is equivalent to minimizing

\[ f(G, H, E, C) = \| Z_e - \hat{Z}_e \|^2 = \| Z_e - GC_e(H' \otimes E') \|^2. \]  

For fixed \( G, H, \) and \( E \) the minimizing \( C_e \) is uniquely defined as

\[ C_e = G'Z_e(H \otimes E) \]  

(Penrose, 1956, p. 18). Hence minimizing (1) reduces to minimizing

\[ g(G, H, E) = \| Z_e - GG'Z_e(HH' \otimes EE') \|^2, \]  

which, in turn, is equivalent to maximizing

\[ p(G, H, E) = \text{tr} \ G'Z_e(HH' \otimes EE')Z_e' G = \text{tr} \ G'PG. \]  

In a completely parallel fashion, it can be shown that

\[ p(G, H, E) = \text{tr} \ H'Z_m(EE' \otimes GG')Z_m' H = \text{tr} \ H'QH, \]  

where \( Z_m \) is the \( m \times \ell n \) matrix containing the \( n \) transposed frontal \( \ell \times m \) planes of \( Z \), and that

\[ p(G, H, E) = \text{tr} \ E'Z_n(GG' \otimes HH')Z_n' E = \text{tr} \ E'RE, \]  

where \( Z_n \) is the \( n \times \ell m \) matrix containing the \( \ell \) horizontal \( n \times m \) planes of \( Z \), (Kroonenberg & de Leeuw, 1980, p. 72).

The TUCKALS-3 solution consists of iteratively improving \( G \) for fixed \( H \) and \( E \), \( H \) for fixed \( G \) and \( E \), and \( E \) for fixed \( G \) and \( H \), starting from Tucker’s final solution for \( G, H \) and \( E \) (Tucker, 1966, p. 297). That is, initially \( G \) consists of the principal \( s \) eigenvectors of \( Z_eZ_e' \); \( H \) consists of the principal \( t \) eigenvectors of \( Z_mZ_m' \), and \( E \) consists of the principal \( u \) eigenvectors of \( Z_nZ_n' \). The procedure terminates when a necessary condition for a maximum is satisfied, that is, when simultaneously \( G \) contains the \( s \) principal eigenvectors of \( P \), \( H \) contains the \( t \) principal eigenvectors of \( Q \), and \( E \) contains the \( u \) principal eigenvectors of \( R \). We shall now rederive the TUCKALS-3 solution from a generalized perspective.

An Alternative Approach to the Least Squares Fitting of the Tucker-3 Model

Kroonenberg and de Leeuw (1980, p. 70) noted that it is merely a matter of convenience to have \( G, H \) and \( E \) constrained to be orthonormal column-wise. This point will now be elaborated in a generalized approach to the Tucker-3 model, in which the orthonormality constraints are omitted. The derivation to be given below applies equally to \( G \),