

UNI-MODE AND PARTIAL UNIQUENESS CONDITIONS FOR CANDECOMP/PARAFAC OF THREE-WAY ARRAYS WITH LINEARLY DEPENDENT LOADINGS*

XIJING GUO[†], SEBASTIAN MIRON[‡], DAVID BRIE[‡], AND ALWIN STEGEMAN[§]

Abstract. In this paper, three sufficient conditions are derived for the three-way CANDECOMP/PARAFAC (CP) model, which ensure uniqueness in one of the three modes (“uni-mode-uniqueness”). Based on these conditions, a partial uniqueness condition is proposed which allows collinear loadings in only one mode. We prove that if there is uniqueness in one mode, then the initial CP model can be uniquely decomposed in a sum of lower-rank tensors for which identifiability can be independently assessed. This condition is simpler and easier to check than other similar conditions existing in the specialized literature. These theoretical results are illustrated by numerical examples.

Key words. uni-mode uniqueness, partial uniqueness, CANDECOMP/PARAFAC, parallel profiles with linear dependencies, PARALIND, constrained factors, CONFAC

AMS subject classifications. 15A69, 62H25

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1. Introduction. In 1927 Hitchcock [13, 14] introduced a canonical polyadic decomposition of a multiway array or tensor. The same decomposition, for three-way arrays, was proposed later independently in psychometrics by Carroll and Chang [4], who named it CANDECOMP (CANonical DECOMPosition) and in phonetics by Harshman [11], who called it PARAFAC (PARAllel FACTor decomposition). In this paper we use the abbreviation CP to address this kind of tensor decomposition, which stands both for canonical polyadic and CANDECOMP/PARAFAC. Because of its versatility and attractive identifiability properties, CP decomposition has been widely used in various fields, such as chemometrics, the food industry [2], telecommunications, and signal processing [22, 21, 9]. For a general overview of CP and its applications, see [18, 1] and the references therein.

CP decomposes a tensor (multiway array) as a sum of rank-one tensors; e.g., for an $I \times J \times K$ three-way array \mathcal{X} , its CP decomposition can be expressed as the sum of R rank-one tensors

$$(1.1) \quad \mathcal{X} = \sum_{r=1}^R (\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r) + \mathcal{E},$$

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[†]Centre de Recherche en Automatique de Nancy (CRAN), Nancy-Université, CNRS, Boulevard des Aiguillettes, B.P. 239, F-54506 Vandœuvre-lès-Nancy, France (xijing.guo@cran.uhp-nancy.fr), and Department of Information and Communication Engineering, Xi’an Jiaotong University, 710049 Xi’an, China.

[‡]Centre de Recherche en Automatique de Nancy (CRAN), Nancy-Université, CNRS, Boulevard des Aiguillettes, B.P. 239, F-54506 Vandœuvre-lès-Nancy, France (sebastian.miron@cran.uhp-nancy.fr, david.brie@cran.uhp-nancy.fr). The work of these authors was supported by the French ANR program through grant ANR-09-BLAN-0336-04.

[§]Heijmans Institute for Psychological Research, University of Groningen, Grote Kruisstraat 2/1, 9712 TS Groningen, The Netherlands (a.w.stegeman@rug.nl, <http://www.gmw.rug.nl/~stegeman>). The work of this author was supported by the Dutch Organisation for Scientific Research (NWO), VIDI grant 452-08-001.

where $(\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r)$ is a rank-one tensor, formulated as the tensor outer products (denoted by \circ) of \mathbf{a}_r ($I \times 1$), \mathbf{b}_r ($J \times 1$), and \mathbf{c}_r ($K \times 1$), namely, the *loading vectors* associated to each of the three modes (dimensions), respectively. The integer R is also frequently referred to as the order of the decomposition. Observe that the CP model (1.1) clearly has two parts, i.e., the “structural part” $\sum_r (\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r)$ and the “residual part” \mathcal{E} ($I \times J \times K$). Since the uniqueness issues studied in this paper concern only the structural part, the residual part \mathcal{E} will be frequently omitted in what follows.

A more concise way to express the CP model (1.1) is

$$(1.2) \quad \mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket,$$

where $\mathbf{A} = [\mathbf{a}_1 \cdots \mathbf{a}_R]$, $\mathbf{B} = [\mathbf{b}_1 \cdots \mathbf{b}_R]$, and $\mathbf{C} = [\mathbf{c}_1 \cdots \mathbf{c}_R]$ are the *loading matrices* for the three modes. It is also frequently formulated as the “unfolded” matrix

$$(1.3) \quad \mathbf{X} \triangleq [\mathbf{X}_1 \cdots \mathbf{X}_K] = \mathbf{A}(\mathbf{C} \odot \mathbf{B})^T,$$

where $\mathbf{X}_k = [x_{ijk}]_{I \times J}$, given x_{ijk} the typical element of \mathcal{X} , and \odot denotes the Khatri-Rao product (columnwise Kronecker product).

CP gained much popularity among the tensor decompositions thanks to its uniqueness properties under mild conditions which are often met in applications. Herein, by uniqueness, we understand “essential uniqueness,” meaning that if another set of matrices $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$, and $\bar{\mathbf{C}}$ verify (1.2), then there exists a permutation matrix $\mathbf{\Pi}$ and three invertible diagonal scaling matrices $(\Delta_1, \Delta_2, \Delta_3)$ satisfying $\Delta_1 \Delta_2 \Delta_3 = \mathbf{I}_R$, where \mathbf{I}_R is the R th-order identity matrix, such that

$$\bar{\mathbf{A}} = \mathbf{A} \mathbf{\Pi} \Delta_1, \quad \bar{\mathbf{B}} = \mathbf{B} \mathbf{\Pi} \Delta_2, \quad \bar{\mathbf{C}} = \mathbf{C} \mathbf{\Pi} \Delta_3.$$

A milestone to the identifiability results of the CP model is the uniqueness condition due to Kruskal [19] relying on the concept of “Kruskal-rank” or simply k-rank. The k-rank of an $I \times R$ matrix \mathbf{A} , denoted by $k_{\mathbf{A}}$, is the maximum value of $\ell \in \mathbb{N}$ such that every ℓ columns of \mathbf{A} are linearly independent. By definition, clearly, the k-rank of a matrix is less than or equal to its rank. Kruskal proved that [19]

$$(1.4) \quad k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2$$

is sufficient for uniqueness of the CP decomposition in (1.2). Furthermore, it becomes a necessary and sufficient condition in the cases $R = 2$ or 3 [29]. More accessible proofs of (1.4) than [19] can be found in [27] and [20]. Recently, a more relaxed uniqueness condition, for the special case where one of the loading matrices has full column rank, was also provided by Jiang and Sidiropoulos [17] and De Lathauwer [6]. These results have been generalized to tensors of an arbitrary order n ($n \geq 3$) by Stegeman [25].

Linear dependence among the loading vectors may violate these uniqueness conditions. In this case, CP decomposition may (but does not necessarily) encounter difficulties. Cases where some loading vectors are uniquely determined, while other subsets of loading vectors are subject to rotational indeterminacies, i.e., “partial uniqueness” phenomena, were first reported by Harshman [11]. Recently, this issue received much attention and some significant results can be found in [28, 3, 5, 26]. In this paper, we will consider only this type of partial uniqueness. More complicated cases of partial uniqueness exist where there is a finite number of solutions only [28].

In this paper, we study the special case where Kruskal’s condition (1.4) is not met and the linear dependencies may take the form of collinear columns in *only one* loading

matrix, say, \mathbf{A} . For this particular case we provide three sufficient conditions ensuring that \mathbf{A} can be uniquely identified. This phenomenon is called uni-mode uniqueness in this paper. Furthermore, we prove that if \mathbf{A} is identifiable, the rank- R CP model can be uniquely decomposed in a sum of lower rank tensors according to a given partition of \mathbf{A} . Identifiability of the loadings can then be assessed independently for each lower rank tensor. It should be pointed out that having collinear loading vectors in \mathbf{A} implies nonuniqueness (or at most partial uniqueness) of the other two modes \mathbf{B} and \mathbf{C} if linear dependency of the corresponding loading vectors of \mathbf{B} and \mathbf{C} does not exist [26, Lemma 4.6].

A systematic treatment of uniqueness for CP with linearly dependent loading vectors according to a fixed pattern is presented in [26]. These types of decompositions are known as PARALIND or CONFAC and are introduced in [3] and [5]. Our uniqueness conditions for CP also hold for PARALIND/CONFAC since the set of alternative CP decompositions includes the set of PARALIND/CONFAC decompositions (with a fixed pattern of linear dependencies in the loading vectors). In the PARALIND/CONFAC framework, we show that our uniqueness results are less restrictive than those in [26] in cases with only one loading matrix having collinear columns and the k-ranks of the other two modes being high. Moreover, if one loading matrix is unique, then the method of splitting up the uniqueness problem into a set of uniqueness problems of lower rank tensors is much more convenient than showing partial uniqueness for the complete decomposition, as was done in [26, section 6].

The remainder of the paper is organized as follows. We present our main results on uni-mode uniqueness in section 2 and on partial uniqueness of the three-way CP model with linear dependent loadings in section 3. Next, in section 4 these theoretical results are illustrated by numerical examples. In section 5.1 we present the PARALIND/CONFAC decompositions, and some uniqueness results for this model derived in [26] are also briefly recalled. In section 5.2 our results are compared to the PARALIND/CONFAC results of [26]. Finally, conclusions are drawn in section 6.

2. Uni-mode uniqueness of the three-way CP with linearly dependent loadings. Let us recall the CP model introduced in the previous section in which only one matrix, namely, \mathbf{A} , may present collinear loadings. Regarding the uniqueness issues, two questions arise naturally. The first is under what conditions essential uniqueness of the first mode loading matrix \mathbf{A} is ensured. The second is whether essential/partial uniqueness holds for the loadings in the other two modes. In this section, we present three sufficient conditions to answer the first question, whereas an answer to the second question will be provided in section 3. Throughout the paper, we assume that \mathbf{B} and \mathbf{C} each have no collinear columns. Meanwhile, no assumptions are made about the dependencies in the columns of \mathbf{A} .

2.1. The uni-mode uniqueness conditions. The first condition for uniqueness of the first mode loadings will be presented in the following theorem.

THEOREM 2.1. *Recall the CP model of a three-way array \mathcal{X} given by (1.2). If \mathbf{A} has no zero columns and the condition*

$$(2.1) \quad \text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2$$

holds, the first mode loading matrix \mathbf{A} is unique up to permutation and scaling of the columns.

Proof. See Appendix A for the proof. \square

As we will see in section 5, condition (2.1) is satisfied in example (5.1). Although $k_{\mathbf{A}} = 1$ as a result of the identical loadings in \mathbf{A} , the rank of \mathbf{A} is 3. On the other

hand, $k_{\mathbf{B}} = k_{\mathbf{C}} = 4$ since both \mathbf{B} and \mathbf{C} have full column rank. The rank and the k-ranks add up to 11 on the left-hand side of (2.1), whereas the sum on the right-hand side is 10. Therefore, by Theorem 2.1, we arrive at the assertion of uniqueness of the first mode loadings (\mathbf{A} is essentially unique).

Observe that if $k_{\mathbf{A}} = \text{rank}(\mathbf{A})$, the condition (2.1) becomes identical to Kruskal's condition (1.4), implying uniqueness of all the loading matrices \mathbf{A} , \mathbf{B} , and \mathbf{C} . In the case where $k_{\mathbf{A}} < \text{rank}(\mathbf{A})$, however, the second and the third mode loading matrices \mathbf{B} and \mathbf{C} may not necessarily be unique, as happens in the example (5.1).

In particular, if

$$(\mathfrak{A}) \quad k_{\mathbf{B}} < \text{rank}(\mathbf{B}) \text{ and } k_{\mathbf{C}} < \text{rank}(\mathbf{C})$$

holds as well, the condition (2.1) can be further weakened, as stated in the following by our second uniqueness condition.

THEOREM 2.2. *Let us recall the CP decomposition problem (1.2). If \mathbf{A} has no zero columns, (\mathfrak{A}) holds, and*

$$(2.2) \quad \text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 1,$$

then the first mode loading matrix \mathbf{A} is unique up to permutation and scaling of the columns.

Proof. See Appendix B for the proof. \square

Both Theorem 2.1 and Theorem 2.2 are generalized by the third condition, as shown below.

THEOREM 2.3. *In the CP decomposition (1.2), if \mathbf{A} has no zero columns and*

$$(2.3) \quad \begin{cases} \text{rank}(\mathbf{A}) + \min(k_{\mathbf{B}}, k_{\mathbf{C}}) \geq R + 2, \\ \text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\text{rank}(\mathbf{B}) - k_{\mathbf{B}}, \text{rank}(\mathbf{C}) - k_{\mathbf{C}}) \geq 2R + 2 \end{cases}$$

both hold, then \mathbf{A} is unique up to permutation and scaling of the columns.

Proof. See Appendix C for the proof. \square

If $\text{rank}(\mathbf{A}) = R$, then (2.3) implies the essential uniqueness of all three matrices \mathbf{A} , \mathbf{B} , and \mathbf{C} , as shown in [24] and [10].

Regarding the relationships between the three sufficient conditions, it is worth noting that

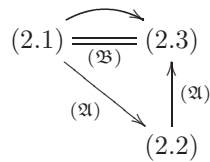
1. though the second condition (2.2) appears to be slightly weaker than the first one (2.1), it is subject to (\mathfrak{A}) ; hence, it cannot completely substitute for (2.1); and
2. the third condition (2.3) is necessary both for (2.1) and for (2.2) under (\mathfrak{A}) .

It should be pointed out that condition (2.1) follows immediately from (2.3) if

$$(\mathfrak{B}) \quad k_{\mathbf{B}} = \text{rank}(\mathbf{B}) \text{ and } k_{\mathbf{C}} = \text{rank}(\mathbf{C})$$

holds.

The following diagram illustrates the relationships between the aforementioned three conditions. In the diagram, we denote by \rightarrow as “being sufficient for” and by $=$ as being “equivalent to.” The notations (\mathfrak{A}) and (\mathfrak{B}) denote the respective conditions under which the sufficiency/equivalence holds.



2.2. Kruskal's early uniqueness results. In this subsection, we compare the uniqueness conditions presented above with two of Kruskal's early results reported in [19].

Before Kruskal arrived at the now well-known uniqueness condition (1.4), he also presented several others (see [19, pp. 114–122]) concerning the uniqueness problem for the loadings of one mode only. Among these uni-mode-uniqueness results, two are similar to the three conditions (2.1), (2.2), and (2.3) proposed in this paper and, hence, draw our attention. Both of these results are reformulated in our terminology as follows. In what follows, we will specify the two conditions as *Kruskal's uni-mode-uniqueness (UM) conditions*, respectively, to distinguish them from Kruskal's condition (1.4).

Kruskal's first UM condition is given by [19, Theorem 3b],

$$(2.4) \quad \begin{cases} \text{rank}(\mathbf{A}) + \min(k_{\mathbf{B}}, k_{\mathbf{C}}) \geq R + 1, \\ \text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\text{rank}(\mathbf{B}) - k_{\mathbf{B}}, \text{rank}(\mathbf{C}) - k_{\mathbf{C}}) \geq 2R + 1, \end{cases}$$

which was claimed to be sufficient to ensure uniqueness of \mathbf{A} in the CP decomposition. Particularly, when (\mathfrak{B}) holds, (2.4) reduces to [19, Theorem 3a]

$$(2.5) \quad \text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 1,$$

which is Kruskal's second UM condition.

Observe that the first Kruskal's UM condition is very close to our third condition (2.3). Moreover, the former seems to be slightly weaker than the latter. Nonetheless, it can be proved by a counterexample using the loading matrices

$$\mathbf{A} = \mathbf{I}_4, \quad \mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & b_1 \\ 0 & 1 & 0 & b_2 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 1 & 0 & 0 & c_1 \\ 0 & 1 & 0 & c_2 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

with b_1 , b_2 , c_1 , and c_2 nonzero, that Kruskal's first UM condition is flawed. This loading matrix configuration was first used by ten Berge and Sidiropoulos in [29]. More details on this counterexample can be found in the reference mentioned above.

Kruskal's second UM condition (2.5) appears to be identical to our condition (2.2), but the former only requires (\mathfrak{B}) , while our condition is restricted to (\mathfrak{A}) . Nevertheless, since (2.5) was derived from (2.4), we claim that (2.5) is also flawed. This can be shown by the following counterexample, which is adapted from the example of ten Berge and Sidiropoulos [29]. Let $\mathbf{A} = \mathbf{I}_3$ and

$$\mathbf{B} = \begin{bmatrix} 1 & 0 & b_1 \\ 0 & 1 & b_2 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 1 & 0 & c_1 \\ 0 & 1 & c_2 \end{bmatrix}$$

with b_1 , b_2 , c_1 , and c_2 nonzero. It is easy to verify that $\text{rank}(\mathbf{A}) = 3$, $\text{rank}(\mathbf{B}) = k_{\mathbf{B}} = 2$, and $\text{rank}(\mathbf{C}) = k_{\mathbf{C}} = 2$. Hence, on the left-hand side of (2.5), $\text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} = 7$ whereas on the right-hand side it equals $2R + 1 = 7$. Clearly, the condition (2.5) is satisfied; thus \mathbf{A} should be unique according to [19]. However, the CP (1.2) does have alternative solutions, e.g., the set

$$\bar{\mathbf{A}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{b_1 c_1}{1+b_2 c_2} & -1 & 1 \end{bmatrix}, \quad \bar{\mathbf{B}} = \begin{bmatrix} 1 & 0 & b_1 c_2 \\ 0 & 1 & 1+b_2 c_2 \end{bmatrix}, \quad \bar{\mathbf{C}} = \begin{bmatrix} 1 & 0 & \frac{b_2 c_1}{1+b_2 c_2} \\ 0 & 1 & 1 \end{bmatrix},$$

which clearly shows that \mathbf{A} is not unique. This matrix configuration can equally be used as a counterexample to Kruskal's first UM condition (2.4).

3. A partial uniqueness condition. Based on Theorems 2.1 through 2.3, a partial uniqueness condition for \mathbf{B} and \mathbf{C} can be proved. Consider first a partition of matrix \mathbf{A} in N submatrices:

$$(3.1) \quad \mathbf{A}\mathbf{\Pi}_A = [\mathbf{A}_1 | \dots | \mathbf{A}_N] \quad \text{with} \quad \sum_{n=1}^N R_n = R,$$

where R_n is the number of columns of the submatrix \mathbf{A}_n and $\mathbf{\Pi}_A$ is a permutation matrix. The partition is such that

$$(3.2) \quad \text{span}(\mathbf{A}) = \text{span}(\mathbf{A}_1) \oplus \dots \oplus \text{span}(\mathbf{A}_N),$$

where \oplus denotes the *direct sum* of the subspaces. Hence, for each $1 \leq n \leq N$ it holds [15]

$$(3.3) \quad \text{span}(\mathbf{A}_n) \cap \left(\bigcup_{\substack{1 \leq i \leq N \\ i \neq n}} \text{span}(\mathbf{A}_i) \right) = \{\mathbf{0}\}.$$

Consider also

$$(3.4) \quad \mathbf{B}\mathbf{\Pi}_A = [\mathbf{B}_1 | \dots | \mathbf{B}_N] \quad \text{and} \quad \mathbf{C}\mathbf{\Pi}_A = [\mathbf{C}_1 | \dots | \mathbf{C}_N],$$

the partitioned matrices for the two other modes corresponding to the partition of \mathbf{A} . Then our partial uniqueness condition on \mathbf{B} and \mathbf{C} can be stated as follows.

THEOREM 3.1. *Consider a partition of \mathbf{A} into N submatrices meeting the conditions above. If \mathbf{A} is essentially unique, then \mathcal{X} can be uniquely decomposed into the sum of N R_n -component lower rank tensors $\llbracket \mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n \rrbracket$. Inside each of these lower rank tensors, the first mode loadings, i.e., the columns of \mathbf{A}_n , can be uniquely determined. The submatrices \mathbf{B}_n and \mathbf{C}_n can be uniquely determined if the R_n -component CP decomposition of $\llbracket \mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n \rrbracket$ is unique.*

Proof. See Appendix D for the proof. \square

In other words, Theorem 3.1 implies that if one of the conditions given by Theorems 2.1 through 2.3 is satisfied, then the identifiability problem of $\llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$ can be divided into N independent identifiability subproblems of lower rank CP models $\llbracket \mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n \rrbracket$, with $n = 1, \dots, N$.

A direct consequence of this theorem is that if a submatrix \mathbf{A}_n in the partition of \mathbf{A} has only one column, then the associated loadings in the second and the third mode are uniquely identifiable. This is obvious since the associated lower rank tensor is a rank-one three-way array which is proved to be essentially unique [12].

Bro et al. [3] and ten Berge [28] explored the cases where \mathbf{B} and \mathbf{C} are full column rank. Obviously, our conditions are not restricted to this case and hold even if the two modes present linear dependencies but only one mode (\mathbf{A}) has proportional loadings. This will be illustrated in the next section by numerical examples. A discussion on the case with collinearity in more than one mode is provided in section 5.2 and in [26].

4. Numerical examples. We provide in this section two numerical examples to validate the theoretical results on the partial uniqueness of the CP model, presented in the previous section. For illustration we use simulated spectroscopy signals to which we added white Gaussian noise with a signal-to-noise ratio of 20 dB. The PARALIND algorithm [3] (see also section 5) with nonnegativity constraints was used to identify the loadings.

Example 1. This first example aims at showing partial uniqueness of CP, as happens in the scenario where the mode one matrix \mathbf{A} has a pair of identical columns. Suppose that there are $R = 6$ components and the first mode matrix \mathbf{A} contains

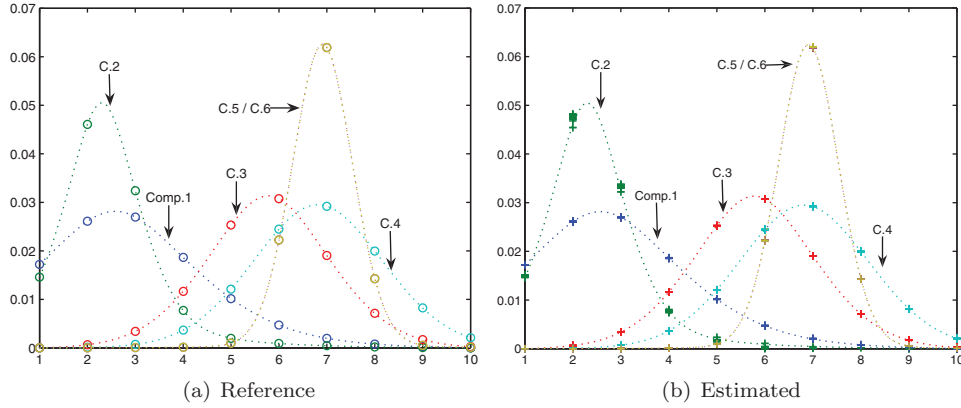


FIG. 4.1. Example 1: Mode one loadings.

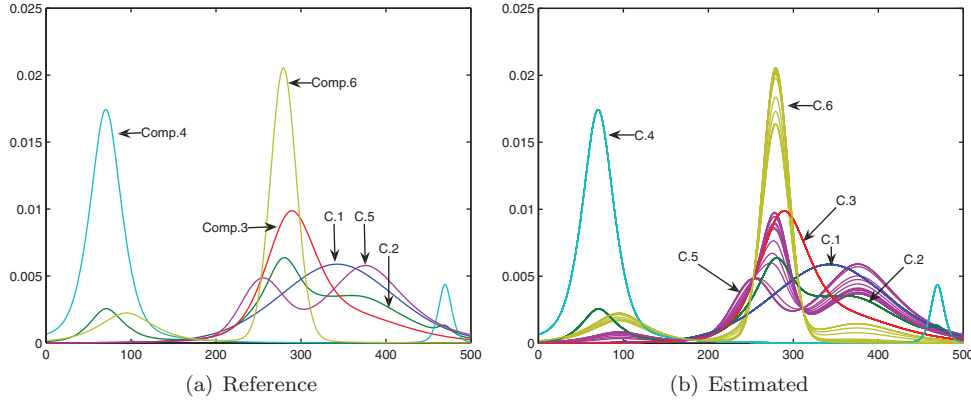


FIG. 4.2. Example 1: Mode two loadings.

$I = 10$ points of the variation profiles of these sources with respect to some physical parameter. The second and third mode matrices \mathbf{B} and \mathbf{C} contain the source variations with respect to some other parameters (e.g., the wavelength for \mathbf{B} and the temperature for \mathbf{C}) and have 500 and 200 rows, respectively. Figure 4.1(a) shows the profiles associated with each of the six components; the samples are marked by o. Herein we assume that $\mathbf{a}_6 = \mathbf{a}_5$ such that $\text{rank}(\mathbf{A}) = 5$ but $k_{\mathbf{A}} = 1$. This example is different from those presented in [3] because we assume that neither \mathbf{B} nor \mathbf{C} has full column rank. We suppose that $\mathbf{b}_6 = \mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4 + \mathbf{b}_5$ and $\mathbf{c}_6 = \mathbf{c}_1 + \mathbf{c}_2 + \mathbf{c}_3 + \mathbf{c}_4$ so that $k_{\mathbf{B}} = 5$ and $k_{\mathbf{C}} = 4$. The second and the third mode loadings are shown in Figures 4.2(a) and 4.3(a), respectively.

Figures 4.1(b), 4.2(b), and 4.3(b) show the estimates obtained from 20 repeated runs for the three modes. As condition (2.1) is met, the results, slightly perturbed by noise, show that the mode one loadings are completely identifiable. For the other two modes, the first four loadings are uniquely identifiable, while the fifth and the sixth are subject to rotational indeterminacies. This follows from dividing the initial CP decomposition into two lower rank tensors according to Theorem 3.1: a first one containing the first four loading vectors and a second one containing loading vectors five and six. For the first lower rank tensor, Kruskal's condition (1.4) is satisfied since the k-ranks are 4, 4, and 4, and 4 components are present. For the second lower

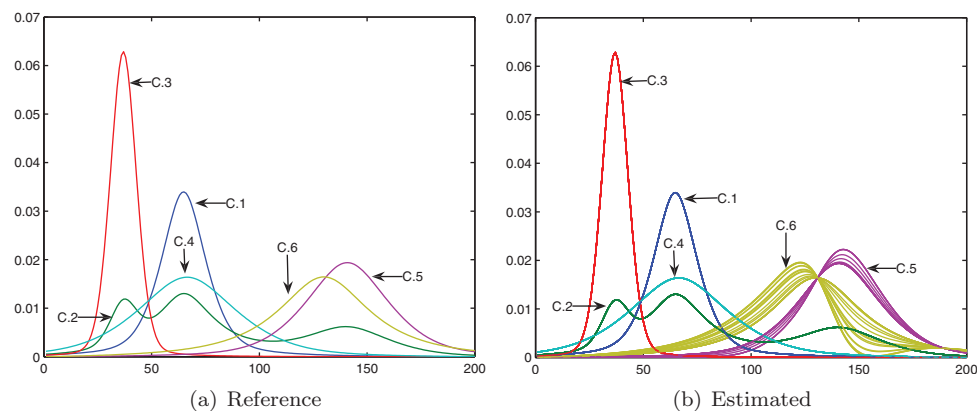


FIG. 4.3. Example 1: Mode three loadings.

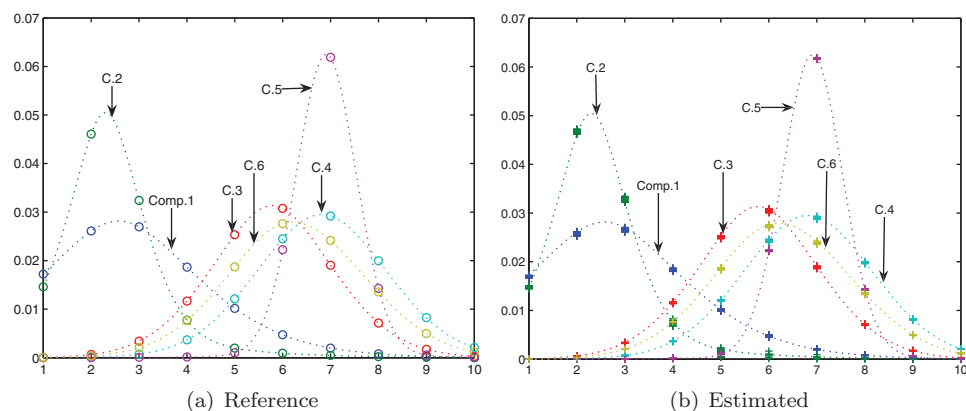


FIG. 4.4. Example 2: Mode one loadings.

rank tensor the k -ranks are 1, 2, and 2, and 2 components are present. Hence, here Kruskal's condition is not satisfied. This explains the numerical results.

Example 2. Now we consider the case where no identical loadings exist in \mathbf{A} , but linear dependence is present. The simulation is different from the previous one only for the first mode for which $\mathbf{a}_6 = \mathbf{a}_3 + \mathbf{a}_4$. The new profiles are shown in Figures 4.4(a), 4.5(a), and 4.6(a). This time, $k_{\mathbf{A}} = 2$, Kruskal's condition (1.4) is still invalid, but condition (2.1) is satisfied. The results (Figures 4.4(b), 4.5(b), and 4.6(b)) show that in this case essential uniqueness is observed for all the three modes. Once again this result can be explained by Theorem 3.1, dividing the initial decomposition into two lower rank tensors: the first one containing the first, second, and fifth loadings and the second containing the remaining loadings. In the first lower rank tensor the k -ranks are 3, 3, and 3, and we have 3 components. In the second lower rank tensor the k -ranks are 2, 3, and 3, and we have 3 components. It can be verified that in both lower rank tensors Kruskal's condition (1.4) is satisfied, which ensures uniqueness for all six loading vectors in each of the three modes. Similar results are obtained if condition (2.2) is used for the simulations.

5. Comparison to the PARALIND/CONFAC uniqueness results. In order to analyze partial uniqueness, Bro et al. [3] and de Almeida, Favier, and Mota [5] proposed to use prespecified matrices, known as constraint matrices, to describe

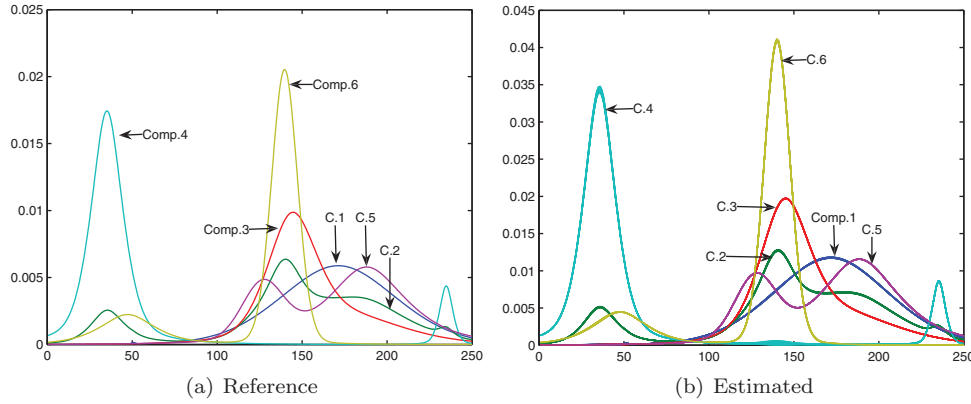


FIG. 4.5. Example 2: Mode two loadings.

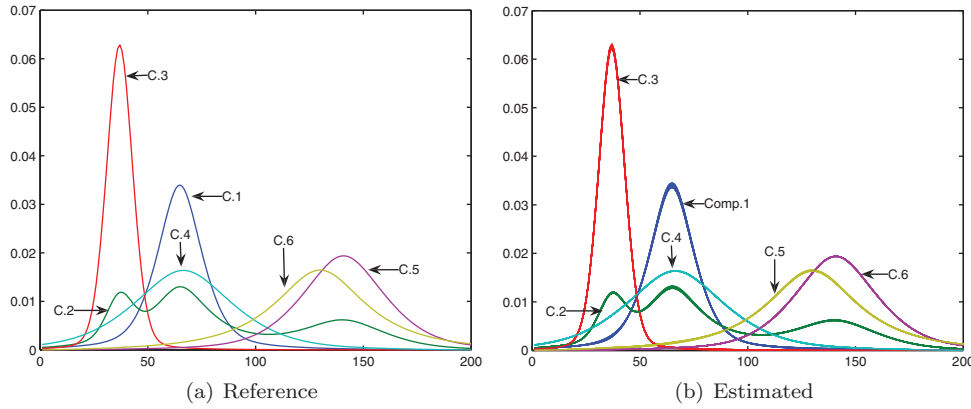


FIG. 4.6. Example 2: Mode three loadings.

the linear dependence patterns in the loading matrices. These new models are called PARAllel profiles with LINEar Dependencies (PARALIND) [3] or CONstrained FACtors (CONFAC) [5]. Instead of $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ in the conventional CP (1.2), the new loading matrices are given by $(\mathbf{A}'\Psi, \mathbf{B}'\Phi, \mathbf{C}'\Omega)$, where \mathbf{A}' , \mathbf{B}' , and \mathbf{C}' are full-column rank matrices and Ψ , Φ , and Ω are fixed constraint matrices containing the patterns of linear dependencies. Note that PARALIND/CONFAC is a special case of CP. Since the set of alternative CP decompositions includes the set of alternative PARALIND/CONFAC decompositions, the uniqueness conditions in sections 2 and 3 also hold for PARALIND/CONFAC, that is, with $\mathbf{A}, \mathbf{B}, \mathbf{C}$ replaced by $\mathbf{A}'\Psi, \mathbf{B}'\Phi, \mathbf{C}'\Omega$.

5.1. Uniqueness results for PARALIND/CONFAC. To illustrate the PARALIND/CONFAC decompositions and the concept of *partial uniqueness*, we give next an intuitive example, similar to the ones that can be found in [28] and [3]. Let $R = 4$ and the rank-three matrix $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \mathbf{a}_3 \ \mathbf{a}_4]$ be the first mode loading matrix. Herein, \mathbf{A} can also be expressed as $\mathbf{A} = \mathbf{A}'\Psi$, i.e., the product of the full-rank matrix $\mathbf{A}' = [\mathbf{a}_1 \ \mathbf{a}_2 \ \mathbf{a}_3]$ and the constraint matrix

$$(5.1) \quad \Psi = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}.$$

Moreover, we assume that the loading matrices of the other two modes, \mathbf{B} and \mathbf{C} , have full column rank. It can be verified that we still have uniqueness for the first two rank-one terms of the CP solution (i.e., $(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1)$ and $(\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2)$) as if no dependence existed. The other two mode one loading vectors (i.e., \mathbf{a}_3 and $\mathbf{a}_4 = \mathbf{a}_3$) are still unique, but the corresponding vectors in the other two modes suffer from rotational freedom.

In [26] several uniqueness results for PARALIND/CONFAC are proved. Below, we will invoke some of them, and in section 5.2 we compare these results to our results obtained in section 2. The main essential uniqueness result of [26] is the following. Let $\omega(\cdot)$ denote the number of nonzero elements of a vector. Define

$$(5.2) \quad N^* = \max_j \left(\text{rank}(\Phi \text{diag}(\psi_j^T) \Omega^T) \right),$$

where ψ_j^T denotes row j of Ψ .

THEOREM 5.1. *For fixed Ψ, Φ, Ω , let $(\mathbf{A}'\Psi, \mathbf{B}'\Phi, \mathbf{C}'\Omega)$ be a PARALIND/CONFAC solution with $\mathbf{A}', \mathbf{B}', \mathbf{C}'$, and $(\Phi \odot \Omega)\Psi^T$ having full column rank. If for any vector \mathbf{d} ,*

$$(5.3) \quad \text{rank}(\Phi \text{diag}(\Psi^T \mathbf{d}) \Omega^T) \leq N^* \quad \text{implies} \quad \omega(\mathbf{d}) \leq 1,$$

then \mathbf{A}' is unique up to permutation and scaling of the columns.

Proof. See [26, Theorem 4.2] for the proof. \square

By interchanging the roles of $\mathbf{A}'\Psi, \mathbf{B}'\Phi$, and $\mathbf{C}'\Omega$, Theorem 5.1 also yields essential uniqueness conditions for \mathbf{B}' and \mathbf{C}' . The following result is useful for proving partial uniqueness.

THEOREM 5.2. *For fixed Ψ, Φ, Ω , let $(\mathbf{A}'\Psi, \mathbf{B}'\Phi, \mathbf{C}'\Omega)$ be a PARALIND/CONFAC solution with $\mathbf{A}', \mathbf{B}', \mathbf{C}'$ having full column rank. If $(\Phi \odot \Omega)\Psi^T$ has full column rank, then the column space of \mathbf{A}' is uniquely determined. That is, for any alternative $\bar{\mathbf{A}}'$ we have $\bar{\mathbf{A}}' = \mathbf{A}' \mathbf{S}$ for some nonsingular \mathbf{S} .*

Proof. See [26, Proposition 3.3] for the proof. \square

5.2. Comparison of uni-mode CP and PARALIND/CONFAC uniqueness conditions. In the PARALIND/CONFAC framework, we compare Theorems 2.1 through 2.3 to Theorem 5.1. First, we consider the examples of section 4. We write the decomposition in Example 1 in PARALIND/CONFAC form with

$$(5.4) \quad \Psi = [\mathbf{I}_5 \mathbf{e}], \quad \Phi = [\mathbf{I}_5 \mathbf{f}], \quad \Omega = [\mathbf{I}_5 \mathbf{g}],$$

where $\mathbf{e} = (0 \ 0 \ 0 \ 0 \ 1)^T$, $\mathbf{f} = (1 \ 1 \ 1 \ 1 \ 1)^T$, and $\mathbf{g} = (1 \ 1 \ 1 \ 1 \ 0)^T$. It can be verified that $N^* = 2$ (see (5.2)) and that

$$(5.5) \quad \Phi \text{diag}(\Psi^T \mathbf{d}) \Omega^T = \begin{bmatrix} d_1 + d_5 & d_5 & d_5 & d_5 & 0 \\ d_5 & d_2 + d_5 & d_5 & d_5 & 0 \\ d_5 & d_5 & d_3 + d_5 & d_5 & 0 \\ d_5 & d_5 & d_5 & d_4 + d_5 & 0 \\ d_5 & d_5 & d_5 & d_5 & d_5 \end{bmatrix},$$

which can have rank 2 for $d_3 = d_4 = d_5 = 0$ and nonzero d_1 and d_2 . Hence, condition (5.3) does not hold, and Theorem 5.1 cannot be used to show uniqueness of \mathbf{A} .

Next, we consider Example 2. We have the same Φ and Ω as above, but now $\Psi = [\mathbf{I}_5 \mathbf{e}]$ with $\mathbf{e} = (0 \ 0 \ 1 \ 1 \ 0)^T$. As in Example 1, we have $N^* = 2$ and $\Phi \text{diag}(\Psi^T \mathbf{d}) \Omega^T$

has rank 2 for $d_3 = d_4 = d_5 = 0$ and nonzero d_1 and d_2 . Again, condition (5.3) does not hold, and Theorem 5.1 cannot be used to show uniqueness of \mathbf{A} . Theorem 5.1 is not as powerful as Theorem 2.1 for these examples because if the constraint matrices Ψ , Φ , or Ω contain columns with only few zeros, then there are few zeros in the matrix $\Phi \text{diag}(\Psi^T \mathbf{d}) \Omega^T$ and it can have low rank without $\omega(\mathbf{d}) \leq 1$ having to hold. Columns with few zeros appear in the constraint matrices in the presence of high k-ranks (for \mathbf{B} and \mathbf{C}), which is to the advantage of condition (2.1). This advantage still holds with Theorems 2.2 and 2.3.

In cases where all three loading matrices have low k-rank, Theorem 5.1 is more powerful. In [26, section 5], the following example is considered. Let $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_1 \ \mathbf{a}_3 \ \mathbf{a}_2]$, $\mathbf{B} = [\mathbf{b}_2 \ \mathbf{b}_2 \ \mathbf{b}_1 \ \mathbf{b}_3]$, and $\mathbf{C} = [\mathbf{c}_1 \ \mathbf{c}_1 \ \mathbf{c}_1 \ \mathbf{c}_2]$. It is shown in [26] that $\mathbf{C}' = [\mathbf{c}_1 \ \mathbf{c}_2]$ is essentially unique, by using Theorem 5.1 translated to mode three. However, since $\text{rank}(\mathbf{C}) = 2$, $k_{\mathbf{A}} = k_{\mathbf{B}} = 1$, $\max(\text{rank}(\mathbf{A}) - k_{\mathbf{A}}, \text{rank}(\mathbf{B}) - k_{\mathbf{B}}) = 2$, and $R = 4$, condition (2.3) translated to mode three does not hold. Since both (2.1) and (2.2) are sufficient for (2.3), the two conditions do not apply, either.

An example from [26, section 5] with moderate k-ranks is the following. Let \mathbf{B} have full column rank, $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_1 \ \mathbf{a}_2 \ \mathbf{a}_2 \ \mathbf{a}_3 \ \mathbf{a}_3]$, and $\mathbf{C} = [\mathbf{c}_1 \mid \mathbf{c}_4 - \mathbf{c}_1 \mid \mathbf{c}_2 \mid \mathbf{c}_4 - \mathbf{c}_2 \mid \mathbf{c}_3 \mid \mathbf{c}_4 - \mathbf{c}_3]$. Using Theorem 5.2, it is shown in [26] that \mathbf{A} is essentially unique. We have $\text{rank}(\mathbf{A}) = 3$, $k_{\mathbf{B}} = 6$, $k_{\mathbf{C}} = 4$, and $R = 6$, which implies that condition (2.1) does not hold; nor does (2.3), which degenerates into (2.1) in this example. Moreover, (2.2) does not apply, either.

The examples above show that Theorem 5.1 and Theorems 2.1 through 2.3 are useful for different types of decompositions. Apart from that, the conditions of Theorems 2.1 through 2.3 are easier to check than the condition of Theorem 5.1.

For checking uniqueness of the lower rank tensors in Theorem 3.1, Kruskal's uniqueness condition (1.4) was used in Examples 1 and 2. However, for the second lower rank tensor of Example 1 this condition was not satisfied. Here, Theorem 5.2 can be used instead. We write the lower rank tensor in PARALIND/CONFAC form with $\Psi = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$ and $\Phi = \Omega = \mathbf{I}_2$. Since $(\Omega \odot \Psi)\Phi^T$ and $(\Psi \odot \Phi)\Omega^T$ both have full column rank, Theorem 5.2 translated to modes two and three yields that $[\mathbf{b}_5 \ \mathbf{b}_6]$ and $[\mathbf{c}_5 \ \mathbf{c}_6]$ are subject to rotational indeterminacies.

In [26, section 6] a partial uniqueness condition is proved that uses the equivalence lemma for partitioned matrices of [7]. However, this condition is rather complicated to check. In case one of the loading matrices is essentially unique, splitting up the decomposition into lower rank tensors is a more convenient way of checking uniqueness.

6. Conclusions. This paper presents three sufficient conditions for *uni-mode* uniqueness of the three-way CP decomposition, which correct some uniqueness results introduced by Kruskal in [19]. These new conditions are formulated similarly to the well-known Kruskal's condition (1.4) with the difference that identical/proportional loadings in one mode are allowed. The mode for which the proportional loadings are allowed is guaranteed to be essentially unique. Based on this, we also proved that if one of these new conditions is met, the identifiability problem of the CP model can be divided into independent lower order CP subproblems, allowing a more refined analysis of the identifiability of the CP loadings.

Within the PARALIND/CONFAC framework of fixed linear dependencies in the loading vectors, our uniqueness conditions are less restrictive than existing results in cases with only one loading matrix having collinear columns and the k-ranks in the other two modes being high. Moreover, if one loading matrix is unique, then our method of splitting up the uniqueness problem into the uniqueness of lower rank

tensors is much simpler than showing partial uniqueness for the global decomposition problem.

As also noted in [26], within the PARALIND/CONFAC framework the uniqueness results in this paper are also relevant for the study of uniqueness of the decomposition in rank- $(L_r, L_r, 1)$ terms, introduced in [8]. In this decomposition, we have $\mathbf{A} = [\mathbf{A}_1 | \dots | \mathbf{A}_N]$, $\mathbf{B} = [\mathbf{B}_1 | \dots | \mathbf{B}_N]$, and $\mathbf{C} = [\mathbf{c}_1 \dots \mathbf{c}_1 | \dots | \mathbf{c}_N \dots \mathbf{c}_N]$, with \mathbf{A}_r and \mathbf{B}_r having L_r linearly independent columns, and \mathbf{c}_r is repeated L_r times in \mathbf{C} , $r = 1, \dots, N$.

Appendix A. Proof of Theorem 2.1. The theorem is proved with the help of the following three lemmas, among which Kruskal's permutation lemma (Lemma A.3) is the key to the proof.

LEMMA A.1 (see Sidiropoulos, Bro, and Giannakis [21]). *For any two matrices $\mathbf{A} (I \times R)$ and $\mathbf{B} (J \times R)$, $\mathbf{A} \odot \mathbf{B}$ has full column rank if $k_{\mathbf{A}} + k_{\mathbf{B}} \geq R + 1$.*

LEMMA A.2 (see Sidiropoulos and Liu [23]). *Let \mathbf{A} be an $I \times R$ matrix and $\tilde{\mathbf{A}}$ be an $I \times n$ matrix consisting of any n columns on \mathbf{A} . Then $\min(n, k_{\mathbf{A}}) \leq k_{\tilde{\mathbf{A}}} \leq n$.*

Recall $\omega(\mathbf{x})$ denotes the number of nonzero elements of a vector \mathbf{x} .

LEMMA A.3 (see Kruskal's permutation lemma [19]). *Given two matrices $\mathbf{A} \in \mathbb{C}^{I \times R}$ and $\tilde{\mathbf{A}} \in \mathbb{C}^{I \times R}$ with $k_{\mathbf{A}} \geq 1$, if for any $\mathbf{x} \in \mathbb{C}^I$ such that $\omega(\mathbf{x}^H \tilde{\mathbf{A}}) \leq R - \text{rank}(\tilde{\mathbf{A}}) + 1$ it holds that $\omega(\mathbf{x}^H \mathbf{A}) \leq \omega(\mathbf{x}^H \tilde{\mathbf{A}})$, then \mathbf{A} and $\tilde{\mathbf{A}}$ are the same up to permutation and scaling of columns.*

Proof of Theorem 2.1. We follow the guidelines of the proof on Kruskal's condition provided by Sidiropoulos, Bro, and Giannakis [22]. See also Stegeman and Sidiropoulos [27]. Assume that there exists another set of matrices $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, and $\tilde{\mathbf{C}}$ that satisfy (1.3):

$$(A.1) \quad \mathbf{A}(\mathbf{C} \odot \mathbf{B})^T = \tilde{\mathbf{A}}(\tilde{\mathbf{C}} \odot \tilde{\mathbf{B}})^T.$$

Then, for all \mathbf{x} that satisfies $\omega(\mathbf{x}^H \tilde{\mathbf{A}}) \leq R - \text{rank}(\tilde{\mathbf{A}}) + 1$, we have

$$(A.2) \quad (\mathbf{C} \odot \mathbf{B})\mathbf{A}^T \mathbf{x}^* = (\tilde{\mathbf{C}} \odot \tilde{\mathbf{B}})\tilde{\mathbf{A}}^T \mathbf{x}^*,$$

which can be equivalently written as

$$(A.3) \quad \mathbf{B} \text{diag}(\mathbf{x}^H \mathbf{A}) \mathbf{C}^T = \tilde{\mathbf{B}} \text{diag}(\mathbf{x}^H \tilde{\mathbf{A}}) \tilde{\mathbf{C}}^T.$$

For such an \mathbf{x} , let $\gamma = \omega(\mathbf{x}^H \mathbf{A})$ and $\bar{\gamma} = \omega(\mathbf{x}^H \tilde{\mathbf{A}})$. Since the rank of the matrix on the right-hand side of (A.3) can be no more than the rank of any of its factors, the following inequality holds:

$$(A.4) \quad \text{rank}[\tilde{\mathbf{B}} \text{diag}(\mathbf{x}^H \tilde{\mathbf{A}}) \tilde{\mathbf{C}}^T] \leq \text{rank}[\text{diag}(\mathbf{x}^H \tilde{\mathbf{A}})] = \bar{\gamma}.$$

We now establish a relationship between γ and the rank of the matrix on the left-hand side of (A.3). Assume, without loss of generality, that the first γ elements of $\mathbf{x}^H \mathbf{A}$ are nonzero and $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ are the corresponding matrices composed of the first γ columns of \mathbf{B} and \mathbf{C} . It follows that

$$(A.5) \quad \begin{aligned} \text{rank}[\mathbf{B} \text{diag}(\mathbf{x}^H \mathbf{A}) \mathbf{C}^T] &\geq \text{rank}(\tilde{\mathbf{B}}) + \text{rank}(\tilde{\mathbf{C}}) - \gamma \\ &\geq \min(\gamma, k_{\mathbf{B}}) + \min(\gamma, k_{\mathbf{C}}) - \gamma, \end{aligned}$$

where the first inequality is a consequence of Sylvester's inequality [16] and the second is due to Lemma A.2.

Combining (A.3), (A.4), and (A.5) one obtains

$$(A.6) \quad \bar{\gamma} \geq \min(\gamma, k_{\mathbf{B}}) + \min(\gamma, k_{\mathbf{C}}) - \gamma.$$

Recall condition (2.1) of our theorem, i.e., $\text{rank}(\mathbf{A}) + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2$. Knowing that $\text{rank}(\mathbf{A}) \leq R$ it follows that $k_{\mathbf{B}} + k_{\mathbf{C}} \geq R + 2$, which by Lemma A.1 implies that $\mathbf{C} \odot \mathbf{B}$ has full column rank and thus

$$(A.7) \quad \text{rank}(\mathbf{A}) = \text{rank}[\mathbf{A}(\mathbf{C} \odot \mathbf{B})^T] = \text{rank}[\bar{\mathbf{A}}(\bar{\mathbf{C}} \odot \bar{\mathbf{B}})^T] \leq \text{rank}(\bar{\mathbf{A}}).$$

The condition (2.1) can also be written as $k_{\mathbf{B}} + k_{\mathbf{C}} - (R + 1) \geq R - \text{rank}(\mathbf{A}) + 1$, which together with (A.7) yields $k_{\mathbf{B}} + k_{\mathbf{C}} - (R + 1) \geq R - \text{rank}(\bar{\mathbf{A}}) + 1$. Using Kruskal's permutation lemma condition $\omega(\mathbf{x}^H \bar{\mathbf{A}}) \leq R - \text{rank}(\bar{\mathbf{A}}) + 1$, we get

$$(A.8) \quad k_{\mathbf{B}} + k_{\mathbf{C}} - (R + 1) \geq \bar{\gamma}.$$

To complete the proof we analyze (A.6) with respect to the values of γ compared to $k_{\mathbf{B}}$ and $k_{\mathbf{C}}$. The following three situations can occur:

1. If $\gamma > \max(k_{\mathbf{B}}, k_{\mathbf{C}})$, then by (A.6) and (A.8) one obtains $k_{\mathbf{B}} + k_{\mathbf{C}} - (R + 1) \geq k_{\mathbf{B}} + k_{\mathbf{C}} - \gamma$, which is impossible since $\gamma < R + 1$.
2. If $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq \max(k_{\mathbf{B}}, k_{\mathbf{C}})$ then (A.6) yields $\bar{\gamma} \geq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$; it follows that $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(k_{\mathbf{B}}, k_{\mathbf{C}}) - (R + 1) = k_{\mathbf{B}} + k_{\mathbf{C}} - (R + 1) \geq \bar{\gamma} \geq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$ as a consequence of (A.8). This implies $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) \geq (R + 1)$, which is also impossible.
3. If $\gamma \leq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, then (A.6) yields $\bar{\gamma} \geq \min(\gamma, k_{\mathbf{B}}) + \min(\gamma, k_{\mathbf{C}}) - \gamma = \gamma$.

So the only possible case is the third one, meaning that $\bar{\gamma} \geq \gamma$, i.e., $\omega(\mathbf{x}^H \bar{\mathbf{A}}) \leq \omega(\mathbf{x}^H \bar{\mathbf{A}})$. This implies by Lemma A.3 that $\bar{\mathbf{A}}$ is essentially the same as \mathbf{A} , which completes the proof. \square

Appendix B. Proof of Theorem 2.2.

Proof. The proof is very similar to the previous one (Appendix A). Suppose that there also exists $[\bar{\mathbf{A}}, \bar{\mathbf{B}}, \bar{\mathbf{C}}] = [\mathbf{A}, \mathbf{B}, \mathbf{C}]$. Then, for all \mathbf{x} that satisfies $\omega(\mathbf{x}^H \bar{\mathbf{A}}) \leq R - \text{rank}(\bar{\mathbf{A}}) + 1$, it can be easily shown by a rationale similar to the one in Appendix A that

$$(B.1) \quad \bar{\gamma} \geq \min(\gamma, k_{\mathbf{B}}) + \min(\gamma, k_{\mathbf{C}}) - \gamma$$

and

$$(B.2) \quad k_{\mathbf{B}} + k_{\mathbf{C}} - R \geq R - \text{rank}(\mathbf{A}) + 1 \geq R - \text{rank}(\bar{\mathbf{A}}) + 1 \geq \bar{\gamma},$$

where $\gamma \triangleq \omega(\mathbf{x}^H \mathbf{A})$ and $\bar{\gamma} \triangleq \omega(\mathbf{x}^H \bar{\mathbf{A}})$.

Let us now examine the possible values for γ . The following three situations are possible:

1. If $\gamma > \max(k_{\mathbf{B}}, k_{\mathbf{C}})$, then it follows from (B.1) and (B.2) that $k_{\mathbf{B}} + k_{\mathbf{C}} - R \geq k_{\mathbf{B}} + k_{\mathbf{C}} - \gamma$. This implies that $\gamma \geq R$. Since $\gamma \leq R$, thus $\gamma = R$. As a result, $\text{diag}(\mathbf{x}^H \mathbf{A})$ has full rank; hence, we obtain

$$(B.3) \quad \bar{\gamma} \geq \text{rank}[\mathbf{B} \text{diag}(\mathbf{x}^H \mathbf{A}) \mathbf{C}^T] \geq \text{rank}(\mathbf{B}) + \text{rank}(\mathbf{C}) - \gamma,$$

where the first inequality can be obtained from (A.3) and (A.4) and the second is derived from Sylvester's inequality [16]. From (B.2) and (B.3) we can deduce that $k_{\mathbf{B}} = \text{rank}(\mathbf{B})$ and $k_{\mathbf{C}} = \text{rank}(\mathbf{C})$, which contradicts our condition (2). Therefore, it is impossible having $\gamma > \max(k_{\mathbf{B}}, k_{\mathbf{C}})$.

2. If $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq \max(k_{\mathbf{B}}, k_{\mathbf{C}})$, then (B.1) yields $\bar{\gamma} \geq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$. Observe that $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(k_{\mathbf{B}}, k_{\mathbf{C}}) - R = k_{\mathbf{B}} + k_{\mathbf{C}} - R \geq \bar{\gamma}$ as a direct consequence of (B.2). It follows that $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(k_{\mathbf{B}}, k_{\mathbf{C}}) - R \geq \bar{\gamma} \geq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, implying $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) \geq R$. This is also impossible because $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) < R$ according to (\mathfrak{A}) .
3. If $\gamma \leq \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, then following (B.1) we obtain that $\bar{\gamma} \geq \min(\gamma, k_{\mathbf{B}}) + \min(\gamma, k_{\mathbf{C}}) - \gamma = \gamma$.

Thus, $\bar{\gamma} \geq \gamma$, i.e., $\omega(\mathbf{x}^H \tilde{\mathbf{A}}) \geq \omega(\mathbf{x}^H \mathbf{A})$, which by Kruskal's permutation lemma (Lemma A.3) implies that $\tilde{\mathbf{A}}$ is essentially the same as \mathbf{A} . The proof is complete. \square

Appendix C. Proof of Theorem 2.3. The following two lemmas are key to the proof.

LEMMA C.1. *Let \mathbf{A} be an $I \times R$ matrix and $\tilde{\mathbf{A}}$ be an $I \times n$ matrix consisting of any n columns of \mathbf{A} . Then $g_{\mathbf{A}}(n) \leq \text{rank}(\tilde{\mathbf{A}}) \leq \min(\text{rank}(\mathbf{A}), n)$, where*

$$(C.1) \quad g_{\mathbf{A}}(n) = \begin{cases} n, & n \leq k_{\mathbf{A}}; \\ k_{\mathbf{A}}, & k_{\mathbf{A}} < n \leq R + k_{\mathbf{A}} - \text{rank}(\mathbf{A}); \\ n + \text{rank}(\mathbf{A}) - R, & n > R + k_{\mathbf{A}} - \text{rank}(\mathbf{A}). \end{cases}$$

Proof. Since the first inequality $\text{rank}(\tilde{\mathbf{A}}) \geq g_{\mathbf{A}}(n)$ has been proved by Kruskal (see [19, Proof that Theorem 3c \Rightarrow Theorem 3b]), herein we only provide some hints for it. On the one hand, if $n \leq k_{\mathbf{A}}$, from the definition of k-rank, we can deduce that $\text{rank}(\tilde{\mathbf{A}}) = n$. Furthermore, once $n > k_{\mathbf{A}}$, then $\text{rank}(\tilde{\mathbf{A}}) \geq k_{\mathbf{A}}$ (see also Lemma A.2). On the other hand, observe that by removing one column from \mathbf{A} the rank cannot be reduced by more than 1. Since $\tilde{\mathbf{A}}$ is \mathbf{A} less $(R - n)$ columns, the worst case for $\text{rank}(\tilde{\mathbf{A}})$ is $\text{rank}(\tilde{\mathbf{A}}) = \text{rank}(\mathbf{A}) - (R - n) = n + \text{rank}(\mathbf{A}) - R$. As n decreases, it reduces to $k_{\mathbf{A}}$ at $n = R + k_{\mathbf{A}} - \text{rank}(\mathbf{A})$. Therefore, it holds that $\text{rank}(\tilde{\mathbf{A}}) \geq g_{\mathbf{A}}(n)$ in general.

Then we verify the second inequality. Since the inequality is obvious for $n \geq \text{rank}(\mathbf{A})$, only the case $n < \text{rank}(\mathbf{A})$ is interesting. As it is already known that $\text{rank}(\tilde{\mathbf{A}}) = n$ for $n < k_{\mathbf{A}}$, we assume without loss of generality that $k_{\mathbf{A}} \leq n < \text{rank}(\mathbf{A})$. Observe that $\text{rank}(\tilde{\mathbf{A}})$ cannot be increased by more than 1 if appending one more column to $\tilde{\mathbf{A}}$. Therefore, $\text{rank}(\tilde{\mathbf{A}}) \leq n$ for $k_{\mathbf{A}} \leq n < \text{rank}(\mathbf{A})$, which completes the proof. \square

Lemma C.1 is also illustrated by Figure C.1: $\text{rank}(\tilde{\mathbf{A}})$ equals n if $n \leq k_{\mathbf{A}}$, whereas for $k_{\mathbf{A}} < n \leq R$, the point $(n, \text{rank}(\tilde{\mathbf{A}}))$ is bounded in the grey area.

LEMMA C.2 (see Guo et al. [10]). *For any two matrices $\mathbf{A}(I \times R)$ and $\mathbf{B}(J \times R)$, if $k_{\mathbf{A}} + k_{\mathbf{B}} + \max(\text{rank}(\mathbf{A}) - k_{\mathbf{A}}, \text{rank}(\mathbf{B}) - k_{\mathbf{B}}) \geq R + 1$, then $\mathbf{A} \odot \mathbf{B}$ has full column rank.*

Proof of Theorem 2.3. As we did for the proofs of Theorems 2.1 and 2.2, suppose that there also exists $[\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}] = [\mathbf{A}, \mathbf{B}, \mathbf{C}]$. For all \mathbf{x} that satisfies $\omega(\mathbf{x}^H \tilde{\mathbf{A}}) \leq R - \text{rank}(\tilde{\mathbf{A}}) + 1$, from

$$\text{rank}[\tilde{\mathbf{B}} \text{diag}(\mathbf{x}^H \tilde{\mathbf{A}}) \tilde{\mathbf{C}}^T] = \text{rank}[\mathbf{B} \text{diag}(\mathbf{x}^H \mathbf{A}) \mathbf{C}^T] \geq \text{rank}(\tilde{\mathbf{B}}) + \text{rank}(\tilde{\mathbf{C}}) - \gamma,$$

and using Lemma C.1, it can be deduced that

$$(C.2) \quad \bar{\gamma} \geq \text{rank}[\tilde{\mathbf{B}} \text{diag}(\mathbf{x}^H \tilde{\mathbf{A}}) \tilde{\mathbf{C}}^T] \geq g_{\mathbf{B}}(\gamma) + g_{\mathbf{C}}(\gamma) - \gamma \triangleq h(\gamma),$$

where γ , $\bar{\gamma}$, $\omega(\cdot)$, $\tilde{\mathbf{B}}$, and $\tilde{\mathbf{C}}$ are defined as in Appendix A. To prove the theorem we must show that $\gamma \leq \bar{\gamma}$.

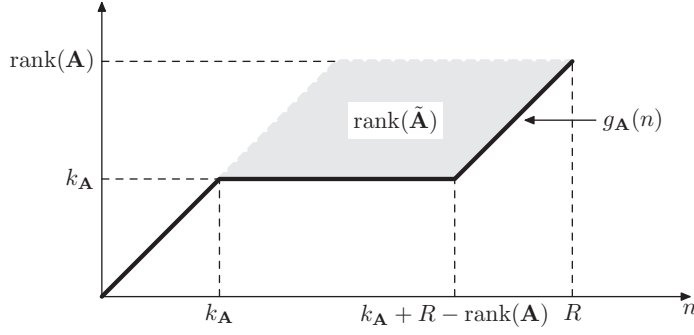


FIG. C.1. Illustration of Lemma C.1.

First observe that the conditions of (2.3) can be reformulated as

$$(C.3) \quad R - \text{rank}(\mathbf{A}) + 1 \leq \min(k_{\mathbf{B}}, k_{\mathbf{C}}, k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R) - 1 \triangleq q,$$

where $\zeta_{\mathbf{B}} \triangleq \text{rank}(\mathbf{B}) - k_{\mathbf{B}}$ and $\zeta_{\mathbf{C}} \triangleq \text{rank}(\mathbf{C}) - k_{\mathbf{C}}$.

The second condition of (2.3) can be rewritten as

$$k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) \geq 2R - \text{rank}(\mathbf{A}) + 2 > R + 1.$$

Based on Lemma C.2, this means that $\mathbf{B} \odot \mathbf{C}$ has full column rank. Therefore, (A.7) also holds in this case, yielding

$$(C.4) \quad \text{rank}(\mathbf{A}) \leq \text{rank}(\bar{\mathbf{A}}).$$

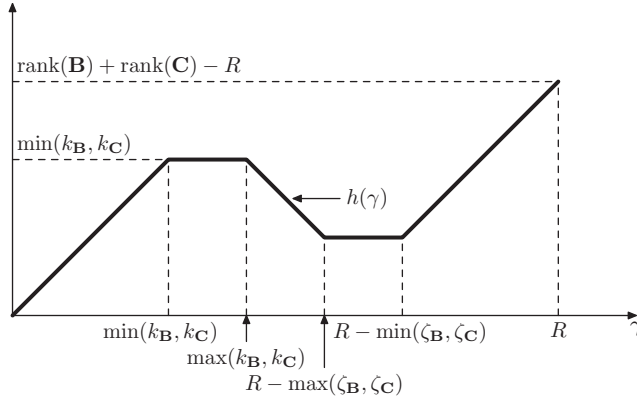
Using the results derived above, it can be easily shown that

$$(C.5) \quad q \geq R - \text{rank}(\mathbf{A}) + 1 \geq R - \text{rank}(\bar{\mathbf{A}}) + 1 \geq \bar{\gamma} \geq h(\gamma),$$

where the second, third, and last inequalities are due to (C.4), the assumption $\bar{\gamma} \leq R - \text{rank}(\bar{\mathbf{A}}) + 1$, and (C.2), respectively.

Next, we will show that (C.5) does not hold for $\gamma > \min(k_{\mathbf{B}}, k_{\mathbf{C}})$. To this end, we will use some piecewise monotony properties of $h(\gamma)$, observed first by Kruskal [19]. Observing that $\text{rank}(\mathbf{B}) \leq R$ and $\text{rank}(\mathbf{C}) \leq R$, it follows that $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq \min(k_{\mathbf{B}} + R - \text{rank}(\mathbf{B}), k_{\mathbf{C}} + R - \text{rank}(\mathbf{C})) = R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$. Similarly, we can derive $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$. The four values, i.e., $\min(k_{\mathbf{B}}, k_{\mathbf{C}})$, $\max(k_{\mathbf{B}}, k_{\mathbf{C}})$, $R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$, and $R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$, are first order discontinuities of $h(\gamma)$ and divide the domain into five intervals on which h is linear, as shown next. Since, clearly, $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq \max(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$, only the following two cases are to be considered with respect to the value of $R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$: the first one corresponds to $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$, whereas for the second case we assume that $R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) < \max(k_{\mathbf{B}}, k_{\mathbf{C}})$. Using the definition (C.1), $h(\gamma)$ can be explicitly expressed as

$$(C.6) \quad h(\gamma) = \begin{cases} \gamma, & \gamma \leq \min(k_{\mathbf{B}}, k_{\mathbf{C}}); \\ \min(k_{\mathbf{B}}, k_{\mathbf{C}}), & \min(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq \max(k_{\mathbf{B}}, k_{\mathbf{C}}); \\ k_{\mathbf{B}} + k_{\mathbf{C}} - \gamma, & \max(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}); \\ k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R, & R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) < \gamma \leq R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}); \\ \text{rank}(\mathbf{B}) + \text{rank}(\mathbf{C}) - 2R + \gamma, & R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) < \gamma \leq R, \end{cases}$$

FIG. C.2. The graph of $h(\gamma)$ in the first case: $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) < R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$.

for the first case (see Figure C.2), and

$$(C.7) \quad h(\gamma) = \begin{cases} \gamma, & \gamma \leq \min(k_{\mathbf{B}}, k_{\mathbf{C}}); \\ \min(k_{\mathbf{B}}, k_{\mathbf{C}}), & \min(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}); \\ \min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R + \gamma, & R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) < \gamma \leq \max(k_{\mathbf{B}}, k_{\mathbf{C}}); \\ k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R, & \max(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}); \\ \text{rank}(\mathbf{B}) + \text{rank}(\mathbf{C}) - 2R + \gamma, & R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) < \gamma \leq R, \end{cases}$$

for the other (see Figure C.3). In what follows we show that $\min_{\gamma > \min(k_{\mathbf{B}}, k_{\mathbf{C}})} h(\gamma) > q$ for both considered cases, which contradicts (C.5).

Case 1. Observe that $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) \leq R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$ can be also expressed as $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R \leq 0$, implying

$$(C.8) \quad \begin{aligned} \min(k_{\mathbf{B}}, k_{\mathbf{C}}) &\geq \min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R \\ &= k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R. \end{aligned}$$

A direct consequence of the above inequality is that $q = k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R - 1$. Now we seek to contradict the inequality $q \geq h(\gamma)$ from (C.5).

Obviously, for $\gamma > \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, the minimum of $h(\gamma)$ occurs when $R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) \leq \gamma < R - \min(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$ and equals (see Figure C.2 and (C.6))

$$(C.9) \quad \bar{h} = k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R > q.$$

Since $h(\gamma) \geq \bar{h}$ for $\gamma > \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, from (C.9) we obtain

$$h(\gamma) > q,$$

which is in contradiction with (C.5).

Case 2. Since $\max(k_{\mathbf{B}}, k_{\mathbf{C}}) > R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$, it holds that

$$(C.10) \quad \begin{aligned} \min(k_{\mathbf{B}}, k_{\mathbf{C}}) &< \min(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(k_{\mathbf{B}}, k_{\mathbf{C}}) + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R \\ &= k_{\mathbf{B}} + k_{\mathbf{C}} + \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}}) - R, \end{aligned}$$

so $q = \min(k_{\mathbf{B}}, k_{\mathbf{C}}) - 1$. Obviously, for $\gamma > \min(k_{\mathbf{B}}, k_{\mathbf{C}})$, the minimum of $h(\gamma)$ is reached (see Figure C.3 and (C.7)) in the interval $\min(k_{\mathbf{B}}, k_{\mathbf{C}}) < \gamma \leq R - \max(\zeta_{\mathbf{B}}, \zeta_{\mathbf{C}})$

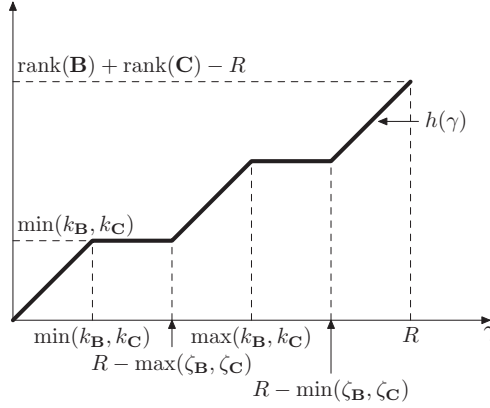


FIG. C.3. The graph of $h(\gamma)$ in the second case: $\max(k_B, k_C) \geq R - \max(\zeta_B, \zeta_C)$.

and is given by

$$(C.11) \quad \bar{h} \triangleq \min_{\gamma > \min(k_B, k_C)} h(\gamma) = \min(k_B, k_C) > q$$

which contradicts (C.5).

Since neither of the above cases is possible, (C.5) holds only if $\gamma \leq \min(k_B, k_C)$, implying $h(\gamma) = \gamma$. Hence, from (C.5), we finally arrive at the assertion $\bar{\gamma} \geq \gamma$, i.e., $\omega(\mathbf{x}^H \bar{\mathbf{A}}) \geq \omega(\mathbf{x}^H \mathbf{A})$. Based on Kruskal's permutation lemma (see Lemma A.3), it means that $\bar{\mathbf{A}}$ is essentially the same as \mathbf{A} . The proof is complete. \square

Appendix D. Proof of Theorem 3.1.

Proof. Recall the unfolded matrix representation of the three-way CP model (1.3)

$$(D.1) \quad \mathbf{X} = \mathbf{A}(\mathbf{C} \odot \mathbf{B})^T.$$

Consider then the following partition of \mathbf{A} (after column permutations), which satisfies (3.2): $\mathbf{A}\Pi_A = [\mathbf{A}_1 | \mathbf{A}_{\{1\}}]$, where $\mathbf{A}_{\{i\}}$ denotes the matrix obtained from $\mathbf{A}\Pi_A$ after the extraction of the \mathbf{A}_i submatrix. Analogously we denote $\mathbf{B}\Pi_A = [\mathbf{B}_1 | \mathbf{B}_{\{1\}}]$, $\mathbf{C}\Pi_A = [\mathbf{C}_1 | \mathbf{C}_{\{1\}}]$, and $\mathbf{C} \odot \mathbf{B} = \mathbf{P} = [\mathbf{P}_1 | \mathbf{P}_{\{1\}}] = [\mathbf{C}_1 \odot \mathbf{B}_1 | \mathbf{C}_{\{1\}} \odot \mathbf{B}_{\{1\}}]$.

The essential uniqueness of \mathbf{A} implies the essential uniqueness of \mathbf{A}_1 and $\mathbf{A}_{\{1\}}$. Suppose now that there exist another two submatrices $\bar{\mathbf{P}}_1 = \bar{\mathbf{C}}_1 \odot \bar{\mathbf{B}}_1$ and $\bar{\mathbf{P}}_{\{1\}} = \bar{\mathbf{C}}_{\{1\}} \odot \bar{\mathbf{B}}_{\{1\}}$ such that

$$(D.2) \quad [\mathbf{A}_1 | \mathbf{A}_{\{1\}}] [\mathbf{P}_1 | \mathbf{P}_{\{1\}}]^T = [\mathbf{A}_1 | \mathbf{A}_{\{1\}}] [\bar{\mathbf{P}}_1 | \bar{\mathbf{P}}_{\{1\}}]^T,$$

or equivalently

$$(D.3) \quad [\mathbf{A}_1 | \mathbf{A}_{\{1\}}] [\mathbf{P}_1 - \bar{\mathbf{P}}_1 | \mathbf{P}_{\{1\}} - \bar{\mathbf{P}}_{\{1\}}]^T = \mathbf{0}.$$

Property (3.3) yields in our case

$$(D.4) \quad \text{span}(\mathbf{A}_1) \cap \text{span}(\mathbf{A}_{\{1\}}) = \{\mathbf{0}\},$$

meaning that (D.3) is equivalent to

$$(D.5) \quad \begin{cases} \mathbf{A}_1(\mathbf{P}_1 - \bar{\mathbf{P}}_1)^T = \mathbf{0}, \\ \mathbf{A}_{\{1\}}(\mathbf{P}_{\{1\}} - \bar{\mathbf{P}}_{\{1\}})^T = \mathbf{0}. \end{cases}$$

Using (D.5), it is straightforward to prove by induction that (D.2) is equivalent to the following set of equations:

$$(D.6) \quad \begin{cases} \mathbf{A}_1(\mathbf{C}_1 \odot \mathbf{B}_1)^T = \mathbf{A}_1(\bar{\mathbf{C}}_1 \odot \bar{\mathbf{B}}_1)^T \\ \vdots \\ \mathbf{A}_N(\mathbf{C}_N \odot \mathbf{B}_N)^T = \mathbf{A}_N(\bar{\mathbf{C}}_N \odot \bar{\mathbf{B}}_N)^T. \end{cases}$$

This means that given the essential uniqueness of $\mathbf{A}_1, \dots, \mathbf{A}_N$, the three-way CP model can be uniquely decomposed into N CP lower rank tensors as follows:

$$(D.7) \quad \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket = \sum_{n=1}^N \llbracket \mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n \rrbracket.$$

For each of these lower rank tensors, the \mathbf{A}_n loading matrix is essentially unique and the uniqueness of \mathbf{B}_n and \mathbf{C}_n can be locally assessed by analyzing the uniqueness of the CP model $\llbracket \mathbf{A}_n, \mathbf{B}_n, \mathbf{C}_n \rrbracket$. \square

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