UNIQUENESS OF THREE-MODE FACTOR MODELS WITH SPARSE CORES:
THE $3 \times 3 \times 3$ CASE

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Three-Mode Factor Analysis (3MFA) and PARAFAC are methods to describe three-way data. Both methods employ models with components for the three modes of a three-way array; the 3MFA model also uses a three-way core array for linking all components to each other. The use of the core array makes the 3MFA model more general than the PARAFAC model (thus allowing a better fit), but also more complicated. Moreover, in the 3MFA model the components are not uniquely determined, and it seems hard to choose among all possible solutions. A particularly interesting feature of the PARAFAC model is that it does give unique components. The present paper introduces a class of 3MFA models in between 3MFA and PARAFAC that share the good properties of the 3MFA model and the PARAFAC model: They fit (almost) as well as the 3MFA model, they are relatively simple and they have the same uniqueness properties as the PARAFAC model.

Key words: three-way methods, PARAFAC.

In the last decades, three-way data have received considerable attention from researchers in various disciplines. Three-way data may consist of measures as diverse as scores of a set of individuals on a set of variables at different occasions (e.g., in the behavioral sciences) or of absorbed energy at various absorption levels on various mixtures of substances that have been exposed to various sorts of light emission (spectroscopy).

Several methods have been proposed for the exploratory analysis of three-way data. Two of the most popular methods are PARAFAC (Carroll & Chang, 1970; Harshman, 1970; Harshman & Lundy, 1984) and Three-Mode Factor Analysis (3MFA; Kroonenberg & de Leeuw, 1980; Tucker, 1966). In fact, PARAFAC can be seen as a constrained variant of 3MFA (as explained below). Due to the constraints used in PARAFAC, the PARAFAC fit is usually less than the 3MFA fit; on the other hand, the PARAFAC model is unique (thanks to the constraints), whereas the 3MFA model is not. In the present paper, we focus on models that are in between the 3MFA model and the PARAFAC model. These models are constrained variants of 3MFA, in which the constraints are less stringent than in PARAFAC. For this reason, one can also view these models as extensions of the PARAFAC model. The main result of the present paper is that a class of such intermediate methods gives unique solutions, just like PARAFAC (and unlike 3MFA). It will thus be shown that, to obtain a unique model, one need not constrain the 3MFA model as heavily as is done in PARAFAC: More relaxed constraints are still sufficient to obtain a unique model.

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Before deriving the uniqueness result, we will discuss PARAFAC and 3MFA in detail, and introduce the intermediate methods. Also, we will indicate why the uniqueness of the intermediate methods is important. This will be illustrated by means of a set of simple exemplary analyses. Subsequently, a description is given of the models for which we prove uniqueness in the present paper, and the uniqueness will be proven. As a byproduct of the uniqueness proof, we propose a numerical procedure for assessing (non)uniqueness of models outside the class of models for which uniqueness is actually proven.

PARAFAC, 3MFA and a Compromise

To facilitate conceptualization of the three modes of a three-way array, in the present section, we will view the first mode (A) as that of the individuals, the second (B) as that of the variables and the third (C) as that of the occasions. In both PARAFAC and 3MFA (implemented in the TUCKALS-3 algorithm by Kroonenberg & de Leeuw, 1980), the data are modeled by components for the three different modes, and the models are fitted to the data in the least squares sense. The PARAFAC model can be written as

$$X_{ijk} = \sum_{r=1}^{R} a_{ir} b_{jr} c_{kr} + e_{ijk},$$

where $x_{ijk}$ denotes the score of individual $i$, on variable $j$, at occasion $k$, $i = 1, \ldots, I$, $j = 1, \ldots, J$, and $k = 1, \ldots, K$; $a_{ir}$, $b_{jr}$, and $c_{kr}$ are elements of the three component matrices $A$, $B$, and $C$, of orders $I \times R$, $J \times R$, and $K \times R$, respectively; and $e_{ijk}$ denotes the error term for observation $x_{ijk}$.

Compared to the PARAFAC model, the 3MFA model uses an additional set of parameters to account for interactions between the three sets of components. The 3MFA model is given by

$$X_{ijk} = \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} g_{pqr} a_{ip} b_{jq} c_{kr} + e_{ijk},$$

where the matrices $A$, $B$, and $C$ are of orders $I \times P$, $J \times Q$, and $K \times R$, and the additional parameters $g_{pqr}$ denote elements of the $P \times Q \times R$ so-called "core array." The matrices $A$, $B$, and $C$ can be considered component matrices for "idealized subjects" (in $A$), "idealized variables" (in $B$), and "idealized occasions" (in $C$), respectively. The elements of the core indicate how the components from the different modes interact.

As has been noted by Carroll and Chang (1970, p. 312), the PARAFAC model can be considered as a version of the 3MFA model where the core is constrained to be "super-diagonal" (which implies that $g_{ijk}$ is unconstrained if $i = j = k$ and $g_{ijk}$ is constrained to 0 otherwise). It follows that, if $P = Q = R$, the 3MFA fit is always at least as good as the PARAFAC fit, because the 3MFA model uses not only the super-diagonal elements of the core, but also the off-super-diagonal elements, which may considerably enhance the fit. To pinpoint the difference between the two models, we use a (simplified) tensorial description of the two models. Considering $x$ as a vectorized version of the modelled three-way array, and $e$ as a vector with error terms, the 3MFA model can be written as

$$x = g_{111}(a_1 \otimes b_1 \otimes c_1) + g_{112}(a_1 \otimes b_1 \otimes c_2) + g_{113}(a_1 \otimes b_1 \otimes c_3) + \cdots + g_{211}(a_2 \otimes b_1 \otimes c_1) + \cdots + g_{PQR}(a_P \otimes b_Q \otimes c_R) + e,$$

where $(a_i \otimes b_j \otimes c_k)$ denotes the triple tensor product of column $i$ of $A$, column $j$ of $B$, and column $k$ of $C$. This tensor product can be viewed as the vectorized version of the three-