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SOME UNIQUENESS RESULTS FOR PARAFAC2

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Whereas the unique axes properties of PARAFAC1 have been examined extensively, little is known about uniqueness properties for the PARAFAC2 model for covariance matrices. This paper is concerned with uniqueness in the rank two case of PARAFAC2. For this case, Harshman and Lundy have recently shown, subject to mild assumptions, that PARAFAC2 is unique when five (covariance) matrices are analyzed. In the present paper, this result is sharpened. PARAFAC2 is shown to be usually unique with four matrices. With three matrices it is not unique unless a certain additional assumption is introduced. If, for instance, the diagonal matrices of weights are constrained to be non-negative, three matrices are enough to have uniqueness in the rank two case of PARAFAC2.

Key words: three-way analysis, stationary component analysis.

Harshman (1972a), also see Harshman and Lundy (1984, p. 136), has introduced the PARAFAC2 model for scalar product matrices derived from distance matrices, and for covariance matrices derived from a common set of variables measured in several populations. This paper emphasizes the latter interpretation. The PARAFAC2 model with rank r decomposes a set of p covariance matrices $S_1, \ldots, S_p$ as

$$S_i = AC_iHC_iA' + E_i, \tag{1}$$

$i = 1, \ldots, p$, where A is an $n \times r$ ($n \geq r$) matrix of factor loadings, C_i is a diagonal matrix of weights for population i, H is a symmetric $r \times r$ matrix of covariances between the factors, and E_i represents the matrix of residual covariances for population i not fit by the model. PARAFAC2 can be considered an indirect fitting variant of PARAFAC1, which is also known as CANDECOMP (Carroll & Chang, 1970). That is, where a threeway data array consisting of p slabs $X_1, \ldots, X_p$ is fit in CANDECOMP/PARAFAC1, it is the sums-of-squares and cross-products matrices $X_i'X_i = S_i$, $i = 1, \ldots, p$, that is fit in PARAFAC2.

Computational methods for fitting the PARAFAC2 model in the least squares sense were first discussed by Harshman (1972a). A complete treatment of fitting this model subject to the constraint that H be a covariance matrix or a correlation matrix has been given by Kiers (1993), who has given algorithms for fitting (1) with or without non-negativity constraints on the diagonal elements of $C_1, \ldots, C_p$.

The purpose of this paper is to establish certain uniqueness results for PARAFAC2, analogous to the well-known unique axes property of the PARAFAC1 model for three-way data (Harshman, 1972b; Kruskal, 1977, 1989), and as a refinement of a result by Harshman and Lundy (1996). Specifically, let $\{A; H; C_1, \ldots, C_p\}$ be a PARAFAC2 solution for a given set of matrices $S_1, \ldots, S_p$.

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Definition 1. A solution $\{B; L; D_1, \ldots, D_p\}$, with B an $n \times r$ matrix, $D_1, \ldots, D_p$ a set of diagonal $r \times r$ matrices, and L an $r \times r$ covariance matrix, is equivalent to $\{A; H; C_1, \ldots, C_p\}$ if and only if, for $i = 1, \ldots, p$,

$$S_i - E_i \equiv AC_iHC_iA' = BD_iLD_iB'. \tag{2}$$

A matrix is called trivial in the sequel when it is the product of a permutation matrix and a nonsingular diagonal matrix.

Definition 2. A solution $\{B; L; D_1, \ldots, D_p\}$ is called trivially equivalent to $\{A; H; C_1, \ldots, C_p\}$ when it satisfies (2) and $B = AT$ and $L = T^{-1}H(T')^{-1}$, for a trivial matrix T.

For any given PARAFAC2 solution, trivially equivalent solutions can easily be constructed. Trivial equivalence reflects the inherent indeterminacy of a PARAFAC2 solution. Although Definition 2 does not yet account for every form of indeterminacy (replacing D_i by $D_i\Lambda^{-1}$ and L by $\Lambda L \Lambda$, where Λ is a nonsingular diagonal matrix, is still permitted), an identification constraint on C_1 and D_1, to be introduced later, will remove this indeterminacy.

Definition 3. Let $\{A; H; C_1, \ldots, C_p\}$ be a given PARAFAC2 solution. This solution is said to be unique when every equivalent solution $\{B; L; D_1, \ldots, D_p\}$ is trivially equivalent.

The question is under what conditions the PARAFAC2 model has a unique solution. Carroll and Wish (1974, pp. 94–96) have pointed out that, whereas two slabs ($p = 2$) is enough for uniqueness in PARAFAC1, more slabs are needed for uniqueness in PARAFAC2. This is because in case $p = 2$ the two symmetric matrices $(S_1 - E_1)$ and $(S_2 - E_2)$ can be diagonalized simultaneously, which provides ample opportunity for constructing nontrivially equivalent solutions.

Harshman and Lundy (1996) have given sufficient conditions for uniqueness in so-called PARATUCK2 models. For the specific case of PARAFAC2 with rank two, they have shown that five slabs are enough to have uniqueness. In the present paper, the same result will be obtained from a slightly different line of proof, and it will be sharpened. Under mild assumptions, PARAFAC2 solutions with rank two will be shown unique with three slabs ($p = 3$) if a nonnegativity restriction on the diagonal matrices $C_1, \ldots, C_p$ is introduced, and nonunique in the unrestricted case. With four slabs, uniqueness holds without the restriction, except when the data belong to a set that has volume zero. To arrive at these results, it is necessary to introduce the assumptions.

A Reformulation of the Problem

Throughout this paper, the following assumptions are adopted:

Assumption 1. The matrix H is positive definite.

Assumption 2. The matrix A has full column rank r. In the particular case when the rank r is 2, to be treated below, this assumption is absolutely necessary, because there is no uniqueness when A has a pair of proportional columns.

Assumption 3. The set of matrices $C_1, \ldots, C_p$ do not contain a proportional pair.

Assumption 4. The matrices $C_1, \ldots, C_p$ are nonsingular. Some results when this condition is not met can be found in Carroll and Wish (1974, pp. 95–96), see Appendix A.

In addition to these assumptions, we set $C_1 = D_1 = I$, for purposes of identification. This can always be achieved by rescaling H and L, respectively. The authors are obliged to Richard Harshman for suggesting this possibility.

We are now in a position to reformulate the definition of equivalence.

Result 1a. Let $\{A; H; C_1, \ldots, C_p\}$ be a given PARAFAC2 solution. For every solution $\{B; L; D_1, \ldots, D_p\}$ that is equivalent to $\{A; H; C_1, \ldots, C_p\}$ there exists a nonsingular $r \times r$ matrix U that satisfies $A = BU$ and

$$UC_iHC_iU' = D_iUHU'D_i, \tag{3}$$

$i = 1, \ldots, p$.

Proof. Let $\{B; L; D_1, \ldots, D_p\}$ be equivalent to $\{A; H; C_1, \ldots, C_p\}$. Then

$$AC_iHC_iA' = BD_iLD_iB', \tag{4}$$

for $i = 1, \ldots, p$. Using Assumptions 1, 2 and 4, it can be shown that B is in the column space of A. Hence there must be a nonsingular matrix N such that $B = AN$. Premultiplying and postmultiplying (4) by $(A'A)^{-1}A'$ and its transpose, respectively, changes (4) into the equivalent expression

$$C_iHC_i = ND_iLD_iN', \tag{5}$$

$i = 1, \ldots, p$. Next, by virtue of the identification constraint $C_1 = D_1 = I$, it can be seen from (5) for $i = 1$ that

$$H = NLN'. \tag{6}$$

Using (6) to eliminate L from (5) we obtain $C_iHC_i = ND_iN^{-1}H(N^{-1})'D_iN'$, which is equivalent to

$$UC_iHC_iU' = D_iUHU'D_i, \tag{7}$$

$i = 1, \ldots, p$, for U defined as N^{-1}. □

Result 1b. Let $\{A; H; C_1, \ldots, C_p\}$ be a given PARAFAC2 solution. Let there be a $\{U; D_1, \ldots, D_p\}$ with $D_1, \ldots, D_p$ diagonal and U nonsingular, that satisfies (3) for $i = 1, \ldots, p$. Then there exists an equivalent solution $\{B; L; D_1, \ldots, D_p\}$ to $\{A; H; C_1, \ldots, C_p\}$ with $D_1, \ldots, D_p$ as given, and with $B = AU^{-1}$ and $L = UHU'$.

Proof. Premultiplying (3) with AU^{-1} and postmultiplying with the transpose of that matrix yields $AC_iHC_iA' = AU^{-1}D_iUHU'D_i(U')^{-1}A'$, from which the result is immediate. □

Combining Result 1a and 1b yields the following simplification of uniqueness:

Corollary 1. Let $\{A; H; C_1, \ldots, C_p\}$ be a given PARAFAC2 solution. This solution is unique if and only if for every $\{U, D_1, \ldots, D_p\}$ that satisfies (3) for $i = 1, \ldots, p$, with U nonsingular and $D_1, \ldots, D_p$ diagonal, U is trivial.

Proof. Let $\{A; H; C_1, \ldots, C_p\}$ be a PARAFAC2 solution, and suppose that (3) is satisfied with U nontrivial. Then Result 1b shows how to construct a solution $\{B; L; D_1, \ldots, D_p\}$, nontrivially equivalent to $\{A; H; C_1, \ldots, C_p\}$. This implies nonuniqueness. Conversely, let $\{A; H; C_1, \ldots, C_p\}$ be nonunique. Then there is an equivalent solution $\{B; L; D_1, \ldots, D_p\}$ with $B = AN$, for a nonsingular N that is nontrivial. It follows from Result 1a that the matrix U defined by $A = BU$ satisfies (3) for $i = 1, \ldots, p$. From $B = AN$ and $A = BU$ it is clear that $U = N^{-1}$. Because N is nontrivial, so is U. □

Corollary 1 allows us to examine uniqueness only in terms of (3) rather than in terms of (2). The corollary will only be used for the case $r = 2$ in the sequel. Because PARAFAC2 is not unique for $p = 2$ (Carroll & Wish, 1974) we shall only consider $p > 2$. We shall examine for what value of $p > 2$ all solutions $\{U; D_1, \ldots, D_p\}$ to (3) involve a matrix U that is trivial.

It is fundamental to the results of this paper that, when $r = 2$, the possibilities of finding solutions $\{U; D_1, \ldots, D_p\}$ for (3), for fixed $\{H; C_1, \ldots, C_p\}$, are completely determined by the possibilities to solve the off-diagonal parts of these equations. This will be explained in the next section.

The Key Role of the Off-Diagonal Elements in (3)

By virtue of Corollary 1, uniqueness conditions for PARAFAC2 can be examined in terms of the set of all possible $\{U; D_1, \ldots, D_p\}$ for which (3) is satisfied, when $\{H; C_1, \ldots, C_p\}$ is given. Let $\mathbf{u}'_1$ and $\mathbf{u}'_2$ stand for the two rows of U; let c_{ij} be the j-th diagonal element of C_i, and d_{ij} the j-th diagonal element of D_i. The key result of this paper is the following:

Result 2. Let $\{A; H; C_1, \ldots, C_p\}$ be a given PARAFAC solution. For any fixed value of i, there exists a pair $\{U; D_i\}$ that satisfies (3), if and only if there exist a matrix U and a scalar σ_i, with $\sigma_i^2 = 1$, such that the off-diagonal element $\mathbf{u}'_1 C_i H C_i \mathbf{u}_2$ of UC_iHC_iU' equals $\sigma_i c_{i1} c_{i2} \mathbf{u}'_1 H \mathbf{u}_2$.

Proof. Let, for any fixed value of i,

$$UC_iHC_iU' = D_iUHU'D_i. \tag{8}$$

By taking determinants on both sides of (8), we find that $\det(C_i^2) = \det(D_i^2)$, and hence also

$$c_{i1}c_{i2} = \sigma_i d_{i1} d_{i2}, \tag{9}$$

where $\sigma_i = 1$ when the determinants of C_i and D_i have the same sign, and $\sigma_i = -1$ otherwise. Note that $\sigma_1 = 1$ due to the identification constraint $C_1 = D_1 = I_2$. Writing $(M)_{kl}$ for the (k, l) entry of any matrix M, we have from (8) that

$$(UC_iHC_iU')_{12} = (D_iUHU'D_i)_{12},$$

hence

$$\mathbf{u}'_1 C_i H C_i \mathbf{u}_2 = d_{i1} d_{i2} \mathbf{u}'_1 H \mathbf{u}_2 = \sigma_i c_{i1} c_{i2} \mathbf{u}'_1 H \mathbf{u}_2, \tag{10}$$

which proves necessity. To prove sufficiency, define H_i as C_iHC_i and write

$$\mathbf{u}'_1 H_i \mathbf{u}_2 = \sigma_i c_{i1} c_{i2} \mathbf{u}'_1 H \mathbf{u}_2, \tag{11}$$

with $\sigma_i = 1$ or -1. We now construct the matrix D_i as a function of U such that (3) is satisfied. Let d_{i1}, the first diagonal element of D_i, be determined as

$$d_{i1} = \left(\frac{\mathbf{u}_1' H_i \mathbf{u}_1}{\mathbf{u}_1' H \mathbf{u}_1}\right)^{1/2}, \tag{12}$$

and determine d_{i2} as

$$d_{i2} = \tau_i \left(\frac{\mathbf{u}_2' H_i \mathbf{u}_2}{\mathbf{u}_2' H \mathbf{u}_2}\right)^{1/2}, \tag{13}$$

where τ_i is the product of σ_i and sgn $[c_{i1}c_{i2}]$, and $\sigma_i = \mathbf{u}_1' H_i \mathbf{u}_2 / (c_{i1}c_{i2}\mathbf{u}_1' H \mathbf{u}_2)$, see (11), assuming that $\mathbf{u}_1' H \mathbf{u}_2$ does not vanish (the case where it does will be treated below). It can be seen that the resulting $D_i UHU'D_i$ has the same diagonal elements as UC_iHC_iU'. It remains to verify, using (12) and (13), that the off-diagonal elements in (8) are also equal. Specifically, it must be shown that

$$\mathbf{u}_1' H_i \mathbf{u}_2 = d_{i1} d_{i2} \mathbf{u}_1' H \mathbf{u}_2. \tag{14}$$

To prove (14), we express the determinant of UC_iHC_iU' in two different ways. We have on the one hand

$$|UC_iHC_iU'| = |UH_iU'| = \mathbf{u}_1' H_i \mathbf{u}_1 \mathbf{u}_2' H_i \mathbf{u}_2 - (\mathbf{u}_1' H_i \mathbf{u}_2)^2 = \mathbf{u}_1' H_i \mathbf{u}_1 \mathbf{u}_2' H_i \mathbf{u}_2 - c_{i1}^2 c_{i2}^2 (\mathbf{u}_1' H \mathbf{u}_2)^2, \tag{15}$$

where (11) has been used. On the other hand, we also have

$$|UC_iHC_iU'| = |C_i|^2 |UHU'| = c_{i1}^2 c_{i2}^2 ((\mathbf{u}_1' H \mathbf{u}_1)(\mathbf{u}_2' H \mathbf{u}_2) - (\mathbf{u}_1' H \mathbf{u}_2)^2). \tag{16}$$

Subtracting (15) from (16) yields

$$c_{i1}^2 c_{i2}^2 = (\mathbf{u}_1' H_i \mathbf{u}_1)(\mathbf{u}_2' H_i \mathbf{u}_2)(\mathbf{u}_1' H \mathbf{u}_1)^{-1}(\mathbf{u}_2' H \mathbf{u}_2)^{-1}, \tag{17}$$

and hence

$$\text{sgn}\,[c_{i1}c_{i2}](c_{i1}c_{i2}) = (\mathbf{u}_1' H_i \mathbf{u}_1)^{1/2}(\mathbf{u}_2' H_i \mathbf{u}_2)^{1/2}(\mathbf{u}_1' H \mathbf{u}_1)^{-1/2}(\mathbf{u}_2' H \mathbf{u}_2)^{-1/2}. \tag{18}$$

Because sgn $[c_{i1}c_{i2}]$ equals $\tau_i/\sigma_i = \sigma_i/\tau_i$ it follows using (12) and (13) that

$$\sigma_i(c_{i1}c_{i2}) = \tau_i(\mathbf{u}_1' H_i \mathbf{u}_1)^{1/2}(\mathbf{u}_2' H_i \mathbf{u}_2)^{1/2}(\mathbf{u}_1' H \mathbf{u}_1)^{-1/2}(\mathbf{u}_2' H \mathbf{u}_2)^{-1/2} = d_{i1} d_{i2}. \tag{19}$$

This yields (9). Combining (9) and (11) shows that (14) is satisfied.

When $\mathbf{u}_1' H \mathbf{u}_2 = 0$, the expression for σ_i used below (13) is not valid, but the proof is much simpler. It is now immediate from (11) that $\mathbf{u}_1' H \mathbf{u}_2 = \mathbf{u}_1' H_i \mathbf{u}_2 = 0$, which means that the off-diagonal part of (3) is satisfied trivially. To construct D_i such that (3) is satisfied, use (12) and (13), with σ_i taken as either 1 or -1. □

The importance of Result 2 is that, in examining solutions for (3) for the rank 2 case, we have also removed D_i, and need only consider U and σ_i, $i = 2, \ldots, p$. Solving the nonlinear "off-diagonal equations" (11) generates the complete set of solutions equivalent to $\{A; H; D_1, \ldots, D_p\}$. The next step is to express these nonlinear equations in terms of linear equations, to see how nontrivial solutions for U may come about, when the rank is 2. This will be done in the next section.

From Nonlinear to Linear Equations

Let U and H have element u_{kl} and h_{kl}, respectively, in row k and column l. Define $\mathbf{c}_i'$ as the row vector $[c_{i1}^2|c_{i1}c_{i2}|c_{i2}^2]$, $i = 1, \ldots, p$. This enables us to rephrase the nonlinear equations of Result 2 into linear equations:

Result 3. For a given H and C_i (i fixed), a matrix U and a scalar σ_i (+1 or −1) that satisfy the off-diagonal equation (11) exist if and only if the vector $\mathbf{c}_i$ is orthogonal to the vector $\mathbf{x}_i$, with elements

$$x_{i1} = h_{11}u_{11}u_{21},$$

$$x_{i2} = h_{12}(u_{11}u_{22} + u_{12}u_{21}) - \sigma_i \mathbf{u}_1' H \mathbf{u}_2, \quad \text{and} \tag{20}$$

$$x_{i3} = h_{22}u_{12}u_{22}.$$

Proof. Equation (11) can be written as $\mathbf{u}_1' H_i \mathbf{u}_2 - \sigma_i c_{i1} c_{i2} \mathbf{u}_1' H \mathbf{u}_2 = 0$, that is, as

$$c_{i1}^2 h_{11}u_{11}u_{21} + c_{i1}c_{i2}h_{12}(u_{11}u_{22} + u_{12}u_{21}) + c_{i2}^2 h_{22}u_{12}u_{22} - \sigma_i c_{i1}c_{i2}\mathbf{u}_1' H \mathbf{u}_2 = \mathbf{c}_i'\mathbf{x}_i = 0. \quad \square$$

From Results 2 and 3 the following corollary is immediate:

Corollary 3. Every $\{U; D_1, \ldots, D_p\}$ satisfying (3) for $i = 1, \ldots, p$ simultaneously satisfies $\mathbf{c}_i'\mathbf{x}_i = 0$ for $i = 1, \ldots, p$ simultaneously.

Corollary (3) is connected to PARAFAC2 uniqueness in the following way: Every solution $\{B; L; D_1, \ldots, D_p\}$, equivalent to $\{A; H; C_1, \ldots, C_p\}$, defines a nonsingular matrix U (by $A = BU$) which may or may not be trivial. This U must satisfy the equations $\mathbf{c}_i'\mathbf{x}_i = 0$ for $i = 1, \ldots, p$. When the latter equations can only be satisfied when U is trivial, uniqueness of $\{A; H; C_1, \ldots, C_p\}$ has been established.

It should be noted that the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_p$ only differ in terms of σ_i and that x_{i1} and x_{i3}, the first and third elements, are constant for $i = 1, \ldots, p$.

Result 4. A PARAFAC2 solution $\{A; H; C_1, \ldots, C_p\}$ is unique if and only if $x_{i1} = x_{i3} = 0$.

Proof. When $x_{i1} = x_{i3} = 0$, then $h_{11}u_{11}u_{21} = 0$ and $h_{22}u_{12}u_{22} = 0$. From Assumption 1 (H positive definite) it follows that $u_{11}u_{21} = 0$ and $u_{12}u_{22} = 0$. Because U is also nonsingular, U is trivial, which implies uniqueness of $\{A; H; C_1, \ldots, C_p\}$. Conversely, when $\{A; H; C_1, \ldots, C_p\}$ is unique, any equivalent solution defines a U that is trivial. Therefore, $u_{11}u_{21} = 0$ and $u_{12}u_{22} = 0$, hence $h_{11}u_{11}u_{21} = 0$ and $h_{22}u_{12}u_{22} = 0$, which means that $x_{i1} = x_{i3} = 0$. $\square$

Define C^* as the $p \times 3$ matrix consisting of the row vectors $\mathbf{c}_i'/c_{i1}^2$, $i = 1, \ldots, p$. This division is legitimate due to Assumption 4. Define $\gamma_i = c_{i2}/c_{i1}$. Then, for $p \geq 3$, the upper 3×3 submatrix $\tilde{C}$ of C^* has the form

$$\tilde{C} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & \gamma_2 & \gamma_2^2 \\ 1 & \gamma_3 & \gamma_3^2 \end{bmatrix}. \tag{22}$$

This is a special case of a Vandermonde matrix, and its determinant is well-known (Jacob & Bailey, 1971, p. 279) to be

$$(\gamma_2 - 1)(\gamma_3 - 1)(\gamma_3 - \gamma_2). \tag{23}$$

This determinant is zero if and only if there is a proportional pair among C_1, C_2 and C_3, a case explicitly excluded at the start of this paper (Assumption 3). It follows that C^* is of full column rank 3.

We now address uniqueness of PARAFAC2 in the rank 2 case, for $p = 3$, $p = 5$, and $p = 4$, respectively.

Result 5. In the rank 2 case, PARAFAC2 solutions are unique when $p = 3$, and σ_2 and σ_3 are constrained to be 1 (rather than +1 or −1).

Proof. When $\sigma_1 = \sigma_2 = \sigma_3$, it can be seen in (20) that $\mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x}_3 \equiv \mathbf{x}$, and this $\mathbf{x}$ is orthogonal to every row of the rank 3 matrix C^*, hence $\mathbf{x}$ must be zero. From Result 4, uniqueness follows. □

Corollary 5. In the rank 2 case, PARAFAC2 solutions are unique for $p \geq 5$.

Proof. When $p \geq 5$, and we have a solution for the off-diagonal equation (11) for $i = 1, \ldots, 5$, there must be three equal values of σ_i among $\sigma_1, \ldots, \sigma_5$. When these equal values are +1, we use the corresponding three rows of C^* in Result 5 to obtain uniqueness. When the three equal values are −1, the proof of Result 5 can still be applied to obtain uniqueness. □

Result 5 implies that uniqueness can be obtained in the rank 2 case for as few as three slabs ($p = 3$) if the additional constraint is adopted that the determinants of D_2 and D_3 in (3) have the same signs as those of C_2 and C_3, respectively. In practical applications of PARAFAC2, it may sometimes be desired to have nonnegative weights only (Harshman, 1972a, p. 38). When such a nonnegativity constraint is used, the determinants of C_2, C_3, D_2, D_3 are positive and PARAFAC2 solutions (rank 2) are unique with as few as three slabs ($p = 3$). However, without a constraint of this sort, PARAFAC2 (rank 2) is not unique when $p = 3$. For example, let

$$H = \begin{bmatrix} 1 & 9/8 \\ 9/8 & 2 \end{bmatrix}, \; C_2 = \begin{bmatrix} 1 & 0 \\ 0 & .5 \end{bmatrix}, \quad \text{and} \quad C_3 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}. \tag{24}$$

Then (3) is satisfied for

$$U = \begin{bmatrix} -3 & 1 \\ -1/3 & 1 \end{bmatrix}, \; D_2 = \begin{bmatrix} 7/\sqrt{34} & 0 \\ 0 & (\sqrt{34})/14 \end{bmatrix}, \quad \text{and} \quad D_3 = \begin{bmatrix} (\sqrt{14})/\sqrt{17} & 0 \\ 0 & -(\sqrt{34})/\sqrt{7} \end{bmatrix}, \tag{25}$$

and $C_1 = D_1 = I_2$, as can readily be verified. It should be noted that $|D_2| = |C_2|$ and $|D_3| = -|C_3|$, so we have a solution with $\sigma_1 = \sigma_2 = 1$ and $\sigma_3 = -1$. In cases where a solution with $\sigma_1 = \sigma_2 = 1$ and $\sigma_3 = -1$ does not exist (solving for U requires a certain quadratic equation to have a nonnegative discriminant), it can be shown that a solution with $\sigma_1 = 1$ and $\sigma_2 = \sigma_3 = -1$ always does exist. Again, this pertains to the $p = 3$, rank 2 situation when there are no constraints on the signs of the determinants of D_1, D_2 and D_3.

PARAFAC2, constrained by the assumption of nonnegative matrices of weights

$C_1, \ldots, C_p$, poses no computational problems, because it can be handled as an option in the program by Kiers (1993). However, this very constraint puts Assumption 4 of this paper in jeopardy: It is likely to introduce zero weights. The case where singular nonnegative matrices of weights are allowed is treated separately in Appendix A.

When $p = 4$, the situation is as follows:

Result 6. In the rank 2 case, PARAFAC2 solutions are usually unique for $p \geq 4$.

Proof. Solutions for (11) with U nontrivial can only exist when, among the values σ_1, σ_2, σ_3 and σ_4, precisely two values are $+1$ and two are -1. Let the slabs be arranged such that $\sigma_1 = \sigma_2 = 1$ and $\sigma_3 = \sigma_4 = -1$. Define $\mathbf{x}$ as the vector orthogonal to the first two rows of C^*, and $\mathbf{y}$ as the vector orthogonal to the last two rows, with C^* defined as

$$C^* = \begin{bmatrix} 1 & 1 & 1 \\ 1 & \gamma_2 & \gamma_2^2 \\ 1 & \gamma_3 & \gamma_3^2 \\ 1 & \gamma_4 & \gamma_4^2 \end{bmatrix}. \tag{26}$$

Then $\mathbf{x}$ is $\lambda[\gamma_2\ (-1 - \gamma_2)\ 1]'$ for some scalar λ, and $\mathbf{y} = \mu[\gamma_3\gamma_4\ -(\gamma_3 + \gamma_4)\ 1]'$, for some scalar μ. Also, $\mathbf{x}$ and $\mathbf{y}$ have the same first and the same third element, see (20). It follows that $\lambda = \mu$ and $\lambda\gamma_2 = \lambda\gamma_3\gamma_4$, so $\lambda C_2 = \lambda C_3 C_4$. Clearly, this means that $\lambda = \mu = 0$, hence $\mathbf{x} = \mathbf{y} = 0$, in all cases where C_2 differs from C_3C_4. It follows that rank two PARAFAC2 solutions with $p = 4$ are unique (see Result 4) except in the case where $C_2 = C_3C_4$. In the latter case, which corresponds to a set of volume zero, nontrivial matrices U can readily be found. For instance, expanding (25) with $D_4 = \begin{bmatrix} .5\sqrt{7} & 0 \\ 0 & -1/(2\sqrt{7}) \end{bmatrix}$, when C_4 is defined as $C_4 = \begin{bmatrix} 1 & 0 \\ 0 & .25 \end{bmatrix}$, provides a case in point.□

Discussion

The results of this paper are limited to the rank 2 case, for H positive definite. Although it seems possible to relax the latter assumption, it would be far more interesting to generalize the results for H positive definite to higher rank. So far, little has been achieved in this direction. The main obstacle is the failure of Result 2 to generalize to rank >2.

Computer simulations for the rank 3 case, using the algorithms by Kiers (1993), suggest that PARAFAC2 is not unique with $p < 5$. For $p \geq 5$, uniqueness does seem to hold. These simulation results differ markedly from those obtained by Carroll and Chang, reported by Carroll and Wish (1974, p. 96). Possibly, these discrepancies are due to different levels of computational accuracy.

Appendix A

When a nonnegativity constraint is introduced for the diagonal matrices $C_1, \ldots, C_p$, PARAFAC2 is likely to produce solutions where some of these diagonal matrices are singular. For this situation, Carroll and Wish (1974, pp. 95–96) have reported some uniqueness results due to Carroll. Specifically, Carroll considered cases with $r = p$ and $C_1, \ldots, C_p$ of rank one. In such cases, there is partial nonuniqueness (A unique, but H nonunique). The nonuniqueness of H disappears if there is one additional $p + 1$-th "subject" with C_{p+1} nonsingular. In this Appendix, it will be examined, for the rank two case only, what is left of the uniqueness results of this paper, when Assumption 1

(H positive definite), Assumption 2 (A of full column rank $r = 2$) and Assumption 3 (no proportional pair among $C_1, \ldots, C_p$) are maintained, but Assumption 4 ($C_1, \ldots, C_p$ nonsingular) is replaced by a nonnegativity assumption on $C_1, \ldots, C_p$.

First, consider the case of only $p = 2$ slabs. Let $\{A; H; C_1, C_2\}$ be a PARAFAC2 solution. When C_1 and C_2 are both of rank one (but non-proportional by virtue of Assumption 3), we have nonuniqueness for H as was pointed out by Carroll. When C_1 is nonsingular and C_2 of rank one, it is possible to diagonalize C_1HC_1 and C_2HC_2 simultaneously, which provides ample room to construct nontrivially equivalent solutions. So there is nonuniqueness both for A and for H in this case. To obtain uniqueness, we need at least $p = 3$. From now on, we only consider the rank two case with $p = 3$, and show that it is unique under the assumptions stated above.

When C_1, C_2 and C_3 happen to be nonsingular, all previous derivations remain valid, and Result 4 implies that PARAFAC2 solutions are unique. The opposite case where C_1, C_2 and C_3 are each of rank one can be discarded due to Assumption 3. What remains is to consider the case where C_1 is nonsingular, C_3 is of rank one (S_1, S_2 and S_3 can be rearranged to achieve this), and C_2 is either of rank one or of rank two. Like before, we set $C_1 = I_2$ and for every solution $\{B; L; D_1, D_2, D_3\}$ equivalent to $\{A; H; C_1, C_2, C_3\}$ we also set $D_1 = I_2$.

In the case where C_2 is of rank one we have C_2 proportional to $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and C_3 proportional to $\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, or vice versa. When $\{B; L; D_1, D_2, D_3\}$ is a solution equivalent to $\{A; H; C_1, C_2, C_3\}$, it is immediate from (2) for $i = 2$ and $i = 3$ that the matrix N satisfying $B = AN$ is diagonal, which means that A is unique (as in Carroll's cases discussed above). From $C_1 = D_1 = I_2$, it can be inferred that H is also unique, see the proof of Result 1. So PARAFAC2 solutions of this type are unique.

Finally, consider the case where only C_3 is a rank one matrix. The element (1, 1) of C_3 is nonzero or it is arranged to be nonzero by a permutation. When $\{B; L; D_1, D_2, D_3\}$ is a solution equivalent to $\{A; H; C_1, C_2, C_3\}$, it is immediate from (2) for $i = 3$ that the matrix N for which $B = AN$ has element $n_{21} = 0$. This means that the element u_{21} of $N^{-1} = U$ is also zero. From this point on, we treat this case as a $p = 2$ case (C_1 and C_2 nonsingular), with the restriction that $u_{21} = 0$. The restriction implies that $x_{i1} = 0$ in (20). Now consider the construction of $\tilde{C}$ as in (22). In the present case, Row 3 is deleted, and because $x_{i1} = 0$, the first column of $\tilde{C}$ can also be deleted. The remaining 2×2 matrix $\begin{bmatrix} 1 & 1 \\ \gamma_2 & \gamma_2^2 \end{bmatrix}$ must be orthogonal to the vectors $\begin{bmatrix} x_{12} \\ x_{13} \end{bmatrix}$ and $\begin{bmatrix} x_{22} \\ x_{23} \end{bmatrix}$. These vectors are equal because $\sigma_1 = \sigma_2$. Because the matrix is nonsingular (Assumption 3), the vector vanishes, and we have also that $x_{i3} = 0$. Uniqueness is now immediate from Result 4.

For the rank two case, it can be concluded that PARAFAC2 solutions with $C_1, \ldots, C_p$ constrained to be nonnegative are unique when $p \geq 3$, under the given assumptions.

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