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UNIQUENESS OF THREE-MODE FACTOR MODELS WITH SPARSE CORES: THE 3 × 3 × 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

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

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 × R, J × R, and K × 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

$$x_{ijk} = \sum_{p=1}^{P} \sum_{q=1}^{Q} \sum_{r=1}^{R} a_{ip} b_{jq} c_{kr} g_{pqr} + e_{ijk}, \tag{2}$$

where the matrices **A**, **B**, and **C** are of orders I × P, J × Q, and K × R, and the additional parameters g_{pqr} denote elements of the P × Q × R socalled "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 "superdiagonal" (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 superdiagonal elements of the core, but also the off-superdiagonal 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

$$\mathbf{x} = g_{111}(\mathbf{a}_1 \otimes \mathbf{b}_1 \otimes \mathbf{c}_1) + g_{112}(\mathbf{a}_1 \otimes \mathbf{b}_1 \otimes \mathbf{c}_2) + g_{113}(\mathbf{a}_1 \otimes \mathbf{b}_1 \otimes \mathbf{c}_3) + \cdots + g_{211}(\mathbf{a}_2 \otimes \mathbf{b}_1 \otimes \mathbf{c}_1) + \cdots + g_{PQR}(\mathbf{a}_P \otimes \mathbf{b}_Q \otimes \mathbf{c}_R) + \mathbf{e}, \tag{3}$$

where $(\mathbf{a}_i \otimes \mathbf{b}_j \otimes \mathbf{c}_k)$ 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-way array that comes about by calculating all possible products of elements from the three different vectors. In the same notation, the PARAFAC model can be written as

$$\mathbf{x} = (\mathbf{a}_1 \otimes \mathbf{b}_1 \otimes \mathbf{c}_1) + (\mathbf{a}_2 \otimes \mathbf{b}_2 \otimes \mathbf{c}_2) + \cdots + (\mathbf{a}_R \otimes \mathbf{b}_R \otimes \mathbf{c}_R) + \mathbf{e}; \tag{4}$$

note that the superdiagonal core elements g_{iii}, $i = 1, \ldots,$ R have been subsumed in one of the parameter matrices. The crucial difference between the models in (3) and (4) is that, whereas the 3MFA model contains all possible tensor products, the PARAFAC model contains only the products $(\mathbf{a}_i \otimes \mathbf{b}_j \otimes \mathbf{c}_k)$ for which $i = j = k$. Clearly, the PARAFAC model is a far more parsimonious model than the 3MFA model. In interpreting the results of a PARAFAC analysis, we have to consider only how A-, B- and C-mode components with the same index contribute jointly to the representation of the data. In interpreting a 3MFA solution, we have to additionally employ *all interactions of components with different indices*. This fact makes the interpretation of 3MFA solutions far more complicated than interpreting a PARAFAC solution.

There is another complication in interpreting the 3MFA solution. Once a 3MFA solution is obtained, we may, without affecting the fit, transform the three component weight matrices by any nonsingular transformation, provided that this is compensated for by applying the inverse transformations to the core array (see Kroonenberg & de Leeuw, 1980, p. 70). This implies that, before interpreting a 3MFA solution, we should decide what transformation of the components to apply. This transformational indeterminacy is similar to that in factor analysis, and one might therefore expect that, as in factor analysis, some kind of simple structure rotation would be convenient to identify the solution. However, for the present problem it is by no means clear what this simple structure rotation should be. One approach is to transform the components such that the core becomes as close as possible to a superdiagonal matrix (see e.g., Kroonenberg, 1983). Another is to apply a set of orthogonal rotations that optimizes a combination of orthomax functions applied to the core (Kiers, in press). However, there is little substantive reason to restrict oneself to orthogonal rotations, and, as has been shown by Kiers (1992), oblique rotation to superdiagonality tends to give ill-defined solutions; other procedures for oblique rotation are still in the stage of development (Kiers, in press; Kruskal, 1988). It can be concluded that the transformational indeterminacy of the 3MFA solution is a serious problem, that has no clear-cut solution.

The PARAFAC model, on the other hand, has no such identification problems. The PARAFAC solution is, under mild assumptions, unique up to scaling and permutations (see Harshman, 1972; Kruskal, 1977, 1989). This implies that the tensor products that contribute to the description of $\mathbf{x}$ are uniquely determined. This difference with 3MFA, added to the above mentioned difference in parsimony of the model descriptions, makes the PARAFAC model more attractive than the 3MFA model. If, for a particular data set, the fit of the PARAFAC model is almost as good as that of the 3MFA model, one will usually prefer the PARAFAC model. The choice becomes difficult if the PARAFAC fit is considerably worse than the 3MFA fit, or if the PARAFAC solution is degenerate. Apparently, in such cases, the tensor products with the same indices are not sufficient to describe the data adequately, and we have to add tensor products with *different* indices (as in the 3MFA model). However, there is no intrinsic reason to take all such tensor products. Adding only a few such terms often appears to increase the fit considerably. In this way, we obtain a model in between the 3MFA model and PARAFAC that has a (much) better fit than PARAFAC, is slightly more complex than the PARAFAC model, but is not nearly as complex as the full 3MFA model, and, as will be seen later, is unique in various cases. In fact, such models strike a compromise between the parsimony of the PARAFAC model and the good fit of the 3MFA model. Technically, such models can be viewed as constrained 3MFA (C3MFA) models, where a majority of the core elements is constrained to zero.

Constrained Three-Mode Factor Analysis (C3MFA)

Above, we introduced Constrained Three-Mode Factor Analysis (C3MFA) as the technique that fits the 3MFA model subject to certain constraints on the core. To fit C3MFA models, Kiers (1992) proposed an iterative algorithm which is a straightforward extension of the PARAFAC algorithm. That is, in this algorithm each component matrix is updated by a regression procedure, as in PARAFAC, and the core is updated by an additional regression step. The algorithm differs considerably from the TUCKALS-3 algorithm for 3MFA (Kroonenberg & de Leeuw, 1980), because in the latter algorithm one can, without affecting the maximum fit, constrain **A**, **B** and **C** to be columnwise orthonormal. In fact, in 3MFA these constraints are merely identification constraints. In C3MFA one can also constrain **A**, **B** and **C** to be columnwise orthonormal, as has been done by Rocci (1992), but in C3MFA these constraints are no longer identification constraints: Using these constraints (usually) decreases the maximum of the fit function. For this reason, Kiers (1992) proposed to drop the orthonormality constraints. In some situations, additional reasons for dropping the orthonormality constraints may arise. For instance, in chemometrical applications the matrices **A**, **B** and **C** should all have nonnegative elements, which is incompatible with the orthonormality constraints. Alternatively, it is conceivable that in certain situations the orthonormality constraints hardly affect the fit, but do make the interpretation of a solution easier. In such cases, Rocci's algorithm is indicated. To keep the results as generally applicable as possible, in the present paper it will be assumed that **A**, **B** and **C** are unconstrained.

Above, it has been mentioned that C3MFA often yields a considerably better fit than PARAFAC. In fact, in numerous analyses of three-way arrays (both empirical and contrived ones) it turned out that the C3MFA fit was approximately or exactly equal to the 3MFA fit, even in cases where a relatively large number of core elements were constrained to zero. Although we will not delve into this in detail, it may be useful to give some of our preliminary results. In case of a $2 \times 2 \times 2$ core, we can constrain at least four elements to zero without affecting the fit. For $3 \times 3 \times 3$ cores, it can be proven that, under mild assumptions, at least 16 of the 27 core elements can be constrained to zero without decrease in fit. Empirical study of several contrived data sets indicates that 18 elements can be constrained to zero without decreasing the fit. Therefore, it seems that the most interesting C3MFA models are those that emerge by adding only a few terms to the PARAFAC model, and the present paper will focus on such models. In the next section, we will illustrate the usefulness of C3MFA models with $3 \times 3 \times 3$ cores with many zero constraints by means of some simple exemplary analyses.

Exemplary Analyses

Lundy, Harshman and Kruskal (1989) report an analysis of their "TV-data" (a three-way array of ratings of 15 television shows by 40 subjects on 16 scales). Their PFCORE procedure produced a PARAFAC solution for **A**, **B** and **C** and a $3 \times 3 \times 3$ core array interrelating the PARAFAC dimensions. Rather than reanalyzing the full data array by C3MFA procedures, we chose to analyze the much simpler $3 \times 3 \times 3$ core array as if it were the original data matrix. That is, we take the interpretation of the components by Lundy et al. as if these interpretations refer to real (rather than idealized) scales, shows and individuals, respectively. The "data" array (see Lundy et al., p. 127) is reported in Table 1.

TABLE 1

"TV" Core Data

	First Idealized Individual		
	Funny Show	Sensitive Show	Violent Show
Humor	1.058	-.257	.301
Sensitivity	-.084	.102	-.216
Violence	-.095	.093	-.057
	Second Idealized Individual		
	Funny Show	Sensitive Show	Violent Show
Humor	.014	-.013	.089
Sensitivity	-.071	.951	.113
Violence	.016	-.049	-.025
	Third Idealized Individual		
	Funny Show	Sensitive Show	Violent Show
Humor	-.125	.485	-.667
Sensitivity	.244	-.099	.194
Violence	.135	.087	1.061

This data set has been analyzed by means of C3MFA with 3 dimensions for all three modes. In this way, obviously, no reduction in dimensionality will be attained, but we hope to obtain a parsimonious representation of this data by using many zero constraints in the core. Specifically, we fitted five C3MFA models (using $3 \times 3 \times 3$ cores with many elements constrained to zero) and the PARAFAC model (in three dimensions). The C3MFA models were all extensions of the PARAFAC model, in that they employed the terms used in the PARAFAC model, plus one or two additional tensor products. The choices of these products may seem somewhat arbitrary; at the end of the present paper, we will explain why these choices were made. In Table 2 the fit percentages (percentages of the total sum of squares explained) of these five models and the PARAFAC model are reported. To describe the five models, we report the core elements corresponding to the tensor products "added" to the PARAFAC model. To interpret the results in Table 2, it should be noted

TABLE 2

Fit Percentages of Five C3MFA Models and PARAFAC fitted to the TV Core Data

Model	Fit Percentage
PARAFAC	93.8 %
PF+g_{121}	93.8 %
PF+g_{121}+g_{211}	93.8 %
PF+g_{321}	94.6 %
PF+g_{321}+g_{231}	98.9 %
PF+g_{321}+g_{132}	98.8 %

that the unconstrained 3MFA model has a fit percentage of 100%. It can be seen that PARAFAC comes rather close to this 100%, and that little can be gained by adding only one tensor product term to the PARAFAC model. However, adding two other terms, as in the last two models, does increase the fit considerably, and raises it close to the maximum of 100%. Hence, it can be seen that the TV core data can be represented very well by a model with five tensor product terms, and that we hardly gain by using the full 3MFA model (with 27 terms) to represent these data.

We will interpret the results of the best fitting model only: PF + g_{321} + g_{231} (see Table 3). The scale components can be interpreted as: "Violence corrected for Humor," "Humor" and "Sensitivity," respectively; the Show components are mainly covered by "Violent Show," "Funny Show" and "Sensitive Show," respectively; the Subject components are virtually identical to "Third Individual," "First Individual" and "Second Individual," respectively. The related constrained core is given in Table 3 as well. It can be seen that, in addition to the three main terms (that relate Corrected Violence, Violent Show and the Third Individual; Humor, Funny Shows and the First Individual; and Sensitivity, Sensitive Shows and the Second Individual), there are two interaction terms, both of which are especially important for the Third Individual: Humor with Sensitive Shows, and Sensitivity with Funny Shows. Looking back at our original data, we had 24 terms that could count as such interaction terms, six of which were relatively large. Thus it has been demonstrated that an important increase in parsimony has been obtained by using the C3MFA model, at very lost costs.

Uniqueness of C3MFA Models

As has been mentioned above, the interpretation of 3MFA solutions is more complicated than of PARAFAC solutions for two reasons: the 3MFA model involves more parameters than the PARAFAC model, and 3MFA gives nonunique solutions. The former

TABLE 3

Component Matrices and Core for C3MFA model "PF+g_{321}+g_{132}"

	Scale Components		
Humor	-.57	.99	.02
Sensitivity	.11	-.13	1.00
Violence	.82	-.10	-.04
	Show Components		
Funny Show	.13	.93	-.06
Sensitive Show	.13	-.23	.99
Violent Show	.98	.28	.12
	Individual Components		
First Individual	-.02	1.00	.04
Second Individual	-.05	.02	1.00
Third Individual	1.00	.00	.01

C3MFA Core

"3rd Individual"	"Violent Show"	"Funny Show"	"Sensitive Show"
"Violence - Humor"	1.33	0	0
"Humor"	0	0	.60
"Sensitivity"	0	.24	0

"1st Individual"	"Violent Show"	"Funny Show"	"Sensitive Show"
"Violence - Humor"	0	0	0
"Humor"	0	1.14	0
"Sensitivity"	0	0	0

"2nd Individual"	"Violent Show"	"Funny Show"	"Sensitive Show"
"Violence - Humor"	0	0	0
"Humor"	0	0	0
"Sensitivity"	0	0	.96

disadvantages of 3MFA can be diminished by constraining a majority of core elements to zero, as has been illustrated in the above example. It is the purpose of the present paper to show that constraining core elements to zero *can also* eliminate the latter disadvantage. Specifically, it will be shown that a class of (sparse) C3MFA models with $3 \times 3 \times 3$ cores has, under mild assumptions, a unique representation. (In the sequel, we will usually contract the phrase that "a model has a (non)unique representation" to "a model is (non)unique.") At the end of the paper we will rediscuss the results for the example in the light of the (non)uniqueness results of the present paper.

The present paper is limited to uniqueness for a class of C3MFA models that employ $3 \times 3 \times 3$ cores. It should be noted that the main results carry over to C3MFA models where **A**, **B**, and or **C** is constrained in some way (e.g., as in Rocci, 1992): All models that are unique when **A**, **B** and **C** are unconstrained, remain unique when constraints on these matrices are imposed. The reason to focus only on $3 \times 3 \times 3$ core arrays is that, among C3MFA models employing smaller core arrays, the only (nontrivial) unique one we encountered in extensive experimentation is the C3MFA model in which the $2 \times 2 \times 2$ core is constrained to be superdiagonal (which is, in fact, the PARAFAC case). On the other hand, among the C3MFA models employing larger cores than $3 \times 3 \times 3$, there may be many unique models, but considering the complexity of the present uniqueness proof, we choose to leave those cases open for further study.

The class of C3MFA models for which uniqueness is proven consists of models in which the $3 \times 3 \times 3$ core **G** is constrained such that the three "superdiagonal" core elements (g_{111}, g_{222} and g_{333}) are unconstrained, the eighteen core elements with two equal indices, denoted as the "plane diagonal elements" (because they are not on the superdiagonal, but they are on the diagonal of a frontal, horizontal, or lateral plane) are constrained to zero, and the six "offdiagonal elements" (i.e., elements with three different indices, which are offdiagonal in all senses) are either unconstrained or constrained to zero. This class of C3MFA models is characterized as those employing a core with frontal planes

$$\mathbf{G}_1 = \begin{pmatrix} x & 0 & 0 \\ 0 & 0 & b \\ 0 & a & 0 \end{pmatrix}, \mathbf{G}_2 = \begin{pmatrix} 0 & 0 & d \\ 0 & y & 0 \\ c & 0 & 0 \end{pmatrix}, \text{and } \mathbf{G}_3 = \begin{pmatrix} 0 & f & 0 \\ e & 0 & 0 \\ 0 & 0 & z \end{pmatrix}, \tag{5}$$

where the elements a, b, c, d, e and f denote the offdiagonal elements, which may or may not be constrained to zero (depending on the model at hand). In the present paper, it will be proven that all C3MFA models in which the core is constrained to be of the form in (5), or a permutation or rescaling thereof, are "unique" under certain mild assumptions. This uniqueness implies that if a set of parameters (**A**, **B**, **C**, **G**) and an alternative set of parameters ($\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$, $\tilde{\mathbf{G}}$), both satisfying the constraints of a particular C3MFA model, give the same representation of the data, then the parameters in **A**, **B** and **C** must be equal up to a permutation and/or rescaling of the columns of $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{C}}$. Note that the columns of **A**, **B** and **C** can always be rescaled arbitrarily, as long as this is compensated by inverse scalings of the "rows," "columns" and "slabs" of the core. (Here "slabs" denote the frontal planes of the core, "rows" denote the horizontal planes of the core, consisting of the rows of the slabs, and "columns" denote the lateral planes of the core, consisting of the columns of the slabs). This explains why uniqueness can only be obtained up to rescalings. Permutations of the columns can sometimes, but not always be compensated by permutations in the core. It will be indicated in a separate section which permutations are and which are not permissible.

A complete description of the uniqueness result to be proven in the present paper is stated in the following Definition and Theorem.

Definition. A set of constraints on the core is called "Extended PARAFAC" (EP) constraints if it specifies all plane diagonal elements to be zero, an arbitrary but fixed set of offdiagonal elements to be zero, and it leaves all superdiagonal elements unconstrained. (This definition implies that all cores that satisfy EP constraints are of the form in (5)).

Note that cases where a superdiagonal element is constrained to zero are excluded by the class of EP constraints. However, by permutations we can always transform each core that has three unconstrained terms in different rows, columns and slabs into the form of (5), and hence subsume such sets of constraints under the class of EP constraints. For ease of notation, we will not treat such cases explicitly in the Uniqueness Theorem.

Uniqueness Theorem. Let $\mathbf{A}$ (I × 3), $\mathbf{B}$ (J × 3) and $\mathbf{C}$ (K × 3) be component matrices, and let $\mathbf{G}$ (3 × 3 × 3) be a core that satisfies a set of EP constraints, with the elements denoted as in (5). Furthermore, let

(i) $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ have full column rank,
(ii) all unconstrained elements of $\mathbf{G}$ be nonzero,
(iii) $(xyz + ade + bcf)^3 \neq 27abcdefxyz$.

Then every set $\{\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}, \tilde{\mathbf{G}}\}$ that gives the same 3MFA representation as $\{\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{G}\}$, hence for which

$$\sum_{p=1}^{3} \sum_{q=1}^{3} \sum_{r=1}^{3} \tilde{a}_{ip}\tilde{b}_{jq}\tilde{c}_{kr}\tilde{g}_{pqr} = \sum_{p=1}^{3} \sum_{q=1}^{3} \sum_{r=1}^{3} a_{ip}b_{jq}c_{kr}g_{pqr},$$

for all i, j, k, and in which $\tilde{\mathbf{G}}$ satisfies the same set of EP constraints, is related to $\{\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{G}\}$ such that the columns of $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{C}}$ are at most rescaled versions of those of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, respectively, possibly in different orders.

To avoid overcomplicating the description of the Uniqueness Theorem, we do not state the precise form the permutations and rescalings may take. The freedom in scaling has already been mentioned above. In a later section, we will offer some details on which permutations are and which are not permissible for the different models. It will also be demonstrated there that the permissible permutations do not affect the interpretation of the components. Since rescalings do not affect the interpretation either, the Uniqueness Theorem can indeed be interpreted as stating that all C3MFA models that use EP constraints give "unique" representations.

The Uniqueness Theorem specifies three conditions that are jointly sufficient for uniqueness. As will be seen in a later section, condition (iii) is necessary for uniqueness as well. As a practical matter, the condition that unconstrained core elements are nonzero (Condition (ii)) can always be assumed to hold. For one thing, with real data, there is zero probability that the fitted value of any unconstrained element will be 0. For another, if such an element should happen to be 0, then the data analyst will immediately switch to a model in which that element is constrained to be 0. The two other uniqueness conditions can be assumed to be satisfied in all practical situations. In fact, violation of Condition (iii) is highly unlikely in practice, since, as can be verified, it requires that either $ade = bcf = xyz$ or $(ade)^{1/3} + (bcf)^{1/3} = -(xyz)^{1/3}$. It should also be noted that we only consider uniqueness *given* the estimates for $\mathbf{X}$. This does not exclude the existence of cases where the estimates themselves are not unique. This restriction to "uniqueness given the estimates" is common in uniqueness proofs, and has, for instance, also been used in uniqueness proofs for the PARAFAC model.

Proof of the Uniqueness Theorem

The bulk of the present paper is devoted to proving the Uniqueness Theorem. We will do so by proving several Lemmas, and linking these to each other. By means of the first

Lemma, all possible sets of EP constraints are classified into ten classes. Constraint sets that are in the same class are shown to define essentially the same C3MFA model. Therefore, it is sufficient to prove uniqueness for these ten cases. The second Lemma shows that **A**, **B** and **C** are related to $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{C}}$ by means of nonsingular transformations (**S**, **T** and **U**, respectively), and it is implied that proving uniqueness of C3MFA models reduces to proving that the transformation matrices are rescaled permutation matrices. Next, lemma 3 specifies a set of six equations for the elements of the matrix **U** (the matrix relating **C** to $\tilde{\mathbf{C}}$ according to $\mathbf{C} = \tilde{\mathbf{C}}\mathbf{U}$), that must hold for all C3MFA models that employ a set of EP constraints. Since these six equations are nonlinear, we cannot simply solve them for the elements of **U**. Instead, we supplement these six equations with 21 other equations and henceforth relate two $3 \times 3 \times 3$ arrays to each other, one of which is of the form of (5). This relation is given in Lemma 4. With these Lemmas, we are in a position to prove that **U** is a rescaled permutation matrix for all ten cases under study (Lemmas 5 and 6). To finish the proof, it is shown that the matrices **S** and **T** (that relate **A** to $\tilde{\mathbf{A}}$, and **B** to $\tilde{\mathbf{B}}$, respectively) must be rescaled permutation matrices as well.

We will now establish the Lemmas used in this uniqueness proof. Elaborate proofs, that do not contribute much to insight in the line of reasoning, will be deferred to an appendix.

Lemma 1. Each of the 2^6 conceivable sets of EP constraints can, by permuting rows, columns or slabs of the array, be subsumed under one of the following ten cases:

Case 0: $a = b = c = d = e = f = 0.$
Case 1: $a \neq 0; b = c = d = e = f = 0.$
Case 2a: $ab \neq 0; c = d = e = f = 0;$
Case 2b: $ad \neq 0; b = c = e = f = 0;$
Case 3a: $abc \neq 0; d = e = f = 0;$
Case 3b: $ade \neq 0; b = c = f = 0;$
Case 4a: $abcd \neq 0; e = f = 0;$
Case 4b: $abde \neq 0; c = f = 0;$
Case 5: $abcde \neq 0; f = 0.$
Case 6: $abcdef \neq 0.$

Proof. See Appendix A.

As shown in Appendix A, the respective cases cover the following situations:

Case 0: The case where all offdiagonal elements are constrained to zero. This case coincides with the PARAFAC model, since we only have the superdiagonal terms in the core.
Case 1: All cases with one unconstrained offdiagonal element.
Case 2: All cases with two unconstrained offdiagonal elements; Case 2a if they are in the same row, column or slab; Case 2b otherwise.
Case 3: All cases with three unconstrained offdiagonal elements; Case 3a if two of them are in the same row, column or slab; Case 3b if they are all in different rows, columns and slabs.
Case 4: All cases with four unconstrained offdiagonal elements; Case 4a if one column, row or slab contains no offdiagonal element; Case 4b otherwise.
Case 5: All cases with five unconstrained offdiagonal elements.
Case 6: The case with six unconstrained offdiagonal elements.

To prove the Uniqueness Theorem, we will first simplify the basic equality

$$\sum_{p=1}^{3} \sum_{q=1}^{3} \sum_{r=1}^{3} \tilde{a}_{ip}\tilde{b}_{jq}\tilde{c}_{kr}\tilde{g}_{pqr} = \sum_{p=1}^{3} \sum_{q=1}^{3} \sum_{r=1}^{3} a_{ip}b_{jq}c_{kr}g_{pqr},$$

$i = 1, \ldots, I, j = 1, \ldots, J, k = 1, \ldots, K$, as

$$\tilde{\mathbf{A}}\left(\sum_{l=1}^{3} \tilde{c}_{kl}\tilde{\mathbf{G}}_l\right)\tilde{\mathbf{B}}' = \mathbf{A}\left(\sum_{l=1}^{3} c_{kl}\mathbf{G}_l\right)\mathbf{B}',$$

$k = 1, \ldots, K$. The following Lemma is used to further simplify this equality.

Lemma 2. If P = Q = R = 3, **G** satisfies a set of EP constraints, and conditions (i) and (ii) in the Uniqueness Theorem are satisfied, then

$$\tilde{\mathbf{A}}\left(\sum_{l=1}^{3} \tilde{c}_{kl}\tilde{\mathbf{G}}_l\right)\tilde{\mathbf{B}}' = \mathbf{A}\left(\sum_{l=1}^{3} c_{kl}\mathbf{G}_l\right)\mathbf{B}', \tag{6}$$

holds for $k = 1, \ldots, K$ if and only if there exist nonsingular matrices **S**, **T** and **U** such that $\mathbf{A} = \tilde{\mathbf{A}}\mathbf{S}$, $\mathbf{B} = \tilde{\mathbf{B}}\mathbf{T}$, $\mathbf{C} = \tilde{\mathbf{C}}\mathbf{U}$, and

$$\tilde{\mathbf{G}}_k = \mathbf{S}\left(\sum_{l=1}^{3} u_{kl}\mathbf{G}_l\right)\mathbf{T}' \equiv \mathbf{S}\bar{\mathbf{G}}_k\mathbf{T}', \tag{7}$$

where we defined $\bar{\mathbf{G}}_k \equiv (\Sigma_{l=1}^{3} u_{kl}\mathbf{G}_l)$, $k = 1, 2, 3$.

Proof. To prove the "only if" part, we can rewrite (6) as $\mathbf{A}(\mathbf{G}_1 \mid \mathbf{G}_2 \mid \mathbf{G}_3)(\mathbf{C}' \otimes \mathbf{B}') = \tilde{\mathbf{A}}(\tilde{\mathbf{G}}_1 \mid \tilde{\mathbf{G}}_2 \mid \tilde{\mathbf{G}}_3)(\tilde{\mathbf{C}}' \otimes \tilde{\mathbf{B}}')$. It follows from Condition (i) that $(\mathbf{C}' \otimes \mathbf{B}')$ is a $9 \times JK$ matrix of full rank 9, and from Condition (ii) that

$$(\mathbf{G}_1 \mid \mathbf{G}_2 \mid \mathbf{G}_3) = \begin{pmatrix} x & 0 & 0 & 0 & 0 & d & 0 & f & 0 \\ 0 & 0 & b & 0 & y & 0 & e & 0 & 0 \\ 0 & a & 0 & c & 0 & 0 & 0 & 0 & z \end{pmatrix}$$

is of full rank 3. Hence, $\mathbf{A} = \tilde{\mathbf{A}}(\tilde{\mathbf{G}}_1 \mid \tilde{\mathbf{G}}_2 \mid \tilde{\mathbf{G}}_3)(\tilde{\mathbf{C}}' \otimes \tilde{\mathbf{B}}')(\mathbf{C}' \otimes \mathbf{B}')^+(\mathbf{G}_1 \mid \mathbf{G}_2 \mid \mathbf{G}_3)^+$, where $^+$ denotes the Moore-Penrose inverse. Because **A** has rank 3, $\tilde{\mathbf{A}}(\tilde{\mathbf{G}}_1 \mid \tilde{\mathbf{G}}_2 \mid \tilde{\mathbf{G}}_3)(\tilde{\mathbf{C}}' \otimes \tilde{\mathbf{B}}')$ must have rank 3 as well, and hence $\tilde{\mathbf{A}}$ must also have rank 3. Because **A** and $\tilde{\mathbf{A}}$ span the same column space, it follows that $\mathbf{A} = \tilde{\mathbf{A}}\mathbf{S}$ for a certain nonsingular matrix **S**. In a completely analogous fashion we find that $\mathbf{B} = \tilde{\mathbf{B}}\mathbf{T}$ and $\mathbf{C} = \tilde{\mathbf{C}}\mathbf{U}$, for nonsingular 3×3 matrices **T** and **U**. Hence it follows from (6) that

$$\tilde{\mathbf{A}}\left(\sum_{l=1}^{3} \tilde{c}_{kl}\tilde{\mathbf{G}}_l\right)\tilde{\mathbf{B}}' = \tilde{\mathbf{A}}\mathbf{S}\left(\sum_{l=1}^{3} [\tilde{\mathbf{C}}\mathbf{U}]_{kl}\mathbf{G}_l\right)\mathbf{T}'\tilde{\mathbf{B}}', \tag{8}$$

$k = 1, \ldots, K$. Premultiplying (8) by $\tilde{\mathbf{A}}^+$ and postmultiplying (8) by $\tilde{\mathbf{B}}'^+$ gives

$$\sum_{l=1}^{3} \tilde{c}_{kl}\tilde{\mathbf{G}}_l = \mathbf{S}\left(\sum_{l=1}^{3} [\tilde{\mathbf{C}}\mathbf{U}]_{kl}\mathbf{G}_l\right)\mathbf{T}', \tag{9}$$

$k = 1, \ldots, K$. Writing both sides of (9) in vectorized form and collecting these vectors (for $k = 1, 2, 3$) in a matrix, we obtain

$$(\text{Vec}(\tilde{\mathbf{G}}_1) \mid \text{Vec}(\tilde{\mathbf{G}}_2) \mid \text{Vec}(\tilde{\mathbf{G}}_3))\tilde{\mathbf{C}}' = (\text{Vec}(\mathbf{S}\mathbf{G}_1\mathbf{T}') \mid \text{Vec}(\mathbf{S}\mathbf{G}_2\mathbf{T}') \mid \text{Vec}(\mathbf{S}\mathbf{G}_3\mathbf{T}'))(\tilde{\mathbf{C}}\mathbf{U})', \tag{10}$$

where Vec (·) denotes the vector containing the columns of the matrix in parentheses below each other. Postmultiplying both sides of (10) by $\tilde{\mathbf{C}}'^+$ yields

$$(\text{Vec}(\tilde{\mathbf{G}}_1) \mid \text{Vec}(\tilde{\mathbf{G}}_2) \mid \text{Vec}(\tilde{\mathbf{G}}_3)) = (\text{Vec}(\mathbf{S}\mathbf{G}_1\mathbf{T}') \mid \text{Vec}(\mathbf{S}\mathbf{G}_2\mathbf{T}') \mid \text{Vec}(\mathbf{S}\mathbf{G}_3\mathbf{T}'))\mathbf{U}', \tag{11}$$

from which (7) follows at once. This proves the "only if" part. To prove the "if" part, we use that the essential steps can validly be made backwards: Rewriting (7) as (11) and postmultiplying both sides of (11) by $\tilde{\mathbf{C}}'$ yields (10), and hence (9); next, pre- and postmultiplying both sides of (9) by $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$, respectively, yields (8), from which (6) follows at once, using $\mathbf{A} = \tilde{\mathbf{A}}\mathbf{S}$, $\mathbf{B} = \tilde{\mathbf{B}}\mathbf{T}$, and $\mathbf{C} = \tilde{\mathbf{C}}\mathbf{U}$. □

The next Lemma specifies a set of equations for the elements of **U** that must be satisfied for (7) to hold, and hence for the basic equality in the Uniqueness Theorem to hold.

Lemma 3. Let $g \equiv \frac{1}{3}(xyz + ade + bcf)$, $h_1 \equiv abx$, $h_2 \equiv cdy$, and $h_3 \equiv efz$. Then a necessary condition for (7) to hold is that the elements of **U** satisfy

$$g(u_{k1}u_{l2}u_{l3} + u_{k2}u_{l1}u_{l3} + u_{k3}u_{l1}u_{l2}) - h_1u_{l1}^2u_{k1} - h_2u_{l2}^2u_{k2} - h_3u_{l3}^2u_{k3} = 0, \quad (12)$$

$k, l = 1, 2, 3, k \neq l$.

Proof. See Appendix B.

The equations in (12) express necessary conditions for (7) to be satisfied by the elements of **U**. These equations form the basis for proving that, if (7) holds, **U** is a rescaled permutation matrix. For this proof, it is convenient to define

$$\mathbf{V}_k \equiv \begin{pmatrix} -h_1u_{k1} & 0 & gu_{k2} \\ gu_{k3} & -h_2u_{k2} & 0 \\ 0 & gu_{k1} & -h_3u_{k3} \end{pmatrix}, \quad k = 1, 2, 3. \quad (13)$$

Corollary 3.1. Let $g \equiv \frac{1}{3}(xyz + ade + bcf)$, $h_1 \equiv abx$, $h_2 \equiv cdy$, and $h_3 \equiv efz$. Then a necessary condition for (7) to hold is that

$$\mathbf{u}_{l.}\mathbf{V}_k\mathbf{u}_{l.}' = 0. \quad (14)$$

$k = 1, 2, 3, l = 1, 2, 3, k \neq l$, where $\mathbf{u}_{l.}$ denotes the l-th row of **U**.

Proof. Immediate from Lemma 3 and the definition in (13). □

The six equations specified in (14) have a very special form. To see this, we define an auxiliary three-way **Y** (depending on the elements of **U** and on a number of constants), with elements $y_{ijk} \equiv \mathbf{u}_{i.}\mathbf{V}_k\mathbf{u}_{j.}'$, and frontal planes $\mathbf{Y}_k = \mathbf{U}\mathbf{V}_k\mathbf{U}'$, $k = 1, 2, 3$. Then the equations in (14) imply that the six elements y_{ijk} of **Y** for which $i = j \neq k$ are zero; these are six of the eighteen plane diagonal elements of **Y**. In the following Lemma, we will establish expressions for the other elements of the auxiliary array **Y**. In particular, Lemma 4 states that **Y** must be of the form displayed by **G** in (5). This result will allow us to prove that **U** must be a rescaled permutation matrix in each of the ten cases under study.

Lemma 4. Let

$$\alpha \equiv -h_1u_{11}u_{21}u_{31} - h_2u_{12}u_{22}u_{32} - h_3u_{13}u_{23}u_{33},$$

$$\beta \equiv u_{11}u_{23}u_{32} + u_{12}u_{21}u_{33} + u_{13}u_{22}u_{31},$$

$$\gamma \equiv u_{11}u_{22}u_{33} + u_{12}u_{23}u_{31} + u_{13}u_{21}u_{32},$$

$$\delta \equiv \alpha + g\beta,$$

$$\varepsilon \equiv \alpha + g\gamma.$$

Then a necessary condition for (7) to hold is that

$$\mathbf{Y}_1 \equiv \mathbf{U}\mathbf{V}_1\mathbf{U}' = \begin{pmatrix} |\bar{\mathbf{G}}_1| & 0 & 0 \\ 0 & 0 & \delta \\ 0 & \varepsilon & 0 \end{pmatrix}; \tag{15a}$$

$$\mathbf{Y}_2 \equiv \mathbf{U}\mathbf{V}_2\mathbf{U}' = \begin{pmatrix} 0 & 0 & \varepsilon \\ 0 & |\bar{\mathbf{G}}_2| & 0 \\ \delta & 0 & 0 \end{pmatrix}; \tag{15b}$$

$$\mathbf{Y}_3 \equiv \mathbf{U}\mathbf{V}_3\mathbf{U}' = \begin{pmatrix} 0 & \delta & 0 \\ \varepsilon & 0 & 0 \\ 0 & 0 & |\bar{\mathbf{G}}_3| \end{pmatrix}, \tag{15c}$$

where $\mathbf{Y}_1$, $\mathbf{Y}_2$ and $\mathbf{Y}_3$ denote the frontal planes of the array $\mathbf{Y}$ defined above.

Proof. For the elements (i, j, k) of $\mathbf{Y}$, we have

$$\begin{aligned} y_{ijk} = \mathbf{u}_{i.}\mathbf{V}_k\mathbf{u}'_{j.} &= (u_{i1}u_{i2}u_{i3})\begin{pmatrix} -h_1u_{k1} & 0 & gu_{k2} \\ gu_{k3} & -h_2u_{k2} & 0 \\ 0 & gu_{k1} & -h_3u_{k3} \end{pmatrix}\begin{pmatrix} u_{j1} \\ u_{j2} \\ u_{j3} \end{pmatrix} \\ &= g(u_{i1}u_{j3}u_{k2} + u_{i2}u_{j1}u_{k3} + u_{i3}u_{j2}u_{k1}) \\ &\quad - h_1u_{i1}u_{j1}u_{k1} - h_2u_{i2}u_{j2}u_{k2} - h_3u_{i3}u_{j3}u_{k3}. \end{aligned} \tag{16}$$

It follows from (16) that

$$\begin{aligned} y_{kll} &= \mathbf{u}_{k.}\mathbf{V}_l\mathbf{u}'_{l.} \\ &= g(u_{k1}u_{l2}u_{l3} + u_{k2}u_{l1}u_{l3} + u_{k3}u_{l1}u_{l2}) \\ &\quad - h_1u_{k1}u_{l1}^2 - h_2u_{k2}u_{l2}^2 - h_3u_{k3}u_{l3}^2, \end{aligned} \tag{17}$$

and

$$\begin{aligned} y_{lkl} &= \mathbf{u}_{l.}\mathbf{V}_l\mathbf{u}'_{k.} \\ &= g(u_{k1}u_{l2}u_{l3} + u_{k2}u_{l1}u_{l3} + u_{k3}u_{l1}u_{l2}) \\ &\quad - h_1u_{k1}u_{l1}^2 - h_2u_{k2}u_{l2}^2 - h_3u_{k3}u_{l3}^2. \end{aligned} \tag{18}$$

Clearly, (17) and (18) equal the left-hand side of (12). Hence, by Lemma 3, it follows from (7) that $y_{kll} = 0$ and $y_{lkl} = 0$, for $k, l = 1, 2, 3$, $k \neq l$. By Corollary 3.1, it follows from (7) that $y_{llk} = 0$ for $k, l = 1, 2, 3$, $k \neq l$. Thus, it has been proven that all eighteen plane diagonal elements of $\mathbf{Y}$ are zero.

Next, we consider the superdiagonal elements of $\mathbf{Y}$. From (16) it follows that

$$y_{kkk} = \mathbf{u}_{k.}\mathbf{V}_k\mathbf{u}'_{k.} = 3gu_{k1}u_{k2}u_{k3} - h_1u_{k1}^3 - h_2u_{k2}^3 - h_3u_{k3}^3, \tag{19}$$

$k = 1, 2, 3$. From the definition of $\bar{\mathbf{G}}_k$, we have

$$\bar{\mathbf{G}}_k \equiv \sum_{l=1}^{3} u_{kl}\mathbf{G}_l = \begin{pmatrix} xu_{k1} & fu_{k3} & du_{k2} \\ eu_{k3} & yu_{k2} & bu_{k1} \\ cu_{k2} & au_{k1} & zu_{k3} \end{pmatrix}, \tag{20}$$

and it is readily verified that $y_{kkk} = |\bar{\mathbf{G}}_k|$.

Finally, we consider the offdiagonal elements of $\mathbf{Y}$. Using expression (16) and the definitions given in Lemma 4, we can verify that

$$y_{123} = y_{231} = y_{312} = \alpha + g\beta \equiv \delta \tag{21a}$$

$$y_{132} = y_{213} = y_{321} = \alpha + g\gamma \equiv \varepsilon, \tag{21b}$$

which completes the proof of Lemma 4. □

Corollary 4.1. Let α, β, γ, δ, and ε be defined as in lemma 4, then a necessary condition for (7) to hold is that $\mathbf{U}$ satisfies

$$\mathbf{Y}_k = \mathbf{U}\left(\sum_{l=1}^{3} u_{kl}\mathbf{W}_l\right)\mathbf{U}',$$

where $\mathbf{W}_l$, $l = 1, 2, 3$, denotes the l-th frontal slab of the three-way array $\mathbf{W}$, defined by

$$\mathbf{W}_1 \equiv \begin{pmatrix} -h_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & g & 0 \end{pmatrix}; \mathbf{W}_2 \equiv \begin{pmatrix} 0 & 0 & g \\ 0 & -h_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \mathbf{W}_3 \equiv \begin{pmatrix} 0 & 0 & 0 \\ g & 0 & 0 \\ 0 & 0 & -h_3 \end{pmatrix}.$$

Proof. It is readily verified that (13) can be written as

$$\mathbf{V}_k = \sum_{l=1}^{3} u_{kl}\mathbf{W}_l,$$

$k = 1, 2, 3$. Then Corollary 4.1 follows at once from Lemma 4. □

Lemma 4 and its Corollary form the basis of our proof that $\mathbf{U}$ is a rescaled permutation matrix. In the Lemmas 5 and 6, the proof will be completed, for two subsets of cases separately.

Lemma 5. Under the Conditions (i), (ii) and (iii) of the Uniqueness Theorem, for Cases 0, 1, 2b and 3b, a necessary condition for (7) to hold is that $\mathbf{U}$ is a rescaled permutation matrix.

Proof. In cases 0, 1, 2b and 3b, we have $|\mathbf{G}_1| = |\mathbf{G}_2| = |\mathbf{G}_3| = |\tilde{\mathbf{G}}_1| = |\tilde{\mathbf{G}}_2| = |\tilde{\mathbf{G}}_3| = 0$, and $h_1 = h_2 = h_3 = 0$, hence

$$\mathbf{V}_k = \begin{pmatrix} 0 & 0 & gu_{k2} \\ gu_{k3} & 0 & 0 \\ 0 & gu_{k1} & 0 \end{pmatrix}. \tag{22}$$

According to (7), we have $\tilde{\mathbf{G}}_k = \mathbf{S}\bar{\mathbf{G}}_k\mathbf{T}'$, $k = 1, 2, 3$. Therefore, from $|\tilde{\mathbf{G}}_1| = |\tilde{\mathbf{G}}_2| = |\tilde{\mathbf{G}}_3| = 0$ it follows that $|\bar{\mathbf{G}}_1| = |\bar{\mathbf{G}}_2| = |\bar{\mathbf{G}}_3| = 0$. Hence, according to Lemma 4, we have

$$\mathbf{U}^{-1}\mathbf{Y}_1 = \mathbf{U}^{-1}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \delta \\ 0 & \varepsilon & 0 \end{pmatrix} = \mathbf{V}_1\mathbf{U}' = g\begin{pmatrix} 0 & 0 & u_{12} \\ u_{13} & 0 & 0 \\ 0 & u_{11} & 0 \end{pmatrix}\mathbf{U}'$$

$$= g\begin{pmatrix} 0 & 0 & u_{12} \\ u_{13} & 0 & 0 \\ 0 & u_{11} & 0 \end{pmatrix}\begin{pmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{pmatrix}; \tag{23a}$$

$$\mathbf{U}^{-1}\mathbf{Y}_2 = \mathbf{U}^{-1}\begin{pmatrix} 0 & 0 & \varepsilon \\ 0 & 0 & 0 \\ \delta & 0 & 0 \end{pmatrix} = \mathbf{V}_2\mathbf{U}' = g\begin{pmatrix} 0 & 0 & u_{22} \\ u_{23} & 0 & 0 \\ 0 & u_{21} & 0 \end{pmatrix}\mathbf{U}'$$

$$= g\begin{pmatrix} 0 & 0 & u_{22} \\ u_{23} & 0 & 0 \\ 0 & u_{21} & 0 \end{pmatrix}\begin{pmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{pmatrix}; \tag{23b}$$

$$\mathbf{U}^{-1}\mathbf{Y}_3 = \mathbf{U}^{-1}\begin{pmatrix} 0 & \delta & 0 \\ \varepsilon & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathbf{V}_3\mathbf{U}' = g\begin{pmatrix} 0 & 0 & u_{32} \\ u_{33} & 0 & 0 \\ 0 & u_{31} & 0 \end{pmatrix}\mathbf{U}'$$

$$= g\begin{pmatrix} 0 & 0 & u_{32} \\ u_{33} & 0 & 0 \\ 0 & u_{31} & 0 \end{pmatrix}\begin{pmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{pmatrix}. \tag{23c}$$

In Cases 0, 1, 2b and 3b, Condition (iii) reduces to $g \neq 0$, because $b = c = f = 0$. From (23), we have that the first column of the matrix in (23a), the second column of the matrix in (23b), and the third column of the matrix in (23c) vanish. Because $g \neq 0$, it follows that

$$u_{12}u_{13} = u_{13}u_{11} = u_{11}u_{12} = 0 \tag{24a}$$

$$u_{22}u_{23} = u_{23}u_{21} = u_{21}u_{22} = 0 \tag{24b}$$

$$u_{32}u_{33} = u_{33}u_{31} = u_{31}u_{32} = 0. \tag{24c}$$

The nonsingularity of **U** implies that every row of **U** has at least one nonzero element. Then it follows from (24) that, in every row, the other elements are zero. Hence, the nonsingularity of **U** implies that **U** is a rescaled permutation matrix. □

Lemma 6. Under the Conditions (i), (ii) and (iii) of the Uniqueness Theorem, for Cases 2a, 3a, 4a, 4b, 5 and 6, equation (7) holds only if **U** is a rescaled permutation matrix.

Proof. By Lemma 4, we have that (7) implies (15). From (15a) and (15b) we can deduce, using the explicit expressions for $\mathbf{V}_1$ and $\mathbf{V}_2$ in (13), the following three results:

$$|u_{21}\mathbf{Y}_1 - u_{11}\mathbf{Y}_2| = |\mathbf{U}(u_{21}\mathbf{V}_1 - u_{11}\mathbf{V}_2)\mathbf{U}'| = |\mathbf{U}|^2|u_{21}\mathbf{V}_1 - u_{11}\mathbf{V}_2| = 0 \tag{25a}$$

$$|u_{22}\mathbf{Y}_1 - u_{12}\mathbf{Y}_2| = |\mathbf{U}(u_{22}\mathbf{V}_1 - u_{12}\mathbf{V}_2)\mathbf{U}'| = |\mathbf{U}|^2|u_{22}\mathbf{V}_1 - u_{12}\mathbf{V}_2| = 0 \tag{25b}$$

$$|u_{23}\mathbf{Y}_1 - u_{13}\mathbf{Y}_2| = |\mathbf{U}(u_{23}\mathbf{V}_1 - u_{13}\mathbf{V}_2)\mathbf{U}'| = |\mathbf{U}|^2|u_{23}\mathbf{V}_1 - u_{13}\mathbf{V}_2| = 0, \tag{25c}$$

where the fact that the determinants are 0 follows from the particular pattern of zeros encountered in the matrices $(u_{2l}\mathbf{V}_1 - u_{1l}\mathbf{V}_2)$, $l = 1, 2, 3$. Elaborating the first terms in (25), using the explicit expression for $\mathbf{Y}_1$ and $\mathbf{Y}_2$ in (15), we find

$$|u_{2l}\mathbf{Y}_1 - u_{1l}\mathbf{Y}_2| = \begin{vmatrix} u_{2l}|\bar{\mathbf{G}}_1| & 0 & -u_{1l}\varepsilon \\ 0 & -u_{1l}|\bar{\mathbf{G}}_2| & u_{2l}\delta \\ -u_{1l}\delta & u_{2l}\varepsilon & 0 \end{vmatrix} = u_{1l}^3|\bar{\mathbf{G}}_2|\delta\varepsilon - u_{2l}^3|\bar{\mathbf{G}}_1|\delta\varepsilon = 0, \tag{26}$$

$l = 1, 2, 3$. It follows that either $\delta\varepsilon = 0$, or

$$u_{1l}|\bar{\mathbf{G}}_2|^{1/3} = u_{2l}|\bar{\mathbf{G}}_1|^{1/3}, \tag{27}$$

$l = 1, 2, 3$. In the Cases $2a$, $3a$, $4a$, $4b$, 5 and 6, we have $|\bar{\mathbf{G}}_1| \neq 0$, hence $|\bar{\mathbf{G}}_1| \neq 0$. Therefore, it follows from (27) that either rows $\mathbf{u}_{1.}$ and $\mathbf{u}_{2.}$ are proportional or row $\mathbf{u}_{2.}$ is zero, both of which would render **U** singular. Hence, because **U** is nonsingular, $\delta\varepsilon = 0$ is the only viable option.

We have proven above that $\delta\varepsilon = 0$. It follows from the definitions of δ and ε (in Lemma 4), that, if $g = 0$, then $\delta = \varepsilon$, hence $\delta\varepsilon = 0$ implies $\delta = \varepsilon = 0$. If $g \neq 0$, then $\delta = 0$ or $\varepsilon = 0$; we cannot have $\delta = \varepsilon = 0$, because then the definitions of δ and ε would imply that $\beta = \gamma$, hence $\gamma - \beta = 0$. Because $\gamma - \beta = |\mathbf{U}|$, as follows directly from the definitions of δ and ε, this would imply that **U** is singular. Hence, we can distinguish three situations:

1. $g = \delta = \varepsilon = 0$
2. $g \neq 0,\ \delta = 0,\ \varepsilon \neq 0$
3. $g \neq 0,\ \varepsilon = 0,\ \delta \neq 0$.

For the three situations distinguished above, we will prove that **U** is a rescaled permutation matrix, by using Corollary 4.1, as follows.

Situation 1. $g = \delta = \varepsilon = 0$. This situation cannot be encountered in Cases 2a, 3a and 4a, because then $e = f = 0$, hence $g = xyz/3 \neq 0$ (by Condition (ii)), nor in Cases 4b and 5 (with $ade \neq 0$ and $f = 0$), because then $g = 0$ (together with $f = 0$) would violate Condition (iii). If $g = \delta = \varepsilon = 0$ for Case 6, we use that

$$\mathbf{Y}_1 = \begin{pmatrix} |\bar{\mathbf{G}}_1| & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};\ \mathbf{Y}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & |\bar{\mathbf{G}}_2| & 0 \\ 0 & 0 & 0 \end{pmatrix};\ \mathbf{Y}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & |\bar{\mathbf{G}}_3| \end{pmatrix} \tag{28}$$

and

$$\mathbf{V}_k \equiv \begin{pmatrix} -h_1 u_{k1} & 0 & 0 \\ 0 & -h_2 u_{k2} & 0 \\ 0 & 0 & -h_3 u_{k3} \end{pmatrix}, \tag{29}$$

with $|\bar{\mathbf{G}}_k| \neq 0$ and $h_k \neq 0$, $k = 1, 2, 3$. It follows that $\mathbf{Y}_k$ has rank 1, hence $\mathbf{V}_k = \mathbf{U}^{-1}\mathbf{Y}_k(\mathbf{U}')^{-1}$ has rank 1, for every k. Using that h_1, h_2 and h_3 are nonzero, we have from (29) that every row of **U** has two zero elements, $k = 1, 2, 3$. Because **U** is nonsingular, **U** must be a (rescaled) permutation matrix.

Situation 2. $g \neq 0$, $\delta = 0$ and $\varepsilon \neq 0$. Then

$$\mathbf{Y}_1 = \begin{pmatrix} |\bar{\mathbf{G}}_1| & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \varepsilon & 0 \end{pmatrix};\ \mathbf{Y}_2 = \begin{pmatrix} 0 & 0 & \varepsilon \\ 0 & |\bar{\mathbf{G}}_2| & 0 \\ 0 & 0 & 0 \end{pmatrix};\ \mathbf{Y}_3 = \begin{pmatrix} 0 & 0 & 0 \\ \varepsilon & 0 & 0 \\ 0 & 0 & |\bar{\mathbf{G}}_3| \end{pmatrix}. \tag{30}$$

Corollary 4.1 specifies that **Y** is related to **W** by

$$\mathbf{Y}_k = \mathbf{U}\left(\sum_{l=1}^{3} u_{kl}\mathbf{W}_l\right)\mathbf{U}'. \tag{31}$$

In Case 6, both **Y** and **W** have six nonzero elements, at the very same positions. In fact, both satisfy the Case 3b constraints. Because (31) is a special case of (7), it follows from Lemma 5 (for Case 3b) that **U** must be a rescaled permutation matrix, unless the uniqueness conditions for the Case 3b model used here are violated. It remains to verify if the uniqueness conditions hold for the present Case 3b model. Condition (i) is satisfied by the mere fact that $\mathbf{U}$ is nonsingular; it follows from $h_k \neq 0$, $k = 1, 2, 3$, and $g \neq 0$, that Condition (ii) is satisfied by $\mathbf{W}$; finally, Condition (iii) is satisfied by $\mathbf{W}$ if $(-h_1h_2h_3 + g^3) \neq 0$, hence if $g^3 \neq h_1h_2h_3$. This condition is equivalent to the Condition (iii) for $\mathbf{G}$ for the Case 6 model that is presently under study, and is hence assumed to hold too. Hence, under the uniqueness conditions for Case 6, it follows from Lemma 5 that $\mathbf{U}$ is a rescaled permutation matrix in this situation.

In Cases 4a and 5, h_1, h_2, $|\bar{\mathbf{G}}_1|$ and $|\bar{\mathbf{G}}_2|$ are nonzero, but $h_3 = efz = 0$ and $|\bar{\mathbf{G}}_3| = 0$ (because $|\mathbf{G}_3| = 0$), as follows from (7). Hence $\mathbf{Y}$ and $\mathbf{W}$ have five nonzero elements, at the same positions, and both arrays satisfy the Case 2b constraints, after permutation. This can be verified most easily by realizing that the ε's will be permuted to the superdiagonal positions and the remaining two elements will be found in different frontal slabs. Hence, the uniqueness properties of Case 2b (Lemma 5) imply that $\mathbf{U}$ must be a (rescaled) permutation matrix. (It is readily verified that the three uniqueness conditions for Case 2b are indeed satisfied).

In Cases 2a, 3a and 4b, h_1 and $|\bar{\mathbf{G}}_1|$ are nonzero, but $h_2 = |\bar{\mathbf{G}}_2| = h_3 = |\bar{\mathbf{G}}_3| = 0$, as follows from (7). Hence $\mathbf{Y}$ and $\mathbf{W}$ have four nonzero elements at the same positions, and, after permutation they satisfy the Case 1 constraints. Hence, again $\mathbf{U}$ must be a (rescaled) permutation matrix according to Lemma 5. (It is readily verified that the three uniqueness conditions for Case 2b are indeed satisfied.)

Situation 3. $g \neq 0$, $\varepsilon = 0$ and $\delta \neq 0$; in this case $\mathbf{Y}$ can be made similar to the array $\mathbf{Y}$ in (30) by interchanging the last two rows, the last two columns and the last two slabs. Denoting this linear operation by $\mathbf{\Pi}$, and denoting the resulting array (of the form of (30)) by $\tilde{\mathbf{Y}}$, we have

$$\tilde{\mathbf{Y}}_1 = \begin{pmatrix} |\bar{\mathbf{G}}_1| & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \delta & 0 \end{pmatrix}; \tilde{\mathbf{Y}}_2 = \begin{pmatrix} 0 & 0 & \delta \\ 0 & |\bar{\mathbf{G}}_3| & 0 \\ 0 & 0 & 0 \end{pmatrix}; \tilde{\mathbf{Y}}_3 = \begin{pmatrix} 0 & 0 & 0 \\ \delta & 0 & 0 \\ 0 & 0 & |\bar{\mathbf{G}}_2| \end{pmatrix}$$

and

$$\tilde{\mathbf{Y}}_k = \mathbf{\Pi}'\mathbf{U}\left(\sum_{l=1}^{3} [\mathbf{\Pi}'\mathbf{U}]_{kl}\mathbf{W}_l\right)\mathbf{U}'\mathbf{\Pi}. \tag{32}$$

Now we can, in a completely analogous way, derive the same results for $\tilde{\mathbf{Y}}$ and $\mathbf{\Pi}'\mathbf{U}$ as we did for $\mathbf{Y}$ and $\mathbf{U}$ in Situation 2. It follows that, under the uniqueness conditions, $\mathbf{U}$ must be a (rescaled) permutation matrix. □

Proof of the Uniqueness Theorem. In the Uniqueness Theorem it is assumed that the uniqueness Conditions (i), (ii) and (iii) hold. Given these conditions, Lemmas 3 through 6 show that in all cases under study it follows from (7) that $\mathbf{U}$ is a rescaled permutation matrix. It remains to prove that (7) also implies that $\mathbf{S}$ and $\mathbf{T}$ are rescaled permutation matrices. This can be done by using Lemmas 5 and 6, as follows.

By interchanging the roles of $\mathbf{S}$ and $\mathbf{U}$ (that is, by writing the rows in slabs, and the slabs in rows), we can rewrite (7) as

$$\bar{\mathbf{H}}_k = \mathbf{U} \sum_{l=1}^{3} s_{kl}\mathbf{H}_l\mathbf{T}' \tag{33}$$

with $\mathbf{H}$ defined as

$$\mathbf{H}_1 = \begin{pmatrix} x & 0 & 0 \\ 0 & 0 & d \\ 0 & f & 0 \end{pmatrix}, \mathbf{H}_2 = \begin{pmatrix} 0 & 0 & b \\ 0 & y & 0 \\ e & 0 & 0 \end{pmatrix}, \text{ and } \mathbf{H}_3 = \begin{pmatrix} 0 & a & 0 \\ c & 0 & 0 \\ 0 & 0 & z \end{pmatrix}, \quad (34)$$

and $\tilde{\mathbf{H}}$ defined analogously, satisfying the same constraints as **H**. Considering **H** as the three-way core under study, the uniqueness conditions (i) and (ii) are the same as for **G**; the Condition (iii) now reads $(xyz + fbc + dea)^3 \neq 27fdebca$, which is also the same as that for **G**. The Cases 0 through 6 will yield arrays **H** that may have zeros at different positions than in **G**, but all belong to the Cases described in Lemma 1. (In fact, it can be verified, by using permutations, that for each Case the array **H** belongs to the same Case as **G**). Hence we can apply Lemmas 3 through 6 to (33), if necessary after permutations of **H** and $\tilde{\mathbf{H}}$ so as to obtain the Cases as specified in Lemma 1. Then it follows that, under the uniqueness conditions, **S** (which now plays the role that **U** played in (7)) is a rescaled permutation matrix, in all ten cases under study.

In a completely analogous fashion, Lemmas 3 through 6 can be used to prove that (7) implies that **T** is a rescaled permutation matrix in all ten cases under study. Together, these results prove that (7) implies that **S**, **T** and **U** are rescaled permutation matrices in all ten cases under study.

We are now in a position to finalize the proof of the Uniqueness Theorem: From Lemma 2 it follows that equality (6), stating that two solutions give equal representations, implies equation (7), where **S**, **T** and **U** specify transformations from the alternative solutions' components matrices to the original component matrices. From Lemmas 3 through 6 it follows that, if (6), and hence (7) holds, **S**, **T** and **U** must be rescaled permutation matrices, in all ten cases specified in Lemma 1. Hence, the columns of $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{C}}$ are at most rescaled and differently ordered versions of those of **A**, **B**, and **C**, respectively. From Lemma 1 it follows that the ten cases under study in the Lemmas 3 through 6 capture all possible sets of EP constraints. Thus it has been proven that, under all possible sets of EP constraints, the C3MFA component matrices are unique up to permutation and rescaling.

Permissible Permutations

The above proven Uniqueness Theorem states that all solutions that give the same C3MFA model representations employ matrices **A**, **B**, and **C** that have the same vectors (up to scaling), albeit in possibly different orders. As mentioned earlier, scaling differences do not affect the residuals (and hence the fit) because they can always be compensated in the core. Differences in ordering of the column, however, could lead to different residuals, and hence affect the fit. We will call combinations of permutations *permissible* if they do not affect the residuals. We will not specify all permissible combinations of permutations, for all possible cases, here. We merely note that for different cases, different sets of permutations are permissible. For instance, in Case 1, no permissible combination of permutations exists; in Case 6, all combinations of permutations are permissible.

Rather than spelling out all permissible permutations, we will study whether or not permissible permutations can lead to solutions that are essentially different (in the sense that they are based on different sets of triple tensor products), and hence lead to different interpretations. For example, suppose we fit the model corresponding to Case 1, that is, the model with four nonzero core elements: g_{111}, g_{222}, g_{333} and g_{321}. If one solution is given by $\mathbf{A} = (\mathbf{a}_1 \mid \mathbf{a}_2 \mid \mathbf{a}_3)$, $\mathbf{B} = (\mathbf{b}_1 \mid \mathbf{b}_2 \mid \mathbf{b}_3)$, and $\mathbf{C} = (\mathbf{c}_1 \mid \mathbf{c}_2 \mid \mathbf{c}_3)$, we can write the full array as

$$\mathbf{x} = g_{111}(\mathbf{a}_1 \otimes \mathbf{b}_1 \otimes \mathbf{c}_1) + g_{222}(\mathbf{a}_2 \otimes \mathbf{b}_2 \otimes \mathbf{c}_2) + g_{333}(\mathbf{a}_3 \otimes \mathbf{b}_3 \otimes \mathbf{c}_3) + g_{321}(\mathbf{a}_3 \otimes \mathbf{b}_2 \otimes \mathbf{c}_1) + \mathbf{e}. \quad (35)$$

Suppose that an alternative solution would be given by $\tilde{\mathbf{A}} = (\mathbf{a}_2 \mid \mathbf{a}_1 \mid \mathbf{a}_3)$, $\tilde{\mathbf{B}} = (\mathbf{b}_2 \mid \mathbf{b}_3 \mid \mathbf{b}_1)$, and $\tilde{\mathbf{C}} = (\mathbf{c}_1 \mid \mathbf{c}_2 \mid \mathbf{c}_3)$ (which differs only by permutations), then we would have

$$\mathbf{x} = \tilde{g}_{111}(\mathbf{a}_2 \otimes \mathbf{b}_2 \otimes \mathbf{c}_1) + \tilde{g}_{222}(\mathbf{a}_1 \otimes \mathbf{b}_3 \otimes \mathbf{c}_2) + \tilde{g}_{333}(\mathbf{a}_3 \otimes \mathbf{b}_1 \otimes \mathbf{c}_3) + \tilde{g}_{321}(\mathbf{a}_3 \otimes \mathbf{b}_3 \otimes \mathbf{c}_1) + \mathbf{e}. \quad (36)$$

The solutions in (35) and (36) involve entirely different tensor products, and hence would lead to entirely different interpretations.

Fortunately, such entirely different solutions can never be obtained by using permissible combinations of permutations, as can be proven as follows. Suppose the solutions {**A**, **B**, **C**, **G**} and {$\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$, $\tilde{\mathbf{G}}$} give the same estimates, and $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ have the same columns as **A**, **B**, **C**, respectively, but in different orders. Noting that $(\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})$ contains all possible triple tensor products between columns of **A**, **B** and **C**, and that $(\tilde{\mathbf{A}} \otimes \tilde{\mathbf{B}} \otimes \tilde{\mathbf{C}})$ contains these in a different order, we can write (3) as

$$\mathbf{x} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathbf{g} + \mathbf{e} = (\tilde{\mathbf{A}} \otimes \tilde{\mathbf{B}} \otimes \tilde{\mathbf{C}})\tilde{\mathbf{g}} + \mathbf{e} = (\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathbf{h} + \mathbf{e}, \quad (37)$$

where **g** and $\tilde{\mathbf{g}}$ are vectorized versions of **G** and $\tilde{\mathbf{G}}$ (that have zero elements at the same positions), and **h** is the permuted version of $\tilde{\mathbf{g}}$ that corresponds to the permutations that transforms $(\tilde{\mathbf{A}} \otimes \tilde{\mathbf{B}} \otimes \tilde{\mathbf{C}})$ into $(\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})$. In fact, the vectors **g** and **h** in (37) indicate which tensor product terms are used to build up the estimates of **x**. If **g** and **h** would have (non)zero elements at different positions, the two models would use different tensor product terms and would lead to different interpretations. However, from the fact that **A**, **B** and **C** have full column rank, it follows at once that $\mathbf{h} = \mathbf{g}$, hence that the alternative solution $(\tilde{\mathbf{A}} \otimes \tilde{\mathbf{B}} \otimes \tilde{\mathbf{C}})\tilde{\mathbf{g}}$ must use exactly the same tensor products as $(\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C})\mathbf{g}$ does, albeit that these tensor products may be ordered differently.

It can be concluded that only those combinations of permutations of **A**, **B** and **C** are permissible that lead to the same set of triple tensor product terms as used in the original C3MFA model. Hence, permissible combinations of permutations will never affect the interpretation of a solution. It follows that all C3MFA models with EP constraints lead to unique solutions with unique interpretations.

Necessity of Condition (iii) for Uniqueness in cases 3b, 4b, 5 and 6

The above uniqueness proof has relied on three uniqueness conditions. As far as the first two are concerned, we do not know if they are necessary conditions for uniqueness. For Condition (iii), we will prove in the present section that it is a necessary condition for uniqueness. Specifically, it will be proven that, if Condition (iii) is violated, the model is not unique. We discuss only the Cases 3b, 4b, 5 and 6, because these are the only cases in which Condition (iii) can be violated.

It is readily verified that for the Cases 3b, 4b and 5 condition (iii) is violated if $ade = -xyz$. It will now be proven that, if $ade = -xyz$, these models are not unique, as follows. First, we scale the array such that $x = y = z = a = d = 1$, hence $e = -1$. Then, choosing

$$\mathbf{S} = \begin{pmatrix} \alpha & 0 & 0 \\ -\beta & 1 & 0 \\ -\alpha & 0 & 1 \end{pmatrix}, \mathbf{T} = \begin{pmatrix} 1 & \alpha & 0 \\ 0 & \alpha & 0 \\ 0 & \beta & 1 \end{pmatrix}, \text{ and } \mathbf{U} = \begin{pmatrix} 1 & 0 & -\beta \\ 0 & 1 & \alpha \\ 0 & 0 & \alpha \end{pmatrix}, \quad (38)$$

we obtain

$$\tilde{\mathbf{G}}_1 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & 0 & b \\ 0 & \alpha & 0 \end{pmatrix}, \tilde{\mathbf{G}}_2 = \begin{pmatrix} 0 & 0 & \alpha \\ 0 & \alpha & 0 \\ c & 0 & 0 \end{pmatrix}, \text{ and } \tilde{\mathbf{G}}_3 = \begin{pmatrix} 0 & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \quad (39)$$

for arbitrary $\alpha \neq 0$ and β. Thus, we have a class of nonsingular matrices **S**, **T** and **U** that yield an array $\tilde{\mathbf{G}}$ that satisfies the constraints of Cases 3b, 4b and 5, respectively. Clearly the matrices **S**, **T** and **U** are not rescaled permutation matrices. This particular class of solutions was given to show that the models are not unique. Incidentally, it is worth noting that this class is by no means the complete class of matrices **S**, **T** and **U** for which $\tilde{\mathbf{G}}$ satisfies the constraints at hand.

For Case 6, the third uniqueness condition is somewhat more complicated. Assuming $x = y = z = a = b = c = d = 1$ (as can always be arranged by scaling of rows, columns and slabs), situations where the condition is violated can be described as those where

$$(1 + e + f)^3 = 27ef. \tag{40}$$

This condition implies that $e = f = 1$, or $f = -(e^{1/3} + 1)^3$ for arbitrary e, as can be verified by factoring the third order polynomial in f.

If the data satisfy (40), Case 6 cannot be guaranteed to give unique solutions. It will be proven now that, under this condition, the model is nonunique, because, here also, classes of solutions where **S** and **T** are not rescaled permutation matrices can be given, as follows. If $e = f = 1$, then taking

$$\mathbf{S} = \begin{pmatrix} 1 & \alpha^2 & -\alpha \\ -\alpha & 1 & \alpha^2 \\ \alpha^2 & -\alpha & 1 \end{pmatrix}, \mathbf{T} = \begin{pmatrix} 1 & 0 & \alpha \\ \alpha & 1 & 0 \\ 0 & \alpha & 1 \end{pmatrix}, \mathbf{U} = \mathbf{I}, \tag{41}$$

for arbitrary $\alpha \neq -1$ gives $\tilde{\mathbf{G}} = (\alpha^3 + 1)\mathbf{G}$, hence $\tilde{\mathbf{G}}$ satisfies the constraints of Case 6 for every choice of α. Also note that **S**, **T** and **U** are nonsingular unless $\alpha = -1$. Again, this is by no means the only class of solutions that yield a $\tilde{\mathbf{G}}$ that satisfies the Case 6 constraints. If, on the other hand, $f = -(e^{1/3} + 1)^3$, with $e \neq 0$ and $f \neq 0$ (because $ef = 0$ would lead to Case 5), we define $\varepsilon = e^{1/3}$ and $\phi = (e^{1/3} + 1)$, hence $e = \varepsilon^3$ and $f = -\phi^3$, and we take

$$\mathbf{S} = \begin{pmatrix} -\varepsilon\alpha & 1 & 0 \\ 1 & 0 & -\phi^2\alpha \\ 0 & \phi\alpha & \varepsilon \end{pmatrix}, \mathbf{T} = \begin{pmatrix} 1 & 0 & \varepsilon\phi\alpha \\ 0 & -\alpha & 1 \\ -\phi^2\alpha & \varepsilon & 0 \end{pmatrix},$$

$$\mathbf{U} = \begin{pmatrix} 0 & -\varepsilon\phi^2\alpha & 1 \\ \phi\alpha & 1 & 0 \\ \varepsilon & 0 & -\alpha \end{pmatrix}, \tag{42}$$

where α is an arbitrary scalar such that $\alpha \neq -\phi^{-1}$. Then, as can be verified, the resulting $\tilde{\mathbf{G}}$ satisfies the constraints of Case 6, and $|\mathbf{S}| = |\mathbf{T}| = |\mathbf{U}| = \varepsilon + \varepsilon\phi^3\alpha^3 \neq 0$, hence **S**, **T** and **U** are nonsingular, but no rescaled permutation matrices. Again, this is not the only class of matrices **S**, **T** and **U** for which $\tilde{\mathbf{G}}$ satisfies the constraints of Case 6.

A Numerical Procedure for Assessing Nonuniqueness for Arbitrary C3MFA Models

The above derived uniqueness result only holds for a special class of C3MFA models. Further study is needed to obtain results on other (classes) of models. Lacking those, however, the practitioner might use an informal procedure which will usually reveal nonuniqueness of a nonunique model, and can therefore be used to examine uniqueness.

As has been shown above, a C3MFA model has (under mild assumptions) a unique representation if and only if (7) is satisfied. Provided that **A**, **B** and **C** have full rank and that the constrained core, after collecting frontal slabs, horizontal slabs or lateral slabs in a supermatrix, yields a full rank matrix, we have the more general result that

$$\tilde{\mathbf{G}}_k = \mathbf{S}\left(\sum_{l=1}^{R} u_{kl}\mathbf{G}_l\right)\mathbf{T}', \tag{43}$$

$k = 1, \ldots, K$, and hence that uniqueness holds iff (43) implies that **S**, **T** and **U** are rescaled permutation matrices. A simple and relatively efficient way to study if a particular model gives (non)unique representations, is to construct (e.g., using random numbers) a $\mathbf{P} \times \mathbf{Q} \times \mathbf{R}$ core array **Z** that satisfies the constraints of the C3MFA model at hand, and to fit the associated C3MFA model to this core (considering it as a data array). The latter amounts to minimizing

$$\sum_{k=1}^{R} \|\mathbf{Z}_k - \mathbf{A}\left(\sum_{l=1}^{R} c_{kl}\mathbf{G}_l\right)\mathbf{B}'\|^2. \tag{44}$$

Because **Z** and **G** satisfy the same constraints, and **A**, **B** and **C** are square matrices, an obvious solution is $\mathbf{G} = \mathbf{Z}$ and $\mathbf{A} = \mathbf{I}$, $\mathbf{B} = \mathbf{I}$ and $\mathbf{C} = \mathbf{I}$. However, if the model is nonunique, other solutions must exist, in which **A**, **B** and/or **C** are not (rescaled) permutation matrices. By using several random starts, one will usually find such deviant solutions if the model is nonunique. If the model is unique, every start will lead to a solution in which **A**, **B** and **C** are rescaled permutation matrices, provided that the global minimum (of 0) is found.

This procedure tends to work fine in practice, but is not absolutely foolproof. On the one hand, it is conceivable that a nonunique model repeatedly gives solutions consisting of rescaled permutation matrices only. It follows that finding only solutions with rescaled permutation matrices does not *necessarily* imply that a model is unique. On the other hand, if we find a solution with at least one matrix unequal to a rescaled permutation matrix (and a perfect fit), then we have proven that the model is nonunique, at least for the particular core constraints at hand. In theory, this does not yet imply that the C3MFA model at hand is unique for all data sets, because, as we saw above, it is possible that certain particular values in the core make the model nonunique. However, such exceptions are unlikely to be encountered in practice. In conclusion, the above sketched procedure for assessing uniqueness gives an indication as to whether or not the model is unique, but guarantees can only be given by *proving* (non)uniqueness for the model at hand.

We have implemented the above sketched procedure in a PCMATLAB program (available from the first author, upon request), and used it for numerous C3MFA models with $3 \times 3 \times 3$ cores. In fact, it has helped us finding the class of unique models discussed in the present paper. It has also indicated that these are the only $3 \times 3 \times 3$ C3MFA models that are unique. Specifically, we have run several hundreds of analyses with randomly created $3 \times 3 \times 3$ core arrays in which 15 or more elements were constrained to zero. In only a few of these runs we found rescaled permutation matrices for **S**, **T** and **U**; in some of those runs, the array corresponded to one of the models for which we have proven uniqueness above; the other arrays turned out to be nonunique after all (as could be proven for those cases).

We also used the numerical procedure for assessing (non)uniqueness for C3MFA models employing other than $3 \times 3 \times 3$ cores. We studied hundreds of $3 \times 3 \times 2$ and $3 \times 2 \times 2$ cores, and never encountered a unique model.

Rediscussion of the Exemplary Analyses

In the exemplary analyses at the beginning of the paper, we used PARAFAC and five C3MFA models. Three of the C3MFA models were chosen because they give unique solutions (as follows from the Uniqueness Theorem); the other two were chosen to demonstrate the implications of using nonunique models. The best of these analyses was the one denoted as PF + g_{321} + g_{231}, which we can now recognize as the Case 2a model. Hence, besides that this model gives a good fit (which is hardly less than that of unconstrained 3MFA), it turns out to be a unique model as well. Therefore, we need not consider rotating or otherwise transforming this solution: The reported solution is the only Case 2a solution available (except for arbitrary rescalings and permutations, that is).

At first sight, it may have come as a surprise that the equally parsimonious model $F + g_{121} + g_{211}$ performs far more poorly. This can, however, be explained by studying its (non)uniqueness. By means of the numerical procedure sketched above, we found that this model is nonunique. In fact, in this case we can easily prove that this model is nonunique, and that nonsingular transformations exist such that we find a core with $\tilde{g}_{121} = 0$ and $\tilde{g}_{211} = 0$. This implies that the model can be transformed into a PARAFAC model, which explains why its fit is no better than that of PARAFAC. It can be concluded that, using the model $PF + g_{121} + g_{211}$, we have inadvertently fitted a redundant description of the PARAFAC model. This demonstrates an obvious advantage of unique models: The very uniqueness of the model excludes the existence of more parsimonious versions of the same model.

Discussion

The present paper describes a range of models that, like the PARAFAC model, give unique representations of the data. This "unique axes property" has a long time been considered a unique feature of the PARAFAC model. The present paper has demonstrated that a series of extensions of this model has the same attractive property.

The class of C3MFA models for which we have proven uniqueness comprises the PARAFAC model as Case 0. Hence, the present paper offers an alternative proof for uniqueness of the PARAFAC components. However, the present uniqueness proof is unduly complicated for proving uniqueness for PARAFAC, and a far more simple proof has been given by Harshman (1972), employing weaker conditions. Uniqueness of the PARAFAC model has been proven under even weaker conditions by Kruskal (1977, 1989). These results indicate that uniqueness in some of the unique C3MFA models may still hold when the condition that **A**, **B** and **C** have full column rank is relaxed.

The Uniqueness Theorem can be used in an exploratory context, because it tells us which models we may choose in order to get unique solutions. By choosing only unique models, we avoid the interpretational problems we would get when using nonunique models. When the solution is not unique, we have to choose which of the different solutions we will interpret. Except in unconstrained 3MFA, it will be difficult to assess the full class of C3MFA solutions for nonunique models, and hence it will be even more difficult to decide which solution we should interpret. In addition, as we saw in the exemplary analyses, nonunique models may not be as parsimonious as one would like. Of course, the Uniqueness Theorem is of limited value only: It establishes uniqueness for C3MFA models using $3 \times 3 \times 3$ cores and EP constraints. In many practical situations, a core size of $3 \times 3 \times 3$ may be too large, and a reduction in one or more directions is often indicated. Our experience indicates that, except for the 1- and 2-dimensional PARAFAC model, such models are nonunique. Another limitation of our Uniqueness Theorem is that it only establishes sufficient conditions for uniqueness of C3MFA models with $3 \times 3 \times 3$ cores: It has not been proven that EP constraints are the only core constraints that make C3MFA models with $3 \times 3 \times 3$ cores unique, although extensive testing suggests that this is indeed the case. For C3MFA models employing larger cores we have neither theoretical nor empirical results.

Another type of applications of C3MFA is in a parameter estimation approach: Especially in chemometrics, applications are found where theory specifies the form of the C3MFA model, and the C3MFA model is used to find the parameters of the model. Unfortunately, it seems rather unlikely to encounter a process where theory exactly prescribes a C3MFA model with EP constraints. Applications do exist where a process can be described by the PARAFAC model (e.g., Leurgans & Ross, 1992) or other C3MFA models (e.g., Smilde, Wang, & Kowalski, 1994). In the latter cases the C3MFA models do not employ EP constraints, but are unique thanks to additional constraints on the parameter matrices. In both cases, the uniqueness of the model is exploited for identifying chemical substances and finding their relative concentrations.

We may conclude that the present Uniqueness Theorem is of limited practical use. Its main value is in demonstrating that PARAFAC is not the only unique three-way model, and that there is a host of parsimonious models in between PARAFAC and 3MFA that are potentially unique. The present results may inspire researchers to find other unique C3MFA models (e.g., employing larger cores, or by imposing constraints on the parameter matrices in addition to constraints on the core). For this purpose one can use some of the Lemmas and derivations established in the present paper (notably Lemma 2). One may use the above sketched numerical approach for studying (non)uniqueness of particular models, before actually proving it.

Appendix A
Proof of Lemma 1

In all sets of EP constraints, the plane diagonal elements are constrained to zero and the superdiagonal elements are unconstrained. Hence, the different sets of EP constraints differ only in terms of the offdiagonal elements a through f. We consider the possibilities systematically:

If all offdiagonal elements are zero, we have Case 0. Then the core is constrained to be superdiagonal, and the resulting C3MFA model is equivalent to the PARAFAC model.

If there is *one* unconstrained offdiagonal element, we can always permute the rows, columns and slabs such that this offdiagonal element is moved to the position of a. Hence, Case 1 describes all cores in which only one offdiagonal element is unconstrained.

If there are *two* unconstrained offdiagonal elements, we distinguish two cases that correspond to the above Cases 2a and 2b. When the two offdiagonal elements are in the same row, column or slab, we can always permute the array such that we find Case 2a. Specifically, if the two offdiagonal elements are in the same row or column, we interchange the first or second mode with the third mode, and obtain a core in which the two offdiagonal elements are in the same slab. If they are located in the second or third slab, we can permute rows and columns such that they will be found on the positions (2, 3) and (3, 2), and next permute slabs such that they are found in the first slab. Thus we have permuted the array to the form of Case 2a.

On the other hand, when the two diagonal elements are in different rows, columns and slabs, we can always obtain Case 2b after permutation of modes and individual rows, columns and/or slabs. To prove this, we note that the unconstrained terms are g_{111}, g_{222}, g_{333}, and two terms from either $\{g_{321}, g_{132}, g_{213}\}$ or $\{g_{123}, g_{312}, g_{231}\}$. If the two additional terms are from the first set, we can always permute rows, columns and slabs by the same permutation (which implies replacing all three indices according to the same prescription) to obtain g_{321} and g_{132}, which corresponds to Case 2b; if the two additional terms are from the second set, we first interchange the first and third mode, thus finding the same set of additional interaction terms as before.

If we have *three* unconstrained offdiagonal elements they can either be all in the different rows, columns and slabs (which will be shown to correspond to Case 3b), or not (Case 3a). If the three offdiagonal elements are in different rows, columns and slabs, they must either be g_{321}, g_{132} and g_{213} (which corresponds to Case 3b), or g_{123}, g_{312} and g_{231}, (which we can permute into Case 3b, by interchanging the first and third mode). If there are two offdiagonal elements in the same row, column, or slab, we can first interchange indices such that they are found in the same slab, and next permute rows, columns and slabs such that they are found in the first slab. Then the third unconstrained offdiagonal element can be in any of the positions of c, d, e, or f. If it is in the position of c, we have

Case 3a directly. If it is in the position of d, we can interchange the first and second mode (which comes down to transposing the slabs) to obtain Case 3a. If it is in the third slab, we first permute rows 2 and 3, columns 2 and 3, and slabs 2 and 3, which moves the offdiagonal element to the second slab, and hence to the position of c or d, which leads to Case 3a.

If there are *four* unconstrained offdiagonal elements, there must be two zero offdiagonal elements. As we saw for Case 2, there are two different situations: The two zeros are in the same row, column or slab, or in different rows, columns and slabs. In the former case, we can always position the zeros in the third slab, and we find Case 4a. In the latter case, we can position the two zeros at the positions of c and f, and we end up with Case 4b.

If there are *five* unconstrained offdiagonal elements, there is one zero offdiagonal element, which can always be positioned at f. Hence this situation is fully covered by Case 5.

We can have *six* unconstrained offdiagonal elements in only one case, Case 6.

Thus it has been proven that all conceivable situations can be reduced to cases described as Case 0 through Case 6 above. □

Appendix B
Proof of Lemma 3

From (7), it follows that

$$\mathbf{S}^{-1}\tilde{\mathbf{G}}_k(\mathbf{T}')^{-1} = \sum_{l=1}^{3} u_{kl}\mathbf{G}_l. \tag{B1}$$

Hence, for an arbitrary vector $\mathbf{m} = (m_1\ m_2\ m_3)'$, we have

$$\begin{aligned}(m_1\mathbf{S}^{-1}\tilde{\mathbf{G}}_1(\mathbf{T}')^{-1} &+ m_2\mathbf{S}^{-1}\tilde{\mathbf{G}}_2(\mathbf{T}')^{-1} + m_3\mathbf{S}^{-1}\tilde{\mathbf{G}}_3(\mathbf{T}')^{-1})\\ &= m_1(u_{11}\mathbf{G}_1 + u_{12}\mathbf{G}_2 + u_{13}\mathbf{G}_3) + m_2(u_{21}\mathbf{G}_1 + u_{22}\mathbf{G}_2 + u_{23}\mathbf{G}_3)\\ &+ m_3(u_{31}\mathbf{G}_1 + u_{32}\mathbf{G}_2 + u_{33}\mathbf{G}_3) \equiv \mathbf{m}'\mathbf{u}_{.1}\mathbf{G}_1 + \mathbf{m}'\mathbf{u}_{.2}\mathbf{G}_2 + \mathbf{m}'\mathbf{u}_{.3}\mathbf{G}_3, \end{aligned}\tag{B2}$$

and $\mathbf{u}_{.1}$, $\mathbf{u}_{.2}$ and $\mathbf{u}_{.3}$ denote the *columns* 1, 2 and 3 of $\mathbf{U}$, respectively. For convenience, we define $\lambda \equiv |\mathbf{ST}|^{-1}$. Taking the determinant of the left-hand side of (B2), using the analog of (5) for $\tilde{\mathbf{G}}$, we find

$$\begin{aligned}|m_1\mathbf{S}^{-1}\tilde{\mathbf{G}}_1(\mathbf{T}')^{-1} + m_2\mathbf{S}^{-1}\tilde{\mathbf{G}}_2(\mathbf{T}')^{-1} + m_3\mathbf{S}^{-1}\tilde{\mathbf{G}}_3(\mathbf{T}')^{-1}| &= \lambda|m_1\tilde{\mathbf{G}}_1 + m_2\tilde{\mathbf{G}}_2 + m_3\tilde{\mathbf{G}}_3|\\ &= \lambda\left|\begin{pmatrix}\tilde{x}m_1 & \tilde{f}m_3 & \tilde{d}m_2\\ \tilde{e}m_3 & \tilde{y}m_2 & \tilde{b}m_1\\ \tilde{c}m_2 & \tilde{a}m_1 & \tilde{z}m_3\end{pmatrix}\right|\\ &= \lambda(m_1m_2m_3(\tilde{x}\tilde{y}\tilde{z} + \tilde{a}\tilde{d}\tilde{e} + \tilde{b}\tilde{c}\tilde{f}) - \tilde{a}\tilde{b}\tilde{x}m_1^3 - \tilde{c}\tilde{d}\tilde{y}m_2^3 - \tilde{e}\tilde{f}\tilde{z}m_3^3). \end{aligned}\tag{B3}$$

The determinant of the right-hand side of (B2) gives

$$\begin{aligned}&|\mathbf{m}'\mathbf{u}_{.1}\mathbf{G}_1 + \mathbf{m}'\mathbf{u}_{.2}\mathbf{G}_2 + \mathbf{m}'\mathbf{u}_{.3}\mathbf{G}_3|\\ &= (\mathbf{m}'\mathbf{u}_{.1})(\mathbf{m}'\mathbf{u}_{.2})\mathbf{m}'\mathbf{u}_{.3})(xyz + ade + bcf) - abx(\mathbf{m}'\mathbf{u}_{.1})^3 - cdy(\mathbf{m}'\mathbf{u}_{.2})^3 - efz(\mathbf{m}'\mathbf{u}_{.3})^3\\ &= 3g(\mathbf{m}'\mathbf{u}_{.1})(\mathbf{m}'\mathbf{u}_{.2})(\mathbf{m}'\mathbf{u}_{.3}) - h_1(\mathbf{m}'\mathbf{u}_{.1})^3 - h_2(\mathbf{m}'\mathbf{u}_{.2})^3 - h_3(\mathbf{m}'\mathbf{u}_{.3})^3. \end{aligned}\tag{B4}$$

Subtracting (B4) from (B3), and using that $\mathbf{m}'\mathbf{u}_{.l} = m_1u_{1l} + m_2u_{2l} + m_3u_{3l}$, $l = 1, 2, 3$, we have

$$\lambda(m_1m_2m_3(\tilde{x}\tilde{y}\tilde{z} + \tilde{a}\tilde{d}\tilde{e} + \tilde{b}\tilde{c}\tilde{f}) - \tilde{a}\tilde{b}\tilde{x}m_1^3 - \tilde{c}\tilde{d}\tilde{y}m_2^3 - \tilde{e}\tilde{f}\tilde{z}m_3^3)$$
$$-3g(m_1u_{11} + m_2u_{21} + m_3u_{31})(m_1u_{12} + m_2u_{22} + m_3u_{32})(m_1u_{13} + m_2u_{23} + m_3u_{33})$$
$$+ h_1(m_1u_{11} + m_2u_{21} + m_3u_{31})^3 + h_2(m_1u_{12} + m_2u_{22} + m_3u_{32})^3$$
$$+ h_3(m_1u_{13} + m_2u_{23} + m_3u_{33})^3 = 0. \quad \text{(B5)}$$

By sorting terms, we can rewrite (B5) as the following polynomial equation in m_1, m_2 and m_3:

$$c_1m_1^3 + c_2m_2^3 + c_3m_3^3 + c_4m_1m_2m_3$$
$$-(3g(u_{21}u_{12}u_{13} + u_{22}u_{11}u_{13} + u_{23}u_{11}u_{12}) - 3h_1u_{11}^2u_{21} - 3h_2u_{12}^2u_{22} - 3h_3u_{13}^2u_{23})m_1^2m_2$$
$$-(3g(u_{31}u_{12}u_{13} + u_{32}u_{11}u_{13} + u_{33}u_{11}u_{12}) - 3h_1u_{11}^2u_{31} - 3h_2u_{12}^2u_{32} - 3h_3u_{13}^2u_{33})m_1^2m_3$$
$$-(3g(u_{11}u_{22}u_{23} + u_{12}u_{21}u_{23} + u_{13}u_{21}u_{22}) - 3h_1u_{21}^2u_{11} - 3h_2u_{22}^2u_{12} - 3h_3u_{23}^2u_{13})m_2^2m_1$$
$$-(3g(u_{31}u_{22}u_{23} + u_{32}u_{21}u_{23} + u_{33}u_{21}u_{22}) - 3h_1u_{21}^2u_{31} - 3h_2u_{22}^2u_{32} - 3h_3u_{23}^2u_{33})m_2^2m_3$$
$$-(3g(u_{11}u_{32}u_{33} + u_{12}u_{31}u_{33} + u_{13}u_{31}u_{32}) - 3h_1u_{31}^2u_{11} - 3h_2u_{32}^2u_{12} - 3h_3u_{33}^2u_{13})m_3^2m_1$$
$$-(3g(u_{21}u_{32}u_{33} + u_{22}u_{31}u_{33} + u_{23}u_{31}u_{32})$$
$$- 3h_1u_{31}^2u_{21} - 3h_2u_{32}^2u_{22} - 3h_3u_{33}^2u_{23})m_3^2m_2 = 0, \quad \text{(B6)}$$

where c_1, c_2, c_3 and c_4 are unspecified expressions depending on **U**, λ, $\tilde{a}$, $\tilde{b}$, $\tilde{c}$, $\tilde{d}$, $\tilde{e}$, $\tilde{f}$, $\tilde{x}$, $\tilde{y}$, $\tilde{z}$, g, h_1, h_2, and h_3. Now we use that (B2), and hence also (B6), holds for every $\mathbf{m} \in \mathbb{R}^3$. To each **m** corresponds a vector **n** with elements m_1^3, m_2^3, m_3^3, $m_1^2m_2$, $m_1^2m_3$, ..., $m_3^2m_2$, $m_1m_2m_3$. We have collected ten choices for **m** and the associated vectors **n** in the rows of the following matrices **M** and **N**

$$\mathbf{M} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix}, \mathbf{N} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & -1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \quad \text{(B7)}$$

For these ten choices of **m**, the ten equations resulting from (B6) can be written as

$$\mathbf{Nw} = \mathbf{0}, \quad \text{(B8)}$$

where **w** is the vector with coefficients for the terms m_1^3, m_2^3, m_3^3, $m_1^2m_2$, $m_1^2m_3$, ..., $m_3^2m_2$, $m_1m_2m_3$; note that the first three elements of **w** are c_1, c_2, c_3, and the last is c_4. The matrix **N** is nonsingular, as can be verified by first subtracting column 4 from column 6, column 5 from column 8 and column 7 from column 9, and next switching columns 6 and 7. The resulting matrix is a lower triangle with nonzero diagonal elements, which is nonsingular, hence, **N** is nonsingular. Because **N** is nonsingular, it follows from (B8) that $\mathbf{w} = \mathbf{0}$, hence all coefficients of the polynomial in (B2) are zero. We only use the coefficients for $m_1^2m_2$, $m_1^2m_3$, ..., $m_3^2m_2$, to obtain

$$3g(u_{21}u_{12}u_{13} + u_{22}u_{11}u_{13} + u_{23}u_{11}u_{12}) - 3h_1u_{11}^2u_{21} - 3h_2u_{12}^2u_{22} - 3h_3u_{13}^2u_{23} = 0 \quad \text{(B9a)}$$

$$3g(u_{31}u_{12}u_{13} + u_{32}u_{11}u_{13} + u_{33}u_{11}u_{12}) - 3h_1u_{11}^2u_{31} - 3h_2u_{12}^2u_{32} - 3h_3u_{13}^2u_{33} = 0 \tag{B9b}$$

$$3g(u_{11}u_{22}u_{23} + u_{12}u_{21}u_{23} + \underline{u_{13}u_{21}u_{22})} - 3h_1u_{21}^2u_{11} - 3h_2u_{22}^2u_{12} - 3h_3u_{23}^2u_{13} = 0 \tag{B9c}$$

$$3g(u_{31}u_{22}u_{23} + u_{32}u_{21}u_{23} + u_{33}u_{21}u_{22}) - \underline{3h_1u_{21}^2u_{31}} - 3h_2u_{22}^2u_{32} - 3h_3u_{23}^2u_{33} = 0 \tag{B9d}$$

$$3g(u_{11}u_{32}u_{33} + u_{12}u_{31}u_{33} + u_{13}u_{31}u_{32}) - 3h_1u_{31}^2u_{11} - 3h_2u_{32}^2u_{12} - 3h_3u_{33}^2u_{13} = 0 \tag{B9e}$$

$$3g(u_{21}u_{32}u_{33} + u_{22}u_{31}u_{33} + u_{23}u_{31}u_{32}) - 3h_1u_{31}^2u_{21} - 3h_2u_{32}^2u_{22} - 3h_3u_{33}^2u_{23} = 0 \tag{B9f}$$

Dividing all equations in (B9) by 3, we obtain (12). □

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