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COUPLED CANONICAL POLYADIC DECOMPOSITIONS AND (COUPLED) DECOMPOSITIONS IN MULTILINEAR RANK-$(L_{r,n}, L_{r,n}, 1)$ TERMS—PART I: UNIQUENESS*

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Abstract. Coupled tensor decompositions are becoming increasingly important in signal processing and data analysis. However, the uniqueness properties of coupled tensor decompositions have not yet been studied. In this paper, we first provide new uniqueness conditions for one factor matrix of the coupled canonical polyadic decomposition (CPD) of third-order tensors. Then, we present necessary and sufficient overall uniqueness conditions for the coupled CPD of third-order tensors. The results demonstrate that improved uniqueness conditions can indeed be obtained by taking into account the coupling between several tensor decompositions. We extend the results to higher-order tensors and explain that the higher-order structure can further improve the uniqueness results. We discuss the special case of coupled matrix-tensor factorizations. We also present a new variant of the coupled CPD model called the coupled block term decomposition (BTD). On one hand, the coupled BTD can be seen as a variant of coupled CPD for the case where the common factor contains collinear columns. On the other hand, it can also be seen as an extension of the decomposition into multilinear rank-$(L_r, L_r, 1)$ terms to coupled factorizations.

Key words. coupled decompositions, higher-order tensor, parallel factor (PARAFAC), canonical decomposition (CANDECOMP), canonical polyadic decomposition, coupled matrix-tensor factorization

AMS subject classifications. 15A22, 15A23, 15A69

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1. Introduction.

The coupled canonical polyadic decomposition (CPD) model (formally defined in subsection 4.1) seems to have been first used in psychometrics [21, 22] as a way of integrating several three-way studies that involve the same stimuli and as a means of coping with missing data in coupled data sets. The technique was also later considered in chemometrics [36]. In recent years coupled canonical polyadic decompositions have had a resurgence in several engineering disciplines. We mention data mining, where they are used as an explorative tool for finding structure in coupled data sets [3, 1], and bioinformatics, where they are used as a tool for fusion of data obtained by different analytical methods such as nuclear magnetic resonance and fluorescence spectroscopy [32, 48]. In chemometrics it has been suggested that coupled matrix-tensor factorizations can be used to fuse data obtained by different analytic methods [2]. We also mention that in biomedical engineering several multisubject or data fusion methods that combine different modalities (fMRI, EEG, MEG, etc.)

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can be interpreted as coupled CPD problems [19, 28, 9, 20, 29, 4]. Despite their importance, to the best of our knowledge, no algebraic studies of coupled tensor decompositions have been provided so far. In particular, no dedicated uniqueness conditions for coupled CPD problems are available.

Several problems in signal processing involve polyadic decompositions that have factor matrices with collinear columns. A particular case is of block term decompositions, which are decompositions of a tensor in terms of low multilinear rank [13]. We mention applications in array processing [34, 38, 39], wireless communication [35, 10, 12, 31, 37], and blind separation of signals that can be modeled as exponential polynomials [14]. There are also applications in chemometrics [6]. Hence, in the study of the coupled CPD model we should pay special attention to collinearity.

The rest of the introduction presents our notation. Sections 2 and 3 briefly review the CPD and the decomposition into multilinear rank-$(L_r, L_r, 1)$ terms. In section 4 we introduce the coupled CPD and study its uniqueness properties. The results are (i) necessary coupled CPD uniqueness conditions, (ii) sufficient uniqueness conditions for the common factor matrix of the coupled CPD, (iii) sufficient overall uniqueness conditions for the coupled CPD, (iv) extensions to tensors of arbitrary order, and (v) a discussion of the uniqueness properties of the coupled matrix-tensor factorization. Section 5 discusses a new coupled CPD model in which the common factor matrix contains collinear components. The paper is concluded in section 6.

1.1. Notation. Vectors, matrices, and tensors are denoted by lowercase boldface, uppercase boldface, and uppercase calligraphic letters, respectively. The rth column vector of $\mathbf{A}$ is denoted by $\mathbf{a}_r$. The symbols $\otimes$ and $\odot$ denote the Kronecker and Khatri–Rao product, defined as

$$\mathbf{A}\otimes\mathbf{B} := \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \dots \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}, \quad \mathbf{A}\odot\mathbf{B} := \begin{bmatrix} \mathbf{a}_1\otimes\mathbf{b}_1 & \mathbf{a}_2\otimes\mathbf{b}_2 & \dots \end{bmatrix},$$

in which $(\mathbf{A})_{mn} = a_{mn}$. The outer product of N vectors $\mathbf{a}^{(n)} \in \mathbb{C}^{I_n}$ is denoted by $\mathbf{a}^{(1)} \circ \mathbf{a}^{(2)} \circ \cdots \circ \mathbf{a}^{(N)} \in \mathbb{C}^{I_1\times I_2\times\cdots\times I_N}$, such that

$$\left(\mathbf{a}^{(1)} \circ \mathbf{a}^{(2)} \circ \cdots \circ \mathbf{a}^{(N)}\right)_{i_1,i_2,\dots,i_N} = a^{(1)}_{i_1} a^{(2)}_{i_2} \cdots a^{(N)}_{i_N}.$$

The identity matrix, all-zero matrix, and all-zero vector are denoted by $\mathbf{I}_M \in \mathbb{C}^{M\times M}$, $\mathbf{0}_{M,N} \in \mathbb{C}^{M\times N}$, and $\mathbf{0}_M \in \mathbb{C}^M$, respectively. The all-ones vector is denoted by $\mathbf{1}_R = [1,\dots,1]^T \in \mathbb{C}^R$.

The transpose, Moore–Penrose pseudo-inverse, Frobenius norm, determinant, range, and kernel of a matrix are denoted by $(\cdot)^T$, $(\cdot)^\dagger$, $\|\cdot\|_F$, $|\cdot|$, range$(\cdot)$, and ker$(\cdot)$, respectively. The cardinality of a set S is denoted by card(S).

MATLAB index notation will be used for submatrices of a given matrix. For example, $\mathbf{A}(1:k,:)$ represents the submatrix of $\mathbf{A}$ consisting of the rows from 1 to k of $\mathbf{A}$. $D_k(\mathbf{A}) \in \mathbb{C}^{J\times J}$ denotes the diagonal matrix holding row k of $\mathbf{A} \in \mathbb{C}^{I\times J}$ on its diagonal. Given $\mathbf{A} \in \mathbb{C}^{I\times J}$, Vec$(\mathbf{A}) \in \mathbb{C}^{IJ}$ will denote the column vector defined by $(\text{Vec}(\mathbf{A}))_{i+(j-1)I} = (\mathbf{A})_{ij}$.

The matrix that orthogonally projects onto the orthogonal complement of the column space of $\mathbf{A} \in \mathbb{C}^{I\times J}$ is denoted by

$$\mathbf{P}_{\mathbf{A}} = \mathbf{I}_I - \mathbf{F}\mathbf{F}^H \in \mathbb{C}^{I\times I},$$

where the column vectors of $\mathbf{F}$ constitute an orthonormal basis for range$(\mathbf{A})$.

The Heaviside step function $H\colon \mathbb{Z} \to \{0,1\}$ is defined as

$$H[n] = \begin{cases} 0\,, & n < 0\,, \\ 1\,, & n \geq 0\,. \end{cases}$$

The rank of a matrix $\mathbf{A}$ is denoted by $r(\mathbf{A})$ or $r_{\mathbf{A}}$. The k-rank of a matrix $\mathbf{A}$ is denoted by $k(\mathbf{A})$ or $k_{\mathbf{A}}$. It is equal to the largest integer $k(\mathbf{A})$ such that every subset of $k(\mathbf{A})$ columns of $\mathbf{A}$ is linearly independent. More generally, the k'-rank of a partitioned matrix $\mathbf{A}$ is denoted by $k'(\mathbf{A})$. It is equal to the largest integer $k'(\mathbf{A})$ such that any set of $k'(\mathbf{A})$ submatrices of $\mathbf{A}$ yields a set of linearly independent columns. The number of nonzero entries of a vector $\mathbf{x}$ is denoted by $\omega(\mathbf{x})$ in the tensor decomposition literature, dating back to the work of Kruskal [26].

Let $C_n^k = \frac{n!}{k!(n-k)!}$ denote the binomial coefficient. The kth compound matrix of $\mathbf{A} \in \mathbb{C}^{m\times n}$ is denoted by $C_k(\mathbf{A}) \in \mathbb{C}^{C_m^k \times C_n^k}$ and its entries correspond to the k-by-k minors of $\mathbf{A}$, ordered lexicographically. As an example, let $\mathbf{A} \in \mathbb{C}^{4\times 3}$; then

$$C_2(\mathbf{A}) = \begin{bmatrix} |\mathbf{A}([1,2],[1,2])| & |\mathbf{A}([1,2],[1,3])| & |\mathbf{A}([1,2],[2,3])| \\ |\mathbf{A}([1,3],[1,2])| & |\mathbf{A}([1,3],[1,3])| & |\mathbf{A}([1,3],[2,3])| \\ |\mathbf{A}([1,4],[1,2])| & |\mathbf{A}([1,4],[1,3])| & |\mathbf{A}([1,4],[2,3])| \\ |\mathbf{A}([2,3],[1,2])| & |\mathbf{A}([2,3],[1,3])| & |\mathbf{A}([2,3],[2,3])| \\ |\mathbf{A}([2,4],[1,2])| & |\mathbf{A}([2,4],[1,3])| & |\mathbf{A}([2,4],[2,3])| \\ |\mathbf{A}([3,4],[1,2])| & |\mathbf{A}([3,4],[1,3])| & |\mathbf{A}([3,4],[2,3])| \end{bmatrix}.$$

See [23, 15] for discussion of compound matrices.

2. Canonical polyadic decomposition. Consider the third-order tensor $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$. We say that $\mathcal{X}$ is a rank-1 tensor if it is equal to the outer product of some nonzero vectors $\mathbf{a} \in \mathbb{C}^I$, $\mathbf{b} \in \mathbb{C}^J$, and $\mathbf{c} \in \mathbb{C}^K$ such that $x_{ijk} = a_i b_j c_k$. Decompositions into a sum of rank-1 terms are called polyadic decompositions (PDs):

$$\mathcal{X} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r\,. \tag{2.1}$$

The rank of a tensor $\mathcal{X}$ is equal to the minimal number of rank-1 tensors that yield $\mathcal{X}$ in a linear combination. Assume that the rank of $\mathcal{X}$ is R; then (2.1) is called the canonical PD (CPD) of $\mathcal{X}$. The CPD is also known as the PARAllel FACtor (PARAFAC) [22] and the CANonical DECOMPosition (CANDECOMP) [7]. Let us stack the vectors $\{\mathbf{a}_r\}$, $\{\mathbf{b}_r\}$, and $\{\mathbf{c}_r\}$ into the matrices

$$\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_R] \in \mathbb{C}^{I\times R}, \quad \mathbf{B} = [\mathbf{b}_1, \ldots, \mathbf{b}_R] \in \mathbb{C}^{J\times R}, \quad \mathbf{C} = [\mathbf{c}_1, \ldots, \mathbf{c}_R] \in \mathbb{C}^{K\times R}.$$

The matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ will be referred to as the factor matrices of the CPD in (2.1). The following subsection presents matrix representations of (2.1) that will be used throughout the paper.

2.1. Matrix representations. Let $\mathbf{X}^{(i\cdot\cdot)} \in \mathbb{C}^{J\times K}$ denote the matrix such that $(\mathbf{X}^{(i\cdot\cdot)})_{jk} = x_{ijk}$; then $\mathbf{X}^{(i\cdot\cdot)} = \mathbf{B} D_i(\mathbf{A}) \mathbf{C}^T$ and

$$\mathbb{C}^{IJ\times K} \ni \mathbf{X}_{(1)} := \left[\mathbf{X}^{(1\cdot\cdot)T}, \ldots, \mathbf{X}^{(I\cdot\cdot)T}\right]^T = (\mathbf{A} \odot \mathbf{B})\,\mathbf{C}^T. \tag{2.2}$$

More generally, the PD or CPD of the higher-order tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times \cdots \times I_M}$ has the matrix representations

$$\mathbf{X}^{(w)} = \left(\bigodot_{p \in \Gamma_w} \mathbf{A}^{(p)} \odot \bigodot_{q \in \Upsilon_w} \mathbf{A}^{(q)} \right) \left(\bigodot_{r \in \Psi_w} \mathbf{A}^{(r)} \right)^T , \tag{2.3}$$

where $\mathbf{A}^{(m)} \in \mathbb{C}^{I_m \times R}$ and the sets Γ_w, Υ_w, and Ψ_w have properties $\Gamma_w \bigcup \Upsilon_w \bigcup \Psi_w = \{1, 2, \ldots, M\}$, $\Gamma_w \bigcap \Upsilon_w = \emptyset$, $\Gamma_w \bigcap \Psi_w = \emptyset$, and $\Upsilon_w \bigcap \Psi_w = \emptyset$.

2.2. Uniqueness conditions for one factor matrix of a CPD. A factor matrix, say $\mathbf{C}$, of the CPD of $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ is said to be unique if it can be determined up to the inherent column scaling and permutation ambiguities from $\mathcal{X}$. More formally, the factor matrix $\mathbf{C}$ is unique if all the triplets $(\widehat{\mathbf{A}}, \widehat{\mathbf{B}}, \widehat{\mathbf{C}})$ satisfying (2.1) also satisfy the condition

$$\widehat{\mathbf{C}} = \mathbf{C}\mathbf{P}\Delta ,$$

where $\mathbf{P}$ is a permutation matrix and Δ is a diagonal matrix. One of the first uniqueness conditions for one factor matrix of a CPD was obtained by Kruskal in [26]. In this paper we will make use of the following result.

THEOREM 2.1. *Consider the PD of* $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ *in* (2.1). *If*

$$\begin{cases} k(\boldsymbol{C}) \geq 1, \\ \min(I, J) \geq R - r(\boldsymbol{C}) + 2, \\ C_{R-r(\boldsymbol{C})+2}(\boldsymbol{A}) \odot C_{R-r(\boldsymbol{C})+2}(\boldsymbol{B}) \ \text{ has full column rank}, \end{cases} \tag{2.4}$$

then the rank of $\mathcal{X}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique* [15].

Condition (2.4) is more relaxed than Kruskal's, and the proof of the theorem admits a constructive interpretation [17].

2.3. Overall uniqueness conditions for CPD. The rank-1 tensors in (2.1) can be arbitrarily permuted without changing the decomposition. The vectors within the same rank-1 tensor can also be arbitrarily scaled provided that the overall rank-1 term remains the same. We say that the CPD is unique when it is only subject to the mentioned indeterminacies. One of the first deep CPD uniqueness results was obtained by Kruskal [26]. For a recent comprehensive study of CPD uniqueness in the third-order case we refer the reader to [15, 16]. Below we state some uniqueness results for CPD that we will extend to the coupled CPD case. The results are summarized in Table 1.

TABLE 1
Full column rank (f.c.r.) requirements for different CPD uniqueness conditions. In the case where $\boldsymbol{C}$ *has f.c.r., we further distinguish between a sufficient (S) and a necessary and sufficient (N and S) condition.*

	Thm. 2.2	Thm. 2.3	Thm. 2.4	Thm. 2.5
Matrices required to have f.c.r.	None	$\mathbf{C}$	$\mathbf{C}$	$\mathbf{C}$ and $\mathbf{A}$
Condition	S	N and S	S	N and S

Together with related results in [16], the following is one of the most relaxed deterministic conditions for CPD uniqueness. It does not require any of the factor matrices to have full column rank.

THEOREM 2.2. *Consider the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ in* (2.1). *Let S denote a subset of $\{1,\ldots,R\}$ and let $S^c = \{1,\ldots,R\} \setminus S$ denote the complementary set. Stack the columns of $\boldsymbol{C}$ with index in S in $\boldsymbol{C}^{(S)} \in \mathbb{C}^{K\times card(S)}$ and stack the columns of $\boldsymbol{C}$ with index in S^c in $\boldsymbol{C}^{(S^c)} \in \mathbb{C}^{K\times(R-card(S))}$. Stack the columns of $\boldsymbol{A}$ (resp., $\boldsymbol{B}$) in the same order such that $\boldsymbol{A}^{(S)} \in \mathbb{C}^{I\times card(S)}$ (resp., $\boldsymbol{B}^{(S)} \in \mathbb{C}^{J\times card(S)}$) and $\boldsymbol{A}^{(S^c)} \in \mathbb{C}^{I\times(R-card(S))}$ (resp., $\boldsymbol{B}^{(S)} \in \mathbb{C}^{J\times(R-card(S))}$) are obtained. If*

$$\begin{cases} k\left(\boldsymbol{C}\right) \geq 2, \\ r\left(C_{R-r_C+2}\left(\boldsymbol{A}\right) \odot C_{R-r_C+2}\left(\boldsymbol{B}\right)\right) = C_R^{R-r_C+2}, \end{cases}$$

and if there exists a subset S of $\{1,\ldots,R\}$ with $0 \leq card(S) \leq r_{\boldsymbol{C}}$ such that [1, 2]

$$\begin{cases} \boldsymbol{C}^{(S)} \text{ has full column rank } \left(r_{\boldsymbol{C}^{(S)}} = card\left(S\right)\right), \\ \boldsymbol{B}^{(S^c)} \text{ has full column rank } \left(r_{\boldsymbol{B}^{(S^c)}} = R - card\left(S\right)\right), \\ r\left(\left[\boldsymbol{P}_{\boldsymbol{C}^{(S)}}\boldsymbol{C}^{(S^c)} \odot \boldsymbol{A}^{(S^c)}, \boldsymbol{P}_{\boldsymbol{C}^{(S)}}\boldsymbol{c}_r^{(S^c)} \otimes \boldsymbol{I}_I\right]\right) = I + R - card\left(S\right) - 1 \quad \forall r \in S^c, \end{cases}$$

then the rank of $\mathcal{X}$ is R and the CPD of $\mathcal{X}$ is unique [40].

If one factor matrix has full column rank, say $\mathbf{C}$, then the following condition is not only sufficient but also necessary.

THEOREM 2.3. *Consider the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ in* (2.1). *Define $\boldsymbol{E}(\boldsymbol{w}) = \sum_{r=1}^{R} w_r \boldsymbol{a}_r \boldsymbol{b}_r^T$. Assume that $\boldsymbol{C}$ has full column rank. The rank of $\mathcal{X}$ is R and the CPD of $\mathcal{X}$ is unique if and only if* [42, 25, 46, 14]

$$r\left(\boldsymbol{E}(\boldsymbol{w})\right) \geq 2 \quad \forall \boldsymbol{w} \in \left\{\boldsymbol{x} \in \mathbb{C}^R \,\middle|\, \omega(\boldsymbol{x}) \geq 2\right\}. \tag{2.5}$$

Generically,[3] *condition* (2.5) *is satisfied and $\boldsymbol{C}$ has full column rank if $R \leq K$ and $R \leq (I-1)(J-1)$* [42].

In practice, condition (2.5) may not be easy to check. Instead we may resort to the following more convenient result in the case where one factor matrix has full column rank.

THEOREM 2.4. *Consider the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ in* (2.1). *If*

$$\begin{cases} \boldsymbol{C} \text{ has full column rank,} \\ C_2\left(\boldsymbol{A}\right) \odot C_2\left(\boldsymbol{B}\right) \text{ has full column rank,} \end{cases} \tag{2.6}$$

then the rank of $\mathcal{X}$ is R and the CPD of $\mathcal{X}$ is unique [25, 11, 46, 15]. *Generically, condition* (2.6) *is satisfied if $R \leq K$ and $2R(R-1) \leq I(I-1)J(J-1)$* [11, 43].

In the case where two factor matrices, say $\mathbf{A}$ and $\mathbf{C}$, have full column rank, Theorems 2.3 and 2.4 simplify to the following.

THEOREM 2.5. *Consider the PD of $\mathcal{X}$ in* (2.1). *Assume that $\boldsymbol{A}$ and $\boldsymbol{C}$ have full column rank. The rank of $\mathcal{X}$ is R and the CPD of $\mathcal{X}$ is unique if and only if $k_{\boldsymbol{B}} \geq 2$ (see, e.g.,* [27]*). Generically, this is satisfied if $R \leq \min(I,K)$ and $2 \leq J$.*

[1]Note that the set S in Theorem 2.2 may be empty, i.e., $\text{card}(S) = 0$ such that $S = \emptyset$. This corresponds to the case where $\mathbf{P}_{\mathbf{C}^{(S)}} = \mathbf{I}_K$.

[2]The last condition states that $\mathbf{M}_r = [\mathbf{P}_{\mathbf{C}^{(S)}}\mathbf{C}^{(S^c)} \odot \mathbf{A}^{(S^c)}, \mathbf{P}_{\mathbf{C}^{(S)}}\mathbf{c}_r^{(S^c)} \otimes \mathbf{I}_I]$ has a one-dimensional kernel for every $r \in S^c$, which is minimal since $[\mathbf{n}_r^T, \mathbf{a}_r^{(S^c)T}]^T \in \ker(\mathbf{M}_r)$ for some $\mathbf{n}_r \in \mathbb{C}^{\text{card}(S^c)}$.

[3]A tensor decomposition property is called generic if it holds with probability one when the entries of the factor matrices are drawn from absolutely continuous probability density measures.

3. CPD with collinearity in a factor matrix. We consider PDs of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ that involve collinearities in the factor matrix $\mathbf{C}$ of the type

$$\mathcal{X} = \sum_{r=1}^{R}\sum_{l=1}^{L_r} \mathbf{a}_l^{(r)} \circ \mathbf{b}_l^{(r)} \circ \mathbf{c}^{(r)} = \sum_{r=1}^{R} \left(\mathbf{A}^{(r)}\mathbf{B}^{(r)T}\right) \circ \mathbf{c}^{(r)}\,, \tag{3.1}$$

where $\mathbf{A}^{(r)} = [\mathbf{a}_1^{(r)}, \ldots, \mathbf{a}_{L_r}^{(r)}] \in \mathbb{C}^{I\times L_r}$, $\mathbf{B}^{(r)} = [\mathbf{b}_1^{(r)}, \ldots, \mathbf{b}_{L_r}^{(r)}] \in \mathbb{C}^{J\times L_r}$. Similarly to $\mathbf{A}^{(r)}$ and $\mathbf{B}^{(r)}$, we may define $\mathbf{C}^{(r)} = \mathbf{1}_{L_r}^T \otimes \mathbf{c}^{(r)} \in \mathbb{C}^{K\times L_r}$, i.e., column vector $\mathbf{c}^{(r)}$ is repeated L_r times. Note that, if $L_r \geq 2$ for some $r \in \{1, \ldots, R\}$, then the PD of $\mathcal{X}$ cannot be unique (see, e.g., [44]). In cases like this, it is impossible to recover the individual columns of the factors $\mathbf{A}^{(r)}$ and $\mathbf{B}^{(r)}$. If the matrices $\mathbf{A}^{(r)}\mathbf{B}^{(r)T}$ have rank L_r, then the decomposition (3.1) is also known as the decomposition into multilinear rank-$(L_r, L_r, 1)$ terms [13].

3.1. Matrix representation. Let us stack the above matrices and vectors into the matrices

$$\mathbf{A} = \left[\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(R)}\right] \in \mathbb{C}^{I\times(\sum_{r=1}^{R} L_r)}, \quad \mathbf{B} = \left[\mathbf{B}^{(1)}, \ldots, \mathbf{B}^{(R)}\right] \in \mathbb{C}^{J\times(\sum_{r=1}^{R} L_r)},$$
$$\mathbf{C} = \left[\mathbf{C}^{(1)}, \ldots, \mathbf{C}^{(R)}\right] \in \mathbb{C}^{K\times(\sum_{r=1}^{R} L_r)}, \quad \mathbf{C}^{(\mathrm{red})} = \left[\mathbf{c}^{(1)}, \ldots, \mathbf{c}^{(R)}\right] \in \mathbb{C}^{K\times R},$$

where "red" stands for reduced. The PD or CPD of the tensor $\mathcal{X}$ in (3.1) with collinear columns in $\mathbf{C}$ admits the following matrix representation:

$$\mathbb{C}^{IJ\times K} \ni \mathbf{X}_{(1)} = \left[\mathbf{X}^{(1\cdot\cdot)T}, \ldots, \mathbf{X}^{(I\cdot\cdot)T}\right]^T$$
$$= (\mathbf{A} \odot \mathbf{B})\, \mathbf{C}^T \tag{3.2}$$
$$= \left[\mathrm{Vec}\left(\mathbf{B}^{(1)}\mathbf{A}^{(1)T}\right), \ldots, \mathrm{Vec}\left(\mathbf{B}^{(R)}\mathbf{A}^{(R)T}\right)\right] \mathbf{C}^{(\mathrm{red})T}. \tag{3.3}$$

3.2. Overall uniqueness conditions for decomposition into multilinear rank-$(L_r, L_r, 1)$ terms. Let $\{\{\widehat{\mathbf{A}}^{(n)}\}, \{\widehat{\mathbf{B}}^{(n)}\}, \widehat{\mathbf{C}}\}$ yield an alternative decomposition of $\mathcal{X}$ into multilinear rank-$(L_r, L_r, 1)$ terms. The multilinear rank-$(L_r, L_r, 1)$ tensors in (3.1) can be arbitrarily permuted, and the vectors within the same coupled multilinear rank-$(L_r, L_r, 1)$ tensor can be arbitrarily scaled provided the overall coupled multilinear rank-$(L_r, L_r, 1)$ term remains the same. We say that the decomposition into multilinear rank-$(L_r, L_r, 1)$ terms is unique when it is only subject to the mentioned indeterminacies.

The following uniqueness condition for decomposition of $\mathcal{X}$ into multilinear rank-$(L_r, L_r, 1)$ terms has been obtained in [13].

THEOREM 3.1. *Consider the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ in* (3.1)*. If*

$$k'(\boldsymbol{A}) = R \quad \text{and} \quad k'(\boldsymbol{B}) + k(\boldsymbol{C}) \geq R + 2\,, \tag{3.4}$$

then the minimal number of multilinear rank-$(L_r, L_r, 1)$ terms is R and the decomposition of $\mathcal{X}$ into multilinear rank-$(L_r, L_r, 1)$ terms is unique.

Other related uniqueness results can be found in [13]. For the case where $\mathbf{C}$ has full column rank, the following necessary and sufficient uniqueness condition for decomposition of $\mathcal{X}$ into multilinear rank-$(L_r, L_r, 1)$ terms has been obtained in [14].

THEOREM 3.2. *Consider the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K}$ in* (3.1)*. Define $\boldsymbol{E}(\boldsymbol{w}) = \sum_{r=1}^{R} w_r \boldsymbol{A}^{(r)}\boldsymbol{B}^{(r)T}$. Assume that $\boldsymbol{C}$ has full column rank. A necessary and sufficient*

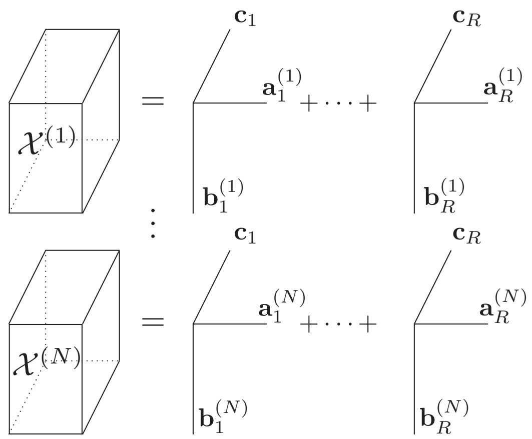

FIG. 1. *Coupled PD of the third-order tensors* $\mathcal{X}^{(1)}, \ldots, \mathcal{X}^{(N)}$.

condition for uniqueness of the decomposition of $\mathcal{X}$ *into multilinear rank-*$(L_r, L_r, 1)$ *terms is that*

$$r\left(\boldsymbol{E}(\boldsymbol{w})\right) > \max_{r|w_r\neq 0} L_r \quad \forall \boldsymbol{w} \in \left\{ \boldsymbol{x} \in \mathbb{C}^R \,\middle|\, \omega(\boldsymbol{x}) \geq 2 \right\}. \tag{3.5}$$

Generalizing CPD results in [8], generic uniqueness bounds for the BTD have been obtained in [50].

4. New results for coupled CPD.

In subsection 4.1 we introduce some definitions and notation associated with the coupled CPD. Subsection 4.2 presents necessary conditions for coupled CPD uniqueness. Subsection 4.3 presents uniqueness conditions for the common factor matrix. In subsection 4.4 we develop sufficient uniqueness conditions for the coupled CPD. Subsection 4.5 briefly explains that the results can be extended to tensors of order greater than three. Subsection 4.6 comments on the coupled matrix-tensor factorization problem.

4.1. Definitions and notation.

We say that a collection of tensors $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \ldots, N\}$, admits an R-term coupled polyadic decomposition if each tensor $\mathcal{X}^{(n)}$ can be written as

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \mathbf{a}_r^{(n)} \circ \mathbf{b}_r^{(n)} \circ \mathbf{c}_r, \quad n \in \{1, \ldots, N\}, \tag{4.1}$$

with factor matrices

$$\begin{aligned}
\mathbf{A}^{(n)} &= \left[\begin{array}{ccc} \mathbf{a}_1^{(n)}, & \ldots & , \mathbf{a}_R^{(n)} \end{array} \right] \in \mathbb{C}^{I_n \times R}, \quad n \in \{1, \ldots, N\}, \\
\mathbf{B}^{(n)} &= \left[\begin{array}{ccc} \mathbf{b}_1^{(n)}, & \ldots & , \mathbf{b}_R^{(n)} \end{array} \right] \in \mathbb{C}^{J_n \times R}, \quad n \in \{1, \ldots, N\}, \\
\mathbf{C} &= \left[\begin{array}{ccc} \mathbf{c}_1, & \ldots & , \mathbf{c}_R \end{array} \right] \in \mathbb{C}^{K \times R}.
\end{aligned}$$

The coupled PD of the third-order tensors $\{\mathcal{X}^{(n)}\}$ is visualized in Figure 1.

We define the coupled rank of $\{\mathcal{X}^{(n)}\}$ as the minimal number of coupled rank-1 tensors that yield $\{\mathcal{X}^{(n)}\}$ in a linear combination. Assume that the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R; then (4.1) will be called the coupled CPD of $\{\mathcal{X}^{(n)}\}$.

It is clear that the coupled rank-1 tensors in (4.1) can be arbitrarily permuted and that the vectors within the same coupled rank-1 tensor can be arbitrarily scaled provided the overall coupled rank-1 term remains the same. We say that the coupled CPD is unique when it is only subject to these trivial indeterminacies.

In this paper we will make use of the matrix representation of $\{\mathcal{X}^{(n)}\}$,

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{(1)} \\ \vdots \\ \mathbf{X}_{(1)}^{(N)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{A}^{(N)} \odot \mathbf{B}^{(N)} \end{bmatrix} \mathbf{C}^T = \mathbf{F}\mathbf{C}^T \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n)\times K}, \tag{4.2}$$

where

$$\mathbf{F} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{A}^{(N)} \odot \mathbf{B}^{(N)} \end{bmatrix} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n)\times R}. \tag{4.3}$$

4.2. Necessary conditions for coupled CPD uniqueness. Propositions 4.1 and 4.2 following generalize well-known necessary uniqueness conditions for CPD (see, e.g., [30, 44]) to the coupled CPD case.

PROPOSITION 4.1. *If the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *in* (4.1) *is unique, then* $k_{\mathbf{C}} \geq 2$.

Proof. Assume that $k(\mathbf{C}) = 1$, say $\mathbf{c}_1$ and $\mathbf{c}_2$ are collinear; then linear combinations of $\mathbf{c}_1$ and $\mathbf{c}_2$ will yield an alternative coupled CPD of $\{\mathcal{X}^{(n)}\}$ that is not related via trivial column scaling and permutation ambiguities. ∎

Note that in contrast to ordinary CPD, Proposition 4.1 does not prevent that $k_{\mathbf{A}^{(n)}} = 1$ and/or $k_{\mathbf{B}^{(n)}} = 1$ for some $n \in \{1, \ldots, N\}$. Indeed, the coupled CPD may be unique in such cases, as will be explained in subsection 4.4.

PROPOSITION 4.2. *If the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *in* (4.1) *is unique, then* $\mathbf{F}$ *has full column rank.*

Proof. The result follows directly from relation (4.2). Indeed, if $\mathbf{F}$ does not have full column rank, then for any $\mathbf{x} \in \ker(\mathbf{F})$ we obtain $\mathbf{X} = \mathbf{F}\mathbf{C}^T = \mathbf{F}(\mathbf{C}^T + \mathbf{x}\mathbf{y}^T)$, where $\mathbf{y} \in \mathbb{C}^K$. ∎

Again, in contrast to ordinary CPD, Proposition 4.2 does not prevent that for some $n \in \{1, \ldots, N\}$ the individual Khatri–Rao product matrices $\mathbf{A}^{(n)} \odot \mathbf{B}^{(n)}$ are rank deficient. This will be further discussed in subsection 4.4.

It is well known that the condition $k_{\mathbf{C}} \geq 2$ is generically satisfied if $K \geq 2$. Based on Lemma 4.3 we explain in Proposition 4.4 that $\mathbf{F}$ generically has full column rank if $\sum_{n=1}^{N} I_n J_n \geq R$. Hence, the necessary conditions stated in Propositions 4.1 and 4.2 are expected to be satisfied under mild conditions.

LEMMA 4.3. *Given an analytic function* $f : \mathbb{C}^n \to \mathbb{C}$, *if there exists an element* $\boldsymbol{x} \in \mathbb{C}^n$ *such that* $f(\boldsymbol{x}) \neq 0$, *then the set* $\{\, \boldsymbol{x} \,|\, f(\boldsymbol{x}) = 0 \,\}$ *is of Lebesgue measure zero (see, e.g.,* [24]*).*

PROPOSITION 4.4. *Consider* $\boldsymbol{F} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n)\times R}$ *given by* (4.3). *For generic matrices* $\{\boldsymbol{A}^{(n)}\}$ *and* $\{\boldsymbol{B}^{(n)}\}$, *the matrix* $\boldsymbol{F}$ *has rank* $\min(\sum_{n=1}^{N} I_n J_n, R)$.

Proof. Due to Lemma 4.3 we just need to find one example where the statement made in this lemma holds. We give an example in the supplementary material. ∎

Another necessary condition for CPD uniqueness is that none of the column vectors of $\mathbf{A} \odot \mathbf{B}$ (similarly for $\mathbf{A} \odot \mathbf{C}$ and $\mathbf{B} \odot \mathbf{C}$) in (2.2) can be written as linear combinations of its remaining column vectors [15, 14]. Proposition 4.5 extends the result to coupled CPD.

PROPOSITION 4.5. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \ldots, N\}$, *in* (4.1). *Define*

$$\boldsymbol{E}^{(n)}(\boldsymbol{w}) = \sum_{r=1}^{R} w_r \boldsymbol{a}_r^{(n)} \boldsymbol{b}_r^{(n)T} \quad \text{and} \quad \Omega = \left\{ \boldsymbol{x} \in \mathbb{C}^R \middle| \, \omega(\boldsymbol{x}) \geq 2 \right\}. \tag{4.4}$$

If the coupled CPD of $\{\mathcal{X}^{(n)}\}$ *in* (4.1) *is unique, then*

$$\forall \boldsymbol{w} \in \Omega \quad \exists n \in \{1, \ldots, N\} : r\left(\boldsymbol{E}^{(n)}(\boldsymbol{w})\right) \geq 2. \tag{4.5}$$

Proof. The necessity of $r(\mathbf{F}) = R$ has already been mentioned in Proposition 4.2. Assume now that there exists a vector $\mathbf{w}^{(r)} \in \mathbb{C}^R$ with $\omega(\mathbf{w}^{(r)}) \geq 2$ such that for some $r \in \{1, \ldots, R\}$ we have

$$\widetilde{\mathbf{a}}_r^{(n)} \otimes \widetilde{\mathbf{b}}_r^{(n)} = \sum_{s=1}^{R} w_s^{(r)} \left(\mathbf{a}_s^{(n)} \otimes \mathbf{b}_s^{(n)} \right) \quad \forall n \in \{1, \ldots, N\}. \tag{4.6}$$

Since $\mathbf{F}$ has full column rank, its column vectors are linearly independent, that is, $\sum_{s \neq r} w_s^{(r)} (\mathbf{a}_s^{(n)} \otimes \mathbf{b}_s^{(n)})$ cannot be proportional to $\mathbf{a}_r^{(n)} \otimes \mathbf{b}_r^{(n)}$ for all $n \in \{1, \ldots, N\}$, and consequently $\widetilde{\mathbf{a}}_r^{(n)} \otimes \widetilde{\mathbf{b}}_r^{(n)}$ is not proportional to $\mathbf{a}_r^{(n)} \otimes \mathbf{b}_r^{(n)}$ for all $n \in \{1, \ldots, N\}$. This means that factor matrices $\{\{\widetilde{\mathbf{A}}^{(n)}\}, \{\widetilde{\mathbf{B}}^{(n)}\}, \widetilde{\mathbf{C}}\}$ with property (4.6) yield an alternative coupled CPD of $\{\mathcal{X}^{(n)}\}$ which is not related to $\{\{\mathbf{A}^{(n)}\}, \{\mathbf{B}^{(n)}\}, \mathbf{C}\}$ via the intrinsic column scaling and permutation ambiguities. ∎

In contrast to ordinary CPD, Proposition 4.5 does not prevent that for some $n \in \{1, \ldots, N\}$ the individual columns of the matrices $\mathbf{A}^{(n)} \odot \mathbf{B}^{(n)}$ may be written as linear combinations of its remaining column vectors.

4.3. Uniqueness conditions for common factor matrix. This subsection presents conditions that guarantee the uniqueness of the common factor $\mathbf{C}$ of the coupled CPD of $\{\mathcal{X}^{(n)}\}$ in (4.1), even in cases where some of the remaining factor matrices $\{\mathbf{A}^{(n)}\}$ and $\{\mathbf{B}^{(n)}\}$ contain all-zero column vectors. This is in contrast with ordinary CPD where $k_{\mathbf{A}^{(n)}} \geq 2$ and $k_{\mathbf{B}^{(n)}} \geq 2$ are necessary conditions.

Proposition 4.6 is a variant of Theorem 2.1 for coupled CPD.

PROPOSITION 4.6. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \ldots, N\}$, *in* (4.1). *W.l.o.g. we assume that* $\min(I_1, J_1) \geq \min(I_2, J_2) \geq \cdots \geq \min(I_N, J_N)$. *Denote* $Q = \sum_{n=1}^{N} H[\min(I_n, J_n) - R + r_{\boldsymbol{C}} - 2]$, *where* $H[\cdot]$ *denotes the Heaviside step function. Define*

$$\boldsymbol{G}^{(m)} = \begin{bmatrix} C_m\left(\boldsymbol{A}^{(1)}\right) \odot C_m\left(\boldsymbol{B}^{(1)}\right) \\ \vdots \\ C_m\left(\boldsymbol{A}^{(Q)}\right) \odot C_m\left(\boldsymbol{B}^{(Q)}\right) \end{bmatrix} \in \mathbb{C}^{\left(\sum_{n=1}^{Q} C_{I_n}^m C_{J_n}^m\right) \times C_R^m}, \tag{4.7}$$

where $m = R - r_{\boldsymbol{C}} + 2$. *If*

$$\begin{cases} k(\boldsymbol{C}) \geq 1, \\ r(\boldsymbol{G}^{(m)}) = C_R^m, \end{cases} \tag{4.8}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique.*

Proof. The result is a technical variant of [15, Proposition 4.3]. It is provided in the supplementary material. ∎

In the case that the common factor matrix $\mathbf{C}$ has full column rank, Proposition 4.6 directly reduces to the following result. (Compare to Theorem 2.4.)

COROLLARY 4.7. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1,\ldots,N\}$, *in* (4.1). *Let* $\boldsymbol{G}^{(2)}$ *be defined as in* (4.7). *If*

$$\begin{cases} \boldsymbol{C} \text{ has full column rank,} \\ \boldsymbol{G}^{(2)} \text{ has full column rank,} \end{cases} \tag{4.9}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique.*

If additionally some of the factor matrices in the set $\{\mathbf{A}^{(n)}\}$ also have full column rank, then Corollary 4.7 further reduces to the following result. (Compare to Theorem 2.5.)

COROLLARY 4.8. *Consider the coupled PD of* $\{\mathcal{X}^{(n)}\}$ *in* (4.1). *Consider also a subset* S *of* $\{1,\ldots,N\}$ *with card*$(S) = Q$. *W.l.o.g., we assume that* $S = \{1,\ldots,Q\}$. *If for some* $Q \in \{1,\ldots,N\}$, *we have*

$$\begin{cases} r_{\boldsymbol{C}} = R\,, \\ r_{\boldsymbol{A}^{(n)}} = R \quad \forall n \in \{1,\ldots,Q\}, \\ \forall r \in \{1,\ldots,R\}, \quad \forall s \in \{1,\ldots,R\} \setminus r, \quad \exists\, n \in \{1,\ldots,Q\} :\, k\left(\left[\boldsymbol{b}_r^{(n)}, \boldsymbol{b}_s^{(n)}\right]\right) = 2\,, \end{cases} \tag{4.10}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique.*

Proof. Due to Corollary 4.7 we know that the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the factor matrix $\mathbf{C}$ is unique. We assume that for some $Q \in \{1,\ldots,N\}$ the matrix

$$\mathbf{G}^{(2)} = \left[\left(C_2\left(\mathbf{A}^{(1)}\right) \odot C_2\left(\mathbf{B}^{(1)}\right)\right)^T, \ldots, \left(C_2\left(\mathbf{A}^{(Q)}\right) \odot C_2\left(\mathbf{B}^{(Q)}\right)\right)^T\right]^T \tag{4.11}$$

has full column rank. As in ordinary CPD [47], we can premultiply each $\mathbf{A}^{(n)}$ by a nonsingular matrix without affecting the rank or the uniqueness of the coupled CPD of $\{\mathcal{X}^{(n)}\}$. Hence, w.l.o.g. we can set $\mathbf{A}^{(n)} = \left[\mathbf{I}_R, \mathbf{0}_{I_n-R,R}^T\right]^T$. Likewise, as in ordinary CPD [45], the premultiplication of $\mathbf{A}^{(n)}$ by a nonsingular matrix does not affect the rank of $\mathbf{G}^{(2)}$. The problem of determining the rank of $\mathbf{G}^{(2)}$ reduces to finding the rank of

$$\mathbf{H} = \begin{bmatrix} C_2\left(\begin{bmatrix} \mathbf{I}_R \\ \mathbf{0}_{I_1-R,R} \end{bmatrix}\right) \odot C_2\left(\mathbf{B}^{(2)}\right) \\ \vdots \\ C_2\left(\begin{bmatrix} \mathbf{I}_R \\ \mathbf{0}_{I_Q-R,R} \end{bmatrix}\right) \odot C_2\left(\mathbf{B}^{(Q)}\right) \end{bmatrix}.$$

After removing the all-zero row-vectors of $\mathbf{H}$ we need to find the rank of

$$\widetilde{\mathbf{H}} = \left[\left(\mathbf{I}_{\frac{R(R-1)}{2}} \odot C_2\left(\mathbf{B}^{(1)}\right)\right)^T, \ldots, \left(\mathbf{I}_{\frac{R(R-1)}{2}} \odot C_2\left(\mathbf{B}^{(Q)}\right)\right)^T\right]^T.$$

Note that $C_2(\mathbf{B}^{(n)}) = [\mathbf{d}^{(n)}_{1,2},\ldots,\mathbf{d}^{(n)}_{1,R},\mathbf{d}^{(n)}_{2,3},\ldots,\mathbf{d}^{(n)}_{2,R},\ldots,\mathbf{d}^{(n)}_{R-2,R-1},\mathbf{d}^{(n)}_{R-2,R},\mathbf{d}^{(n)}_{R-1,R}]$, where $\mathbf{d}^{(n)}_{p,q} = C_2([\mathbf{b}^{(n)}_p,\mathbf{b}^{(n)}_q]) \in \mathbb{C}^{J_n(J_n-1)/2}$. Note also that $\widetilde{\mathbf{H}}$ corresponds to a row-permuted version of a block-diagonal matrix holding the column vectors $\{\widetilde{\mathbf{d}}_{p,q}\}$ defined as $\widetilde{\mathbf{d}}_{p,q} = [\mathbf{d}^{(1)T}_{p,q},\ldots,\mathbf{d}^{(N)T}_{p,q}]^T \in \mathbb{C}^{(\sum_{n=1}^N J_n(J_n-1)/2)}$ on its block-diagonal. It is now clear that $\widetilde{\mathbf{H}}$ has full column rank if for every pair $(r,s)\in\{1,\ldots,R\}^2$ with $r\neq s$ there exists an $n\in\{1,\ldots,Q\}$ such that $\omega(\mathbf{d}^{(n)}_{r,s})\geq 1$. Equivalently, for every pair $(r,s)\in\{1,\ldots,R\}^2$ with $r\neq s$ there should exist an $n\in\{1,\ldots,Q\}$ such that $k([\mathbf{b}^{(n)}_r,\mathbf{b}^{(n)}_s]) = 2$. ∎

In the case where $\mathbf{C}$ has full column rank we have the following necessary and sufficient uniqueness condition for the common factor. (Compare to Theorem 2.3.)

Proposition 4.9. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n\in\{1,\ldots,N\}$, *in* (4.1). *Define* $\boldsymbol{E}^{(n)}(\boldsymbol{w})$ *and* Ω *as in* (4.4). *Assume that* $\boldsymbol{C}$ *has full column rank. The coupled rank of* $\{\mathcal{X}^{(n)}\}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique if and only if condition* (4.5) *is satisfied.*

Proof. The necessity of condition (4.5) has already been demonstrated in Proposition 4.5. Let us now prove the sufficiency of condition (4.5) in the case where $\mathbf{C}$ has full column rank. Note that (4.5) implies that $\mathbf{F}$ has full column rank. Indeed, if $\mathbf{F}$ is rank deficient, then there exists a vector $\mathbf{x}\in\mathbb{C}^R$ with property $\omega(\mathbf{x})\geq 2$ such that $\sum_{r=1}^R x_r\mathbf{f}_r = \mathbf{0}$. This will contradict (4.5). Let $\{\{\widetilde{\mathbf{A}}^{(n)}\},\{\widetilde{\mathbf{B}}^{(n)}\},\widetilde{\mathbf{C}}\}$ denote the factor matrices of an alternative coupled CPD of $\mathcal{X}^{(n)}$, $n\in\{1,\ldots,N\}$, where $\widetilde{\mathbf{A}}^{(n)}\in\mathbb{C}^{I_n\times\widetilde{R}}$, $\widetilde{\mathbf{B}}^{(n)}\in\mathbb{C}^{J_n\times\widetilde{R}}$, and $\widetilde{\mathbf{C}}\in\mathbb{C}^{K\times\widetilde{R}}$ with $\widetilde{R}\leq R$. Further, let $\widetilde{\mathbf{F}}\in\mathbb{C}^{(\sum_{n=1}^N I_nJ_n)\times\widetilde{R}}$ denote the alternative $\mathbf{F}$ constructed from $\{\widetilde{\mathbf{A}}^{(n)}\}$ and $\{\widetilde{\mathbf{B}}^{(n)}\}$ such that

$$\mathbf{X} = \mathbf{F}\mathbf{C}^T = \widetilde{\mathbf{F}}\widetilde{\mathbf{C}}^T. \tag{4.12}$$

Since $\mathbf{F}$ has full column rank and $\mathbf{C}$ has full column rank by assumption, we know from (4.12) that $R=\widetilde{R}$, that $\widetilde{\mathbf{C}}$ and $\widetilde{\mathbf{F}}$ have full column rank, and that $\text{range}(\mathbf{C}) = \text{range}\left(\widetilde{\mathbf{C}}\right)$.

We obtain from (4.12) the relation

$$\mathbf{F}\mathbf{H} = \widetilde{\mathbf{F}}, \tag{4.13}$$

where $\mathbf{H} = \mathbf{C}^T(\widetilde{\mathbf{C}}^T)^\dagger \in \mathbb{C}^{R\times R}$ is nonsingular. This may be expressed in a columnwise manner as

$$\widetilde{\mathbf{a}}^{(n)}_r \otimes \widetilde{\mathbf{b}}^{(n)}_r = \sum_{s=1}^R h_{sr}\left(\mathbf{a}^{(n)}_s\otimes\mathbf{b}^{(n)}_s\right), \quad r\in\{1,\ldots,R\},\ n\in\{1,\ldots,N\}. \tag{4.14}$$

Combination of (4.5) and (4.14) now yields that the nonsingular matrix $\mathbf{H}$ has exactly one nonzero entry in every column. This implies that $\mathbf{H}=\mathbf{P}\mathbf{D}$, where $\mathbf{P}\in\mathbb{C}^{R\times R}$ is a permutation matrix and $\mathbf{D}\in\mathbb{C}^{R\times R}$ is a nonsingular diagonal matrix. From (4.12) we obtain that $\widetilde{\mathbf{C}} = \mathbf{C}\mathbf{P}\mathbf{D}^{-1}$. We conclude that the common factor $\mathbf{C}$ is unique. ∎

While Proposition 4.9 provides a necessary and sufficient condition for the case where $\mathbf{C}$ has full column rank, Corollaries 4.7 and 4.8 may be easier to check in practice.

4.4. Sufficient uniqueness conditions for coupled CPD. We first present a condition in Proposition 4.10 and Theorem 4.11 for the case where at least one of the involved CPDs is unique. Next, in Theorem 4.12 we extend Theorem 2.2 to coupled CPD. It is a more relaxed condition than Proposition 4.10 and Theorem 4.11 since it requires only that the overall coupled CPD be unique, i.e., none of the individual CPDs are required to be unique. In Corollary 4.13 and Theorem 4.15 we extend Theorems 2.3 and 2.4 to the coupled CPD case in which the common factor matrix has full column rank. Finally, in Corollary 4.14 we extend Theorem 2.5 to coupled CPD. Table 2 summarizes the organization and structure.

TABLE 2

Relations between uniqueness conditions for the single CPD and coupled CPD for different rank properties of the common factor matrix $\mathbf{C}$*. The coupled CPD, case* 1*, corresponds to the cases where one of the individual CPDs is unique, while the coupled CPD, case* 2*, corresponds to the cases where none of the individual CPDs are required to be unique. In the case where* $\mathbf{C}$ *has full column rank, we further distinguish between sufficient (S) conditions and necessary and sufficient (N and S) conditions.*

	(S) $k(\mathbf{C}) \geq 2$	(N and S) $r(\mathbf{C}) = R$	(S) $r(\mathbf{C}) = R$	(S) $r(\mathbf{C}) = R$
Single CPD	Thm. 2.2	Thm. 2.3	Thm. 2.4	Thm. 2.5
Coupled CPD, case 1	Thm. 4.11	Prop. 4.10	Prop. 4.10	Cor. 4.14
Coupled CPD, case 2	Thm. 4.12	Thm. 4.15	Cor. 4.13	Cor. 4.14

PROPOSITION 4.10. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$*,* $n \in \{1, \ldots, N\}$*, in* (4.1)*. If* [4]

$$\exists\, n \in \{1, \ldots, N\} : \text{the rank of } \mathcal{X}^{(n)} \text{ is } R \text{ and the CPD of } \mathcal{X}^{(n)} \text{ is unique},$$

and if $\mathbf{C}$ *has full column rank, then the coupled rank of* $\{\mathcal{X}^{(n)}\}$ *is* R *and the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. If there exists an integer $n \in \{1, \ldots, N\}$ such that the rank of $\mathcal{X}^{(n)}$ is R and the CPD of $\mathcal{X}^{(n)}$ is unique, then obviously the common factor matrix $\mathbf{C}$ is unique. Compute $\mathbf{Y}^{(n)} = \mathbf{X}^{(n)}(\mathbf{C}^T)^{\dagger}$; then the remaining factor matrices are obtained by recognizing that the columns of $\mathbf{Y}^{(n)}$ are vectorized rank-1 matrices:

$$\min_{\mathbf{a}_r^{(n)}, \mathbf{b}_r^{(n)}} \left\| \mathbf{y}_r^{(n)} - \mathbf{a}_r^{(n)} \otimes \mathbf{b}_r^{(n)} \right\|_F^2, \quad r \in \{1, \ldots, R\}, n \in \{1, \ldots, N\}.$$

Hence, the coupled CPD of $\{\mathcal{X}^{(n)}\}$ is unique and the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R. ∎

Proposition 4.10 tells us that a coupled CPD in which the common factor matrix has full column rank is unique if one of the involved CPDs is unique. This simple observation already demonstrates that a coupled CPD can be unique even if some of the involved CPDs are individually nonunique. For instance, Proposition 4.10 does not prevent in the coupled CPD that some of the Khatri–Rao products are rank deficient, which is not allowed in the ordinary CPD. As an example, we consider

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{(1)} \\ \mathbf{X}_{(1)}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \odot \mathbf{B}^{(2)} \end{bmatrix} \mathbf{C}^T,$$

[4] As an example, Theorem 2.4 states that if $r(C_2(\mathbf{A}^{(n)}) \odot C_2(\mathbf{B}^{(n)})) = \frac{R(R-1)}{2}$, then the rank of $\mathcal{X}^{(n)}$ is R and the CPD of $\mathcal{X}^{(n)}$ is unique. Alternatively, Theorem 2.3 states that if $r(\mathbf{E}^{(n)}(\mathbf{w})) = \sum_{r=1}^{R} w_r \mathbf{a}_r^{(n)} \mathbf{b}_r^{(n)T} \geq 2$ for all $\mathbf{w} \in \Omega = \{\mathbf{x} \in \mathbb{C}^R | \, \omega(\mathbf{x}) \geq 2\}$, then the rank of $\mathcal{X}^{(n)}$ is R and the CPD of $\mathcal{X}^{(n)}$ is unique.

where $\mathbf{A}^{(1)} \in \mathbb{C}^{3\times 4}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{3\times 4}$, $\mathbf{B}^{(1)} \in \mathbb{C}^{3\times 4}$, $\mathbf{B}^{(2)} \in \mathbb{C}^{3\times 4}$, and $\mathbf{C} \in \mathbb{C}^{4\times 4}$. Further, let $\mathbf{a}_1^{(2)} \otimes \mathbf{b}_1^{(2)} = \mathbf{a}_2^{(2)} \otimes \mathbf{b}_2^{(2)}$; then generically $r(\mathbf{A}^{(2)} \odot \mathbf{B}^{(2)}) = 3$, and consequently the CPD of $\mathcal{X}^{(2)}$ is not unique [30]. However, Proposition 4.10 tells us that the coupled CPD of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ is generically unique.

Theorem 4.11 considers the more general case where $\mathbf{C}$ does not necessarily have full column rank.

THEOREM 4.11. *Consider the coupled PD of $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \ldots, N\}$, in* (4.1). *Let S_n denote a subset of $\{1, \ldots, R\}$, and let $S_n^c = \{1, \ldots, R\} \setminus S_n$ denote the complementary set. Stack the columns of $\boldsymbol{C}$ with index in S_n in $\boldsymbol{C}^{(S_n)} \in \mathbb{C}^{K \times card(S_n)}$ and stack the columns of $\boldsymbol{C}$ with index in S_n^c in $\boldsymbol{C}^{(S_n^c)} \in \mathbb{C}^{K \times (R - card(S_n))}$. Stack the columns of $\boldsymbol{A}^{(n)}$ (resp., $\boldsymbol{B}^{(n)}$) in the same order such that $\boldsymbol{A}^{(n,S_n)} \in \mathbb{C}^{I_n \times card(S_n)}$ (resp., $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n \times card(S_n)}$) and $\boldsymbol{A}^{(n,S_n^c)} \in \mathbb{C}^{I_n \times (R - card(S_n))}$ (resp., $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n \times (R - card(S_n))}$) are obtained. If* [5]

$$\exists\, n \in \{1, \ldots, N\} : \textit{the rank of } \mathcal{X}^{(n)} \textit{ is } R \textit{ and CPD of } \mathcal{X}^{(n)} \textit{ is unique,} \tag{4.15a}$$

and for all $n \in \{1, \ldots, N\}$ there exist an index set S_n with $0 \le card(S_n) \le r_{\boldsymbol{C}}$ such that $\boldsymbol{C}^{(S_n)}$ has full column rank and

$$\begin{cases} \boldsymbol{B}^{(n,S_n^c)} \textit{ has full column rank,} \\ r\left(\left[\boldsymbol{P}_{\boldsymbol{C}^{(S_n)}} \boldsymbol{C}^{(S_n^c)} \odot \boldsymbol{A}^{(n,S_n^c)}, \boldsymbol{P}_{\boldsymbol{C}^{(S_n)}} \boldsymbol{c}_r^{(S_n^c)} \otimes \boldsymbol{I}_{I_n}\right]\right) = \alpha_n \quad \forall r \in S_n^c, \end{cases} \tag{4.15b}$$

where $\alpha_n = I_n + R - card(S_n) - 1$, or

$$\begin{cases} \boldsymbol{A}^{(n,S_n^c)} \textit{ has full column rank,} \\ r\left(\left[\boldsymbol{P}_{\boldsymbol{C}^{(S_n)}} \boldsymbol{C}^{(S_n^c)} \odot \boldsymbol{B}^{(n,S_n^c)}, \boldsymbol{P}_{\boldsymbol{C}^{(S_n)}} \boldsymbol{c}_r^{(S_n^c)} \otimes \boldsymbol{I}_{J_n}\right]\right) = \beta_n \quad \forall r \in S_n^c, \end{cases} \tag{4.15c}$$

where $\beta_n = J_n + R - card(S_n) - 1$, then the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the coupled CPD of $\{\mathcal{X}^{(n)}\}$ is unique. Generically, condition (4.15b) *or* (4.15c) *is satisfied if for all $n \in \{1, \ldots, N\}$ we have*

$$\begin{cases} R \le \min\left(V_n + \min(K, R), \frac{V_n(W_n - 1) + W_n(K-1) + 1}{W_n}\right) & \textit{when} \quad V_n < R, \\ R \le (K-1)W_n + 1 & \textit{when} \quad V_n \ge R, \end{cases} \tag{4.16}$$

where $V_n = \max(I_n, J_n)$ and $W_n = \min(I_n, J_n)$.

Proof. We assume that the rank of $\mathcal{X}^{(p)}$ is R and the CPD of $\mathcal{X}^{(p)}$ is unique for some $p \in \{1, \ldots, N\}$. The overall uniqueness of the CPD of $\mathcal{X}^{(p)}$ implies that the common factor matrix $\mathbf{C}$ is unique with property $k(\mathbf{C}) \ge 2$. We now consider the individual CPDs of the tensors $\{\mathcal{X}^{(n)}\}$ with matrix representations

$$\mathbf{X}_{(1)}^{(n)} = \left(\mathbf{A}^{(n)} \odot \mathbf{B}^{(n)}\right) \mathbf{C}^T, \quad n \in \{1, \ldots, N\},$$

as CPDs with a known factor matrix. We know from [40, Theorem 4.8] that the CPD of the tensor $\mathcal{X}^{(n)}$ with known factor $\mathbf{C}$ is unique if condition (4.15b) or (4.15c) is

[5]As an example, if the conditions stated in Theorem 2.2 are satisfied for some $p \in \{1, \ldots, N\}$ in which the roles of $\mathbf{A}^{(p)}$, $\mathbf{B}^{(p)}$, and $\mathbf{C}$ may be interchanged, then the rank of $\mathcal{X}^{(p)}$ is R and the CPD of $\mathcal{X}^{(p)}$ is unique.

satisfied. We also know from [40, Theorem 4.8] that the CPD of the tensor $\mathcal{X}^{(n)}$ with known factor $\mathbf{C}$ is generically unique if conditions (4.16) are satisfied. We conclude that the coupled CPD of $\{\mathcal{X}^{(n)}\}$ linked via the matrix $\mathbf{C}$ is unique and the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R. ∎

Theorem 4.11 tells us that a coupled CPD is unique under more relaxed conditions than the individually involved ordinary CPDs even in cases where $\mathbf{C}$ does not have full column rank. This also means that some of the involved CPDs are allowed to be individually nonunique. As an example, we consider

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}^{(1)}_{(1)} \\ \mathbf{X}^{(2)}_{(1)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \odot \mathbf{B}^{(2)} \end{bmatrix} \mathbf{C}^T,$$

where $\mathbf{A}^{(1)} \in \mathbb{C}^{4\times 5}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{4\times 5}$, $\mathbf{B}^{(1)} \in \mathbb{C}^{4\times 5}$, $\mathbf{B}^{(2)} \in \mathbb{C}^{4\times 5}$, and $\mathbf{C} \in \mathbb{C}^{4\times 5}$. Furthermore, let $\mathbf{b}_1^{(2)} = \mathbf{b}_2^{(2)}$; then generically $k(\mathbf{B}^{(2)}) = 1$ and consequently the CPD of $\mathcal{X}^{(2)}$ is not unique (see, e.g., [44]). Since $\mathbf{C}$ does not have full column rank, Proposition 4.10 does not apply. However, Theorem 4.11 tells us that the coupled CPD of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ is generically unique. Note that this result is not obtained by inverting $\mathbf{C}$ as in the proof of Proposition 4.10.

THEOREM 4.12. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1,\dots,N\}$ *in* (4.1). *Let* S_n *denote a subset of* $\{1,\dots,R\}$, *and let* $S_n^c = \{1,\dots,R\}\setminus S_n$ *denote the complementary set. Stack the columns of* $\boldsymbol{C}$ *with index in* S_n *in* $\boldsymbol{C}^{(S_n)} \in \mathbb{C}^{K\times card(S_n)}$ *and stack the columns of* $\boldsymbol{C}$ *with index in* S_n^c *in* $\boldsymbol{C}^{(S_n^c)} \in \mathbb{C}^{K\times(R-card(S_n))}$. *Stack the columns of* $\boldsymbol{A}^{(n)}$ *(resp.,* $\boldsymbol{B}^{(n)}$*) in the same order such that* $\boldsymbol{A}^{(n,S_n)} \in \mathbb{C}^{I_n\times card(S_n)}$ *(resp.,* $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n\times card(S_n)}$*) and* $\boldsymbol{A}^{(n,S_n^c)} \in \mathbb{C}^{I_n\times(R-card(S_n))}$ *(resp.,* $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n\times(R-card(S_n))}$*) are obtained.*

If $\boldsymbol{C}$ *is unique*[6] *with property* $k(\boldsymbol{C}) \geq 2$, *and if for all* $n \in \{1,\dots,N\}$ *there exists an index set* S_n *with* $0 \leq card(S_n) \leq r_{\boldsymbol{C}}$ *such that* $\boldsymbol{C}^{(S_n)}$ *has full column rank and condition* (4.15b) *or* (4.15c) *is satisfied, then the coupled rank of* $\{\mathcal{X}^{(n)}\}$ *is* R *and the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. The necessity of $k(\mathbf{C}) \geq 2$ has already been mentioned in Proposition 4.1. Assuming that the common factor matrix $\mathbf{C}$ is unique with $k(\mathbf{C}) \geq 2$, we can consider the individual CPDs of the tensors $\{\mathcal{X}^{(n)}\}$ as CPDs with a known factor matrix $\mathbf{C}$. We know from [40, Theorem 4.8] that the CPD of the tensor $\mathcal{X}^{(n)}$ with known factor $\mathbf{C}$ is unique if condition (4.15b) or (4.15c) is satisfied. We can now conclude that the coupled CPD of $\{\mathcal{X}^{(n)}\}$ linked via the matrix $\mathbf{C}$ is unique and the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R. ∎

Note that Theorem 4.12, unlike Proposition 4.10 and Theorem 4.11, does not assume that the CPD of one of the individual tensors $\mathcal{X}^{(n)}$ is unique. As an example, we consider

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}^{(1)}_{(1)} \\ \mathbf{X}^{(2)}_{(1)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \odot \mathbf{B}^{(2)} \end{bmatrix} \mathbf{C}^T,$$

where $\mathbf{A}^{(1)} \in \mathbb{C}^{4\times 5}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{4\times 5}$, $\mathbf{B}^{(1)} \in \mathbb{C}^{4\times 5}$, $\mathbf{B}^{(2)} \in \mathbb{C}^{4\times 5}$, and $\mathbf{C} \in \mathbb{C}^{4\times 5}$. Further, let $\mathbf{b}_1^{(1)} = \mathbf{b}_2^{(1)}$ and $\mathbf{b}_3^{(2)} = \mathbf{b}_4^{(2)}$; then generically $k(\mathbf{B}^{(1)}) = 1$ and $k(\mathbf{B}^{(2)}) = 1$. Consequently the individual CPDs of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ are not unique, which means

[6] As an example, if the conditions (4.8) stated in Proposition 4.6 are satisfied, then the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the common factor matrix $\mathbf{C}$ is unique.

that neither Proposition 4.10 nor Theorem 4.11 can be used to establish coupled CPD uniqueness. However, Proposition 4.6, together with Theorem 4.12, tells us that the coupled CPD of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ is generically unique.

The above example explains that in some cases it is better to first establish uniqueness of the common factor matrix $\mathbf{C}$ via, for instance, Proposition 4.6, and thereafter establish coupled CPD uniqueness of $\{\mathcal{X}^{(n)}\}$ by treating the individual CPDs of $\{\mathcal{X}^{(n)}\}$ as CPDs with a known factor $\mathbf{C}$. However, in other cases it is better to first establish CPD uniqueness of one of the individual tensors, say $\mathcal{X}^{(p)}$, via, for instance, Theorem 2.2, and thereafter establish coupled CPD uniqueness of $\{\mathcal{X}^{(n)}\}$ by treating the individual CPDs of $\{\mathcal{X}^{(n)}\}$ as CPDs with a known factor $\mathbf{C}$. As an example, we consider

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}^{(1)}_{(1)} \\ \mathbf{X}^{(2)}_{(1)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \odot \mathbf{B}^{(2)} \end{bmatrix} \mathbf{C}^T,$$

where $\mathbf{A}^{(1)} \in \mathbb{C}^{4\times 6}$, $\mathbf{A}^{(2)} \in \mathbb{C}^{4\times 6}$, $\mathbf{B}^{(1)} \in \mathbb{C}^{6\times 6}$, $\mathbf{B}^{(2)} \in \mathbb{C}^{5\times 6}$, and $\mathbf{C} \in \mathbb{C}^{3\times 6}$. For this problem Proposition 4.6 cannot be used since the matrix $\mathbf{G}^{(5)}$ is not defined. On the other hand, Theorem 2.2, together with Theorem 4.11, tells us that the coupled CPD of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ is generically unique.

Let us now assume that the common factor matrix $\mathbf{C}$ has full column rank. In that case, Theorem 4.12 reduces to Corollary 4.13, which in turn can be understood as an extension of Theorem 2.4 to coupled CPD. Corollary 4.13 can also be seen as a generalization of Proposition 4.10 to the case where none of the involved CPDs are required to be unique.

COROLLARY 4.13. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1,\dots,N\}$, *in* (4.1). *Let* $\boldsymbol{G}^{(2)}$ *be defined as in* (4.7). *If*

$$\begin{cases} \boldsymbol{C} \text{ has full column rank,} \\ \boldsymbol{G}^{(2)} \text{ has full column rank,} \end{cases} \tag{4.17}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. Due to Corollary 4.7 we know that the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the common factor matrix $\mathbf{C}$ is unique when condition (4.17) is satisfied. Assuming that $\mathbf{C}$ has full column rank, the remaining factors follow from rank-1 approximations as explained in the proof of Proposition 4.10. ∎

If additionally some of the factor matrices in the set $\{\mathbf{A}^{(n)}\}$ also have full column rank, then we may use the Corollary 4.14 following, which can be understood as an extension of Theorem 2.5 to coupled CPD.

COROLLARY 4.14. *Consider the coupled PD of* $\{\mathcal{X}^{(n)}\}$ *in* (4.1). *Consider also a subset* S *of* $\{1,\dots,N\}$ *with* $card(S) = Q$. *W.l.o.g., we assume that* $S = \{1,\dots,Q\}$. *If for some* $Q \in \{1,\dots,N\}$ *we have*

$$\begin{cases} r_{\boldsymbol{C}} = R\,, \\ r_{\boldsymbol{A}^{(n)}} = R \quad \forall n \in \{1,\dots,Q\}, \\ \forall r \in \{1,\dots,R\}, \quad \forall s \in \{1,\dots,R\}\setminus r, \quad \exists\, n \in \{1,\dots,Q\} :\ k\left(\left[\boldsymbol{b}_r^{(n)}, \boldsymbol{b}_s^{(n)}\right]\right) = 2\,, \end{cases} \tag{4.18}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. Due to Corollary 4.8 we know that the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the common factor $\mathbf{C}$ is unique. Since $\mathbf{C}$ is unique and has full column rank, the remaining factors follow from rank-1 approximations as explained in the proof of Proposition 4.10. ∎

Comparison of Theorem 2.5 with condition (4.19) shows that the coupling has relaxed the uniqueness condition.

Finally, we generalize the necessary and sufficient uniqueness condition (2.5) stated in Theorem 2.3 to the coupled CPD problem.

THEOREM 4.15. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \ldots, N\}$, *in* (4.1). *Assume that* $\boldsymbol{C}$ *has full column rank. The coupled rank of* $\{\mathcal{X}^{(n)}\}$ *is* R *and the coupled CPD of* $\{\mathcal{X}^{(n)}\}$ *is unique if and only if*

$$\forall \boldsymbol{w} \in \Omega\,, \quad \exists\, n \in \{1, \ldots, N\}\, :\, r\left(\boldsymbol{E}^{(n)}(\boldsymbol{w})\right) \geq 2\,, \tag{4.19}$$

where $\boldsymbol{E}^{(n)}$ *and* Ω *are defined as in* (4.4).

Proof. Due to Proposition 4.9 we know that the coupled rank of $\{\mathcal{X}^{(n)}\}$ is R and the common factor $\mathbf{C}$ is unique if and only if the condition (4.19) is satisfied. Since the common factor $\mathbf{C}$ is unique and has full column rank, the remaining factors follow from rank-1 approximations as explained in the proof of Proposition 4.10. ∎

As in the case of ordinary CPD, the conditions in Theorem 4.15 may be harder to check than those in Corollary 4.13 or Corollary 4.14.

4.5. Extension to tensors of arbitrary order. The uniqueness properties of the CPD of higher-order tensors are not just a straightforward generalization of those for third-order tensors. As a matter of fact, they are conceptually quite different. We note that the idea of simultaneously considering different matrix representations of the CPD of a single higher-order tensor for the case where one factor matrix has full column rank was first considered in [46]. As our contribution, first we generalize the idea to cases where none of the involved factor matrices are required to have full column rank. In fact, based on the connection between coupled CPD and higher-order tensors, we even demonstrate that the (coupled) CPD of a higher-order tensor(s) can be unique despite collinearities in all factor matrices. Second, we extend the coupled CPD framework in subsections 4.3 and 4.4 to tensors of arbitrary order. More specifically, we demonstrate that by taking into account both the coupled and higher-order structures, improved uniqueness conditions are obtained.

We consider coupled PDs of $\mathcal{X}^{(n)} \in \mathbb{C}^{I_{1,n} \times \cdots \times I_{M_n,n} \times K}$, $n \in \{1, \ldots, N\}$, of the form

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \mathbf{a}_r^{(1,n)} \circ \cdots \circ \mathbf{a}_r^{(M_n,n)} \circ \mathbf{c}_r, \quad n \in \{1, \ldots, N\}. \tag{4.20}$$

The factor matrices are

$$\mathbf{A}^{(m,n)} = \left[\ \mathbf{a}_1^{(m,n)}, \quad \ldots \quad, \mathbf{a}_R^{(m,n)}\ \right] \in \mathbb{C}^{I_{m,n} \times R}, \quad m \in \{1, \ldots, M_n\},\ n \in \{1, \ldots, N\},$$
$$\mathbf{C} = \left[\ \mathbf{c}_1, \quad \ldots \quad, \mathbf{c}_R\ \right] \in \mathbb{C}^{K \times R}.$$

The coupled PD of tensors $\{\mathcal{X}^{(n)}\}$ of arbitrary order is visualized in Figure 2.

Note that the tensors $\mathcal{X}^{(n)}$ may have different orders M_n and different sizes $I_{m,n}$. As a special case, we have the case of a single tensor ($N = 1$) of order $M \geq 4$. Our key idea is that, if one or more tensors have order $M_n \geq 4$, then we may combine

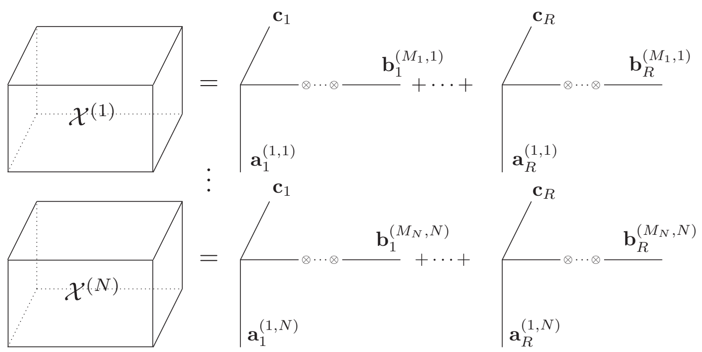

FIG. 2. *Coupled PD of tensors* $\mathcal{X}^{(1)},\ldots,\mathcal{X}^{(N)}$ *in which* $\mathbf{b}_r^{(M_n,n)} = \mathbf{a}_r^{(2,n)} \otimes \cdots \otimes \mathbf{a}_r^{(M_n,n)}$.

the coupled third-order CPD results discussed in subsections 4.2–4.4 with results for higher-order tensors [46]. More precisely, uniqueness results may be obtained by reducing the associated higher-order PDs to coupled third-order PDs. Namely, we simultaneously consider several matrix representations of the form

$$\mathbf{X}^{(w,n)} = \left(\bigodot_{p\in\Gamma_{w,n}} \mathbf{A}^{(p,n)} \odot \bigodot_{q\in\Upsilon_{w,n}} \mathbf{A}^{(q,n)} \right) \mathbf{C}^T = \left(\mathbf{A}^{[w,n]} \odot \mathbf{B}^{[w,n]}\right)\mathbf{C}^T, \tag{4.21}$$

where $\mathbf{A}^{[w,n]} = \bigodot_{p\in\Gamma_{w,n}} \mathbf{A}^{(p,n)} \in \mathbb{C}^{\hat{I}_{w,n}\times R}$ with $\hat{I}_{w,n} = \prod_{p\in\Gamma_{w,n}} I_{p,n}$, $\mathbf{B}^{[w,n]} = \bigodot_{q\in\Upsilon_{w,n}} \mathbf{A}^{(q,n)} \in \mathbb{C}^{\hat{J}_{w,n}\times R}$ with $\hat{J}_{w,n} = \prod_{q\in\Upsilon_{w,n}} I_{q,n}$, and the sets $\Gamma_{w,n}$ and $\Upsilon_{w,n}$ have properties $\Gamma_{w,n} \bigcup \Upsilon_{w,n} = \{1,2,\ldots,M_n\}$ and $\Gamma_{w,n} \bigcap \Upsilon_{w,n} = \emptyset$. Let us assume that there are W_n sets $\{\Gamma_{w,n}\}$ and $\{\Upsilon_{w,n}\}$ for each $n \in \{1,\ldots,N\}$. We collect the matrices $\{\mathbf{X}^{(w,n)}\}$ into the matrix

$$\mathbf{X} = \left[\mathbf{X}^{(1)T}, \mathbf{X}^{(2)T}, \ldots, \mathbf{X}^{(N)T}\right]^T, \quad \mathbf{X}^{(n)} = \left[\mathbf{X}^{(1,n)T}, \mathbf{X}^{(2,n)T}, \ldots, \mathbf{X}^{(W_n,n)T}\right]^T,$$

such that

$$\mathbf{X} = \mathbf{F}\mathbf{C}^T, \quad \mathbf{F} = \begin{bmatrix} \mathbf{F}^{(1)} \\ \mathbf{F}^{(2)} \\ \vdots \\ \mathbf{F}^{(N)} \end{bmatrix}, \quad \mathbf{F}^{(n)} = \begin{bmatrix} \mathbf{A}^{[1,n]} \odot \mathbf{B}^{[1,n]} \\ \mathbf{A}^{[2,n]} \odot \mathbf{B}^{[2,n]} \\ \vdots \\ \mathbf{A}^{[W_n,n]} \odot \mathbf{B}^{[W_n,n]} \end{bmatrix}. \tag{4.22}$$

We now ignore the Khatri–Rao structure of $\mathbf{A}^{[w,n]}$ and $\mathbf{B}^{[w,n]}$ and treat (4.22) as a matrix representation of a set of coupled third-order CPDs.

For establishing uniqueness, we may resort to the different results in subsection 4.4. For the results that make use of $\mathbf{G}^{(R-r_{\mathbf{C}}+2)}$, we may work with the following generalization. We limit ourselves to the $\widetilde{W}_n$ sets $\{\Gamma_{w,n}\}$ and $\{\Upsilon_{w,n}\}$ for each $n \in \{1,\ldots,N\}$ in which $\min(\prod_{p\in\Gamma_{w,n}} I_{p,n}, \prod_{q\in\Upsilon_{w,n}} I_{q,n}) \geq R - r_{\mathbf{C}} + 2$. Define

$\mathbf{G}^{(R-r_{\mathbf{C}}+2,\widetilde{W}_n)} \in \mathbb{C}^{(\sum_{w=1}^{\widetilde{W}_n} C^{R-r_{\mathbf{C}}+2}_{\prod_{p\in\Gamma_{w,n}} I_{p,n}} C^{R-r_{\mathbf{C}}+2}_{\prod_{q\in\Upsilon_{w,n}} I_{q,n}})\times C^{R-r_{\mathbf{C}}+2}_R}$ as follows:

$$\mathbf{G}^{(R-r_{\mathbf{C}}+2,\widetilde{W}_n)} = \begin{bmatrix} C_{R-r_{\mathbf{C}}+2}\left(\mathbf{A}^{[1,n]}\right) \odot C_{R-r_{\mathbf{C}}+2}\left(\mathbf{B}^{[1,n]}\right) \\ \vdots \\ C_{R-r_{\mathbf{C}}+2}\left(\mathbf{A}^{[\widetilde{W}_n,n]}\right) \odot C_{R-r_{\mathbf{C}}+2}\left(\mathbf{B}^{[\widetilde{W}_n,n]}\right) \end{bmatrix}, \quad n \in \{1,\ldots,N\}.$$

The following matrix generalizes $\mathbf{G}^{(R-r_{\mathbf{C}}+2)}$ in (4.7):

$$\mathbf{G}^{(m)} = \begin{bmatrix} \mathbf{G}^{(m,\widetilde{W}_1)} \\ \vdots \\ \mathbf{G}^{(m,\widetilde{W}_N)} \end{bmatrix} \in \mathbb{C}^{\sum_{n=1}^{N}(\sum_{w=1}^{\widetilde{W}_n} C^m_{\prod_{p\in\Gamma_{w,n}} I_{p,n}} C^m_{\prod_{q\in\Upsilon_{w,n}} I_{q,n}})\times C^m_R}, \tag{4.23}$$

where $m = R - r_{\mathbf{C}} + 2$. In the extensions of Theorems 4.11 and 4.12, it suffices to check condition (4.15b) or (4.15c) for one of the $\widetilde{W}_n$ matrix representations.

As an example, consider the fourth-order tensors $\mathcal{X}^{(n)} \in \mathbb{C}^{I\times J\times K\times L}$, $n \in \{1, 2\}$, with PDs,

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \mathbf{a}_r^{(n)} \circ \mathbf{b}_r^{(n)} \circ \mathbf{c}_r^{(n)} \circ \mathbf{d}_r, \quad n \in \{1, 2\}, \tag{4.24}$$

in which $I = 4$, $J = 5$, $K = 4$, $L = 3$, $R = 4$, $\mathbf{a}_2^{(1)} = \mathbf{a}_3^{(1)}$, $\mathbf{b}_1^{(1)} = \mathbf{b}_3^{(1)}$, $\mathbf{c}_1^{(1)} = \mathbf{c}_2^{(1)}$, $\mathbf{c}_3^{(1)} = \mathbf{c}_4^{(1)}$, $\mathbf{a}_1^{(2)} = \mathbf{a}_4^{(2)}$, $\mathbf{b}_1^{(2)} = \mathbf{b}_2^{(2)} = \mathbf{b}_3^{(2)}$, and $\mathbf{c}_3^{(2)} = \mathbf{c}_4^{(2)}$. Note that generically $k_{\mathbf{A}^{(1)}} = k_{\mathbf{B}^{(1)}} = k_{\mathbf{C}^{(1)}} = k_{\mathbf{A}^{(2)}} = k_{\mathbf{B}^{(2)}} = k_{\mathbf{C}^{(2)}} = 1$ and $k_{\mathbf{D}} \geq 2$. The existing CPD uniqueness conditions for higher-order tensors stated in [33, 46, 5] do not apply. Similarly, the uniqueness conditions for coupled CPD based on third-order tensors (i.e., if we ignore the fourth-order structure by combining two modes) discussed in subsection 4.4 do not apply either. We now explain that by simultaneously exploiting both the higher-order and coupled structures of the PDs in (4.24), coupled CPD uniqueness can be established. Generically $\mathbf{D}$ has rank 3. Denote

$$\mathbf{G}^{(n)} = \begin{bmatrix} C_3\left(\mathbf{A}^{(n)}\right) \odot C_3\left(\mathbf{B}^{(n)} \odot \mathbf{C}^{(n)}\right) \\ C_3\left(\mathbf{B}^{(n)}\right) \odot C_3\left(\mathbf{C}^{(n)} \odot \mathbf{A}^{(n)}\right) \\ C_3\left(\mathbf{C}^{(n)}\right) \odot C_3\left(\mathbf{A}^{(n)} \odot \mathbf{B}^{(n)}\right) \end{bmatrix}.$$

Using Lemma 4.3 it can be verified that, although the matrices $\mathbf{G}^{(1)}$ and $\mathbf{G}^{(2)}$ are rank deficient, the matrix $\mathbf{G} = [\mathbf{G}^{(1)T}, \mathbf{G}^{(2)T}]^T$ generically has full column rank. Thus, Proposition 4.6 tells us that by taking into account the higher-order structure and the coupling between $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$, uniqueness of $\mathbf{D}$ can be established. Using Lemma 4.3 it also can be verified that $\mathbf{E}^{(1)} = \mathbf{B}^{(1)} \odot \mathbf{C}^{(1)}$ and $\mathbf{E}^{(2)} = \mathbf{B}^{(2)} \odot \mathbf{C}^{(2)}$ generically have full column rank and that the matrix $[\mathbf{D} \odot \mathbf{A}^{(n)}, \mathbf{d}_r \otimes \mathbf{I}_I]$ generically has a one-dimensional kernel for every $r \in \{1, 2, 3, 4\}$ and $n \in \{1, 2\}$. Invoking Theorem 4.12 we can conclude that the coupled CPD of $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ (in which the Khatri–Rao structure of $\mathbf{E}^{(1)}$ and $\mathbf{E}^{(2)}$ has been ignored) is unique. Consequently, the factors $\{\mathbf{A}^{(n)}\}$, $\{\mathbf{E}^{(n)}\}$, and $\mathbf{D}$ are unique despite the collinearities in the factor matrices. Finally, the rank-1 structure of the columns of $\mathbf{E}^{(n)} = \mathbf{B}^{(n)} \odot \mathbf{C}^{(n)}$ implies that $\{\mathbf{B}^{(n)}\}$ and $\{\mathbf{C}^{(n)}\}$ are also unique.

We now demonstrate that (coupled) CPD of higher-order tensors can even be unique despite collinearities in *all* factor matrices; i.e., the factor matrices of the PDs of $\{\mathcal{X}^{(n)}\}$ in (4.20) may satisfy $k_{\mathbf{C}} = 1$ and $k_{\mathbf{A}^{(m,n)}} = 1$ for all $m \in \{1, \ldots, M_n\}$, for all $n \in \{1, \ldots, N\}$. For this reason Proposition 4.1 does not extend to higher-order tensors in an obvious manner. Note that the existing CPD uniqueness conditions for higher-order tensors stated in [33, 46, 5] do not apply in this case. As an example, consider $N = 1$ and the PD of $\mathcal{X} \in \mathbb{C}^{I\times J\times K\times L}$ given by

$$\mathcal{X} = \sum_{r=1}^{R} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \circ \mathbf{d}_r \,, \tag{4.25}$$

in which $\mathbf{a}_1 = \mathbf{a}_2$, $\mathbf{b}_1 = \mathbf{b}_3$, $\mathbf{c}_3 = \mathbf{c}_4$, $\mathbf{d}_2 = \mathbf{d}_3$, and $I = J = K = L = R = 4$. Since $k_{\mathbf{A}} = k_{\mathbf{B}} = k_{\mathbf{C}} = k_{\mathbf{D}} = 1$ the results discussed in subsection 4.4 cannot be applied in a direct manner. We will establish uniqueness by reducing the fourth-order PD to a coupled third-order PD and by following a deflation argument. Generically $r_{\mathbf{A}} = 3$. Using Lemma 4.3 it can be verified that

$$\begin{bmatrix} C_{R-r_{\mathbf{A}}+2}(\mathbf{B}) \odot C_{R-r_{\mathbf{A}}+2}(\mathbf{C}\odot\mathbf{D}) \\ C_{R-r_{\mathbf{A}}+2}(\mathbf{C}) \odot C_{R-r_{\mathbf{A}}+2}(\mathbf{B}\odot\mathbf{D}) \\ C_{R-r_{\mathbf{A}}+2}(\mathbf{D}) \odot C_{R-r_{\mathbf{A}}+2}(\mathbf{B}\odot\mathbf{C}) \end{bmatrix} = \begin{bmatrix} C_3(\mathbf{B}) \odot C_3(\mathbf{C}\odot\mathbf{D}) \\ C_3(\mathbf{C}) \odot C_3(\mathbf{B}\odot\mathbf{D}) \\ C_3(\mathbf{D}) \odot C_3(\mathbf{B}\odot\mathbf{C}) \end{bmatrix}$$

generically has full column rank. Proposition 4.6 implies that the factor matrix $\mathbf{A}$ is unique. The next step is to demonstrate that the rank-1 term $\mathbf{a}_4 \circ \mathbf{b}_4 \circ \mathbf{c}_4 \circ \mathbf{d}_4$ is unique. The PD of $\mathcal{X}$ in (4.25) has matrix representation

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

Lemma 4.3 can also tell us that $\mathbf{E}$ generically has full column rank and that generically

$$r([\mathbf{A}\odot\mathbf{B}, \mathbf{a}_r \otimes \mathbf{I}_J]) = R + J - \Gamma_r(\mathbf{A}),$$

where $\Gamma_1(\mathbf{A}) = \Gamma_2(\mathbf{A}) = 2$ and $\Gamma_3(\mathbf{A}) = \Gamma_4(\mathbf{A}) = 1$. Since $\Gamma_4(\mathbf{A}) = 1$, [41, Proposition 5.2] tells us that the vectors $\mathbf{b}_4$ and $\mathbf{e}_4$ are unique. As a consequence of the rank-1 structure of $\mathbf{e}_4$ we also know that $\mathbf{c}_4$ and $\mathbf{d}_4$ are unique. We subtract the unique rank-1 term,

$$\mathcal{Y} = \mathcal{X} - \mathbf{a}_4 \circ \mathbf{b}_4 \circ \mathbf{c}_4 \circ \mathbf{d}_4 = \sum_{r=1}^{3} \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \circ \mathbf{d}_r \,.$$

The PD of $\mathcal{Y}$ has the factor matrices $\mathbf{A}^{(2)} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]$, $\mathbf{B}^{(2)} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3]$, $\mathbf{C}^{(2)} = [\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3]$, and $\mathbf{D}^{(2)} = [\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3]$. The matrix $\mathbf{C}^{(2)}$ generically has full column rank. Using Lemma 4.3 it can be verified that

$$\begin{bmatrix} C_2\left(\mathbf{A}^{(2)}\right) \odot C_2\left(\mathbf{B}^{(2)}\odot\mathbf{D}^{(2)}\right) \\ C_2\left(\mathbf{B}^{(2)}\right) \odot C_2\left(\mathbf{D}^{(2)}\odot\mathbf{A}^{(2)}\right) \\ C_2\left(\mathbf{D}^{(2)}\right) \odot C_2\left(\mathbf{A}^{(2)}\odot\mathbf{B}^{(2)}\right) \end{bmatrix}$$

generically has full column rank. Due to Corollary 4.13 we now know that the remaining factors $\mathbf{A}^{(2)}$, $\mathbf{B}^{(2)}$, $\mathbf{C}^{(2)}$, and $\mathbf{D}^{(2)}$ are unique.

More generally, for the case of coupled CPD of higher-order tensors it is possible in some cases to establish coupled CPD uniqueness via a sequence of deflation steps. See the supplementary material for a brief discussion.

4.6. Coupled matrix-tensor factorization. A simple case of coupled decompositions is the coupled matrix-tensor factorization, admitting a matrix representation of the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{(1)} \\ \mathbf{X}_{(1)}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \end{bmatrix} \mathbf{C}^T. \tag{4.26}$$

Because of its simplicity, (4.26) is common in the analysis of multiview data [49, 1, 18, 2]. Note that coupled matrix-tensor factorization is a special case of coupled CPD. Indeed, define $\mathbf{B}^{(2)} = [1, 1, \ldots, 1] \in \mathbb{C}^{1\times R}$; then (4.26) can also be written as

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{(1)} \\ \mathbf{X}_{(1)}^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \mathbf{A}^{(2)} \odot \mathbf{B}^{(2)} \end{bmatrix} \mathbf{C}^T,$$

which is of form (4.2), so that several of the results presented in this paper can be applied.

A notable limitation of the coupled matrix-tensor factorization (4.26) is that in order to guarantee the uniqueness of $\mathbf{A}^{(2)}$, the common factor $\mathbf{C}$ must have full column rank. More precisely, if $\mathbf{C}$ has full column rank, then $\mathbf{A}^{(2)}$ follows from $\mathbf{A}^{(2)} = \mathbf{X}_{(1)}^{(2)}(\mathbf{C}^T)^\dagger$. On the other hand, if $\mathbf{C}$ does not have full column rank, then there will be an intrinsic indeterminacy between $\mathbf{A}^{(2)}$ and $\mathbf{C}$. Indeed, when $\mathbf{C}$ does not have full column rank, the null space of $\mathbf{C}$ is not empty. Any vector $\mathbf{y} \in \ker(\mathbf{C})$ will generate an alternative coupled matrix-tensor factorization $\mathbf{X}$ in which $\mathbf{X}_{(1)}^{(2)} = (\mathbf{A}^{(2)} + \mathbf{x}\mathbf{y}^T)\mathbf{C}^T$, where $\mathbf{x} \in \mathbb{C}^{I_2}$.

5. Coupled CPD with collinearity in common factor. We consider coupled PDs of $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1, \ldots, N\}$, of the following form:

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \sum_{l=1}^{L_{r,n}} \mathbf{a}_l^{(r,n)} \circ \mathbf{b}_l^{(r,n)} \circ \mathbf{c}^{(r)} = \sum_{r=1}^{R} \left(\mathbf{A}^{(r,n)}\mathbf{B}^{(r,n)T}\right) \circ \mathbf{c}^{(r)}. \tag{5.1}$$

On one hand, this is an extension of (3.1) to the coupled case. On the other hand, it is a variant of the coupled PD in (4.1) for collinearity constrained $\mathbf{C}$. If the matrices $\mathbf{A}^{(r,n)}\mathbf{B}^{(r,n)T}$ have rank $L_{r,n}$, then (5.1) is a coupled decomposition into multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ terms. We will briefly call this a coupled block term decomposition (BTD). The coupled BTD of the third-order tensors $\{\mathcal{X}^{(n)}\}$ is visualized in Figure 3.

The coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ tensors in (5.1) can be arbitrarily permuted, and the vectors/matrices within the same coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ tensor can be arbitrarily scaled provided the overall coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ term remains the same. We say that the coupled BTD is unique when it is only subject to the mentioned indeterminacies.

In this section we limit the exposition to third-order tensors. Analogous to the coupled CPD in subsection 4.5, the coupled BTD and its associated properties can be extended to tensors of arbitrary order. In the supplementary material we briefly explain that it can be reduced to a set of coupled BTDs of third-order tensors.

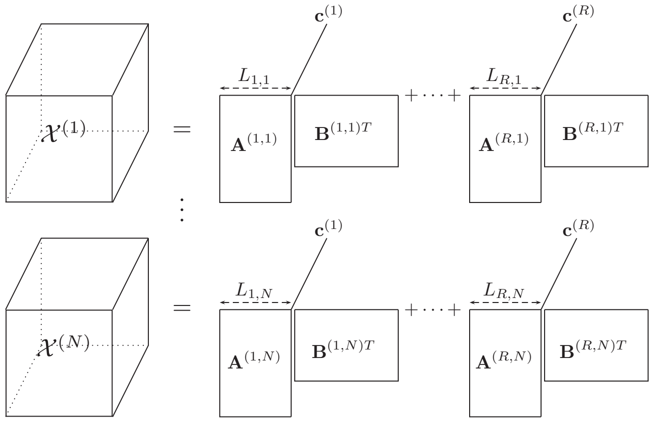

FIG. 3. *Coupled BTD of the third-order tensors* $\mathcal{X}^{(1)},\dots,\mathcal{X}^{(N)}$.

5.1. Matrix representation. Denote $R_{\text{tot},n} = \sum_{r=1}^{R} L_{r,n}$. The coupled PD of the tensors $\{\mathcal{X}^{(n)}\}$ of the form (5.1) has the factor matrices

$$\mathbf{A}^{(r,n)} = \left[\ \mathbf{a}_1^{(r,n)}, \ \dots \ , \mathbf{a}_{L_{r,n}}^{(r,n)}\ \right] \in \mathbb{C}^{I_n \times L_{r,n}},$$

$$\mathbf{A}^{(n)} = \left[\ \mathbf{A}^{(1,n)}, \ \dots \ , \mathbf{A}^{(R,n)}\ \right] \in \mathbb{C}^{I_n \times R_{\text{tot},n}}, \quad n \in \{1,\dots,N\},$$

$$\mathbf{B}^{(r,n)} = \left[\ \mathbf{b}_1^{(r,n)}, \ \dots \ , \mathbf{b}_{L_{r,n}}^{(r,n)}\ \right] \in \mathbb{C}^{J_n \times L_{r,n}},$$

$$\mathbf{B}^{(n)} = \left[\ \mathbf{B}^{(1,n)}, \ \dots \ , \mathbf{B}^{(R,n)}\ \right] \in \mathbb{C}^{J_n \times R_{\text{tot},n}}, \quad n \in \{1,\dots,N\},$$

$$\mathbf{C}^{(\text{red})} = \left[\ \mathbf{c}^{(1)}, \ \dots \ , \mathbf{c}^{(R)}\ \right] \in \mathbb{C}^{K \times R}, \tag{5.2}$$

$$\mathbf{C}^{(n)} = \left[\mathbf{1}_{L_{r,n}}^T \otimes \mathbf{c}^{(1)}, \dots, \mathbf{1}_{L_{R,n}}^T \otimes \mathbf{c}^{(R)}\right] \in \mathbb{C}^{K \times R_{\text{tot},n}}, \tag{5.3}$$

and matrix representation

$$\mathbf{X} = \left[\mathbf{X}_{(1)}^{(1)T}, \dots, \mathbf{X}_{(1)}^{(N)T}\right]^T = \mathbf{F}^{(\text{red})}\mathbf{C}^{(\text{red})T} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times K}, \tag{5.4}$$

where $\mathbf{F}^{(\text{red})} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times R}$ is given by

$$\mathbf{F}^{(\text{red})} = \begin{bmatrix} \text{Vec}\left(\mathbf{B}^{(1,1)}\mathbf{A}^{(1,1)T}\right) & \cdots & \text{Vec}\left(\mathbf{B}^{(R,1)}\mathbf{A}^{(R,1)T}\right) \\ \vdots & \ddots & \vdots \\ \text{Vec}\left(\mathbf{B}^{(1,N)}\mathbf{A}^{(1,N)T}\right) & \cdots & \text{Vec}\left(\mathbf{B}^{(R,N)}\mathbf{A}^{(R,N)T}\right) \end{bmatrix}. \tag{5.5}$$

Denote $L_{r,\max} = \max_{n \in \{1,\dots,N\}} L_{r,n}$ and $R_{\text{ext}} = \sum_{r=1}^{R} L_{r,\max}$, where "ext" stands for extended. By appending all-zero column vectors to $\mathbf{A}^{(r,n)}$ and $\mathbf{B}^{(r,n)}$, (5.4) may also be expressed as

$$\mathbf{X} = \mathbf{F}^{(\text{ext})}\mathbf{C}^{(\text{ext})T} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times K}, \tag{5.6}$$

where

$$\mathbf{F}^{(\mathrm{ext})} = \left[\left(\widetilde{\mathbf{A}}^{(1)} \odot \widetilde{\mathbf{B}}^{(1)} \right)^T, \ldots, \left(\widetilde{\mathbf{A}}^{(N)} \odot \widetilde{\mathbf{B}}^{(N)} \right)^T \right]^T \in \mathbb{C}^{(\sum_{n=1}^N I_n J_n) \times R_{\mathrm{ext}}}, \tag{5.7}$$

$$\mathbf{C}^{(\mathrm{ext})} = \left[\mathbf{1}_{L_{1,\max}}^T \otimes \mathbf{c}^{(1)}, \ldots, \mathbf{1}_{L_{R,\max}}^T \otimes \mathbf{c}^{(R)} \right] \in \mathbb{C}^{K \times R_{\mathrm{ext}}}, \tag{5.8}$$

in which

$$\begin{aligned}
\widetilde{\mathbf{A}}^{(r,n)} &= \left[\mathbf{A}^{(r,n)}, \mathbf{0}_{I_n,(L_{r,\max}-L_{r,n})} \right] \in \mathbb{C}^{I_n \times L_{r,\max}}, \\
\widetilde{\mathbf{A}}^{(n)} &= \left[\widetilde{\mathbf{A}}^{(1,n)}, \ldots, \widetilde{\mathbf{A}}^{(R,n)} \right] \in \mathbb{C}^{I_n \times R_{\mathrm{ext}}}, \quad n \in \{1, \ldots, N\}, \\
\widetilde{\mathbf{B}}^{(r,n)} &= \left[\mathbf{B}^{(r,n)}, \mathbf{0}_{J_n,(L_{r,\max}-L_{r,n})} \right] \in \mathbb{C}^{J_n \times L_{r,\max}}, \\
\widetilde{\mathbf{B}}^{(n)} &= \left[\widetilde{\mathbf{B}}^{(1,n)}, \ldots, \widetilde{\mathbf{B}}^{(R,n)} \right] \in \mathbb{C}^{J_n \times R_{\mathrm{ext}}}, \quad n \in \{1, \ldots, N\}.
\end{aligned}$$

5.2. Uniqueness conditions for coupled CPD with collinearity in common factor. Let $\{\{\widehat{\mathbf{A}}^{(r,n)}\}, \{\widehat{\mathbf{B}}^{(r,n)}\}, \{\widehat{\mathbf{c}}^{(r)}\}\}$ yield an alternative coupled BTD of the tensors $\{\mathcal{X}^{(n)}\}$ in (5.1). We say that the coupled BTD of $\{\mathcal{X}^{(n)}\}$ is unique if it is unique up to a permutation of the coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ terms $\{(\widehat{\mathbf{A}}^{(r,n)}\widehat{\mathbf{B}}^{(r,n)T}) \circ \widehat{\mathbf{c}}^{(r)}\}$ and up to the following indeterminacies within each term:

$$\widehat{\mathbf{A}}^{(r,n)} = \alpha^{(r,n)}\mathbf{A}^{(r,n)}\mathbf{H}_{r,n}\,, \;\; \widehat{\mathbf{B}}^{(r,n)} = \beta^{(r,n)}\mathbf{B}^{(r,n)}\mathbf{H}_{r,n}^{-1}\,, \;\; \widehat{\mathbf{c}}^{(r)} = \gamma^{(r)}\mathbf{c}^{(r)},$$

where $\mathbf{H}_{r,n} \in \mathbb{C}^{L_{r,n} \times L_{r,n}}$ are nonsingular matrices and $\alpha^{(r,n)}, \beta^{(r,n)}, \gamma^{(r)} \in \mathbb{C}$ are scalars satisfying $\alpha^{(r,n)}\beta^{(r,n)}\gamma^{(r)} = 1$, $r \in \{1, \ldots, R\}$, $n \in \{1, \ldots, N\}$. From (5.4) it is clear that uniqueness requires $k_{\mathbf{C}^{(\mathrm{red})}} \geq 2$. From (5.4) it is also clear that $\mathbf{F}^{(\mathrm{red})}$ must have full column rank in order to guarantee the uniqueness of the coupled BTD of $\{\mathcal{X}^{(n)}\}$. Proposition 5.1 below extends the necessary conditions stated in Propositions 4.1, 4.2, and 4.5 to coupled BTD.

PROPOSITION 5.1. *Consider the coupled PD of* $\mathcal{X}^{(n)}$, $n \in \{1, \ldots, N\}$, *in* (5.1). *Define* $\boldsymbol{E}^{(n)}(\boldsymbol{w}) = \sum_{r=1}^R w_r \boldsymbol{A}^{(r,n)}\boldsymbol{B}^{(r,n)T}$ *and* $\Omega = \left\{\boldsymbol{x} \in \mathbb{C}^R \middle| \, \omega(\boldsymbol{x}) \geq 2\right\}$. *If the coupled BTD of* $\{\mathcal{X}^{(n)}\}$ *in* (5.1) *is unique, then*

(i) $k_{\boldsymbol{C}^{(\mathrm{red})}} \geq 2$,
(ii) $\boldsymbol{F}^{(\mathrm{red})}$ *has full column rank,*
(iii) *for all* $\boldsymbol{w} \in \Omega\,, \exists\, n \in \{1, \ldots, N\} \,:\, r(\boldsymbol{E}^{(n)}(\boldsymbol{w})) > \max_{r|w_r \neq 0} L_{r,n}$.

Proof. The proof is analogous to that of Propositions 4.1, 4.2, and 4.5. ∎

Proposition 5.2 tells us that this is generically true if $\mathbf{F}^{(\mathrm{red})}$ has at least as many rows as columns.

PROPOSITION 5.2. *Consider* $\boldsymbol{F}^{(\mathrm{red})} \in \mathbb{C}^{(\sum_{n=1}^N I_n J_n) \times R}$ *given by* (5.5). *For generic matrices* $\{\boldsymbol{A}^{(r,n)}\}$ *and* $\{\boldsymbol{B}^{(r,n)}\}$, *the matrix* $\boldsymbol{F}^{(red)}$ *has rank* $\min(\sum_{n=1}^N I_n J_n, R)$.

Proof. Due to Lemma 4.3 we just need to find one example for which the proposition holds. Since the coupled CPD (4.1) is a particular case of (5.4), a particular example is the matrix $\mathbf{F}^{(\mathrm{red})}$ in (4.3). (Formally, we take $\mathbf{a}_l^{(r,n)} = \mathbf{0}_{I_n}$ for all $l \in \{2, \ldots, L_{r,n}\}$, for all $r \in \{1, \ldots, R\}$, for all $n \in \{1, \ldots, N\}$.) The proposition now follows directly from Proposition 4.4. ∎

We will now discuss extensions of Theorems 4.11, 4.12, and 4.15 to the case where the common factor matrix contains collinear components. The generalizations of Proposition 4.10 and Corollary 4.13 follow immediately and are therefore not considered in this section.

Theorem 5.3 can be seen as a version of Theorem 4.11 for the case where the common factor matrix contains collinear columns.

THEOREM 5.3. *Consider the coupled PD of* $\mathcal{X}^{(n)}$, $n \in \{1,\ldots,N\}$, *in* (5.1). *Let* S_n *denote a subset of* $\{1,\ldots,R\}$, *and let* $S_n^c = \{1,\ldots,R\} \setminus S_n$ *denote the complementary set. Stack the columns of* $\boldsymbol{C}^{(\text{red})}$ *with index in* S_n *in* $\boldsymbol{C}^{(\text{red},S_n)} \in \mathbb{C}^{K\times card(S_n)}$ *and stack the columns of* $\boldsymbol{C}^{(\text{red})}$ *with index in* S_n^c *in* $\boldsymbol{C}^{(\text{red},S_n^c)} \in \mathbb{C}^{K\times(R-card(S_n))}$. *Stack* $\boldsymbol{A}^{(r,n)}$ *(resp.,* $\boldsymbol{B}^{(r,n)}$ *and* $\boldsymbol{C}^{(r,n)}$*) in the same order such that* $\boldsymbol{A}^{(n,S_n)} \in \mathbb{C}^{I_n\times(\sum_{p\in S_n} L_{p,n})}$ *(resp.,* $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n\times(\sum_{p\in S_n} L_{p,n})}$ *and* $\boldsymbol{C}^{(n,S_n)} \in \mathbb{C}^{K\times(\sum_{p\in S_n} L_{p,n})}$*) and* $\boldsymbol{A}^{(n,S_n^c)} \in \mathbb{C}^{I_n\times(\sum_{p\in S_n^c} L_{p,n}t)}$ *(resp.,* $\boldsymbol{B}^{(n,S_n^c)} \in \mathbb{C}^{J_n\times(\sum_{p\in S_n^c} L_{p,n})}$ *and* $\boldsymbol{C}^{(n,S_n^c)} \in \mathbb{C}^{K\times(\sum_{p\in S_n^c} L_{p,n})}$*) are obtained. Denote* $\boldsymbol{D}^{(n,S_n^c)} = \boldsymbol{P}_{\boldsymbol{C}^{(\text{red},S_n)}} \boldsymbol{C}^{(n,S_n^c)}$. *If* [7]

$$\text{(5.9a)} \qquad \begin{cases} \exists\, p \in \{1,\ldots,N\} : \textit{the minimal number of rank-}(L_{r,p}, L_{r,p}, 1) \\ \quad \textit{terms in } \mathcal{X}^{(p)} \textit{ is } R \textit{ and the decomposition of } \mathcal{X}^{(p)} \textit{ into} \\ \quad \textit{rank-}(L_{r,p}, L_{r,p}, 1) \textit{ terms is unique,} \end{cases}$$

and for every $n \in \{1,\ldots,N\}$ *there exists an index set* $S_n \subseteq \{1,\ldots,R\}$ *with property* $0 \le card(S_n) \le r_{\boldsymbol{C}^{(\text{red})}}$, *such that*

$$\text{(5.9b)} \qquad \begin{cases} \boldsymbol{B}^{(n,S_n^c)} \textit{ has full column rank } \left(r_{\boldsymbol{B}^{(n,S_n^c)}} = \sum_{p\in S_n^c} L_{p,n} \right), \\ r\left(\left[\boldsymbol{D}^{(n,S_n^c)} \odot \boldsymbol{A}^{(n,S_n^c)}, \boldsymbol{d}_r^{(n,S_n^c)} \otimes \boldsymbol{I}_{I_n} \right] \right) = \alpha_{r,n} \quad \forall r \in S_n^c, \end{cases}$$

where $\alpha_{r,n} = I_n + \sum_{p\in S_n^c} L_{p,n} - L_{r,n}$, *or*

$$\text{(5.9c)} \qquad \begin{cases} \boldsymbol{A}^{(n,S_n^c)} \textit{ has full column rank } \left(r_{\boldsymbol{A}^{(n,S_n^c)}} = \sum_{p\in S_n^c} L_{p,n} \right), \\ r\left(\left[\boldsymbol{D}^{(n,S_n^c)} \odot \boldsymbol{B}^{(n,S_n^c)}, \boldsymbol{d}_r^{(n,S_n^c)} \otimes \boldsymbol{I}_{J_n} \right] \right) = \beta_{r,n} \quad \forall r \in S_n^c, \end{cases}$$

where $\beta_{r,n} = J_n + \sum_{p\in S_n^c} L_{p,n} - L_{r,n}$, *then the minimal number of coupled multilinear rank-*$(L_{r,n}, L_{r,n}, 1)$ *terms is* R *and the coupled BTD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. Assume that there exists an integer $p \in \{1,\ldots,N\}$ such that the minimal number of rank-$(L_{r,p}, L_{r,p}, 1)$ terms in $\mathcal{X}^{(p)}$ is R and the decomposition of $\mathcal{X}^{(p)}$ into rank-$(L_{r,p}, L_{r,p}, 1)$ terms is unique. Since $\mathbf{C}^{(\text{red})}$ is unique and the condition (5.9b) or (5.9c) is satisfied for every $n \in \{1,\ldots,N\}$, we know from [41, Proposition 5.2] that the coupled BTD of $\{\mathcal{X}^{(n)}\}$ is unique and the minimal number of coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ terms is R. ∎

Theorem 5.4 below can be interpreted as a version of Theorem 4.12 for the case where the common factor matrix contains collinear columns.

THEOREM 5.4. *Consider the coupled PD of* $\mathcal{X}^{(n)}$, $n \in \{1,\ldots,N\}$, *in* (5.1). *Let* S_n *denote a subset of* $\{1,\ldots,R\}$ *and let* $S_n^c = \{1,\ldots,R\} \setminus S_n$ *denote the complementary*

[7] As an example, if $r(C_{R_{\text{tot},p}-r_{\mathbf{C}^{(\text{red})}}+2}(\mathbf{A}^{(p)}) \odot C_{R_{\text{tot},p}-r_{\mathbf{C}^{(\text{red})}}+2}(\mathbf{B}^{(p)})) = C_{R_{\text{tot},p}}^{R_{\text{tot},p}-r_{\mathbf{C}^{(\text{red})}}+2}$, then Theorem 2.1 tells us that the rank of $\mathcal{X}^{(p)}$ is $\sum_{r=1}^{R} L_{r,p}$ and the factor $\mathbf{C}^{(p)}$ is unique up to a column permutation and scaling. The uniqueness of the decomposition of $\mathcal{X}^{(p)}$ into rank-$(L_{r,p}, L_{r,p}, 1)$ terms now follows from condition (5.9b) or (5.9c), as explained by Proposition 5.2 in [41].

set. Stack the columns of $\boldsymbol{C}^{(\mathrm{red})}$ *with index in* S_n *in* $\boldsymbol{C}^{(\mathrm{red},S_n)} \in \mathbb{C}^{K\times card(S_n)}$ *and stack the columns of* $\boldsymbol{C}^{(\mathrm{red})}$ *with index in* S_n^c *in* $\boldsymbol{C}^{(\mathrm{red},S_n^c)} \in \mathbb{C}^{K\times(R-card(S_n))}$*. Stack* $\boldsymbol{A}^{(r,n)}$ *(resp.,* $\boldsymbol{B}^{(r,n)}$ *and* $\boldsymbol{C}^{(r,n)}$*) in the same order such that* $\boldsymbol{A}^{(n,S_n)} \in \mathbb{C}^{I_n\times(\sum_{p\in S_n} L_{p,n})}$ *(resp.,* $\boldsymbol{B}^{(n,S_n)} \in \mathbb{C}^{J_n\times(\sum_{p\in S_n} L_{p,n})}$ *and* $\boldsymbol{C}^{(n,S_n)} \in \mathbb{C}^{K\times(\sum_{p\in S_n} L_{p,n})}$*) and* $\boldsymbol{A}^{(n,S_n^c)} \in \mathbb{C}^{I_n\times(\sum_{p\in S_n^c} L_{p,n})}$ *(resp.,* $\boldsymbol{B}^{(n,S_n^c)} \in \mathbb{C}^{J_n\times(\sum_{p\in S_n^c} L_{p,n})}$ *and* $\boldsymbol{C}^{(n,S_n^c)} \in \mathbb{C}^{K\times(\sum_{p\in S_n^c} L_{p,n})}$*) are obtained.*

If $\boldsymbol{C}^{(\mathrm{red})}$ *is unique*[8] *with property* $k(\boldsymbol{C}^{(\mathrm{red})}) \geq 2$ *and if for every* $n \in \{1,\ldots,N\}$ *there exists an index set* $S_n \subseteq \{1,\ldots,R\}$ *with property* $0 \leq card(S_n) \leq r_{\boldsymbol{C}^{(\mathrm{red})}}$*, such that condition* (5.9b) *or* (5.9c) *is satisfied, then the minimal number of coupled multilinear rank-*$(L_{r,n}, L_{r,n}, 1)$ *terms is* R *and the coupled BTD of* $\{\mathcal{X}^{(n)}\}$ *is unique.*

Proof. We assume that the common factor matrix $\mathbf{C}^{(\mathrm{ext})}$ is unique. Since $k(\mathbf{C}^{(\mathrm{red})}) \geq 2$ we can remove repeated column vectors of $\mathbf{C}^{(\mathrm{ext})}$ so that $\mathbf{C}^{(\mathrm{red})}$ is obtained up to an intrinsic column permutation and scaling. From [41, Proposition 5.2] we know that when $\mathbf{C}^{(\mathrm{red})}$ is unique and condition (5.9b) or (5.9c) is satisfied for every $n \in \{1,\ldots,N\}$, the coupled BTD of $\{\mathcal{X}^{(n)}\}$ is unique and the minimal number of coupled multilinear rank-$(L_{r,n}, L_{r,n}, 1)$ terms is R. ∎

Let us now assume that the common factor $\mathbf{C}^{(\mathrm{red})}$ has full column rank. We formulate the generalization of the necessary and sufficient uniqueness condition stated in Theorem 4.15 to the coupled BTD case.

THEOREM 5.5. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1,\ldots,N\}$ *in* (5.1). *Define* $\boldsymbol{E}^{(n)}(\boldsymbol{w}) = \sum_{r=1}^{R} w_r \boldsymbol{A}^{(r,n)}\boldsymbol{B}^{(r,n)T}$ *and* $\Omega = \left\{\boldsymbol{x} \in \mathbb{C}^R \middle| \, \omega(\boldsymbol{x}) \geq 2\right\}$. *Assume that* $\boldsymbol{C}^{(red)}$ *has full column rank. The decomposition of* $\{\mathcal{X}^{(n)}\}$ *into coupled multilinear rank-*$(L_{r,n}, L_{r,n}, 1)$ *terms is unique if and only if*

$$\forall \boldsymbol{w} \in \Omega \quad \exists\, n \in \{1,\ldots,N\} : r\left(\boldsymbol{E}^{(n)}(\boldsymbol{w})\right) > \max_{r|w_r\neq 0} L_{r,n} \,. \tag{5.10}$$

Proof. The proof is analogous to that of Theorem 4.15. ∎

6. Conclusion. Coupled tensor decompositions are currently gaining interest in several engineering disciplines. However, a firm algebraic framework for coupled tensor decompositions had not yet been presented in the literature. The existing uniqueness conditions for single tensor decompositions are not sufficient for the coupled case. In this paper we have derived necessary and sufficient conditions for the uniqueness of a coupled CPD. The conditions are more relaxed than their single tensor counterparts. We have considered variants for tensors of order greater than three and for coupled matrix-tensor decompositions.

In several signal processing problems the common factor matrix contains collinear columns. To cope with collinearity, we introduced the coupled BTD, which can be seen as a variant of the coupled CPD but also as an extension of the decomposition into multilinear rank-$(L_r, L_r, 1)$ terms to the coupled case. For the coupled BTD, we provided several necessary and sufficient uniqueness conditions as well.

It is also important to take into account the coupling in the actual computation of the decompositions. Computation is addressed in the companion paper [41].

[8]For working with Proposition 4.6, denote $Q = \sum_{n=1}^{N} H[\min(I_n, J_n) - R_{\mathrm{ext}} + r_{\mathbf{C}^{(\mathrm{red})}} - 2]$ and define $\mathbf{G} \in \mathbb{C}^{(\sum_{n=1}^{Q} C_{I_n}^{R_{\mathrm{ext}}-r_{\mathbf{C}^{(\mathrm{red})}}+2} C_{J_n}^{R_{\mathrm{ext}}-r_{\mathbf{C}^{(\mathrm{red})}}+2})\times C_{R_{\mathrm{ext}}}^{R_{\mathrm{ext}}-r_{\mathbf{C}^{(\mathrm{red})}}+2}}$ as in (4.7) and built from the zero-padded matrices $\{\widetilde{\mathbf{A}}^{(n)}\}$ and $\{\widetilde{\mathbf{B}}^{(n)}\}$. Proposition 4.6 tells us that if $r(\mathbf{G}) = C_{R_{\mathrm{ext}}}^{R_{\mathrm{ext}}-r_{\mathbf{C}^{(\mathrm{red})}}+2}$ and $k(\mathbf{C}^{(\mathrm{red})}) \geq 1$, then the coupled rank of $\{\mathbf{X}^{(n)}\}$ is R_{ext} and the common factor $\mathbf{C}^{(\mathrm{ext})}$ is unique.

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COUPLED CANONICAL POLYADIC DECOMPOSITIONS AND (COUPLED) DECOMPOSITIONS IN MULTILINEAR RANK-$(L_{r,n}, L_{r,n}, 1)$ TERMS — PART I: UNIQUENESS SUPPLEMENTARY MATERIAL

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Recall that a collection of tensors $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1, \dots, N\}$, admits an R-term coupled polyadic decomposition if each tensor $\mathcal{X}^{(n)}$ can be written as

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \mathbf{a}_r^{(n)} \circ \mathbf{b}_r^{(n)} \circ \mathbf{c}_r , \quad n \in \{1, \dots, N\}, \tag{S.0.1}$$

with factor matrices

$$\begin{aligned} \mathbf{A}^{(n)} &= \left[\begin{array}{ccc} \mathbf{a}_1^{(n)}, & \dots & ,\mathbf{a}_R^{(n)} \end{array} \right] \in \mathbb{C}^{I_n \times R}, \quad n \in \{1, \dots, N\}, \\ \mathbf{B}^{(n)} &= \left[\begin{array}{ccc} \mathbf{b}_1^{(n)}, & \dots & ,\mathbf{b}_R^{(n)} \end{array} \right] \in \mathbb{C}^{J_n \times R}, \quad n \in \{1, \dots, N\}, \\ \mathbf{C} &= \left[\begin{array}{ccc} \mathbf{c}_1, & \dots & ,\mathbf{c}_R \end{array} \right] \in \mathbb{C}^{K \times R}. \end{aligned}$$

we will make use of the following matrix representation of $\{\mathcal{X}^{(n)}\}$:

$$\mathbf{X} = \left[\begin{array}{c} \mathbf{X}_{(1)}^{(1)} \\ \vdots \\ \mathbf{X}_{(1)}^{(N)} \end{array} \right] = \left[\begin{array}{c} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{A}^{(N)} \odot \mathbf{B}^{(N)} \end{array} \right] \mathbf{C}^T = \mathbf{F}\mathbf{C}^T \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times K}, \tag{S.0.2}$$

where

$$\mathbf{F} = \left[\begin{array}{c} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{A}^{(N)} \odot \mathbf{B}^{(N)} \end{array} \right] \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times R}. \tag{S.0.3}$$

S.1. Supplementary material related to Proposition 4.4. Consider $\mathbf{F} \in \mathbb{C}^{(\sum_{n=1}^{N} I_n J_n) \times R}$ given by (S.0.3). For generic matrices $\{\mathbf{A}^{(n)}\}$ and $\{\mathbf{B}^{(n)}\}$, the matrix $\mathbf{F}$ has rank $\min\left(\sum_{n=1}^{N} I_n J_n, R\right)$.

Proof. Due to [3, Lemma 4.3] we just need to find one example where the statement made in this lemma holds.

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By way of example, let

$$\mathbf{a}_r^{(n)} = \begin{bmatrix} 1 \\ z_r^{J_n} \\ z_r^{2J_n} \\ \vdots \\ z_r^{(I_n-1)J_n} \end{bmatrix} z_r^{\prod_{p<n} I_p J_p} \in \mathbb{C}^{I_n} \quad \text{and} \quad \mathbf{b}_r^{(n)} = \begin{bmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{(J_n-1)} \end{bmatrix} \in \mathbb{C}^{J_n}. \tag{S.1.1}$$

By inserting (S.1.1) into (S.0.3) we obtain

$$\mathbf{F} = \begin{bmatrix} \mathbf{A}^{(1)} \odot \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{A}^{(N)} \odot \mathbf{B}^{(N)} \end{bmatrix} = \begin{bmatrix} 1 & \cdots & 1 \\ z_1^1 & \cdots & z_R^1 \\ z_1^2 & \cdots & z_R^2 \\ \vdots & \ddots & \vdots \\ z_1^{\sum_{n=1}^N I_n J_n - 1} & \cdots & z_R^{\sum_{n=1}^N I_n J_n - 1} \end{bmatrix}. \tag{S.1.2}$$

The Vandermonde matrix $\mathbf{F}$ given by (S.1.2) has rank $\min\left(\sum_{n=1}^N I_n J_n, R\right)$ if the generators $\{z_r\}$ are distinct. By invoking [3, Lemma 4.3] we conclude that the matrix $\mathbf{F}$ given by (S.0.3) generically has rank $\min\left(\sum_{n=1}^N I_n J_n, R\right)$. ◻

S.2. Supplementary material related to Proposition 4.6. In Proposition S.2.3 we briefly explain how Proposition 4.3 in [1] for CPD can be extended to coupled CPD. The proof of Proposition S.2.3 makes use of the following two lemmas.

LEMMA S.2.1 (Kruskal's Permutation Lemma). *Let* $\widetilde{\boldsymbol{C}} \in \mathbb{C}^{K\times\widetilde{R}}$ *and* $\boldsymbol{C} \in \mathbb{C}^{K\times R}$ *in which* $\widetilde{R} \le R$ *and* $k(\boldsymbol{C}) \ge 1$. *If*

$$\omega\left(\widetilde{\boldsymbol{C}}^T \boldsymbol{x}\right) \le \widetilde{R} - r\left(\widetilde{\boldsymbol{C}}\right) + 1 \Rightarrow \omega\left(\boldsymbol{C}^T \boldsymbol{x}\right) \le \omega\left(\widetilde{\boldsymbol{C}}^T \boldsymbol{x}\right), \quad \forall \boldsymbol{x} \in \mathbb{C}^K,$$

then $\widetilde{R} = R$ *and there exists a unique permutation matrix* $\boldsymbol{P} \in \mathbb{C}^{R\times R}$ *and a unique nonsingular diagonal matrix* $\boldsymbol{D} \in \mathbb{C}^{R\times R}$ *such that* $\widetilde{\boldsymbol{C}} = \boldsymbol{C}\boldsymbol{P}\boldsymbol{D}$.

Proof. The original proof can be found in [2] and a discussion of the result can be found in [5]. ◻

LEMMA S.2.2. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1,\dots,N\}$ *in* (S.0.1). *W.l.o.g. we assume that* $\min(I_1,J_1) \ge \min(I_2,J_2) \ge \cdots \ge \min(I_N,J_N)$. *Denote* $Q = \sum_{n=1}^N H\left[\min(I_n,J_n) - R + r_{\boldsymbol{C}} - 2\right]$. *Define*

$$\boldsymbol{G}^{(m)} = \begin{bmatrix} C_m\left(\boldsymbol{A}^{(1)}\right) \odot C_m\left(\boldsymbol{B}^{(1)}\right) \\ \vdots \\ C_m\left(\boldsymbol{A}^{(Q)}\right) \odot C_m\left(\boldsymbol{B}^{(Q)}\right) \end{bmatrix} \in \mathbb{C}^{\left(\sum_{n=1}^Q C_{I_n}^m C_{J_n}^m\right)\times C_R^m}, \tag{S.2.1}$$

where $m = R - r_{\boldsymbol{C}} + 2$. *If* $\boldsymbol{G}^{(m)}$ *has full column rank, then* $\boldsymbol{G}^{(m-1)}, \boldsymbol{G}^{(m-2)}, \dots, \boldsymbol{G}^{(1)} = \boldsymbol{F}$ *all have full column rank.*

Proof. The result is analogous to Lemma 3.6 in [1]. ◻

PROPOSITION S.2.3. *Consider the coupled PD of* $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n\times J_n\times K}$, $n \in \{1,\dots,N\}$ *in* (S.0.1). *Let* $\boldsymbol{G}^{(m)}$ *be defined as in* (S.2.1). *If*

$$\begin{cases} k(\boldsymbol{C}) \ge 1 \\ r\left(\boldsymbol{G}^{(R-r_C+2)}\right) = C_R^{R-r_C+2}, \end{cases} \tag{S.2.2}$$

then the coupled rank of $\{\mathcal{X}^{(n)}\}$ *is* R *and the factor matrix* $\boldsymbol{C}$ *is unique.*

Proof. Let $\left\{\{\widetilde{\mathbf{A}}^{(n)}\},\{\widetilde{\mathbf{B}}^{(n)}\},\widetilde{\mathbf{C}}\right\}$ denote the factor matrices of an alternative coupled CPD of $\mathcal{X}^{(n)}$, $n\in\{1,\ldots,N\}$, where $\widetilde{\mathbf{A}}^{(n)}\in\mathbb{C}^{I_n\times\widetilde{R}}$, $\widetilde{\mathbf{B}}^{(n)}\in\mathbb{C}^{J_n\times\widetilde{R}}$ and $\widetilde{\mathbf{C}}\in\mathbb{C}^{K\times\widetilde{R}}$. This implies that $\widetilde{R}\leq R$ and

$$\left(\widetilde{\mathbf{A}}^{(n)}\odot\widetilde{\mathbf{B}}^{(n)}\right)\widetilde{\mathbf{C}}^T=\left(\mathbf{A}^{(n)}\odot\mathbf{B}^{(n)}\right)\mathbf{C}^T,\quad n\in\{1,\ldots,N\}\,. \tag{S.2.3}$$

Denote

$$\widetilde{\mathbf{F}}=\left[\left(\widetilde{\mathbf{A}}^{(1)}\odot\widetilde{\mathbf{B}}^{(1)}\right)^T,\ldots,\left(\widetilde{\mathbf{A}}^{(N)}\odot\widetilde{\mathbf{B}}^{(N)}\right)^T\right]^T\in\mathbb{C}^{(\sum_{n=1}^N I_nJ_n)\times\widetilde{R}}.$$

Due to Lemma S.2.2 we know that condition (S.2.2) implies that $\mathbf{F}$ has full column rank. Since we know that $\mathbf{F}$ has full column rank we also know that

$$r\left(\mathbf{C}\right)=r\left(\mathbf{F}\mathbf{C}^T\right)=r\left(\widetilde{\mathbf{F}}\widetilde{\mathbf{C}}^T\right)\leq r\left(\widetilde{\mathbf{C}}\right). \tag{S.2.4}$$

Let $\mathbf{x}\in\mathbb{C}^K$ be a vector such that $\omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right)\leq\widetilde{R}-r\left(\widetilde{\mathbf{C}}\right)+1$. Due to inequalities $\widetilde{R}\leq R$ and (S.2.4) we also know that $\omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right)\leq\widetilde{R}-r\left(\widetilde{\mathbf{C}}\right)+1\leq R-r\left(\mathbf{C}\right)+1=R-r_{\mathbf{C}}+1$.

From (S.2.3) we obtain

$$\widetilde{\mathbf{A}}^{(n)}D_1\left(\mathbf{x}^T\widetilde{\mathbf{C}}\right)\widetilde{\mathbf{B}}^{(n)T}=\mathbf{A}^{(n)}D_1\left(\mathbf{x}^T\mathbf{C}\right)\mathbf{B}^{(n)T},\quad n\in\{1,\ldots,N\}\,. \tag{S.2.5}$$

Denote $\gamma=\omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right)+1$. Like Proposition 4.3 in [1], the result will be based on Lemmas 2.4 and 2.5 in [1], as explained next. Lemma 2.4 in [1] tells us that $C_\gamma\left(\mathbf{AB}\right)=C_\gamma\left(\mathbf{A}\right)C_\gamma\left(\mathbf{B}\right)$ while Lemma 2.5 in [1] states that $\omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right)<\gamma\Leftrightarrow C_\gamma\left(D_1\left(\mathbf{x}^T\widetilde{\mathbf{C}}\right)\right)=\mathbf{0}$. Consequently from (S.2.5) we obtain the relations

$$\begin{aligned}C_\gamma\left(\widetilde{\mathbf{A}}^{(n)}D_1\left(\mathbf{x}^T\widetilde{\mathbf{C}}\right)\widetilde{\mathbf{B}}^{(n)T}\right)&=C_\gamma\left(\widetilde{\mathbf{A}}^{(n)}\right)C_\gamma\left(D_1\left(\mathbf{x}^T\widetilde{\mathbf{C}}\right)\right)C_\gamma\left(\widetilde{\mathbf{B}}^{(n)T}\right)\\&=C_\gamma\left(\mathbf{A}^{(n)}\right)C_\gamma\left(D_1\left(\mathbf{x}^T\mathbf{C}\right)\right)C_\gamma\left(\mathbf{B}^{(n)T}\right)\\&=\mathbf{0},\quad n\in\{1,\ldots,N\}\,,\end{aligned} \tag{S.2.6}$$

where the last equality follows from the fact that $C_\gamma\left(D_1\left(\mathbf{x}^T\widetilde{\mathbf{C}}\right)\right)=\mathbf{0}$. Let us collect the relations (S.2.6) as follows

$$\mathbf{G}^{(\gamma)}\mathrm{Vecd}\left(C_\gamma\left(D_1\left(\mathbf{x}^T\mathbf{C}\right)\right)\right)=\mathbf{0}\,, \tag{S.2.7}$$

where $\mathbf{G}^{(\gamma)}\in\mathbb{C}^{\left(\sum_{n=1}^{Q}C_{I_n}^{\gamma}C_{J_n}^{\gamma}\right)\times C_R^{\gamma}}$ is given by (S.2.1). Since we assume that $\mathbf{G}^{(R-r_{\mathbf{C}}+2)}$ has full column rank, we also known from Lemma S.2.2 that $\mathbf{G}^{(R-r_{\mathbf{C}}+1)},\mathbf{G}^{(R-r_{\mathbf{C}})},\ldots,\mathbf{G}^{(1)}$ all have full column rank. We can now conclude from (S.2.7) that

$$\mathrm{Vecd}\left(C_\gamma\left(D_1\left(\mathbf{x}^T\mathbf{C}\right)\right)\right)=\mathbf{0}.$$

Hence, for any vector $\mathbf{x} \in \mathbb{C}^K$ with property $\omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right) \leq \widetilde{R} - r\left(\widetilde{\mathbf{C}}\right) + 1$ we have $\omega\left(\mathbf{C}^T\mathbf{x}\right) \leq \omega\left(\widetilde{\mathbf{C}}^T\mathbf{x}\right)$. By invoking Lemma S.2.1 we can conclude that $\widetilde{R} = R$ and there exists a unique permutation matrix $\mathbf{P} \in \mathbb{C}^{R\times R}$ and a unique diagonal matrix $\mathbf{D} \in \mathbb{C}^{R\times R}$ such that $\widetilde{\mathbf{C}} = \mathbf{CPD}$. ☐

S.3. Supplementary material related to subsection 4.5. We consider coupled PDs of $\mathcal{X}^{(n)} \in \mathbb{C}^{I_{1,n}\times\cdots\times I_{M_n,n}\times K}$, $n \in \{1,\ldots,N\}$ of the form

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R} \mathbf{a}_r^{(1,n)} \circ \cdots \circ \mathbf{a}_r^{(M_n,n)} \circ \mathbf{c}_r\,, \quad n \in \{1,\ldots,N\}. \tag{S.3.1}$$

We will here explain in a bit more detail how to combine the uniqueness results presented in [3, 4] with a deflation argument in order to establish coupled CPD uniqueness of higher-order tensors of the form (S.3.1).

Let $\{Q_t\}_{t=1}^{T}$ denote a disjoint partitioning of $\{1,\ldots,R\}$, i.e., $Q_t \cap Q_u = \emptyset$, $\forall t \neq u$ and $\cup_{t=1}^{T} Q_t = \{1,\ldots,R\}$. Denote $R_q = \operatorname{card}\left(\cup_{t=q}^{T} Q_t\right)$, meaning that

$$\begin{aligned}
R_1 &= \operatorname{card}(Q_1) + \operatorname{card}(Q_2) + \operatorname{card}(Q_3) + \cdots + \operatorname{card}(Q_T)\\
R_2 &= \operatorname{card}(Q_2) + \operatorname{card}(Q_3) + \cdots + \operatorname{card}(Q_T)\\
&\;\;\vdots\\
R_T &= \operatorname{card}(Q_T)\,.
\end{aligned}$$

Note that $R = R_1$. Define for $t \in \{1,\ldots,T\}$ the following coupled PDs

$$\mathbb{C}^{I_{1,n}\times\cdots\times I_{M_n,n}\times K} \ni \mathcal{X}^{(n,t)} = \sum_{r\in Q_t} \mathbf{a}_{\sigma_t(r)}^{(1,n)} \circ \cdots \circ \mathbf{a}_{\sigma_t(r)}^{(M_n,n)} \circ \mathbf{c}_{\sigma_t(r)}, \quad n \in \{1,\ldots,N\},$$

with factor matrices

$$\begin{aligned}
\mathbf{A}^{(m,n,t)} &= \left[\mathbf{a}_{\sigma_t(1)}^{(m,n)}, \ldots, \mathbf{a}_{\sigma_t(\operatorname{card}(Q_t))}^{(m,n)}\right] \in \mathbb{C}^{I_{m,n}\times \operatorname{card}(Q_t)},\\
\mathbf{C}^{(t)} &= \left[\mathbf{c}_{\sigma_t(1)}, \ldots, \mathbf{c}_{\sigma_t(\operatorname{card}(Q_t))}\right] \in \mathbb{C}^{K\times \operatorname{card}(Q_t)},
\end{aligned}$$

where $\{\sigma_t(r)\}$ denotes the indexing of the rank-1 terms associated with the set Q_t. Note that we have partitioned $\mathcal{X}^{(n)}$, $n \in \{1,\ldots,N\}$, in (S.3.1) as follows

$$\mathcal{X}^{(n)} = \mathcal{X}^{(n,1)} + \mathcal{X}^{(n,2)} + \cdots + \mathcal{X}^{(n,T)}, \quad n \in \{1,\ldots,N\}. \tag{S.3.2}$$

Denote

$$\mathcal{Y}^{(n,t)} = \mathcal{X}^{(n,t)} + \mathcal{X}^{(n,t+1)} + \cdots + \mathcal{X}^{(n,T)}, \quad n \in \{1,\ldots,N\}. \tag{S.3.3}$$

Note that $\mathcal{X}^{(n)} = \mathcal{Y}^{(n,1)}$. The idea is to process $\mathcal{Y}^{(n,t)}$ consecutively for increasing t. Several results in [3, 4] can be used to establish coupled CPD uniqueness for $\{\mathcal{X}^{(n,1)}\}$ (involving $\operatorname{card}(Q_1)$ coupled rank-1 tensors) by working on $\{\mathcal{Y}^{(n,1)}\}$ (involving R coupled rank-1 tensors). In several cases the uniqueness of $\mathbf{A}^{(m,n,1)}$ can be demonstrated after proving uniqueness of the overall matrix $\mathbf{C}$. See subsection 4.5 in [3] for an example. If coupled CPD uniqueness of $\{\mathcal{X}^{(n,1)}\}$ can be proven, then we deflate:

$$\mathcal{Y}^{(n,2)} = \mathcal{Y}^{(n,1)} - \mathcal{X}^{(n,1)}, \quad n \in \{1,\ldots,N\}.$$

Likewise, if we can establish coupled CPD uniqueness of $\{\mathcal{X}^{(n,2)}\}$ (involving card (Q_2) coupled rank-1 tensors) by working on $\{\mathcal{Y}^{(n,2)}\}$ (involving R_2 coupled rank-1 tensors), then we deflate:

$$\mathcal{Y}^{(n,3)} = \mathcal{Y}^{(n,2)} - \mathcal{X}^{(n,2)}, \quad n \in \{1,\ldots,N\}.$$

In general, if there exists a disjoint partitioning $\{Q_t\}_{t=1}^{T}$ of $\{1,\ldots,R\}$ such that we can establish coupled CPD uniqueness of $\{\mathcal{X}^{(n,t)}\}$ (involving card (Q_t) coupled rank-1 tensors) by working on $\{\mathcal{Y}^{(n,t)}\}$ (involving R_t coupled rank-1 tensors) for every $t \in \{1,\ldots,T\}$, then overall coupled CPD uniqueness of $\{\mathcal{X}^{(n)}\}$ in (S.3.1) follows.

S.4. Supplementary material related to section 5. We consider coupled PDs of $\mathcal{X}^{(n)} \in \mathbb{C}^{I_n \times J_n \times K}$, $n \in \{1,\ldots,N\}$ of the following form:

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R}\sum_{l=1}^{L_{r,n}} \mathbf{a}_l^{(r,n)} \circ \mathbf{b}_l^{(r,n)} \circ \mathbf{c}^{(r)} = \sum_{r=1}^{R} \left(\mathbf{A}^{(r,n)}\mathbf{B}^{(r,n)T}\right) \circ \mathbf{c}^{(r)}. \qquad \text{(S.4.1)}$$

We now explain how to extend (S.4.1) to tensors $\mathcal{X}^{(n)} \in \mathbb{C}^{I_{1,n}\times\cdots\times I_{M_n,n}\times K}$ of arbitrary order:

$$\mathcal{X}^{(n)} = \sum_{r=1}^{R}\sum_{l=1}^{L_{r,n}} \mathbf{a}_l^{(r,1,n)} \circ \cdots \circ \mathbf{a}_l^{(r,M_n,n)} \circ \mathbf{c}_r\,, \quad n \in \{1,\ldots,N\}\,. \qquad \text{(S.4.2)}$$

Tensor $\mathcal{X}^{(n)}$ of order $M_n \geq 4$ admits several matrix representations of the form

$$\mathbf{X}^{(w,n)} = \left(\bigodot_{p\in\Gamma_{w,n}} \mathbf{A}^{(p,n)} \odot \bigodot_{q\in\Upsilon_{w,n}} \mathbf{A}^{(q,n)}\right)\mathbf{C}^{(n)T} = \left(\mathbf{A}^{[w,n]} \odot \mathbf{B}^{[w,n]}\right)\mathbf{C}^{(n)T}, \qquad \text{(S.4.3)}$$

where $\Gamma_{w,n}$ and $\Upsilon_{w,n}$ are disjoint sets such that $\Gamma_{w,n}\bigcup\Upsilon_{w,n} = \{1,2,\ldots,M_n\}$ and $\Gamma_{w,n}\bigcap\Upsilon_{w,n} = \emptyset$. Assume that there are W_n such sets for every $n \in \{1,\ldots,N\}$. The factor matrices in (S.4.3) are of the form:

$$\begin{aligned}
\mathbf{A}^{(r,m,n)} &= \left[\mathbf{a}_1^{(r,m,n)},\ldots,\mathbf{a}_{L_{r,n}}^{(r,m,n)}\right] \in \mathbb{C}^{I_{m,n}\times L_{r,n}},\\
\mathbf{A}^{(m,n)} &= \left[\mathbf{A}^{(1,m,n)},\ldots,\mathbf{A}^{(R,m,n)}\right] \in \mathbb{C}^{I_{m,n}\times R_{\text{tot},n}},\\
\mathbf{A}^{[w,n]} &= \bigodot_{p\in\Gamma_{w,n}} \mathbf{A}^{(p,n)} \in \mathbb{C}^{\hat{I}_{w,n}\times R_{\text{tot},n}}, \quad \hat{I}_{w,n} = \prod_{p\in\Gamma_{w,n}} I_{p,n},\\
\mathbf{B}^{[w,n]} &= \bigodot_{q\in\Upsilon_{w,n}} \mathbf{A}^{(q,n)} \in \mathbb{C}^{\hat{J}_{w,n}\times R_{\text{tot},n}}, \quad \hat{J}_{w,n} = \prod_{q\in\Upsilon_{w,n}} I_{q,n},\\
\mathbf{C}^{(n)} &= \left[\mathbf{1}_{L_{r,n}}^T \otimes \mathbf{c}^{(1)},\ldots,\mathbf{1}_{L_{R,n}}^T \otimes \mathbf{c}^{(R)}\right] \in \mathbb{C}^{K\times R_{\text{tot},n}},
\end{aligned}$$

where $R_{\text{tot},n} = \sum_{r=1}^{R} L_{r,n}$. Let

$$\mathbf{C}^{(\text{red})} = \left[\mathbf{c}^{(1)},\ldots,\mathbf{c}^{(R)}\right] \in \mathbb{C}^{K\times R}$$

and define $\mathbf{F}^{(\mathrm{red})} \in \mathbb{C}^{\left(\sum_{n=1}^{N} W_n \prod_{m=1}^{M_n} I_{m,n}\right)\times R}$ as follows

$$\mathbf{F}^{(\mathrm{red})} = \begin{bmatrix} \mathbf{F}^{(1)} \\ \mathbf{F}^{(2)} \\ \vdots \\ \mathbf{F}^{(N)} \end{bmatrix}, \quad \mathbf{F}^{(n)} = \begin{bmatrix} \mathrm{Vec}\left(\mathbf{D}^{[1,1,n]}\right) & \dots & \mathrm{Vec}\left(\mathbf{D}^{[R,1,n]}\right) \\ \mathrm{Vec}\left(\mathbf{D}^{[1,2,n]}\right) & \dots & \mathrm{Vec}\left(\mathbf{D}^{[R,2,n]}\right) \\ \vdots & \ddots & \vdots \\ \mathrm{Vec}\left(\mathbf{D}^{(1,W_N,N)}\right) & \dots & \mathrm{Vec}\left(\mathbf{D}^{(R,W_N,N)}\right) \end{bmatrix},$$

where $\mathbf{D}^{[r,w,n]} = \mathbf{B}^{[r,w,n]}\mathbf{A}^{[r,w,n]T}$, then we obtain the overall matrix representation

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{(1)}^{(1,1)} \\ \mathbf{X}_{(1)}^{(2,1)} \\ \vdots \\ \mathbf{X}_{(1)}^{(W_N,N)} \end{bmatrix} = \mathbf{F}^{(\mathrm{red})}\mathbf{C}^{(\mathrm{red})} \in \mathbb{C}^{\left(\sum_{n=1}^{N} W_n \prod_{m=1}^{M_n} I_{m,n}\right)\times K}. \tag{S.4.4}$$

Alternatively, by appending all-zero column vectors to $\mathbf{A}^{[w,n]}$ and $\mathbf{B}^{[w,n]}$ we can also express (S.4.4) as follows

$$\mathbf{X} = \mathbf{F}^{(\mathrm{ext})}\mathbf{C}^{(\mathrm{ext})T}, \tag{S.4.5}$$

where

$$\mathbf{C}^{(\mathrm{ext})} = \left[\mathbf{1}_{L_{1,\max}}^{T} \otimes \mathbf{c}^{(1)}, \dots, \mathbf{1}_{L_{R,\max}}^{T} \otimes \mathbf{c}^{(R)}\right] \in \mathbb{C}^{K\times R_{\mathrm{ext}}},$$

and $\mathbf{F}^{(\mathrm{ext})} \in \mathbb{C}^{\left(\sum_{n=1}^{N} W_n \prod_{m=1}^{M_n} I_{m,n}\right)\times R_{\mathrm{ext}}}$ is given by

$$\mathbf{F}^{(\mathrm{ext})} = \begin{bmatrix} \mathbf{F}^{(\mathrm{ext},1)} \\ \mathbf{F}^{(\mathrm{ext},2)} \\ \vdots \\ \mathbf{F}^{(\mathrm{ext},N)} \end{bmatrix}, \quad \mathbf{F}^{(\mathrm{ext},n)} = \begin{bmatrix} \widetilde{\mathbf{A}}^{[1,n]} \odot \widetilde{\mathbf{B}}^{[1,n]} \\ \widetilde{\mathbf{A}}^{[2,n]} \odot \widetilde{\mathbf{B}}^{[2,n]} \\ \vdots \\ \widetilde{\mathbf{A}}^{[W_n,n]} \odot \widetilde{\mathbf{B}}^{[W_n,n]} \end{bmatrix},$$

in which

$$\begin{aligned} L_{r,\max} &= \max_{n\in\{1,\dots,N\}} L_{r,n}, \\ R_{\mathrm{ext}} &= \sum_{r=1}^{R} L_{r,\max}, \\ \widetilde{\mathbf{A}}^{(r,m,n)} &= \left[\mathbf{A}^{(r,m,n)}, \mathbf{0}_{I_{m,n},(L_{r,\max}-L_{r,n})}\right] \in \mathbb{C}^{I_{m,n}\times L_{r,\max}}, \\ \widetilde{\mathbf{A}}^{(m,n)} &= \left[\widetilde{\mathbf{A}}^{(1,n)}, \dots, \widetilde{\mathbf{A}}^{(R,n)}\right] \in \mathbb{C}^{I_{m,n}\times R_{\mathrm{ext}}}, \\ \widetilde{\mathbf{A}}^{[w,n]} &= \bigodot_{p\in\Gamma_{w,n}} \widetilde{\mathbf{A}}^{(p,n)} \in \mathbb{C}^{\hat{I}_{w,n}\times R_{\mathrm{ext}}}, \quad \hat{I}_{w,n} = \prod_{p\in\Gamma_{w,n}} I_{p,n}, \\ \widetilde{\mathbf{B}}^{[w,n]} &= \bigodot_{q\in\Upsilon_{w,n}} \widetilde{\mathbf{A}}^{(q,n)} \in \mathbb{C}^{\hat{J}_{w,n}\times R_{\mathrm{ext}}}, \quad \hat{J}_{w,n} = \prod_{q\in\Upsilon_{w,n}} I_{q,n}. \end{aligned}$$

From (S.4.4) and (S.4.5) it is clear that the uniqueness results presented in subsection 5.2 can be extended to coupled tensors of arbitrary order by treating them as a set of coupled third-order tensors.

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