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# Blind Multilinear Identification 

Lek-Heng Lim* and Pierre Comon ${ }^{\ddagger}$, Fellow, IEEE


#### Abstract

We discuss a technique that allows blind recovery of signals or blind identification of mixtures in instances where such recovery or identification were previously thought to be impossible: (i) closely located or highly correlated sources in antenna array processing, (ii) highly correlated spreading codes in CDMA radio communication, (iii) nearly dependent spectra in fluorescent spectroscopy. This has important implications in the case of antenna array processing, it allows for joint localization and extraction of multiple sources from the measurement of a noisy mixture recorded on multiple sensors in an entirely deterministic manner. In the case of CDMA, it allows the possibility of having a number of users larger than the spreading gain. In the case of fluorescent spectroscopy, it allows for detection of nearly identical chemical constituents. The proposed technique involves the solution of a bounded coherence low-rank tensor approximation problem. We show that bounded coherence allows us to establish existence and uniqueness of the recovered solution. We will provide some statistical motivation for the approximation problem and discuss greedy approximation bounds. To provide the theoretical underpinnings for this technique, we develop a corresponding theory of sparse separable decompositions of functions, including notions of rank and Schatten norms that specialize to the usual one for matrices and operators but applies to also hypermatrices and tensors.


## I. InTRODUCTION

THERE are two simple ideas for reducing the complexity or dimension of a problem that are widely applicable because of their simplicity and generality:

- Sparsity: resolving a complicated entity, represented by a function $f$, into a sum of a small number of simple or elemental constituents:

$$
f=\sum_{p=1}^{r} \alpha_{p} g_{p} .
$$

- Separability: decoupling a complicated entity, represented by a function $g$, that depends on multiple factors into a product of simpler constituents, each depending only on one factor:

$$
g\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}\right)=\prod_{k=1}^{d} \varphi_{k}\left(\mathbf{x}_{k}\right)
$$

The two ideas underlie some of the most useful techniques in engineering and science - Fourier, wavelets, and other orthogonal or sparse representations of signals and images, singular value and eigenvalue decompositions of matrices, separation-of-variables, Fast Fourier Transform, mean field

[^0]approximation, etc. This article examines the model that combines these two simple ideas:
\[

$$
\begin{equation*}
f\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}\right)=\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\left(\mathbf{x}_{k}\right) \tag{1}
\end{equation*}
$$

\]

and we are primarily interested in its inverse problem, i.e. identification of the factors $\varphi_{k p}$ based on noisy measurements of $f$. We shall see that this is a surprisingly effective method for a wide range of identification problems.

Here $f$ is approximately encoded by $r$ scalars, $\boldsymbol{\alpha}=$ $\left(\alpha_{1}, \ldots, \alpha_{r}\right) \in \mathbb{C}^{r}$, and $d r$ functions, $\varphi_{k p}, k=1, \ldots, d ;$ $p=1, \ldots, r$. Since $d$ and $r$ are both assumed to be small, we expect (1) to be a very compact, possibly approximate, representation of $f$. We will assume that all these functions live in some Hilbert spaces and that $\varphi_{k p}$ are of unit norm (clearly possible since the norm of $\varphi_{k p}$ can be 'absorbed into' the coefficient $\alpha_{p}$ in (1)).

Let $\mu_{k}=\max _{p \neq q}\left|\left\langle\varphi_{k p}, \varphi_{k q}\right\rangle\right|$ and define the relative incoherence $\omega_{k}=\left(1-\mu_{k}\right) / \mu_{k}$ for $k=1, \ldots, d$. Note that $\mu_{k} \in[0,1]$ and $\omega_{k} \in[0, \infty]$. We will show in this article that if $d \geq 3$, and

$$
\begin{equation*}
\sum_{k=1}^{d} \omega_{k} \geq 2 r-1 \tag{2}
\end{equation*}
$$

then the decomposition in (1) is essentially unique and sparsest possible, i.e. $r$ is minimal. Hence we may in principle identify $\varphi_{k p}$ based only on measurements of the mixture $f$.

One of the keys in the identifiability requirement is that $d \geq 3$ or otherwise (when $d=1$ or 2 ) the result would not hold. We will show that the condition $d \geq 3$ however leads to a difficulty (that does not happen when $d=1$ or 2 ). Since it is rarely, if not never, the case that one has the exact values of $f$, the decomposition (1) is only useful in an idealized scenario. In reality, one has $\hat{f}=f+\varepsilon$, an estimate of $f$ corrupted by noise $\varepsilon$. Solving the inverse problem to (1) would require that we solve a best approximation problem. For example, with the appropriate noise models (see Section V), the best approximation problem often takes the form

$$
\begin{equation*}
\underset{\alpha \in \mathbb{C}^{r},\left\|\varphi_{k p}\right\|=1}{\operatorname{argmin}}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\|, \tag{3}
\end{equation*}
$$

with $\|\cdot\|$ an $L^{2}$-norm. Now the trouble is that when $d \geq 3$, this best approximation problem may not have a solution because the infimum of the loss function is unattainable in general, as we will discuss in Section VIII-A. In view of this, our next result is that when

$$
\begin{equation*}
\prod_{k=1}^{d}\left(1+\omega_{k}\right)>r \tag{4}
\end{equation*}
$$

the infimum in (3) is always attainable, thereby alleviating the aforementioned difficulty. A condition that meets both (2) and (4) is easy to obtain because of the arithmetic-geometric mean inequality

$$
\left[\prod_{k=1}^{d}\left(1+\omega_{k}\right)\right]^{1 / d} \leq 1+\frac{1}{d} \sum_{k=1}^{d} \omega_{k}
$$

## II. Sparse separable decompositions

The notion of sparsity dates back to harmonic analysis [64], [71], [50] and approximation theory [65], and has received a lot of recent attention in compressive sensing [25], [10], [28], [15]. The notion of separability is also classical - the basis behind the separation-of-variables technique in partial differential equations [6] and special functions [53], fast Fourier transforms on arbitrary groups [51], mean field approximations in statistical physics [44], and the naïve Bayes model in machine learning [5], [46]. We describe a simple model that incorporates the two notions.

The function $f: X \rightarrow \mathbb{C}$ or $\mathbb{R}$ to be resolved into simpler entities will be referred to as our target function. We will treat the discrete ( $X$ is finite or countably infinite) and continuous ( $X$ is a continuum) cases on an equal footing. The discrete cases are when $f$ is a vector (if $X=\left[n_{1}\right]=\left\{1, \ldots, n_{1}\right\}$ ), a matrix (if $X=\left[n_{1}\right] \times\left[n_{2}\right]$ ), a hypermatrix (if $X=$ $\left[n_{1}\right] \times\left[n_{2}\right] \times \cdots \times\left[n_{d}\right]$ ), while the usual continuous cases are when $f$ is a function on some domain $X=\Omega \subseteq \mathbb{R}^{m}$ or $\mathbb{C}^{m}$. In the discrete cases, the set of target functions under consideration are identified with $\mathbb{C}^{n_{1}}, \mathbb{C}^{n_{1} \times n_{2}}, \mathbb{C}^{n_{1} \times n_{2} \times \cdots \times n_{d}}$ respectively whereas in the continuous cases, we usually impose some additional regularity structures such integrability or differentability, so that the set of target functions under consideration are $L^{2}(\Omega)$ or $C^{\infty}(\Omega)$ or $H^{k}(\Omega)=W^{k, 2}(\Omega)$, etc. We will only assume that the space of target functions is a Hilbert space. Note that the requirement $d \geq 3$ implies that $f$ is at least a 3-dimensional hypermatrix in discrete case or a function of at least three continuous variables, i.e. $m \geq 3$, in the continuous case. The identifiability does not work for (usual 2-dimensional) matrices or bivariate functions. With (1) in mind, we will call $f$ a $d$-partite or multipartite function if we wish to partition its arguments into $d$ blocks of variables.

We will briefly examine the decompositions and approximations of our target function into a sum or integral of separable functions, adopting a tripartite notation for simplicity. There are three cases:

- Continuous:

$$
\begin{equation*}
f(\mathbf{x}, \mathbf{y}, \mathbf{z})=\int_{T} \theta(\mathbf{x}, \mathbf{t}) \varphi(\mathbf{y}, \mathbf{t}) \psi(\mathbf{z}, \mathbf{t}) d \nu(\mathbf{t}) \tag{5}
\end{equation*}
$$

Here we assume that $\nu$ is some given Borel measure and that $T$ is compact.

- Semidiscrete:

$$
\begin{equation*}
f(\mathbf{x}, \mathbf{y}, \mathbf{z})=\sum_{p=1}^{r} \theta_{p}(\mathbf{x}) \varphi_{p}(\mathbf{y}) \psi_{p}(\mathbf{z}) \tag{6}
\end{equation*}
$$

This may be viewed as a discretization of the continuous case in the $\mathbf{t}$ variable, i.e. $\theta_{p}(\mathbf{x})=\theta\left(\mathbf{x}, \mathbf{t}_{p}\right), \varphi_{p}(\mathbf{y})=$ $\varphi\left(\mathbf{y}, \mathbf{t}_{p}\right), \psi_{p}(\mathbf{z})=\psi\left(\mathbf{z}, \mathbf{t}_{p}\right)$.

## - Discrete:

$$
\begin{equation*}
a_{i j k}=\sum_{p=1}^{r} u_{i p} v_{j p} w_{k p} \tag{7}
\end{equation*}
$$

This may be viewed as a further discretization of the semidiscrete case, i.e. $a_{i j k}=f\left(\mathbf{x}_{i}, \mathbf{y}_{j}, \mathbf{z}_{k}\right), u_{i p}=\theta_{p}\left(\mathbf{x}_{i}\right)$, $v_{j p}=\varphi_{p}\left(\mathbf{y}_{j}\right), w_{k p}=\psi_{p}\left(\mathbf{z}_{k}\right)$.
It is clear that when $i, j, k$ take finitely many values, the discrete decomposition (7) is always possible with a finite $r$ since the space is of finite dimension. If $i, j, k$ could take infinitely many values, then the finiteness of $r$ requires that equality be replaced by approximation to any arbitrary precision $\varepsilon>0$ in some suitable norm. This follows from the following observation about the semidiscrete decomposition: The space of functions with a semidiscrete representation as in (6), with $r$ finite, is dense in $C^{0}(\Omega)$, the space of continuous functions. This is just a consequence of the Stone-Weierstrass theorem [21]. Discussion of the most general case (5) would require us to go into integral operators, which we will not do as in the present framework we are interested in applications that rely on the inverse problems corresponding to (6) and (7). Nonetheless (5) is expected to be useful and we state it here for completeness. Henceforth, we will drop the adjective 'semidiscrete' or 'discrete' and simply refer to (6) or (7) as a decomposition into a sum of separable functions (SS). Note that SS decompositions have been already proposed in the past and received many different names. In particular, in finite dimension, the acronym CP is now widely used, and stands either for Candecomp/Parafac or for Canonical Polyadic decompositions.

We will also frame our discussions in terms of the semidiscrete case (6), since this also includes the discrete case (7) (when $\mathbf{x}, \mathbf{y}, \mathbf{z}$ take only finite discrete values).

Example 1. SS decompositions arise in many contexts. For example, in machine learning and nonparametric statistics, a fact of note is that Gaussians are separable

$$
\exp \left(x^{2}+y^{2}+z^{2}\right)=\exp \left(x^{2}\right) \exp \left(y^{2}\right) \exp \left(z^{2}\right)
$$

More generally for symmetric positive-definite $A \in \mathbb{R}^{n \times n}$ with eigenvalues $\Lambda=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{n}\right)$,

$$
\exp \left(\mathbf{x}^{\top} A \mathbf{x}\right)=\exp \left(\mathbf{z}^{\top} \Lambda \mathbf{z}\right)=\prod_{i=1}^{n} \exp \left(\lambda_{i} z_{i}^{2}\right)
$$

under a linear change of coordinates $\mathbf{z}=Q^{\top} \mathbf{x}$ where $A=$ $Q \Lambda Q^{\top}$. Hence, Gaussian mixture models of the form

$$
f(\mathbf{x})=\sum_{j=1}^{m} \alpha_{j} \exp \left[\left(\mathbf{x}-\boldsymbol{\mu}_{j}\right)^{\top} A_{j}\left(\mathbf{x}-\boldsymbol{\mu}_{j}\right)\right]
$$

where $A_{i} A_{j}=A_{j} A_{i}$ for all $i \neq j$ (and therefore $A_{1}, \ldots, A_{m}$ have a common eigenbasis) may likewise be transformed with a suitable linear change of coordinates into a SS decomposition as in (6).

We will later see several more examples from signal processing and spectroscopy.

## A. Modeling

The SS decomposition - an additive decomposition into multiplicatively decomposable components - is extremely simple but models a wide range of phenomena in signal processing and spectroscopy. The main message of this article is that the corresponding inverse problem - recovering the factors $\theta_{p}, \varphi_{p}, \psi_{p}$ from noisy measurements of $f$ can be solved under mild assumptions and yields a class of techniques for a range of applications (cf. Section IX) that we shall collectively call multilinear identification. We wish to highlight in particular that multilinear identification gives a determistic approach for solving the problem of joint localization and estimation of radiating sources with short data lengths. Previous approaches based on cumulants [18] require not only longer data lengths but also sources to be statistically independent.

The experienced reader would probably guess that such a powerful technique must be fraught with difficulties and he would be right. The inverse problem to (6), like most other inverse problems, faces issues of existence, uniqueness, and computability. The approximation problem involved can be illposed in the worst possible way (cf. Section III). Fortunately, prompted by study of the restricted isometry property in compressed sensing (interpreted in a broad sense, encompassing not only the ideas covered in [10], [9], [15], [25], [26], [32] but also in [7], [8], [29], [33]), we will show here that mild assumptions on coherence could allow one to overcome most of these difficulties (cf. Section VIII)

## III. Finite rank multipartite functions

In this section, we will discuss the notion of rank, which measures the sparsity of a SS decomposition, and the notion of Kruskal rank, which measures the uniqueness of a SS decomposition in a somewhat more restrictive sense. Why is uniqueness important? It can be answered in one word: Identifiability. More specifically, a unique decomposition means that we may in principle identify the factors. To be completely precise, we will first need to define the terms in the previous sentence, namely, 'unique', 'decomposition', and 'factor'. Before we do that, we will introduce the tensor product notation. It is not necessary to know anything about tensor product of Hilbert spaces to follow what we present below. We shall assume that all our Hilbert spaces are separable and so there is no loss of generality in assuming at the outset that they are just $L^{2}(X)$ for some $\sigma$-finite $X$.

Let $X_{1}, \ldots, X_{d}$ be $\sigma$-finite measurable spaces. There is a natural Hilbert space isomorphism

$$
\begin{equation*}
L^{2}\left(X_{1} \times \cdots \times X_{d}\right) \cong L^{2}\left(X_{1}\right) \otimes \cdots \otimes L^{2}\left(X_{d}\right) \tag{8}
\end{equation*}
$$

In other words, every $d$-partite $L^{2}$-function $f: X_{1} \times \cdots \times$ $X_{d} \rightarrow \mathbb{C}$ may be expressed as ${ }^{1}$

$$
\begin{equation*}
f\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}\right)=\sum_{p=1}^{\infty} \varphi_{1 p}\left(\mathbf{x}_{1}\right) \cdots \varphi_{d p}\left(\mathbf{x}_{d}\right) \tag{9}
\end{equation*}
$$

[^1]with $\varphi_{k p} \in L^{2}\left(X_{k}\right)$. The tensor product of functions $\varphi_{1} \in$ $L^{2}\left(X_{1}\right), \ldots, \varphi_{d} \in L^{2}\left(X_{d}\right)$ is denoted by $\varphi_{1} \otimes \cdots \otimes \varphi_{d}$ and is the function in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ defined by
$$
\varphi_{1} \otimes \cdots \otimes \varphi_{d}\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}\right)=\varphi_{1}\left(\mathbf{x}_{1}\right) \cdots \varphi_{d}\left(\mathbf{x}_{d}\right)
$$

With this notation, we may rewrite (9) as

$$
f=\sum_{p=1}^{\infty} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}
$$

A point worth noting here is that:

> "Multipartite functions are infinite-dimensional tensors."

Finite-dimensional tensors are simply the special case when $X_{1}, \ldots, X_{d}$ are all finite sets (see Example 6). In particular, a multivariate function ${ }^{2} f \in L^{2}\left(\mathbb{R}^{d}\right)$ is a an infinite-dimensional tensor that can expressed as an infinite sum of a tensor product of $\varphi_{1 p}, \ldots, \varphi_{d p} \in L^{2}(\mathbb{R})$ and $L^{2}\left(\mathbb{R}^{d}\right) \cong L^{2}(\mathbb{R}) \otimes \cdots \otimes L^{2}(\mathbb{R})$. We shall have more to say about this later in conjunction with Kolmogorov's superposition principle for multivariate functions.

In this paper, functions having a finite decomposition will play a central role; for these we define

$$
\begin{equation*}
\operatorname{rank}(f):=\min \left\{r \in \mathbb{N}: f=\sum_{p=1}^{r} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\} \tag{10}
\end{equation*}
$$

provided $f \neq 0$. The zero function is defined to have rank 0 and we say $\operatorname{rank}(f)=\infty$ if such a decomposition is not possible.

We will call a function $f$ with $\operatorname{rank}(f) \leq r$ a rank- $r$ function. Such a function may be written as a sum of $r$ separable functions but possibly fewer. A decomposition of the form

$$
\begin{equation*}
f=\sum_{p=1}^{r} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p} \tag{11}
\end{equation*}
$$

will be called an rank- $r$ SS decomposition. Note that the qualificative 'rank- $r$ ' will always mean 'rank not more than $r^{\prime}$. If we wish to refer to a function $f$ with rank exactly $r$, we will just specify that $\operatorname{rank}(f)=r$. In this case, the rank- $r$ SS decomposition in (11) is of mininum length and we call it a rank revealing $S S$ decomposition of $f$.

A rank-1 function is both non-zero and decomposable, i.e., of the form $\varphi_{1} \otimes \cdots \otimes \varphi_{d}$ where $\varphi_{k} \in L^{2}\left(X_{k}\right)$. This agrees precisely with the notion of a separable function. Observe that the inner product (and therefore the norm) on $L^{2}\left(X_{1} \times \cdots \times\right.$ $X_{d}$ ) of a rank-1 function splits into a product

$$
\begin{equation*}
\left\langle\varphi_{1} \otimes \cdots \otimes \varphi_{d}, \psi_{1} \otimes \cdots \otimes \psi_{d}\right\rangle=\left\langle\varphi_{1}, \psi_{1}\right\rangle_{1} \cdots\left\langle\varphi_{d}, \psi_{d}\right\rangle_{d} \tag{12}
\end{equation*}
$$

where $\langle\cdot, \cdot\rangle_{p}$ denotes the inner product of $L^{2}\left(X_{p}\right)$. This inner product extends linearly to finite-rank elements of $L^{2}\left(X_{1} \times\right.$

[^2]$\left.\cdots \times X_{d}\right)$ : for $f=\sum_{p=1}^{r} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}$ and $g=\sum_{q=1}^{s} \psi_{1 q} \otimes$ $\cdots \otimes \psi_{d q}$, we have
$$
\langle f, g\rangle=\sum_{p, q=1}^{r, s}\left\langle\varphi_{1 p}, \psi_{1 q}\right\rangle_{1} \cdots\left\langle\varphi_{d p}, \psi_{d q}\right\rangle_{d}
$$

In fact this is how a tensor product of Hilbert spaces (the right hand side of (8)) is usually defined, namely, as the completion of the set of finite-rank elements of $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ under this inner product.

When $X_{1}, \ldots, X_{d}$ are finite sets, then all functions in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ are of finite rank (and may in fact be viewed as hypermatrices or tensors as discussed in Section II). Otherwise there will be functions in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ of infinite rank. However, since we have assumed that $X_{1}, \ldots, X_{d}$ are $\sigma$-finite measurable spaces, the set of all finite-rank $f$ will always be dense in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ by the Stone-Weierstrass theorem.

The next statement is a straightforward observation about rank-revealing SS decompositions of finite-rank functions but since it is central to this article we state it as a theorem. It is also tempting to call the decomposition a 'singular value decomposition' given its similarities with the usual matrix singular value decomposition (cf. Example 4).

Theorem 2 ('Singular value decomposition' for multipartite functions). Let $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ be of finite rank. Then there exists a rank-r SS decomposition

$$
\begin{equation*}
f=\sum_{p=1}^{r} \sigma_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p} \tag{13}
\end{equation*}
$$

such that

$$
\begin{equation*}
r=\operatorname{rank}(f) \tag{14}
\end{equation*}
$$

the functions $\varphi_{k p} \in L^{2}\left(X_{p}\right)$ are of unit norm,

$$
\begin{equation*}
\left\|\varphi_{k p}\right\|=1 \quad \text { for all } k=1, \ldots, d, \quad p=1, \ldots, r \tag{15}
\end{equation*}
$$

the coefficients $\sigma_{1}, \ldots, \sigma_{r}$ are real positive, and

$$
\begin{equation*}
\sigma_{1} \geq \sigma_{2} \geq \cdots \geq \sigma_{r}>0 \tag{16}
\end{equation*}
$$

Proof: This requires nothing more than rewriting the sum in (11) as a linear combination with the positive $\sigma_{p}$ 's accouning for the norms of the summands and then re-indexing them in descending order of magnitudes.

While the usual singular value decomposition of a matrix would also have properties (14), (15), and (16), the one crucial difference here is that our 'singular vectors' $\varphi_{k 1}, \ldots, \varphi_{k r}$ in (13) will only be of unit norms but will not in general be orthonormal. Given this, we will not expect properties like the Eckhart-Young theorem, or that $\sigma_{1}^{2}+\cdots+\sigma_{r}^{2}=\|f\|^{2}$, etc, to hold for (13) (cf. Section VI for more details).

One may think of the SS decomposition (13) as being similar in spirit, although not in substance, to Kolmogorov's superposition principle [39]; the main message of which is that:
"There are no true multivariate functions."
More precisely, the principle states that continuous functions in multiple variables can be expressed as a composition of a
univariate function with other univariate functions. For readers not familiar with this remarkable result, we state a version of it here due to Kahane [38]
Theorem 3 (Kolmogorov superposition). Let $f:[0,1]^{d} \rightarrow \mathbb{R}$ be continuous. Then there exists constants $\lambda_{1}, \ldots, \lambda_{d} \in \mathbb{R}$ and Lipschitz continuous functions $\varphi_{1}, \ldots, \varphi_{d}:[0,1] \rightarrow[0,1]$ such that

$$
f\left(x_{1}, \ldots, x_{d}\right)=\sum_{p=1}^{2 d+1} g\left(\lambda_{1} \varphi_{p}\left(x_{1}\right)+\cdots+\lambda_{d} \varphi_{p}\left(x_{d}\right)\right)
$$

It is in general not easy to determine $g$ and $\varphi_{1}, \ldots, \varphi_{2 d+1}$ given such a function $f$. A SS decomposition of the form (13) alleviates this by allowing $g$ to be the simplest multivariate function, namely, the product function,

$$
\begin{equation*}
g\left(t_{1}, \ldots, t_{d}\right)=t_{1} t_{2} \cdots t_{d} \tag{17}
\end{equation*}
$$

and unlike the univariate $g$ in Theorem 3, the $g$ in (17) works universally for any function $f$ - only the $\varphi_{p}$ 's need to be constructed. Furthermore, (13) applies more generally to functions on a product of general domains $X_{1}, \ldots, X_{d}$ whereas Theorem 3 only applies if they are compact intervals of $\mathbb{R}$.

At this stage, it would be instructive to give a few examples for concreteness.

Example 4. Let $A \in \mathbb{C}^{m \times n}$ be a matrix of rank $r$. Then it can be decomposed in infinitely many ways into a sum of rank-1 terms as

$$
\begin{equation*}
A=\sum_{p=1}^{r} \sigma_{p} \mathbf{u}_{p} \mathbf{v}_{p}^{*} \tag{18}
\end{equation*}
$$

where $\mathbf{u}_{p} \in \mathbb{C}^{m}$ and $\mathbf{v}_{p} \in \mathbb{C}^{n}$ are unit-norm vectors and $\sigma_{1} \geq \cdots \geq \sigma_{r}>0$. Note that if we regard $A$ as a complexvalued function on its row and column indices $i$ and $j$ as described earlier in Section II, then (18) may be written as

$$
a(i, j)=\sum_{p=1}^{r} \sigma_{p} u_{p}(i) v_{p}(j)
$$

which clearly is the same as (9). The singular value decomposition (SVD) of A yields one such decomposition, where $\left\{\mathbf{u}_{1}, \ldots, \mathbf{u}_{r}\right\}$ and $\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{r}\right\}$ are both orthonormal. But in general a rank-revealing decomposition of the form (13) will not have such a property.

Example 5. The previous example can be generalized to infinite dimensions. Let $A: \mathbb{H}_{1} \rightarrow \mathbb{H}_{2}$ be a compact operator (also known as a completely continuous operator) between two separable Hilbert spaces. Then the Schmidt decomposition theorem says that there exist orthonormal basis $\left\{\varphi_{p} \in \mathbb{H}_{2}\right.$ : $p \in \mathbb{N}\}$ and $\left\{\psi_{p} \in \mathbb{H}_{1}: p \in \mathbb{N}\right\}$ so that

$$
\begin{equation*}
A f=\sum_{p=1}^{\infty} \sigma_{p}\left\langle\psi_{p}, f\right\rangle \varphi_{p} \tag{19}
\end{equation*}
$$

for every $f \in \mathbb{H}_{1}$. In tensor product notation, (19) becomes

$$
A=\sum_{p=1}^{\infty} \sigma_{p} \varphi_{p} \otimes \psi_{p}^{*}
$$

where $\psi_{p}^{*}$ denotes the dual form of $\psi_{p}$.
Examples 4 and 5 are well-known but they are bipartite examples, i.e. $d=2$ in (13). This article is primarily concerned with the $d$-partite case where $d \geq 3$, which has received far less attention. As we have alluded to in the previous section, the identification techniques in this article will rely crucially on the fact that $d \geq 3$.

Example 6. Let $A \in \mathbb{C}^{l \times m \times n}$ be a 3 -dimensional hypermatrix. The outer product of three vectors $\mathbf{u} \in \mathbb{C}^{l}, \mathbf{v} \in \mathbb{C}^{m}$, $\mathbf{w} \in \mathbb{C}^{n}$ is defined by

$$
\mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w}=\left(u_{i} v_{j} w_{k}\right)_{i, j, k=1}^{l, m, n} \in \mathbb{C}^{l \times m \times n}
$$

The rank of $A$ is defined to be the minimum $r \in \mathbb{N}$ such that $A$ can be written in the form

$$
\begin{equation*}
A=\sum_{p=1}^{r} \sigma_{p} \mathbf{u}_{p} \otimes \mathbf{v}_{p} \otimes \mathbf{w}_{p} \tag{20}
\end{equation*}
$$

and if $A=0$, then its rank is set to be 0 . This agrees of course with our use of the word rank in (10), the only difference is notational, since (20) may be written in the form

$$
a(i, j, k)=\sum_{p=1}^{r} \sigma_{p} u_{p}(i) v_{p}(j) w_{p}(k) .
$$

This definition of rank is invariant under the natural action of $\mathrm{GL}(l) \times \mathrm{GL}(m) \times \mathrm{GL}(n)$ on $\mathbb{C}^{l \times m \times n}$ [22, Lemma 2.3], i.e. for any $X \in \mathrm{GL}(l), Y \in \mathrm{GL}(m), Z \in \mathrm{GL}(n)$,

$$
\begin{equation*}
\operatorname{rank}((X, Y, Z) \cdot A)=\operatorname{rank}(A) \tag{21}
\end{equation*}
$$

The definition also extends easily to d-dimensional hypermatrices in $\mathbb{C}^{n_{1} \times \cdots \times n_{d}}$ and when $d=2$ reduces to the usual definition in Example 4 for matrix rank. This definition is due to F. L. Hitchcock [36] and is often called tensor rank. The only difference here is that our observation in Theorem 2 allows us to impose the conditions

$$
\sigma_{1} \geq \sigma_{2} \geq \cdots \geq \sigma_{r}
$$

and

$$
\begin{equation*}
\left\|\mathbf{u}_{p}\right\|=\left\|\mathbf{v}_{p}\right\|=\left\|\mathbf{w}_{p}\right\|=1, \quad p=1, \ldots, r \tag{22}
\end{equation*}
$$

while leaving $\operatorname{rank}(A)$ unchanged, thus bringing (20) closer in form to its matrix cousin (18). What is lost here is that the sets $\left\{\mathbf{u}_{1}, \ldots, \mathbf{u}_{r}\right\},\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{r}\right\},\left\{\mathbf{w}_{1}, \ldots, \mathbf{w}_{r}\right\}$ can no longer be chosen to be orthonormal as in Example 4, the unit norm condition (22) is as far as we may go. In fact for a generic $A \in \mathbb{C}^{l \times m \times n}$, we will always have

$$
r>\max (l, m, n)
$$

and $\left\{\mathbf{u}_{1}, \ldots, \mathbf{u}_{r}\right\},\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{r}\right\},\left\{\mathbf{w}_{1}, \ldots, \mathbf{w}_{r}\right\}$ will be overcomplete sets in $\mathbb{C}^{l}, \mathbb{C}^{m}, \mathbb{C}^{n}$ respectively.

Perhaps it is worthwhile saying a word concerning our use of the words 'tensor' and 'hypermatrix': A $d$-tensor or order$d$ tensor is an element of a tensor product of $d$ vector spaces $\mathbb{V}_{1} \otimes \cdots \otimes \mathbb{V}_{d} ;$ a $d$-dimensional hypermatrix is an element of $\mathbb{C}^{n_{1} \times \cdots \times n_{d}}$. If we choose bases on $\mathbb{V}_{1}, \ldots, \mathbb{V}_{d}$, then any $d$-tensor $\mathbf{A} \in \mathbb{V}_{1} \otimes \cdots \otimes \mathbb{V}_{d}$ will have a unique coordinate representation as a $d$-dimensional hypermatrix $A \in \mathbb{C}^{n_{1} \times \cdots \times n_{d}}$,
where $n_{k}=\operatorname{dim}\left(\mathbb{V}_{k}\right)$. A notion defined on a hypermatrix is only defined on the tensor (that is represented in coordinates by the hypermatrix) if that notion is independent of the choice of bases. So the use of the word 'tensor rank' is in fact well justified because of (21). For more details, we refer the reader to [45].

## IV. Uniqueness of SS decompositions

In Theorem 2, we chose the coefficients to be in descending order of magnitude and require the factors in each separable term to be of unit norm. This is largely to ensure as much uniqueness in the SS decomposition as generally possible. However there remain two obvious ways to obtain trivially different SS decompositions: (i) one may scale the factors $\varphi_{1 p}, \ldots, \varphi_{d p}$ by arbitrary unimodulus complex numbers as long as their product is 1 ; (ii) when two or more successive coefficients are equal, their orders in the sum may be arbitrarily permuted. We will call a SS decomposition of $f$ that meets the conditions in Theorem 2 essentially unique if the only other such decompositions of $f$ differ in one or both of these manners.

It is perhaps astonishing that when $d>2$, a sufficient condition for essential uniqueness can be derived with relatively mild conditions on the factors. This relies on the notion of Kruskal rank, which we will now define.
Definition 7. Let $\Phi=\left\{\varphi_{1}, \ldots, \varphi_{r}\right\}$ be a finite collection of vectors of unit norm in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$. The Kruskal rank of $\Phi$, denoted $\operatorname{krank} \Phi$, is the largest $k \in \mathbb{N}$ so that every $k$-element subset of $\Phi$ contains linearly independent elements.

This notion was originally introduced in [40]. It is related to the notion of spark introduced in compressed sensing [26], [32], defined as the smallest $k \in \mathbb{N}$ so that there is at least one $k$-element subset of $\Phi$ that is linearly dependent. The relation is simple to describe, $\operatorname{spark} \Phi=\operatorname{krank} \Phi+1$, and it follows immediately from the respective definitions. It is clear that $\operatorname{dim} \operatorname{span} \Phi \geq \operatorname{krank} \Phi$.

We now generalize Kruskal's famous result [40], [59] to tensor products of arbitrary Hilbert spaces, possibly of infinite dimensions. But first let us be more specific about essential uniqueness.

Definition 8. We shall say that a SS decomposition of the form (13) (satisfying both (16) and (15)) is essentially unique if given another such decomposition,

$$
\sum_{p=1}^{r} \sigma_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}=f=\sum_{p=1}^{r} \lambda_{p} \psi_{1 p} \otimes \cdots \otimes \psi_{d p}
$$

we must have (i) the coefficients $\sigma_{p}=\lambda_{p}$ for all $p=1, \ldots, r$; and (ii) the factors $\varphi_{1 p}, \ldots, \varphi_{d p}$ and $\psi_{1 p}, \ldots, \psi_{d p}$ differ at most via unimodulus scaling, i.e.

$$
\begin{equation*}
\varphi_{1 p}=e^{i \theta_{1 p}} \psi_{1 p}, \ldots, \varphi_{d p}=e^{i \theta_{d p}} \psi_{d p} \tag{23}
\end{equation*}
$$

where $\theta_{1 p}+\cdots+\theta_{d p} \equiv 0 \bmod 2 \pi$, for all $p=1, \ldots, r$. In the event when successive coefficients are equal, $\sigma_{p-1}>\sigma_{p}=$ $\sigma_{p+1}=\cdots=\sigma_{p+q}>\sigma_{p+q+1}$, the uniqueness of the factors in (ii) is only up to relabelling of indices, i.e. $p, \ldots, p+q$.

Lemma 9. Let $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$. Then a SS decomposition of the form

$$
\begin{equation*}
f=\sum_{p=1}^{r} \sigma_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p} \tag{24}
\end{equation*}
$$

is both essentially unique and rank-revealing, i.e. $r=\operatorname{rank} f$, if the following condition is satisfied:

$$
\begin{equation*}
2 r+d-1 \leq \sum_{k=1}^{d} \operatorname{krank} \Phi_{k} \tag{25}
\end{equation*}
$$

where $\Phi_{k}=\left\{\varphi_{k 1}, \ldots, \varphi_{k r}\right\}$ for $k=1, \ldots, d$.
Proof: Consider the subspaces $\mathbb{V}_{k}=\operatorname{span}\left(\varphi_{k 1}, \ldots, \varphi_{k r}\right)$ in $L^{2}\left(X_{k}\right)$ for each $k=1, \ldots, d$. Observe that $f \in \mathbb{V}_{1} \otimes \cdots \otimes$ $\mathbb{V}_{d}$. Clearly $\operatorname{dim}\left(\mathbb{V}_{k}\right) \leq r$ and so $\operatorname{dim}\left(\mathbb{V}_{1} \otimes \cdots \otimes \mathbb{V}_{d}\right) \leq r^{d}$. Now if we could apply Kruskal's result [40] to the finitedimensional space $\mathbb{V}_{1} \otimes \cdots \otimes \mathbb{V}_{d}$, then we may immediately deduce both the uniqueness and rank-revealing property of (24). However there is one caveat: We need to show that Kruskal rank does not change under restriction to a subspace, i.e. the value of $\operatorname{krank}\left\{\varphi_{k 1}, \ldots, \varphi_{k r}\right\}$ in (25) is the same whether we regard $\varphi_{k 1}, \ldots, \varphi_{k r}$ as elements of $L^{2}\left(X_{k}\right)$ or as elements of the subspace $\mathbb{V}_{k}$. But this just follows from the simple fact that linear independence has precisely this property, i.e. if $v_{1}, \ldots, v_{n} \in \mathbb{U} \subseteq \mathbb{V}$ are linearly independent in the vector space $\mathbb{V}$, then then they are linearly independent in the subspace $\mathbb{U}$.

It follows immediately why we usually need $d \geq 3$ for identifiability.

## Corollary 10. A necessary condition for Kruskal's inequality

 (25) to hold is that $d \geq 3$.Proof: If $d=2$, then $2 r+d-1=2 r+1>\operatorname{krank} \Phi_{1}+$ krank $\Phi_{2}$ since the Kruskal rank of of $r$ vectors cannot exceed $r$. Likewise for $d=1$.

Lemma 9 shows that the condition in (25) is sufficient to ensure uniqueness and it is known that the condition is not necessary. In an appropriate sense, the condition is sharp [24]. We should note that the version of Lemma 9 that we state here for general $d \geq 3$ is due to Sidiropoulos and Bro [59]. Kruskal's original version [40] is only for $d=3$.

The main problem with Lemma 9 is that the condition (25) is difficult to check since the right-hand side cannot be readily computed. In fact Kruskal rank is known to be NP-complete over a field of two elements [70]. We conjecture that it is NP-hard over $\mathbb{R}$ and $\mathbb{C}$.

Kruskal's result also does not tell us how often are SS decompositions unique. In the event when the sets $X_{1}, \ldots, X_{d}$ are finite, $L^{2}\left(X_{1} \times \cdots \times X_{d}\right) \cong \mathbb{C}^{n_{1} \times \cdots \times n_{d}}$ where $n_{1}=$ $\# X_{1}, \ldots, n_{d}=\# X_{d}$, and there is a simple result on uniqueness based simply on a dimension count. Note that the dimension of $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ is the product $n_{1} \cdots n_{d}$ and the number of parameters needed to describe a separable element of the form $\lambda \varphi_{1} \otimes \cdots \otimes \varphi_{d}$ where $\varphi_{1}, \ldots, \varphi_{d}$ are of unit norm is $n_{1}+\cdots+n_{d}-d+1$ (each $\varphi_{k}$ requires $n_{k}-1$ parameters because of the unit norm constraint, the last ' +1 '
accounts for the coefficient $\lambda$ ). We call the number

$$
\left\lceil\frac{\prod_{k=1}^{d} n_{k}}{1-d+\sum_{k=1}^{d} n_{k}}\right\rceil
$$

the expected rank of $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$, since it is heuristically the minimum $r$ expected for a SS decomposition (13).

Proposition 11. Let the notations be as above. If $f \in L^{2}\left(X_{1} \times\right.$ $\cdots \times X_{d}$ ) has rank smaller than the expected rank, i.e.

$$
\operatorname{rank}(f)<\left\lceil\frac{\prod_{k=1}^{d} n_{k}}{1-d+\sum_{k=1}^{d} n_{k}}\right\rceil
$$

then $f$ admits at most a finite number of distinct rank revealing decompositions.

This proposition has been proved in several cases, including symmetric tensors [14], but the proof still remains incomplete for tensors of most general form [13], [1].

## V. Estimation of SS decompositions

In practice we would only have at our disposal $\hat{f}$, a measurement of $f$ corrupted by noise. Recall that our model for $f$ takes the form

$$
\begin{equation*}
f\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}\right)=\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\left(\mathbf{x}_{k}\right) \tag{26}
\end{equation*}
$$

Then we would often have to solve an approximation problem corresponding to (26) of the form

$$
\begin{equation*}
\underset{\alpha \in \mathbb{C}^{r},\left\|\varphi_{k p}\right\|=1}{\operatorname{argmin}}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\|, \tag{27}
\end{equation*}
$$

which we will call a best rank-r approximation problem. A solution to (27), if exists, will be called a best rank-r approximation of $\hat{f}$.

In this section, we will give some motivations as to why such an approximation is reasonable. Assuming that the norm in (27) is the $L^{2}$-norm and that the factors $\varphi_{k p}, p=1, \ldots r$ and $k=1, \ldots d$, have been determined in advance and we are just trying to estimate the parameters $\alpha_{1}, \ldots, \alpha_{r}$ from $\hat{f}^{(1)}, \ldots, \hat{f}^{(N)}$ a finite sample of size $N$ of measurements of $f$ corrupted by noise, then the solution of the approximation problem in (27) is in fact (i) a maximum likelihood estimator (MLE) if the noise is zero mean Gaussian, and (ii) a best linear unbiased estimator (BLUE) if the noise has zero mean and finite variance. Of course in our identification problems, the factors $\varphi_{k p}$ 's are not known and have to be estimated too. A probabilistic model in this situation would take us too far afield. Note that even for the case $d=2$ and where $X_{1}$ and $X_{2}$ are finite sets, a case that essentially reduces to principal components analysis (PCA), a probabilistic model along the lines of [67] require several strong assumptions and was only developed as late as 1999. The lack of a formal probabilistic model has not stopped PCA, proposed in 1901 [56], to be an invaluable tool in the intervening century.

## VI. Existence of best SS approximation

As we mentioned in the previous section, in realistic situation where measurements are corrupted by additive noise, one has to extract the factors $\varphi_{k p}$ 's and $\alpha_{p}$ through solving an approximation problem (27), that we now write in a slightly different (but equivalent) form,

$$
\begin{equation*}
\underset{\alpha \in[0, \infty)^{r},\left\|\varphi_{k p}\right\|=1}{\operatorname{argmin}}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\| . \tag{28}
\end{equation*}
$$

Note that by Theorem 2, we may assume that the coefficients $\boldsymbol{\alpha}=\left(\alpha_{1}, \ldots, \alpha_{r}\right)$ are real and nonnegative valued without any loss of generality. Such a form is also natural in applications given that $\alpha_{p}$ usually captures the magnitude of whatever quantity that is represented by the $p$ summand.

We will see this problem, whether in the form (27) or (28), has no solution in general. We will first observe a somewhat unusual phenomenon in SS decomposition of $d$ partite functions where $d \geq 3$, namely, a sequence of rank$r$ functions (each with an rank- $r$ SS decomposition) can converge to a limit that is not rank-r (has no rank-r SS decomposition).
Example 12 (SS approximation of functions). For linearly independent $\varphi_{1}, \psi_{1}: X_{1} \rightarrow \mathbb{C}, \varphi_{2}, \psi_{2}: X_{2} \rightarrow \mathbb{C}, \varphi_{3}, \psi_{3}:$ $X_{3} \rightarrow \mathbb{C}$, let $\hat{f}: X_{1} \times X_{2} \times X_{3} \rightarrow \mathbb{C}$ be

$$
\begin{aligned}
& \hat{f}\left(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}\right):=\psi_{1}\left(\mathbf{x}_{1}\right) \varphi_{2}\left(\mathbf{x}_{2}\right) \varphi_{3}\left(\mathbf{x}_{3}\right) \\
& \quad+\varphi_{1}\left(\mathbf{x}_{1}\right) \psi_{2}\left(\mathbf{x}_{2}\right) \varphi_{3}\left(\mathbf{x}_{3}\right)+\varphi_{1}\left(\mathbf{x}_{1}\right) \varphi_{2}\left(\mathbf{x}_{2}\right) \psi_{3}\left(\mathbf{x}_{3}\right)
\end{aligned}
$$

For $n \in \mathbb{N}$, define

$$
\begin{aligned}
& f_{n}\left(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}\right):= \\
& n\left[\varphi_{1}\left(\mathbf{x}_{1}\right)+\frac{1}{n} \psi_{1}\left(\mathbf{x}_{1}\right)\right]\left[\varphi_{2}\left(\mathbf{x}_{2}\right)+\frac{1}{n} \psi_{2}\left(\mathbf{x}_{2}\right)\right]\left[\varphi_{3}\left(\mathbf{x}_{3}\right)+\frac{1}{n} \psi_{3}\left(\mathbf{x}_{3}\right)\right] \\
& \\
& -n \varphi_{1}\left(\mathbf{x}_{1}\right) \varphi_{2}\left(\mathbf{x}_{2}\right) \varphi_{3}\left(\mathbf{x}_{3}\right) .
\end{aligned}
$$

## Then

$$
\left.\begin{array}{rl}
\hat{f}\left(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}\right)-f_{n}\left(\mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}\right) & =\frac{1}{n}\left[\psi_{1}\left(\mathbf{x}_{1}\right) \psi_{2}\left(\mathbf{x}_{2}\right) \varphi_{3}\left(\mathbf{x}_{3}\right)\right. \\
+ & \psi_{1}\left(\mathbf{x}_{1}\right) \varphi_{2}\left(\mathbf{x}_{2}\right) \psi_{3}
\end{array}+\varphi_{1}\left(\mathbf{x}_{1}\right) \psi_{2}\left(\mathbf{x}_{2}\right) \psi_{3}\left(\mathbf{x}_{3}\right)\right] .
$$

## Hence

$$
\begin{equation*}
\left\|\hat{f}-f_{n}\right\|=O\left(\frac{1}{n}\right) \tag{29}
\end{equation*}
$$

Lemma 13. In Example 12, $\operatorname{rank}(\hat{f})=3$ iff $\varphi_{i}, \psi_{i}$ are linearly independent, $i=1,2,3$. Furthermore, it is clear that $\operatorname{rank}\left(f_{n}\right) \leq 2$ and

$$
\lim _{n \rightarrow \infty} f_{n}=\hat{f}
$$

Note that our fundamental approximation problem may be regarded as the approixmation problem

$$
\begin{equation*}
\operatorname{argmin}\{\|\hat{f}-f\|: \operatorname{rank}(f) \leq r\} \tag{30}
\end{equation*}
$$

followed by a decomposition problem

$$
f=\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}
$$

which always exists for an $f$ with $\operatorname{rank}(f) \leq r$. The discussion above shows that there are $f$ for which

$$
\operatorname{argmin}\{\|\hat{f}-f\|: \operatorname{rank}(f) \leq r\}=\varnothing
$$

and thus (28) or (30) does not need to have a solution in general. This is such a crucial point that we are obliged to formally state it.

Theorem 14. For $d \geq 3$, the best approximation of a d-partite function by a sum of $p$ products of $d$ separable functions does not exist in general.

Proof: Take the tripartite function $\hat{f} \in L^{2}\left(X_{1} \times X_{2} \times X_{3}\right)$ in Example 12. Suppose we seek a best rank-2 approximation, in other words, we seek to solve the minimization problem

$$
\underset{\left\|g_{k}\right\|=\left\|h_{k}\right\|=1, \gamma, \eta \geq 0}{\operatorname{argmin}}\left\|\hat{f}-\gamma g_{1} \otimes g_{2} \otimes g_{3}-\eta h_{1} \otimes h_{2} \otimes h_{3}\right\|
$$

Now the infimum,
$\inf _{\left\|g_{k}\right\|=\left\|h_{k}\right\|=1, \gamma, \eta \geq 0}\left\|\hat{f}-\gamma g_{1} \otimes g_{2} \otimes g_{3}-\eta h_{1} \otimes h_{2} \otimes h_{3}\right\|=0$
since we may choose $n \in \mathbb{N}$ sufficiently large,

$$
g_{k}=\frac{\varphi_{k}+n^{-1} \psi_{k}}{\left\|\varphi_{k}+n^{-1} \psi_{k}\right\|}, \quad h_{k}=\frac{\varphi_{k}}{\left\|\varphi_{k}\right\|}
$$

for $k=1,2,3$,

$$
\begin{aligned}
\gamma & =n\left\|\varphi_{1}+n^{-1} \psi_{1}\right\|\left\|\varphi_{2}+n^{-1} \psi_{2}\right\|\left\|\varphi_{3}+n^{-1} \psi_{3}\right\| \\
\eta & =n\left\|\varphi_{1}\right\|\left\|\varphi_{2}\right\|\left\|\varphi_{3}\right\|
\end{aligned}
$$

so as make $\left\|\hat{f}-\gamma g_{1} \otimes g_{2} \otimes g_{3}-\eta h_{1} \otimes h_{2} \otimes h_{3}\right\|$ as small as we desired by virtue of (29). However there is no rank-2 function $\gamma g_{1} \otimes g_{2} \otimes g_{3}-\eta h_{1} \otimes h_{2} \otimes h_{3}$ for which

$$
\left\|\hat{f}-\gamma g_{1} \otimes g_{2} \otimes g_{3}-\eta h_{1} \otimes h_{2} \otimes h_{3}\right\|=0
$$

In other words, the zero infimum can never be attained.
Our construction above is based on an earlier construction in [22]. The first such example was given in [4], which also contains the very first definiton of border rank. We will define it here for $d$-partite functions. When $X_{1}, \ldots, X_{d}$ are finite sets, this reduces to the original definiton in [4] for hypermatrices.
Definition 15. Let $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$. The border rank of $f$ is defined as

$$
\begin{aligned}
& \overline{\operatorname{rank}}(f)=\min \{r \in \mathbb{N}: \inf \|f-g\|=0 \\
& \quad \text { over all } g \text { with } \operatorname{rank}(g)=r\} .
\end{aligned}
$$

Clearly we would always have that

$$
\overline{\operatorname{rank}}(f) \leq \operatorname{rank}(f)
$$

The discussions above show that strict inequality can occur. In fact, for the $\hat{f}$ in Example 12, $\overline{\operatorname{rank}}(\hat{f})=2$ while $\operatorname{rank}(\hat{f})=$ 3.

We would like to mention here that this problem applies to operators too. Approximation of an operator by a sum of tensor/Kronecker products of lower-dimensional operators is in general an ill-posed problem whose existence cannot be guaranteed.

Example 16 (SS approximation of operators). For linearly independent operators $\Phi_{i}, \Psi_{i}: V_{i} \rightarrow W_{i}, i=1,2,3$, let $\widehat{T}$ : $V_{1} \otimes V_{2} \otimes V_{3} \rightarrow W_{1} \otimes W_{2} \otimes W_{3}$ be

$$
\begin{equation*}
\widehat{T}:=\Psi_{1} \otimes \Phi_{2} \otimes \Phi_{3}+\Phi_{1} \otimes \Phi_{2} \otimes \Psi_{3}+\Phi_{1} \otimes \Phi_{2} \otimes \Psi_{3} \tag{31}
\end{equation*}
$$

If $\Phi_{i}, \Psi_{i}$ 's are all finite-dimensional and represented in coordinates as matrices, then ' $\otimes$ ' may be taken to be Kronecker product of matrices. For $n \in \mathbb{N}$,

$$
\begin{aligned}
T_{n}:=n\left[\Phi_{1}+\frac{1}{n} \Psi_{1}\right] \otimes\left[\Phi_{2}+\frac{1}{n} \Psi_{2}\right] & {\left[\Phi_{3}+\frac{1}{n} \Psi_{3}\right] } \\
& -n \Phi_{1} \otimes \Phi_{2} \otimes \Phi_{3} .
\end{aligned}
$$

## Then

$$
\lim _{n \rightarrow \infty} T_{n}=\widehat{T}
$$

An example of an operator that has the form in (31) is the $3 m$-dimensional Laplacian $\Delta_{3 m}$, which can be expressed in terms of the m-dimensional Laplacian $\Delta_{m}$ as

$$
\Delta_{3 m}=\Delta_{m} \otimes I \otimes I+I \otimes \Delta_{m} \otimes I+I \otimes I \otimes \Delta_{m}
$$

There are several simple but artificial ways to alleviate the issue of non-existent best approximant. Observe from the proof of Theorem 14 that the coefficients in the approximant $\gamma, \eta$ becomes unbounded in the limit. Likewise we see this happening in Example 16. In fact this must always happen in the event when a function or operator is approximated by a rank- $r$ function, i.e.

$$
\begin{equation*}
\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\| \quad \text { or } \quad\left\|\widehat{T}-\sum_{p=1}^{r} \alpha_{p} \bigotimes_{k=1}^{d} \Phi_{k p}\right\|, \tag{32}
\end{equation*}
$$

and if a best approximation does not exist, then the $r$ coefficients $\alpha_{1}, \ldots, \alpha_{r}$ must all diverge in magnitude to $+\infty$ as the approximant converges to the infimum of the norm loss function in (32). This result was first established in [22, Proposition 4.9].

So a simple but artificial way to prevent the nonexistence issue is to simply limit the sizes of the coefficients $\alpha_{1}, \ldots, \alpha_{r}$ in the approximant. One way to achieve this is regularization [55], [46] - adding a regularization term to our objective function in (28) to penalize large coefficients. A common choice is Tychonoff regularization, which uses a sum-ofsquares regularization term:

$$
\begin{equation*}
\underset{\alpha \in[0, \infty)^{r},\left\|\varphi_{k p}\right\|=1}{\operatorname{argmin}}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\|+\lambda \sum_{p=1}^{r}\left|\alpha_{p}\right|^{2} . \tag{33}
\end{equation*}
$$

Here $\lambda$ is an arbitrarily chosen regularization parameter. It can be seen that this is equivalent to constraining the sizes $\alpha_{1}, \ldots, \alpha_{r}$ to $\sum_{p=1}^{r}\left|\alpha_{p}\right|^{2}=\rho$, with $\rho$ being determined a posteriori from $\lambda$. The main drawback of such constraints is that $\rho$ and $\lambda$ are arbitrary, and that they generally have no physical meaning.

More generally, one may alleviate the nonexistence issue by restricting the optimization problem (30) to a compact subset of its non-compact feasible set

$$
\left\{f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right): \operatorname{rank}(f) \leq r\right\}
$$

Limiting the sizes of $\alpha_{1}, \ldots, \alpha_{r}$ is a special case but there are several other simple (but also artificial) strategies. In [17], the factors $\varphi_{k 1}, \ldots, \varphi_{k p}$ are required to be orthogonal for all $k \in\{1, \ldots, d\}$, i.e.

$$
\begin{equation*}
\left\langle\varphi_{k p}, \varphi_{k q}\right\rangle_{k}=\delta_{p q}, \quad p, q=1, \ldots, r, \quad k=1, \ldots, d \tag{34}
\end{equation*}
$$

This remedy is acceptable only in very restrictive conditions. In fact a necessary condition for this to work is that

$$
r \leq \min _{k=1, \ldots, d} \operatorname{dim} L^{2}\left(X_{k}\right)
$$

It is also trivial to see that imposing orthogonality between the separable factors removes this problem

$$
\begin{equation*}
\left\langle\varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}, \varphi_{1 q} \otimes \cdots \otimes \varphi_{d q}\right\rangle=\delta_{p q}, \quad p, q=1, \ldots, r \tag{35}
\end{equation*}
$$

This constraint is slightly less restrictive - by (12), it is equivalent to requiring (34) for some $k \in\{1, \ldots, d\}$. Both (34) and (35) are nonetheless so restrictive as to exclude the most useful circumstances for the model (13), which usually involves factors that have no reason to be orthogonal, as we will see in Section IX. In fact, Kruskal's uniqueness condition is such a potent tool precisely because it does not require orthogonality.
The conditions (34), (35), and (33) all limit the feasible sets for the original approximation (28) to a much smaller compact subset of the original feasible set. This is not the case for nonnegative constraints. In [46] it was shown that the following best rank- $r$ approximation problem for a nonnegativevalued $\hat{f}$ and where the coefficients $\alpha_{p}$ and factors $\varphi_{k p}$ of the approximants are also nonnegative valued, i.e.

$$
\underset{\boldsymbol{\alpha} \in[0, \infty)^{r},\left\|\varphi_{k p}\right\|=1, \varphi_{k p} \geq 0}{\operatorname{argmin}}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\|,
$$

always has a solution. The feasible set in this case is noncompact and has nonempty interior within the feasible set of our original problem (28). The nonnegativity constraints are natural in some applications, such as the fluorescence spectroscopy one described in Section IX-F, where $\varphi_{k p}$ represent intensities and concentrations, and are therefore nonnegative valued.

There are two major problems with imposing artificial constraints simply to force a solution: How do we know a priori that the solution that we seek would meet those constraints? But more importantly, perhaps the model is ill-posed and a solution indeed should not exist? To illustrate the case in point with a more commonplace example, suppose we want to find a maximum likelihood estimator $X \in \mathbb{R}^{n \times n}$ for the covariance $\Sigma$ of independent samples $\mathbf{y}_{1}, \ldots, \mathbf{y}_{m} \sim N(0, \Sigma)$. This would lead us to a semi-definite programming problem

$$
\begin{equation*}
\underset{X \succ 0}{\operatorname{argmin}} \operatorname{tr}\left(X^{-1} Y\right)-\log \operatorname{det}(X) \tag{36}
\end{equation*}
$$

where $Y=\frac{1}{m} \sum_{i=1}^{m} \mathbf{y}_{i} \mathbf{y}_{i}^{\top}$. However the problem will not have a solution when the number of samples is smaller than the dimension, i.e. $m<n$, as the infimum of the loss function in (36) cannot be attained by any $X$ in the feasible set. This is an indication that we should seek more samples (so that we could get $m \geq n$, which will guarantee the attainment of
the infimum) or use a different model (e.g. determine if $X^{-1}$ might perhaps have some a priori zero entries due to statistical independence of the variables). It is usually unwise to impose artificial constraints on the covariance matrix $X$ just so that the loss function in (36) would attain an infimum on a smaller feasible set - the thereby obtained 'solution' may bear no relation to the true solution that we want.

Our goal in Section VIII-A is to define a type of physically meaningful constraints via the notion of coherence. It ensures the existence of a unique minimum, but not via an artificial limitation of the optimization problem to a convenient subset of the feasible set. In the applications we discuss in Section IX, we will see that it is natural to expect existence of a solution when coherence is small enough, but not otherwise. So when our model is ill-posed or ill-conditioned, we are warned by the size of the coherence and could seek other remedies (collect more measurements, use a different model, etc) instead of forcing a 'solution' that bears no relation to reality. But before we get to that we will examine another method based on an approximation of rank by a ratio of Schatten 1- and $\infty$-norms.

## VII. Schatten and Ky Fan norms

We introduce the notion of Schatten norms and Ky Fan norms for multipartite functions and see how a condition involving the Schatten 1 -norm and Schatten $\infty$-norm allows us to alleviate the problem discussed in Section VI, namely, that a $d$-partite function may not have a best approximation by a sum of $r$ separable functions.

The definition of Schatten norm follows naturally from the definition of rank in Section III, and from which the definiton of Ky Fan norm is immediate.

Definition 17. For any $1 \leq s<\infty$, we define the Schatten $s$-norm of $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ as

$$
\begin{align*}
& \|f\|_{*, s}:=\inf \left\{\left[\sum_{p=1}^{\infty} \lambda_{p}^{s}\right]^{1 / s}:\right. \\
& \left.f=\sum_{p=1}^{\infty} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p},\left\|\varphi_{k p}\right\|=1, \lambda_{p} \geq \lambda_{p+1}>0\right\} \tag{37}
\end{align*}
$$

with the usual modification (replace sum by supremum) for the case $s=\infty$.

Definition 18. For any $1 \leq s<\infty$ and any $k \in \mathbb{N}$, we define the Ky Fan $(s, k)$-norm of $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ as

$$
\begin{align*}
& \|f\|_{*, s, k}:=\inf \left\{\left[\sum_{p=1}^{k} \lambda_{p}^{s}\right]^{1 / s}:\right. \\
& \left.f=\sum_{p=1}^{\infty} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p},\left\|\varphi_{k p}\right\|=1, \lambda_{p} \geq \lambda_{p+1}>0\right\} \tag{38}
\end{align*}
$$

with again the usual modification for the case $s=\infty$.
The letters $s$ and $k$ are of course chosen to remind us of the respective eponymous norms. The fact that (37) and (38)
define norms on $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ follows from the standard Minkowski gauge argument [23]. The Ky Fan and Schatten norms are related by $\|f\|_{*, s, \infty}=\|f\|_{*, s}$. When $X_{1}, \ldots, X_{d}$ are finite sets of cardinalities $n_{1}, \ldots, n_{d} \in \mathbb{N}$, the Schatten 1-norm for the unipartite case $(d=1)$ is just the usual $\ell^{1}$ norm for vectors in $\mathbb{C}^{n_{1}}=L^{2}\left(X_{1}\right)$; the Schatten $s$-norm for the bipartite case $(d=2)$ agrees with the usual Schatten $s$ norm for matrices in $\mathbb{C}^{n_{1} \times n_{2}}=L^{2}\left(X_{1} \times X_{2}\right)$. In particular, the bipartite Schatten 1,2 , and $\infty$-norms are respectively the nuclear, Frobenius, and spectral norms of a matrix. For $d \geq 3$, Definitions 17 and 18 yield notions of Schatten and Ky Fan norms for hypermatrices in $\mathbb{C}^{n_{1} \times \cdots \times n_{d}}=L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ when $X_{k}$ are finite sets (with $n_{k}$ elements) for all $k=1, \ldots, d$.

Example 19 (Nuclear norm for 3-tensors). Let $T \in$ $\mathbb{C}^{n_{1} \times n_{2} \times n_{3}}$. Then by Definition 17, we have

$$
\|T\|_{*, 1}=\inf \left\{\sum_{p=1}^{r} \lambda_{p}: T=\sum_{p=1}^{r} \lambda_{p} \mathbf{x}_{p} \otimes \mathbf{y}_{p} \otimes \mathbf{z}_{p}\right\}
$$

where the infimum is taken over all linear combinations of complex vectors of unit 2 -norm $\mathbf{x}_{p} \in \mathbb{C}^{n_{1}}, \mathbf{y}_{p} \in \mathbb{C}^{n_{2}}, \mathbf{z}_{p} \in$ $\mathbb{C}^{n_{3}}$, with real positive coefficientss $\lambda_{p} \in[0, \infty)$, and $p=$ $1, \ldots, r$, with $r \in \mathbb{N}$.

Note that we used the term tensors, as opposed to hypermatrices, in the above example. In fact, Definitions 17 and 18 define Schatten and Ky Fan norms for the tensors, not just their coordinate representations as hypermatrices (see our discussion after Example 6), because of the following invariant properties.

Lemma 20. The Schatten and Ky Fan norms as defined in (37) and (38) for $\mathbb{C}^{n_{1} \times \cdots \times n_{d}}$ are unitarily invariant, i.e. invariant under the natural action of $U\left(n_{1}\right) \times \cdots \times U\left(n_{d}\right)$ where $U(n)$ denotes the group of unitary matrices in $\mathbb{C}^{n \times n}$.

Proof: To avoid the clutter of indices, we will assume that $d=3$. It is easy, although notationally cumbersome, to extend this to general $d \geq 3$. Let $(U, V, W) \in U\left(n_{1}\right) \times U\left(n_{2}\right) \times U\left(n_{3}\right)$ and $T \in \mathbb{C}^{n_{1} \times n_{2} \times n_{3}}$. The natural action, given in coordinates by

$$
(U, V, W) \cdot T=\left[\sum_{i, j, k=1}^{n_{1}, n_{2}, n_{3}} u_{a i} v_{b j} w_{c k} t_{i j k}\right]_{a, b, c=1}^{n_{1}, n_{2}, n_{3}}
$$

has the property that if $T$ has a SS decomposition of the form

$$
T=\sum_{p=1}^{r} \lambda_{p} \mathbf{x}_{p} \otimes \mathbf{y}_{p} \otimes \mathbf{z}_{p}
$$

then

$$
\begin{equation*}
(U, V, W) \cdot T=\sum_{p=1}^{r} \lambda_{p}\left(U \mathbf{x}_{p}\right) \otimes\left(V \mathbf{y}_{p}\right) \otimes\left(W \mathbf{z}_{p}\right) \tag{39}
\end{equation*}
$$

(39) is obvious when $r=1$ and for general $r$ follows from the linearity of the action (i.e. $(U, V, W) \cdot(S+T)=(U, V, W)$. $S+(U, V, W) \cdot T)$. We also need the simple fact that $U\left(n_{1}\right) \times$ $U\left(n_{2}\right) \times U\left(n_{3}\right)$ acts transitively on unit-norm rank-1 tensors, i.e. take any $\mathbf{x} \in \mathbb{C}^{n_{1}}, \mathbf{y} \in \mathbb{C}^{n_{2}}, \mathbf{z} \in \mathbb{C}^{n_{3}}$ of unit norm, then every other unit-norm rank-1 tensor may be written as
$U \mathbf{x} \otimes V \mathbf{y} \otimes W \mathbf{z}$ for some $(U, V, W) \in U\left(n_{1}\right) \times U\left(n_{2}\right) \times U\left(n_{3}\right)$. With these, it follows immediately from Definition 17 that Schatten norms satisfy

$$
\|(U, V, W) \cdot T\|_{*, s}=\|T\|_{*, 1}
$$

and likewise for Ky Fan norms.
If we allow $0<s<1$, then (37) and (38) no longer define norms although the Schatten and Ky Fan quasinorms

$$
\begin{aligned}
& \|f\|_{*, s, k}=\inf \left\{\sum_{p=1}^{k} \lambda_{p}^{s}:\right. \\
& \left.f=\sum_{p=1}^{\infty} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p},\left\|\varphi_{k p}\right\|=1, \lambda_{p} \geq \lambda_{p+1}>0\right\}
\end{aligned}
$$

are nonetheless still interesting measures of nearness. Observe that we have dropped the $1 / s$ power here. In particular, the limiting case as $s \rightarrow 0$ yields the Schatten 0-quasinorm,

$$
\begin{aligned}
& \|f\|_{*, 0}:=\inf \left\{\sum_{p=1}^{\infty} \lambda_{p}^{0}:\right. \\
& \left.f=\sum_{p=1}^{\infty} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p},\left\|\varphi_{k p}\right\|=1, \lambda_{p} \geq \lambda_{p+1}>0\right\}
\end{aligned}
$$

where we adopt the convention that $0^{0}=0$.
Lemma 21. For any $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$, we have $\|f\|_{*, 0}=$ $\operatorname{rank}(f)$ and

$$
\begin{equation*}
\|f\|_{*, 1} \leq \operatorname{rank}(f) \times\|f\|_{*, \infty} \tag{40}
\end{equation*}
$$

In other words, the Schatten 1-norm is a convex underestimator of rank on the Schatten $\infty$-norm unit ball $\left\{f:\|f\|_{*, \infty} \leq\right.$ $1\}$. In fact, (40) may be sharpened to have border rank in place of rank

$$
\begin{equation*}
\|f\|_{*, 1} \leq \overline{\operatorname{rank}}(f) \times\|f\|_{*, \infty} \tag{41}
\end{equation*}
$$

Proof: Let $\operatorname{rank}(f)=r$ and $f=\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes$ $\varphi_{d p}$ be a SS decomposition as in Theorem 2. Therefore $\left\|\varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|_{*, 1}=\left\|\varphi_{1 p}\right\| \cdots\left\|\varphi_{d p}\right\|=1$ for all $p=$ $1, \ldots, r$. The triangle inequality immediate yields $\|f\|_{*, 1} \leq$ $\sum_{p=1}^{r}\left|\lambda_{p}\right|\left\|\varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|_{*, 1}=\sum_{p=1}^{r}\left|\lambda_{p}\right| \leq r\|f\|_{*, \infty}$. For the border rank version, let $\overline{\operatorname{rank}}(f)=r$, then there exists a sequence $f_{n}$ where $\operatorname{rank}\left(f_{n}\right)=r$ and $\lim _{n \rightarrow \infty} f_{n}=f$. By what we have just proved,

$$
\left\|f_{n}\right\|_{*, 1} \leq \operatorname{rank}\left(f_{n}\right) \times\left\|f_{n}\right\|_{*, \infty}=r\left\|f_{n}\right\|_{*, \infty}
$$

Taking limits and using the continuity of norms immediately yields (41).

It is known that the $\ell^{1}$-norm is the largest convex underestimator ${ }^{3}$ of the 0 -quasinorm on the $\ell^{\infty}$-norm unit ball [43] and that the nuclear norm is the largest convex underestimator of rank on spectral norm unit ball [29]. We suspect that a vast generalization of this observation is true, namely, the Schatten 1 -norm as defined in (37) is the largest convex underestimator of the rank function as defined in (10). We are however unable to prove nor disprove this stronger version of Lemma 21, i.e., with 'largest convex underestimator' in place of 'convex underestimator'.

The condition (40) in Lemma 21 provides a simple way for alleviating the fact that by replacing the condition $\operatorname{rank}(f) \leq r$

[^3]by the condition $\|f\|_{*, 1} \leq r\|f\|_{*, \infty}$. Recall that the discussion in Section VI shows that there are $\hat{f}$ for which
$$
\operatorname{argmin}\{\|\hat{f}-f\|: \operatorname{rank}(f) \leq r\}=\varnothing
$$
which really results from the fact that
$$
\left\{f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right): \operatorname{rank}(f) \leq r\right\}
$$
is not a closed set. The condition (40) we derived may then be used as a work-around relaxation where we have the ratio $\|f\|_{*, 1} /\|f\|_{*, \infty}$ as a 'proxy' in place of $\operatorname{rank}(f)$.
Theorem 22. Let $\hat{f} \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$. For any $r \in \mathbb{N}$, the optimization problem
$$
\operatorname{argmin}\left\{\|\hat{f}-f\|:\|f\|_{*, 1} \leq r\|f\|_{*, \infty}\right\}
$$
always has a solution.
Proof: The follows from the fact that the set
$$
\left\{f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right):\|f\|_{*, 1} \leq r\|f\|_{*, \infty}\right\}
$$
is closed, which follows easily from the continuity of the realvalued function $\|\cdot\|_{*, 1}-r\|\cdot\|_{*, \infty}$ on $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$, which in turn follows easily from the fact that all norms are continuous functions.

We would like to add a few words about the ratio

$$
\frac{\|f\|_{*, 1}}{\|f\|_{*, \infty}}
$$

Note that this gives a crude notion of 'numerical rank' for a $d$ partite function. Recall that when $d=2$ and $X_{1}, X_{2}$ are finite, bipartite functions may be regarded as matrices, i.e. $L^{2}\left(X_{1} \times\right.$ $\left.X_{2}\right) \cong \mathbb{C}^{n_{1} \times n_{2}}$ where $\# X_{1}=n_{1}, \# X_{2}=n_{2}$. In this case, the ratio of the Frobenius norm to the spectral norm and the ratio of the nuclear norm to the spectral norm are occasionally used as proxies for matrix rank, often in scenarios where the use of matrix rank would be computational intractable. These ratios are used because of bounds that are the analogues of (40),

$$
\|A\|_{F} \leq \sqrt{\operatorname{rank}(A)}\|A\|_{2} \quad \text { and } \quad\|A\|_{*} \leq \operatorname{rank}(A)\|A\|_{2}
$$

for $A \in \mathbb{C}^{n_{1} \times n_{2}}$. In fact the inequality on the right is exactly (40) applied to the case of bipartite functions, i.e. matrices.

Theorem 22 represents a simple, elegant solution to the nonexistence problem in Section VI but we do not find it useful for the applications that we consider here. Instead another workaround that uses the notion of coherence, discussed in the next section, is more naturally applicable in our situtations.

## VIII. COHERENCE

We will show in this section that a simple measure of angular constriant called coherence, or rather, the closely related notion of relative incoherence, allows us to alleviate two problems simultaneously: the computational intractability of checking for uniqueness discussed in Section IV and the non-existence of a best approximant in Section VI.

Definition 23. Let $\mathbb{H}$ be a Hilbert space provided with scalar product $\langle\cdot, \cdot\rangle$, and let $\Phi \subseteq \mathbb{H}$ be a set of elements of unit norm in $\mathbb{H}$. The coherence of $\Phi$ is defined as

$$
\mu(\Phi)=\sup _{\varphi \neq \psi}|\langle\varphi, \psi\rangle|
$$

where the supremum is taken over all distinct pairs $\varphi, \psi \in \mathbb{H}$. If $\Phi=\left\{\varphi_{1}, \ldots, \varphi_{r}\right\}$ is finite, we also write $\mu\left(\varphi_{1}, \ldots, \varphi_{r}\right):=$ $\max _{p \neq q}\left|\left\langle\varphi_{p}, \varphi_{q}\right\rangle\right|$.

We adopt the convention that whenever we write $\mu(\Phi)$ (resp. $\mu\left(\varphi_{1}, \ldots, \varphi_{r}\right)$ ) as in Definition 23, it is implicitly implied that all elements of $\Phi$ (resp. $\varphi_{1}, \ldots, \varphi_{r}$ ) are of unit norm.

Th notion of coherence has received different names in the literature: mutual incoherence of two dictionaries [26], mutual coherence of two dictionaries [9], the coherence of a subspace projection [8], etc. The version here follows that of [32]. Usually, dictionaries are finite or countable, but we have here a continuum of atoms. Clearly, $0 \leq \mu(\Phi) \leq 1$, and $\mu(\Phi)=0$ iff $\varphi_{1}, \ldots, \varphi_{r}$ are orthonormal. Also, $\mu(\Phi)=1$ iff $\Phi$ contains at least a pair of collinear elements, i.e. $\varphi_{p}=\lambda \varphi_{q}$ for some $p \neq q, \lambda \neq 0$.

We find it useful to introduce a closely related notion that we call relative incoherence. It allows us to formulate some of our results slightly more elegantly.
Definition 24. Let $\Phi \subseteq \mathbb{H}$ be a set of elements of unit norm. The relative incoherence of $\Phi$ is defined as

$$
\omega(\Phi)=\frac{1-\mu(\Phi)}{\mu(\Phi)}
$$

For a finite set of unit vectors $\Phi=\left\{\varphi_{1}, \ldots, \varphi_{r}\right\}$, we will also write $\omega\left(\varphi_{1}, \ldots, \varphi_{r}\right)$ occasionally.

It follows from our observation about coherence that $0 \leq$ $\omega(\Phi) \leq \infty, \omega(\Phi)=\infty$ iff $\varphi_{1}, \ldots, \varphi_{r}$ are orthonormal, and $\omega(\Phi)=0$ iff $\Phi$ contains at least a pair of collinear elements.

In the next few subsections, we will see respectively how coherence can inform us about the existence (Section VIII-A), uniqueness (Section VIII-B), as well as both existence and uniqueness (Section VIII-C) of a solution to the best rank-r SS approximation problem (28). We will also see how it can be used for establishing exact recoverability (Section VIII-D) and approximation bounds (Section VIII-E) in greedy algorithms.

## A. Existence via coherence

The goal is to prevent the phenomenon we observed in Example 12 to occur, by imposing natural and weak constraints; we do not want to reduce the search to a compact set. It is clear that the objective is not coercive, which explains why the minimum may not exist. But with an additional condition on the coherence, we shall be able to prove existence thanks to coercivity.

The following shows that a solution to the bounded coherence best rank- $r$ approximation problem always exists:
Proposition 25. Let $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ be a d-partite function. If

$$
\begin{equation*}
\prod_{k=1}^{d}\left(1+\omega_{k}\right)>r-1 \tag{42}
\end{equation*}
$$

or equivalently if

$$
\begin{equation*}
\prod_{k=1}^{d} \mu_{k}<\frac{1}{r-1} \tag{43}
\end{equation*}
$$

then

$$
\begin{gather*}
\eta=\inf \left\{\left\|f-\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|:\right. \\
\left.\lambda \in \mathbb{C}^{r}, \mu\left(\varphi_{k 1}, \ldots, \varphi_{k r}\right) \leq \mu_{k}\right\}  \tag{44}\\
=\inf \left\{\left\|f-\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|:\right. \\
\left.\lambda \in \mathbb{C}^{r}, \omega\left(\varphi_{k 1}, \ldots, \varphi_{k r}\right) \geq \omega_{k}\right\}
\end{gather*}
$$

is attained. Here $\|\cdot\|$ denotes the $L^{2}$-norm on $L^{2}\left(X_{1} \times \cdots \times\right.$ $\left.X_{d}\right)$ and $\boldsymbol{\lambda}=\left(\lambda_{1}, \ldots, \lambda_{r}\right)$. If desired, we may assume that $\boldsymbol{\lambda} \in \mathbb{R}^{r}$ and $\lambda_{1} \geq \cdots \geq \lambda_{r}>0$ by Theorem 2.

Proof: The equivalence between (42) and (43) follows from Definition 24. We show that if either of these conditions are met, then the loss function is coercive. We have the following inequalities

$$
\begin{aligned}
\left\|\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|^{2}= & \sum_{p, q=1}^{r} \lambda_{p} \bar{\lambda}_{q} \prod_{k=1}^{d}\left\langle\varphi_{k p}, \varphi_{k q}\right\rangle \\
\geq & \sum_{p=1}^{r} \lambda_{p} \bar{\lambda}_{p} \prod_{k=1}^{d}\left\|\varphi_{k p}\right\|^{2} \\
& \quad-\sum_{p \neq q}^{r}\left|\lambda_{p} \bar{\lambda}_{q} \prod_{k=1}^{d}\left\langle\varphi_{k p}, \varphi_{k q}\right\rangle\right| \\
\geq & \sum_{p=1}^{r}\left|\lambda_{p}\right|^{2}-\prod_{k=1}^{d} \mu_{k} \sum_{p \neq q}\left|\lambda_{p} \bar{\lambda}_{q}\right| \\
\geq & \|\boldsymbol{\lambda}\|_{2}^{2}-(r-1)\|\boldsymbol{\lambda}\|_{2}^{2} \prod_{k=1}^{d} \mu_{k}
\end{aligned}
$$

where the last inequality follows from
$\sum_{p \neq q}\left|\lambda_{p} \bar{\lambda}_{q}\right|=2 \sum_{p<q}\left|\lambda_{p} \bar{\lambda}_{q}\right| \leq \sum_{p<q}\left(\left|\lambda_{p}\right|^{2}+\left|\bar{\lambda}_{q}\right|^{2}\right)=(r-1)\|\boldsymbol{\lambda}\|_{2}^{2}$.
This yields

$$
\begin{equation*}
\left\|\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|^{2} \geq\left[1-(r-1) \prod_{k=1}^{d} \mu_{k}\right]\|\boldsymbol{\lambda}\|_{2}^{2} \tag{45}
\end{equation*}
$$

Since by assumption $(r-1) \prod_{k=1}^{d} \mu_{k}<1$, it is clear that the left hand side of (45) tends to infinity as $\|\boldsymbol{\lambda}\|_{2} \rightarrow \infty$. And because $f$ is fixed, $\left\|f-\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}\right\|$ also tends to infinity as $\|\boldsymbol{\lambda}\|_{2} \rightarrow \infty$. This proves coercivity of the loss function and hence the existential statement.

The condition (42) or, equivalently, (43), in Proposition 25 is sharp in an appropriate sense. Proposition 25 shows that the condition (43) is sufficient in the sense that it guarantees a best rank- $r$ approximation when the condition is met. We show that it is also necessary in the sense that if (43) does not hold, then
there are examples where a best rank- $r$ approximation fails to exist.

In fact, let $\hat{f}$ be as in Example 12. As demonstrated in the proof of Theorem 14, the infimum for the case $d=3$ and $r=2$,

$$
\inf _{\left\|g_{k}\right\|=\left\|h_{k}\right\|=1, \lambda, \mu \geq 0}\left\|\hat{f}-\lambda g_{1} \otimes g_{2} \otimes g_{3}-\mu h_{1} \otimes h_{2} \otimes h_{3}\right\|
$$

is not attained. Since

$$
g_{k}=\frac{\varphi_{k}+n^{-1} \psi_{k}}{\left\|\varphi_{k}+n^{-1} \psi_{k}\right\|}, \quad h_{k}=\frac{\varphi_{k}}{\left\|\varphi_{k}\right\|}
$$

for $k=1,2,3$, the corresponding coherence

$$
\mu\left(g_{k}, h_{k}\right) \geq\left|\left\langle g_{k}, h_{k}\right\rangle\right| \rightarrow 1
$$

as $n \rightarrow \infty$. For any values of $\mu_{1}, \mu_{2}, \mu_{3} \in[0,1]$ such that (43) holds, i.e. $\mu_{1} \mu_{2} \mu_{3}<1 /(r-1)=1$, we cannot possibly have $\mu\left(g_{k}, h_{k}\right) \leq \mu_{k}$ for all $k=1,2,3$ since

$$
\mu\left(g_{1}, h_{1}\right) \mu\left(g_{2}, h_{2}\right) \mu\left(g_{3}, h_{3}\right) \rightarrow 1
$$

as $n \rightarrow \infty$.

## B. Uniqueness via coherence

In order to prove uniqueness, we need a simple observation and the notion of Kruskal rank introduced in Definition 7.

Lemma 26. Let $\Phi \subseteq L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ be finite. Then

$$
\begin{equation*}
\operatorname{krank} \Phi \geq \frac{1}{\mu(\Phi)} \tag{46}
\end{equation*}
$$

Proof: Let $s=\operatorname{krank} \Phi+1$. Then there exists a subset of $s$ distinct unit vectors in $\Phi,\left\{\Phi_{1}, \ldots, \Phi_{s}\right\}$ such that $\alpha_{1} \Phi_{1}+$ $\cdots+\alpha_{s} \Phi_{s}=0$ with $\left|\alpha_{1}\right|=\max \left\{\left|\alpha_{1}\right|, \ldots,\left|\alpha_{s}\right|\right\}>0$. Taking inner product with $\Phi_{1}$ we get $\alpha_{1}=-\alpha_{2}\left\langle\Phi_{2}, \Phi_{1}\right\rangle-\cdots-$ $\alpha_{s}\left\langle\Phi_{s}, \Phi_{1}\right\rangle$ and so $\left|\alpha_{1}\right| \leq\left(\left|\alpha_{2}\right|+\cdots+\left|\alpha_{s}\right|\right) \mu(V)$. Dividing by $\left|\alpha_{1}\right|$ then yields $1 \leq(s-1) \mu(\Phi)$.

We now characterize the uniqueness of the rank revealing decomposition in terms of coherence introduced in Definition 23.

Proposition 27. Let $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ have a rank-r SS decomposition

$$
f=\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}
$$

where $\Phi_{k}:=\left\{\varphi_{k 1}, \ldots, \varphi_{k r}\right\}$ are elements in $L^{2}\left(X_{k}\right)$ of unit norm for all $k=1, \ldots, d$. Let $\omega_{k}=\omega\left(\Phi_{k}\right)$. If

$$
\begin{equation*}
\sum_{k=1}^{d} \omega_{k} \geq 2 r-1 \tag{47}
\end{equation*}
$$

then $r=\operatorname{rank}(f)$ and the decomposition is essentially unique.
Proof: Inequality (47) implies that $\sum_{k=1}^{d} \mu_{k}^{-1} \geq 2 r+$ $d-1$, where $\mu_{k}$ denotes $\mu\left(\Phi_{k}\right)$. If it is satisfied, then so is Kruskal's condition (25) thanks to Lemma 26. The result hence directly follows from Lemma 9.

Note that unlike the $k$-ranks in (25), the coherences in (47) are trivial to compute. In addition to uniqueness, an easy but important consequence of Proposition 27 is that it provides a readily checkable sufficient condition for tensor rank, which is NP-hard over any field [41], [42].

## C. Existence and uniqueness via coherence

Now the following existence and uniqueness sufficient condition can be deduced from Propositions 25 and 27.
Corollary 28. If $d \geq 3$ and if coherences $\mu_{k}$ satisfy

$$
\begin{equation*}
\left(\prod_{k=1}^{d} \mu_{k}\right)^{1 / d} \leq \frac{d}{2 r+d-1} \tag{48}
\end{equation*}
$$

then the bounded coherence best rank-r approximation problem has a unique solution up to unimodulus scaling.

Proof: The existence in the case $r=1$ is ensured, because the set of separable functions $\left\{\varphi_{1} \otimes \cdots \otimes \varphi_{d}: \varphi_{k} \in L^{2}\left(X_{k}\right)\right\}$ is closed. Consider thus the case $r \geq 2$. Since the function $f(x)=\frac{1}{x}-\left(\frac{d}{2 x+d-1}\right)^{d}$ is strictly positive for $x \geq 2$ and $d \geq 3$, condition (48) implies that $\prod_{k=1}^{d} \mu_{k}$ is smaller than $1 / r$, which permits to claim that the solution exists by calling for Proposition 25. Next in order to prove uniqueness, we use the inequality between harmonic and geometric means: if (48) is verified, then we also necessarily have $d\left(\sum_{k=1}^{d} \mu_{k}^{-1}\right)^{-1} \leq$ $\frac{d}{2 r+d-1}$. Hence $\sum_{k=1}^{d} \mu_{k}^{-1} \geq 2 r+d-1$ and we can apply Proposition 27.

In practice, simpler expressions than (48) can be more attractive for computational purposes. These can be derived from the inequalities between means:
$\left(\frac{1}{d} \sum_{k=1}^{d} \mu_{k}^{-1}\right)^{-1} \leq\left(\prod_{k=1}^{d} \mu_{k}\right)^{1 / d} \leq \frac{1}{d} \sum_{k=1}^{d} \mu_{k} \leq\left(\frac{1}{d} \sum_{k=1}^{d} \mu_{k}^{2}\right)^{1 / 2}$
Examples of weaker sufficient conditions that could be used in place of (48) include

$$
\begin{align*}
& \sum_{k=1}^{d} \mu_{k} \leq \frac{d^{2}}{2 r+d-1}  \tag{49}\\
& \sum_{k=1}^{d} \mu_{k}^{2} \leq d\left(\frac{d}{2 r+d-1}\right)^{2} \tag{50}
\end{align*}
$$

Another simplification can be performed, which yields differentiable expressions of the constraints if (50) is to be used. In fact, noting that for any set of numbers $x_{1}, \ldots, x_{n} \in \mathbb{C}$, $\max _{i=1, \ldots, n}\left|x_{i}\right| \leq \sqrt{\sum_{i=1}^{n}\left|x_{i}\right|^{2}}$, a sufficient condition ensuring that (50) is satisfied, and hence (48), is

$$
\sum_{k=1}^{d} \sum_{p<q}\left|\left\langle\varphi_{k p}, \varphi_{k q}\right\rangle\right|^{2} \leq d\left(\frac{d}{2 r+d-1}\right)^{2}
$$

## D. Exact recoverability via coherence

We now describe a result that follows from the remarkable work of Temlyakov. It allows us to in principle determine the SS decomposition meeting the type of coherence conditions in Section VIII-A.

Some additional notations would be useful. We let $\Phi \subseteq$ $\left\{f \in L^{2}\left(X_{1} \times \cdots \times X_{d}: \operatorname{rank}(f)=1\right\}\right.$ be a dictionary ${ }^{4}$ of

[^4]separable functions (i.e. rank-1) in $L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ that meets a bounded coherence condition, i.e.
\[

$$
\begin{equation*}
\mu(\Phi)<\mu \tag{51}
\end{equation*}
$$

\]

for some $\mu \in[0,1)$ to be chosen later. Recall that the elements of $\Phi$ are implictly assumed to be of unit norm (cf. remark after Definition 23). Note that in Proposition 25, we had $\mu=$ $\prod_{k=1}^{d} \mu_{k}$ but we would not impose this here.

Let $t \in(0,1]$. The weakly orthogonal greedy algorithm (WOGA) is simple to describe: Set $f_{0}=f$. For each $m \in \mathbb{N}$, we inductively define a sequence of $f_{m}$ 's as follows:

1) $g_{m} \in \Phi$ is any element satisfying

$$
\left|\left\langle f_{m-1}, g_{m}\right\rangle\right| \geq t \sup _{g \in \mathcal{D}}\left|\left\langle f_{m-1}, g\right\rangle\right|
$$

2) $h_{m} \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ is a projection of $f$ onto $\operatorname{span}\left(g_{1}, \ldots, g_{m}\right)$, i.e.

$$
\begin{equation*}
h_{m} \in \operatorname{argmin}\left\{\|f-g\|: g \in \operatorname{span}\left(g_{1}, \ldots, g_{m}\right)\right\} \tag{52}
\end{equation*}
$$

3) $f_{m} \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ is a deflation of $f$ by $h_{m}$, i.e.

$$
f_{m}=f-h_{m}
$$

Note that by Proposition 25, the projection in (52) is welldefined, i.e. a minimizer $h_{m}$ always exist. The following result, adpated here for our purpose, was proved for any arbitrary dictionary in [66]. Also note that deflation generally does not work to compute SS decompositions, as pointed out in [63].
Theorem 29 (Temlyakov). Suppose $f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ has a SS decomposition

$$
f=\sum_{p=1}^{r} \lambda_{p} \varphi_{1 p} \otimes \cdots \otimes \varphi_{d p}
$$

with $\varphi_{1 p} \otimes \cdots \otimes \varphi_{d p} \in \Phi$ and the condition that

$$
r<\frac{t}{1+t}\left(1+\frac{1}{\mu}\right)
$$

for some $t \in(0,1]$ and $\mu=\prod_{k=1}^{d} \mu_{k}$. Then the WOGA algorithm recovers the factors exactly, or more precisely, $f_{r}=0$ and thus $f=h_{r}$.

So $h_{r}$, by its definition in (52) and our choice of $\Phi$, is given in the form of a linear combination of rank-1 functions, i.e. an rank-r SS decomposition.

## E. Greedy approximation bounds via coherence

This discussion in Section VIII-D pertains to exact recovery of a rank-r SS decomposition although our main problem really takes the form of a best rank- $r$ approximation more often than not. We will describe some greedy approximation bounds for the approximation problem in this section.

We let

$$
\sigma_{r}(\hat{f}):=\inf _{\alpha \in \mathbb{C}^{r},\left\|\varphi_{k p}\right\|=1}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \prod_{k=1}^{d} \varphi_{k p}\right\|
$$

By our definition of rank and border rank,

$$
\begin{aligned}
\sigma_{r}(\hat{f}) & =\inf \{\|\hat{f}-f\|: \operatorname{rank}(f) \leq r\} \\
& =\min \{\|\hat{f}-f\|: \overline{\operatorname{rank}}(f) \leq r\}
\end{aligned}
$$

It would be wonderful if greedy algorithms along the lines of what we discussed in Section VIII-D could yield an approximant within some provable bounds that is a factor of $\sigma_{r}(\hat{f})$. However this is too much to hope for mainly because a dictionary comprising all separable functions, i.e. $\{f$ : $\operatorname{rank}(f)=1\}$ is far too large to be amenable to such analysis. This does not prevent us from considering somewhat more restrictive dictionaries like what we did in the previous section. So again, let $\Phi \subseteq\left\{f \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right): \operatorname{rank}(f)=1\right\}$ be such that

$$
\mu(\Phi)<\mu
$$

for some given $\mu \in[0,1)$ to be chosen later. Let us instead define

$$
s_{r}(\hat{f})=\inf _{\boldsymbol{\alpha} \in \mathbb{C}^{r}, \varphi_{p} \in \Phi}\left\|\hat{f}-\sum_{p=1}^{r} \alpha_{p} \varphi_{p}\right\|
$$

Clearly

$$
\begin{equation*}
\sigma_{r}(\hat{f}) \leq s_{r}(\hat{f}) \tag{53}
\end{equation*}
$$

since the infimum is taken over a smaller dictionary.
The special case where $t=1$ in the woGA described in Section VIII-D is also called the orthogonal greedy algorithm (OGA). The result we state next comes from the work of a number of people done over the last decade: (54) is due to Gilbert, Muthukrisnan, and Strauss in 2003 [31]; (55) is due to Tropp in 2004 [68]; (56) is due to Dohono, Elad, and Temlyakov in 2006 [27]; and (57) is due to Livshitz in 2012 [48]. We merely apply it to our approximation problem here.
Theorem 30. Let $\hat{f} \in L^{2}\left(X_{1} \times \cdots \times X_{d}\right)$ and $f_{r}$ be the rth iterate as defined in WOGA with $t=1$ and input $\hat{f}$.

1) If $r<\frac{1}{32} \mu^{-1}$, then

$$
\begin{equation*}
\left\|\hat{f}-f_{r}\right\| \leq 8 r^{1 / 2} s_{r}(\hat{f}) \tag{54}
\end{equation*}
$$

2) If $r<\frac{1}{3} \mu^{-1}$, then

$$
\begin{equation*}
\left\|\hat{f}-f_{r}\right\| \leq(1+6 r)^{1 / 2} s_{r}(\hat{f}) \tag{55}
\end{equation*}
$$

3) If $r \leq \frac{1}{20} \mu^{-2 / 3}$, then

$$
\begin{equation*}
\left\|\hat{f}-f_{r \log r}\right\| \leq 24 s_{r}(\hat{f}) \tag{56}
\end{equation*}
$$

4) If $r \leq \frac{1}{20} \mu^{-1}$, then

$$
\begin{equation*}
\left\|\hat{f}-f_{2 r}\right\| \leq 3 s_{r}(\hat{f}) \tag{57}
\end{equation*}
$$

It would be marvelous if one could instead establish bounds in (54), (55), (56), and (57) with $\sigma_{r}(\hat{f})$ in place of $s_{r}(\hat{f})$ and $\{f: \operatorname{rank}(f)=1\}$ in place of $\Phi$, dropping the coherence $\mu$ altogether. In which case one may estimate how well the $r$ th OGA iterates $f_{r}$ approximates the best rank- $r$ approximation. This appears to be beyond present capabilites.

## IX. Applications

Various applications, many under the headings of CANDECOMP [12] and PARAFAC [35], have appeared in psychometrics and, more recently, also other data analytic applications. We found that many of such applications suffer from a regretable defect - there are no compelling reasons nor rigorous arguments that support the use of a rank- $r$ SS decomposition model. The mere fact that a data set may be cast in the form of a $d$-dimensional array $A \in \mathbb{C}^{n_{1} \times \cdots \times n_{d}}$ does not mean that (13) would be the right or even just a reasonable thing to do. In particular, how would one even interpret the factors $\varphi_{k p}$ 's when $d>2$ ? When $d=2$, one could arguably interpret these as principal or varimax components when orthonormality is imposed but for general $d>2$, a convincing application of a model based on the rank-r SS decomposition (13) must rely on careful arguments that follow from first principles.

The goal of this section is two-fold. First we would like to provide a selection of applications where the rank-r SS decomposition (13) arises naturally via considerations of first principles (in electrodynamics, quantum mechanics, wave propagation, etc). Secondly we want to also demonstrate that the coherence conditions discussed extensively in Section VIII invariably have reasonable interpretations in terms of physical quantities.

The use of a rank-r SS decomposition model in signal processing via the higher-order statistics has a long history [57], [30], [16], [11], [58]. Our signal processing applications here are of a different nature, they are based on geometrical properties of sensor arrays instead of considerations of higherorder statistics. This line of argument first appeared in the work of Sidiropoulos and Bro [60], which is innovative and well-motivated by first principles. However, like all other applications considered thus far, whether in data analysis, signal processing, psychometrics, or chemometrics, it does not address the serious nonexistence problem that we discussed at length in Section VIII-A. Without any guarantee that a solution to (28) exists, one can never be sure when the model would yield a solution. Another issue of concern is that the Kruskal uniqueness condition in Lemma 9 has often been invoked to provide evidence of a unique solution but as we have discussed in Section IV, this condition is impossible to check since there is no known way to efficiently computing the Kruskal rank. The applications considered below would use the coherence conditions developed in Section VIII to avoid these difficulties. More precisely, Proposition 25, Proposition 27, and Corollary 28 are invoked to guarantee the existence of a solution to the approximation problem and provide readily checkable conditions for uniqueness of the solution, all via the notion of coherence.

In this section, applications are presented in finite dimension. In order to avoid any confusion, ${ }^{*},{ }^{H}$ and ${ }^{\top}$ will denote complex conjugation, hermitian transposition, and transposition, respectively.

## A. Joint channel and source estimation

Consider a narrow band transmission problem in the far field. We assume here that we are in the context of wireless
telecommunications, but the same principle could apply in other fields. Let $r$ signals impinge on an array, so that their mixture is recorded. It is wished to recover the original signals, and to estimate their directions of arrival and respective powers at the receiver. If the channel is specular, some of these signals can correspond to different propagation paths of the same radiating source, and are hence correlated. In other words, $r$ does not denote the number of sources, but the total number of distinct paths viewed from the receiver.

In the present framework, we assume that channels can be time-varying, but that they can be assumed constant over a sufficiently short observation length. The goal is hence to be able to work with extremely short samples.

In order to face this challenge, we assume that the sensor array is structured, as in [60]. More precisely, the sensor array is composed of a reference array containing $n_{1}$ sensors, whose location is defined by a vector $\mathbf{b}_{i} \in \mathbb{R}^{3}$, and $n_{2}-1$ other subarrays, deduced from the reference array by a translation in space defined by a vector $\boldsymbol{\Delta}_{j} \in \mathbb{R}^{3}, 1<j \leq n_{2}$. The reference subarray is numbered with $j=1$ in the remainder.

Under these assumptions, the signal received at discrete time $t_{k}, k=1, \ldots, n_{3}$, on the $i$ th sensor of the reference subarray can be written as:

$$
s_{i, 1}(k)=\sum_{p=1}^{r} \sigma_{p}\left(t_{k}\right) \exp \left(\psi_{i, p}\right)
$$

with $\psi_{i, p}=\jmath \frac{\omega}{C}\left(\mathbf{b}_{i}^{\top} \mathbf{d}_{p}\right)$ where the dotless $\jmath$ denotes $\sqrt{-1}$, vector $\mathbf{d}_{p}$ is unit norm and denotes the direction of arrival of the $p$ th path. Next, on the $j$ th subarray, $j>1$, we have

$$
\begin{equation*}
s_{i, j}(k)=\sum_{p=1}^{r} \sigma_{p}\left(t_{k}\right) \exp \left(\psi_{i, j, p}\right) \tag{58}
\end{equation*}
$$

with $\psi_{i, j, p}=\jmath \frac{\omega}{C}\left(\mathbf{b}_{i}^{\top} \mathbf{d}_{p}+\boldsymbol{\Delta}_{j}^{\top} \mathbf{d}_{p}\right)$. If we let $\boldsymbol{\Delta}_{1}$ be the null vector, then (58) also applies for the reference subarray. The interest of this structure is that variables $i$ and $j$ decouple in function $\exp \left(\psi_{i, j, p}\right)$, yielding a relation resembling the rank revealing SS decomposition:

$$
s_{i, j}(k)=\sum_{p=1}^{r} \lambda_{p} u_{i p} v_{j p} w_{k p}
$$

where $u_{i p}=\exp \left(\jmath \frac{\omega}{C} \mathbf{b}_{i}^{\top} \mathbf{d}_{p}\right), v_{j p}=\exp \left(\jmath \frac{\omega}{C} \boldsymbol{\Delta}_{j}^{\top} \mathbf{d}_{p}\right)$ and $w_{k p}=\sigma_{p}\left(t_{k}\right) /\left\|\boldsymbol{\sigma}_{p}\right\|, \lambda_{p}=\left\|\boldsymbol{\sigma}_{p}\right\|$.

Hence, by computing the rank revealing decomposition of the tensor $\mathbf{S}=\left(s_{i, j}(k)\right) \in \mathbb{C}^{n_{1} \times n_{2} \times n_{3}}$, it is possible to jointly estimate: (i) signal waveforms $\sigma_{p}(k)$, and (ii) the directions of arrival $\mathbf{d}_{p}$ of each propagation path if $\mathbf{b}_{i}$ or $\boldsymbol{\Delta}_{j}$ are known.
However, the observation model (58) is not realistic, and an additional error term should be added in order to stand for modeling inaccuracies and background noise. It is customary (and realistic thanks to the central limit theorem) to assume that this additive error has a continuous probability distribution, so that tensor $\mathbf{S}$ has a generic rank. Yet, the generic rank takes values at least as large as $\left\lceil n_{1} n_{2} n_{3} /\left(n_{1}+n_{2}+n_{3}-2\right)\right\rceil$, which is always larger than Kruskal's bound [20]. Therefore, we have to face the problem of approximating tensor $\mathbf{S}$ by another of rank $r$. And we have seen that the angular
constraint imposed in Section VIII permits to deal with a wellposed problem. In order to see the physical meaning of this constraint, it is convenient to define first the tensor product between subarrays.

## B. Tensor product between sensor subarrays

The sensor arrays we cope with are structured, in the sense that the whole array is generated by one subarray, defined by the collection of vector locations $\left\{\mathbf{b}_{i} \in \mathbb{R}^{3}: 1 \leq i \leq n_{1}\right\}$, and a collection of translations in space, $\left\{\boldsymbol{\Delta}_{j} \in \mathbb{R}^{3}: 1 \leq j \leq n_{2}\right\}$. If we define vectors

$$
\begin{align*}
\mathbf{u}_{p} & =\frac{1}{\sqrt{n_{1}}}\left[\exp \left(\jmath \frac{\omega}{C} \mathbf{b}_{i}^{\top} \mathbf{d}_{p}\right)\right]_{i=1}^{n_{1}} \\
\mathbf{v}_{p} & =\frac{1}{\sqrt{n_{2}}}\left[\exp \left(\jmath \frac{\omega}{C} \boldsymbol{\Delta}_{j}^{\top} \mathbf{d}_{p}\right)\right]_{j=1}^{n_{2}}  \tag{59}\\
\mathbf{w}_{p} & =\frac{\boldsymbol{\sigma}_{p}}{\left\|\boldsymbol{\sigma}_{p}\right\|}
\end{align*}
$$

then this means that we may see all measurements as the superimposition of decomposable tensors:

$$
\lambda_{p} \mathbf{u}_{p} \otimes \mathbf{v}_{p} \otimes \mathbf{w}_{p}
$$

The geometry of the sensor array is contained in $\mathbf{u}_{p} \otimes \mathbf{v}_{p}$, whereas $\lambda_{p}$ and $\mathbf{w}_{p}$ contain energy and time information on each path $p$, respectively. Note that the reference subarray and the set of translations play symmetric roles, in the sense that $\mathbf{u}_{p}$ and $\mathbf{v}_{p}$ could be interchanged without changing the whole array. This will become clear with a few examples.

When we are given a structured sensor array, there can be several ways of splitting it into a tensor product of two (or more) subarrays, as now shown by simple examples.

Example 31. Define the matrix of sensor locations

$$
\left[\mathbf{b}_{1}, \mathbf{b}_{2}, \mathbf{b}_{3}\right]=\left[\begin{array}{ccc}
0 & 0 & 1 \\
0 & 1 & 1
\end{array}\right]
$$

This subarray is depicted in Figure 1.b. By translating it according to the translation defined in Figure 1.c one obtains another subarray. The union of the two subarrays yields the array of Figure 1.a. The same array is obtained by interchanging the roles of the two subarrays, i.e. three subarrays of two sensors deduced from each other by two translations.
(a)






Fig. 1. Antenna array (a) is obtained as the tensor product between subarrays (b) and (c)

Example 32. Define the array by

$$
\left[\mathbf{b}_{1}, \mathbf{b}_{2}, \ldots, \mathbf{b}_{6}\right]=\left[\begin{array}{cccccc}
0 & 1 & 2 & 0 & 1 & 2 \\
0 & 0 & 0 & 1 & 1 & 1
\end{array}\right]
$$

This array, depicted in Figure 2.a, can be obtained either by the union of subarray of Figure 2.6 and its translation
defined by Figure 2.c, or by the array of Figure 2.c translated three times according to Figure 2.b. We agree to express this relationship by the equation:

Another decomposition may be obtained as

$$
\underset{0-0}{0-0}=i_{0} \otimes \ldots
$$

 it is important to stress that the various decompositions of the whole array into tensor products of subarrays are not equivalent from the point of view of performance. In particular, the Kruskal's bound can be different, as will be pointed out next.
(a) (b)


(c)


Fig. 2. Antenna array (a) is obtained as the tensor product between subarrays (b) and (c)

Similar observations can be made for grid arrays in general.
Example 33. Take an array of 9 sensors located at $(x, y) \in$ $\{1,2,3\} \times\{1,2,3\}$. We have the relations

among others.
Let's now have a look at the maximal number of sources $r_{\text {max }}$ that can be extracted from a $n_{1} \times n_{2} \times n_{3}$. A sufficient condition is that the total number of paths, $r$, is smaller than Kruskal's bound (25). We shall simplify the bound by making two assumptions: (a) the loading matrices are generic, that is, they are full rank, and (b) the number of paths is larger than the sizes $n_{1}$ and $n_{2}$ of the two subarrays entering the array tensor product, and smaller than the number of time samples, $n_{3}$. Under these simplifying assumptions, Kruskal's bound becomes $2 r_{\max } \leq n_{1}+n_{2}+r_{\max }-2$, or:

$$
\begin{equation*}
r_{\max }=n_{1}+n_{2}-2 \tag{60}
\end{equation*}
$$

The table below illustrates the fact that the choice of subarrays has an impact on this bound.

| Array | Subarray product | $n_{1}$ | $n_{2}$ | $r_{\text {max }}$ |
| :---: | :---: | :---: | :---: | :---: |
| $a^{-\infty}$ | $0^{-\infty} \otimes$ | 3 | 2 | 3 |
| a-0 | $1-9 \otimes 00$ | 4 | 2 | 4 |
|  | $!\otimes 0-0$ | 2 | 3 | 3 |
| ancoand$0-3$ | $!\otimes 0-0$ | 3 | 3 | 4 |
|  | ?-9-? $\otimes$ ! | 6 | 2 | 6 |
|  | d-0 $\otimes$ and | 4 | 4 | 6 |

## C. Significance of the angular constraint

We are now in a position to interpret the meaning of angular constraints proposed in Section VIII. According to the notations given in (59), the first coherence

$$
\mu_{1}=\max _{p \neq q}\left|\mathbf{u}_{p}^{\mathrm{H}} \mathbf{u}_{q}\right|
$$

corresponds to the angular separation viewed from the reference subarray. In fact, vectors $\mathbf{b}_{i}$ and $\mathbf{d}_{p}$ having a unit norm, as well as vectors $\mathbf{u}_{p}$, the quantity $\left|\mathbf{u}_{p}^{\mathrm{H}} \mathbf{u}_{q}\right|$ may be seen as a measure of angular separation between $\mathbf{d}_{p}$ and $\mathbf{d}_{q}$, as we shall now subsequently show in Proposition 35.

Definition 34. We shall say that a collection of vectors $\left\{\mathbf{b}_{1}, \ldots, \mathbf{b}_{n}\right\}$ is resolvent with respect to a direction $\mathbf{v} \in \mathbb{R}^{3}$ if there exist two indices $k$ and $l$ such that $\mathbf{v}=\mathbf{b}_{k}-\mathbf{b}_{l}$ and

$$
\begin{equation*}
0<\|\mathbf{v}\|<\frac{\lambda}{2} \tag{61}
\end{equation*}
$$

where $\lambda=\frac{2 \pi C}{\omega}$ denotes the wavelength.
Let $\mathbf{b}_{i}, \mathbf{d}_{p}$ and $\mathbf{u}_{q}$ be defined as in (59), $1 \leq i \leq n_{1}$, $1 \leq p, q \leq n_{2}$. Then we have [19]:

Proposition 35. If $\left\{\mathbf{b}_{1}, \ldots, \mathbf{b}_{n}\right\}$ is resolvent with respect to three linearly independent directions, then

$$
\left|\mathbf{u}_{p}^{\mathrm{H}} \mathbf{u}_{q}\right|=1 \Leftrightarrow \mathbf{d}_{p}=\mathbf{d}_{q} .
$$

Proof: Assume $\left|\mathbf{u}_{p}^{\mathrm{H}} \mathbf{u}_{q}\right|=1$. Then because they are unit norm, vectors $\mathbf{u}_{p}$ and $\mathbf{u}_{q}$ are collinear with a unit modulus proportionality factor. Hence from (59), for all $j, k$, $1 \leq j, k \leq n_{1},\left(\mathbf{b}_{j}-\mathbf{b}_{k}\right)^{\top}\left(\mathbf{d}_{p}-\mathbf{d}_{q}\right) \in \lambda \mathbb{Z}$, where $\lambda$ is defined in Definition 61. Since $\left\{\mathbf{b}_{1}, \ldots, \mathbf{b}_{n}\right\}$ is resolvant, there exist ( $k, l$ ) such that $0<\left\|\mathbf{b}_{k}-\mathbf{b}_{l}\right\|<\lambda / 2$. Hence, because vectors $\mathbf{d}_{p}$ are unit norm, $\left\|\mathbf{d}_{p}-\mathbf{d}_{q}\right\| \leq 2$ so that we necessarily have that $\left(\mathbf{b}_{k}-\mathbf{b}_{l}\right)^{\top}\left(\mathbf{d}_{p}-\mathbf{d}_{q}\right)=0$. Vector $\left(\mathbf{d}_{p}-\mathbf{d}_{q}\right)$ is consequently orthogonal to $\left(\mathbf{b}_{k}-\mathbf{b}_{l}\right)$. The same reasoning can be carried out with two other independent vectors. Eventually, vector $\left(\mathbf{d}_{p}-\mathbf{d}_{q}\right)$ is null because it is orthogonal to three linearly independent vectors in $\mathbb{R}^{3}$. The converse is immediate, by the definition of $\mathbf{u}_{q}$.

Note that the condition of Definition 61 is not very restrictive, since sensor arrays usually contain sensors separated by half a wavelength or less. Thanks to Proposition 35, we now
know that uniqueness of the matrix factor $\mathbf{U}=\left[\mathbf{u}_{1}, \ldots, \mathbf{u}_{r}\right]$ and identifiability of the directions of arrival $\mathbf{d}_{p}$ are equivalent. And from the results of Section VIII, they are ensured by a constraint on coherence such as (48).

From Section IX-B, one can claim that a similar interpretation can be put forward for the second coherence, which measures the minimal angular separation between paths, viewed from the subarray defining translations.

The third coherence is nothing else but the maximal correlation coefficient between signals received from various paths on the array:

$$
\mu_{3}=\max _{p \neq q} \frac{\left|\boldsymbol{\sigma}_{p}^{\mathrm{H}} \boldsymbol{\sigma}_{q}\right|}{\left\|\boldsymbol{\sigma}_{p}\right\|\left\|\boldsymbol{\sigma}_{q}\right\|}
$$

As a conclusion, the tensor approximation exists and is unique if either signals propagating through various paths are not too much correlated, or if their direction of arrival are not too close. By "not too" it should be understood that the product of coherencies need to satisfy inequality (48) of Corollary 28. In other words, one can separate paths with high correlation provided they are sufficiently well separated in space.

Hence, the decomposition of an array into a tensor product of two (or more) subarrays should not only take into account Kruskal's bound, as elaborated in Section IX-B, but also the ability of the latter subarrays to separate two distinct directions of arrival (cf. Proposition 35).

## D. CDMA communications

The application to antenna array processing we described in Section IX-A is one among many others, including Sparse Component Analysis and Compressed Sensing. Actually, the present framework also applies to all Source Separation problems, as those reported in [18], provided an additional diversity is available. For example, one can mention the case of Code Division Multiple Access (CDMA) communications. In fact, as already pointed out in [61], it is possible to distinguish between symbol and chip diversities. In order to be more explicit, let's detail a little further the latter example.

Consider a downlink CDMA communication with $r$ users, each assigned a spreading sequence $C_{p}(k), 1 \leq p \leq r, 1 \leq$ $k \leq n$. Next, denote $A_{i p}$ the complex gain between sensor $i$, $i=1, \ldots, m$, and user $p, S_{j p}$ the symbol sequence transmitted by user $p, j \in \mathbb{Z}$, and $H_{p}(k)$ the channel impulse response of user $p$. Then, the signal received on sensor $i$ during the $k$ th chip of the $j$ th symbol period takes the form:

$$
T_{i j k}=\sum_{p=1}^{r} A_{i p} S_{j p} B_{k p}
$$

where $B_{k p}=\sum_{t} H_{p}(k-t) C_{p}(t)$ denotes the output of the $p$ th channel excited by the $p$ th coding sequence, after removal of the guard chips (which may be affected by two different consecutive symbols) [61].

The columns of matrix B are often referred to as "effective codes", and coincide with spreading codes if the channel is memoryless and noiseless. In practice, the receiver filter is matched to the transmitter shaping filter combined with the propagation channel, so that effective and spreading codes are
ideally proportional. Under these conditions, the coherence $\mu_{C}$ accounts for the angular separation between spreading sequences: $\mu_{C}=0$ means that they are orthogonal. On the other hand, $\mu_{A}=0$ means that symbol sequences are all uncorrelated. Lastly, as seen in Proposition 35, $\mu_{B}=1$ means directions of arrival are collinear.

Yet, in order to avoid multiple access interferences, spreading sequences are usually chosen uncorrelated for all delays, which implies among others that they are orthogonal. Hence the results obtained in this paper show that spreading sequences do not need to be orthogonal, nor symbol sequences need to be uncorrelated, if directions of arrival are not collinear. In particular, shorter spreading sequences may be used for the same number of users, which would increase the throughput. Alternatively, one could increase the number of users for a given spreading gain. This is made possible because the constraint of having almost orthogonal spreading sequences is relaxed. In addition, some directions of arrival may be collinear if the corresponding spreading sequences are sufficiently angularly separated. However, these conclusions are essentially valid when users are synchronized, that is, for downlink communications.

## E. Polarization

The exploitation of polarization as an additional diversity takes its roots in the paper by Nehorai and Paldi [54]. Several attempts to use this diversity in the frame of tensorbased source localization and estimation can be found in the literature. A good account of the existing approaches can be found in [34].

In this framework, we consider again an array of $n_{1}$ sensors, whose location is defined by a 3-dimensional real vector $\mathbf{b}_{i}$, and we assume a narrow-band transmission in the far field (i.e. sources - or source paths - are all seen as plane waves at the receiver sensor array). The difference with Section IX-B is that the translation diversity is not mandatory anymore, provided impinging waves are polarized, and provided their polarization is neither linear nor circular. One measures the electric and magnetic fields at each sensor as a function of time, so that $n_{2}=6$. More precisely, vector $\mathbf{v}_{p}$ of Equation (59) is replaced by:

$$
\begin{equation*}
\mathbf{v}_{p}=\mathbf{B}_{p} \mathbf{g}_{p} \tag{62}
\end{equation*}
$$

where $\mathbf{B}_{p}$ is a $6 \times 2$ matrix depending only on the direction of arrival $\mathbf{d}_{p}$ (defined in Section IX-B), and a vector $\mathbf{g}_{p}$ depending on the orientation and ellipticity of the polarization of the $p$ th wave.

Coherences $\mu_{1}$ and $\mu_{3}$ are the same as in Section IX-B, and represent respectively the angular separation between directions of arrival, and correlation coefficient between arriving sources. It is slightly more involved to capture the significance of the coherence associated with polarization, $\mu_{2}$.

With this goal, we need to go into more details. Referring to [54], and denoting $\alpha_{p}$ and $\beta_{p}$ the orientation and ellipticity angles of the polarization of the $p$ th wave, $\alpha_{p} \in(-\pi / 2, \pi / 2]$,
$\beta_{p} \in(-\pi / 4, \pi / 4)-\{0\}$, we have:

$$
\begin{gathered}
\mathbf{B}_{p}=\frac{1}{\sqrt{2}}\left[\begin{array}{cc}
\mathbf{e}_{p} & \mathbf{f}_{p} \\
\mathbf{f}_{p} & -\mathbf{e}_{p}
\end{array}\right] \\
\mathbf{g}_{p}=\mathbf{Q}\left(\alpha_{p}\right) \mathbf{h}_{p}
\end{gathered}
$$

with

$$
\begin{gathered}
\mathbf{e}_{p}=\left[\begin{array}{c}
-\sin \theta_{p} \\
\cos \theta_{p} \\
0
\end{array}\right], \mathbf{f}_{p}=\left[\begin{array}{c}
-\cos \theta_{p} \sin \chi_{p} \\
-\sin \theta_{p} \sin \chi_{p} \\
\cos \chi_{p}
\end{array}\right] \\
\mathbf{Q}(\alpha)=\left[\begin{array}{rr}
\cos \alpha & \sin \alpha \\
-\sin \alpha & \cos \alpha
\end{array}\right], \mathbf{h}_{p}=\binom{\cos \beta_{p}}{\jmath \sin \beta_{p}}
\end{gathered}
$$

where $\theta_{p} \in[0,2 \pi)$ and $\chi_{p} \in(-\pi / 2, \pi / 2]$ denote respectively the azimuth and elevation of the direction of arrival of the $p$ th path. In particular, the unit vector defining the $p$ th direction of arrival is:

$$
\mathbf{d}_{p}=\left(\begin{array}{c}
\cos \theta_{p} \cos \chi_{p} \\
\sin \theta_{p} \cos \chi_{p} \\
\sin \chi_{p}
\end{array}\right)
$$

so that the triplet $\left(\mathbf{d}_{p}, \mathbf{e}_{p}, \mathbf{f}_{p}\right)$ forms a right orthonormal triad.
Lemma 36. $\left|\mathbf{g}_{p}^{H} \mathbf{g}_{q}\right|=1$ if and only if $\alpha_{p}=\alpha_{q}+k \pi$ and $\beta_{p}=\beta_{q}, k \in \mathbb{Z}$.
Proposition 37. $\left|\mathbf{v}_{p}^{H} \mathbf{v}_{q}\right| \leq 1$, with equality if and only if $\alpha_{p}=$ $\alpha_{q}+k \pi, \beta_{p}=\beta_{q}, \theta_{p}=\theta_{q}+k^{\prime} \pi$ and $\chi_{p}=\chi_{q}, k, k^{\prime} \in \mathbb{Z}$.

Proofs are given in appendix. This proposition proves that a constraint on coherence $\mu_{2}$ imposes sources paths to have either different directions of arrival or to have different polarizations. The constraint $\mu_{2}<1$ has hence a clear physical meaning. It is also interesting to note that $\mu_{2}<1$ contributes to satisfy $\mu_{1}<1$, because $\mu_{1}$ also involves directions of arrival.

## F. Fluorescence spectral analysis

Here an another application to fluorescence spectral analysis [62]. We refer the reader to Example 6 for the notations used here. Suppose we have $l$ samples with an unknown number of pure substances in different concentration that are fluorescent. If $a_{i j k}$ is the measured fluorescence emission intensity at wavelength $\lambda_{j}^{\mathrm{em}}$ of $i$ th sample excited with light at wavelength $\lambda_{k}^{\mathrm{ex}}$. The measured data is a 3 -dimensional hypermatrix $A=\left(a_{i j k}\right) \in \mathbb{R}^{l \times m \times n}$. At low concentrations, Beer's law of spectroscopy (which in turn is a consequence of fundamental principles in quantum mechanics) can be linearized [49], and yields a rank-revealing decomposition:

$$
A=\mathbf{x}_{1} \otimes \mathbf{y}_{1} \otimes \mathbf{z}_{1}+\cdots+\mathbf{x}_{r} \otimes \mathbf{y}_{r} \otimes \mathbf{z}_{r}
$$

This can reveal the true chemical factors responsible for the data: $r=\operatorname{rank}(A)$ would be the number of pure substances in the mixtures, $\mathbf{x}_{p}=\left(x_{1 p}, \ldots, x_{l p}\right)$ would be the relative concentrations of $p$ th substance in specimens $1, \ldots, l ; \mathbf{y}_{p}=$ $\left(y_{1 p}, \ldots, y_{m p}\right)$ the excitation spectrum of $p$ th substance; $\mathbf{z}_{p}=$ $\left(z_{1 p}, \ldots, z_{n p}\right)$ the emission spectrum of $p$ th substance. The spectra would then allow one to identify the pure substances.

Of course this is only valid in an idealized situation when the measurements are performed perfectly without error and noise. Under realistic noisy circumstances, one would then need to a find best rank- $r$ approximation.

## G. Statistical independence induces diversity

When measurements are recorded only as a function of two variables (e.g. time and space), the present framework can apply if at least one additional diversity is taken into account. We have seen already several instances of additional diversities in the previous subsections. We shall point out now a quite different way to build a function of more than two variables, which makes sense from the physical point of view.

Assume the linear model below

$$
\begin{equation*}
\mathbf{x}(t)=U \mathbf{s}(t) \tag{63}
\end{equation*}
$$

where only signal $\mathbf{x}(t)$ is observed, $U=\left[\mathbf{u}_{1}, \ldots, \mathbf{u}_{r}\right]$ is an unknown $N \times r$ matrix, and $\mathbf{s}(t)$ is of dimension $r$ with mutuallly statistically independent components, $s_{i}(t)$. Then one can build the $d$ th order cumulant tensor of $\mathbf{x}(t), \mathbf{T}$, and the latter will satisfy the SS model [52]:

$$
\mathbf{T}=(U, \ldots, U) \cdot \boldsymbol{\Lambda}=\sum_{p=1}^{r} \lambda_{p} \mathbf{u}_{p} \otimes \cdots \otimes \mathbf{u}_{p}
$$

where $\boldsymbol{\Lambda}$ denotes the cumulant tensor of s . Yet, because of statistical independence, $\boldsymbol{\Lambda}$ is diagonal [18]. If $d \geq 3$, and if at most one entry of $\boldsymbol{\Lambda}$ is null, then matrix $U$ and the entries $\Lambda_{p \cdots p}=\lambda_{p}$ can be identified. The uniqueness of the solution is subject to identifiability conditions evoked earlier.

As pointed out in [18] and references therein, this kind of problems generalizes to convolutive mixtures as well, and finds applications in telecommunications, radar, sonar, speech processing, and biomedical engineering, among others.

## H. Nonstationarity induces diversity

If a signal $x(t)$ is nonstationary, its time-frequency transform, defined by

$$
X(t, f)=\int x(u) \kappa(u-t ; f) d u
$$

for some given kernel $\kappa$, bears information. If variables $t$ and $f$ are discretized, then the values of $X(t, f)$ can be stored in a matrix $X$, and the more nonstationary $x(t)$, the larger the rank of $X$. A similar statement can be made on a signal $y(\mathbf{z})$ depending on a space variable $\mathbf{z}$. The discrete values of the space-wavevector transform $Y(\mathbf{z}, \mathbf{w})$ of a field $y(\mathbf{z})$ can be stored in a matrix $Y$. And the less homogeneous the field $y(\mathbf{z})$, the larger the rank of $Y$. This is probably the reason why algorithms proposed in [69], [3] permit to localize and extract dipole contributions in the brains by identifying a multilinear model, provided the have distinct time-frequency or spacewavevector patterns. Nevertheless, localization is guaranteed to be successful only under restrictive assumptions.

## X. Future work

A separate article discussing practical algorithms for the bounded coherence best rank- $r$ SS approximation is under preparation with additional coauthors. These algorithms follow the general strategy of the greedy approximations WOGA and ogA discussed in Sections VIII-D and VIII-E but contain other elements exploiting the special separable structure of our problem. Extensive numerical experiments will be provided in the forthcoming article.

## Appendix

Proof of Lemma 36. First note that $\mathbf{Q}\left(\alpha_{p}\right)^{H} \mathbf{Q}\left(\alpha_{q}\right)=$ $\mathbf{Q}\left(\alpha_{q}-\alpha_{p}\right)$. Hence $\mathbf{g}_{p} \mathbf{H}_{q}$ can be of unit modulus only if $\mathbf{h}_{p}$ and $\mathbf{Q}\left(\alpha_{q}-\alpha_{p}\right) \mathbf{h}_{q}$ are collinear. But the first entry of $\mathbf{h}_{p}$ is real and the second is pure imaginary. Hence, corresponding imaginary and real parts of $\mathbf{Q}\left(\alpha_{q}-\alpha_{p}\right) \mathbf{h}_{q}$ must be zero, which implies that $\sin \left(\alpha_{q}-\alpha_{p}\right)=0$. Consequently $\mathbf{Q}\left(\alpha_{q}-\alpha_{p}\right)= \pm \mathbf{I}$, which yields $\mathbf{h}_{p}= \pm \mathbf{h}_{q}$. But because angle $\beta$ lies in the interval $(-\pi / 4, \pi / 4)$, only the positive sign is acceptable.

Proof of Proposition 37. We have $\left|\mathbf{v}_{p}^{\mathrm{H}} \mathbf{v}_{q}\right|=\left|\mathbf{g}_{p}^{\mathrm{H}} \mathbf{B}_{p}^{\top} \mathbf{B}_{q} \mathbf{g}_{q}\right|$. Notice that matrix $\mathbf{B}_{p}^{\top} \mathbf{B}_{q}$ is of the form

$$
\mathbf{B}_{p}^{\top} \mathbf{B}_{q}=\left(\begin{array}{rr}
\gamma & \eta \\
-\eta & \gamma
\end{array}\right)
$$

where $\gamma$ and $\eta$ are real, $\gamma=\frac{1}{2}\left(\mathbf{e}_{p}^{\top} \mathbf{e}_{q}+\mathbf{f}_{p}^{\top} \mathbf{f}_{q}\right)$ and $\eta=\frac{1}{2}\left(\mathbf{e}_{p}^{\top} \mathbf{f}_{q}-\right.$ $\mathbf{f}_{p}^{\top} \mathbf{e}_{q}$ ). Yet, since vectors $\mathbf{g}_{p}$ and $\mathbf{g}_{q}$ are of unit modulus, $\left|\mathbf{v}_{p}^{\mathrm{H}} \mathbf{v}_{q}\right|$ can be of unit modulus only if matrix $\mathbf{B}_{p}^{\top} \mathbf{B}_{q}$ has an eigenvalue of unit modulus, which requires that $\gamma^{2}+\eta^{2}=1$. Let us prove that we have $\gamma^{2}+\eta^{2} \leq 1$ with equality if and only if results of Proposition 37 are satisfied.

With this goal, define the three 6-dimensional vectors:

$$
\mathbf{z}=\frac{1}{\sqrt{2}}\left[\begin{array}{c}
\mathbf{e}_{p} \\
\mathbf{f}_{p}
\end{array}\right], \mathbf{w}=\frac{1}{\sqrt{2}}\left[\begin{array}{c}
\mathbf{e}_{q} \\
\mathbf{f}_{q}
\end{array}\right], \mathbf{w}^{\prime}=\frac{1}{\sqrt{2}}\left[\begin{array}{c}
\mathbf{f}_{q} \\
-\mathbf{e}_{q}
\end{array}\right]
$$

Then $\gamma=\mathbf{z}^{\top} \mathbf{w}$ and $\gamma=\mathbf{z}^{\top} \mathbf{w}^{\prime}$. Now decompose vector $\mathbf{z}$ into two orthogonal parts: $\mathbf{z}=\mathbf{z}_{0}+\mathbf{z}_{1}$, with $\mathbf{z}_{0} \in \operatorname{Span}\left\{\mathbf{w}, \mathbf{w}^{\prime}\right\}$ and $\mathbf{z}_{0} \perp \mathbf{z}_{1}$. Clearly, $\gamma^{2}+\eta^{2}=\left\|\mathbf{z}_{0}\right\|^{2}$. It is also bounded by one because $\left\|z_{0}\right\|^{2} \leq\|\mathbf{z}\|^{2}=1$, with equality if and only if $\mathbf{z} \in \operatorname{Span}\left\{\mathbf{w}, \mathbf{w}^{\prime}\right\}$. By inspection of the definitions of $\mathbf{e}_{p}$ and $\mathbf{e}_{q}$, we see that the third entry of $\mathbf{z}$ and $\mathbf{w}$ is null. Hence $\mathbf{z} \in \operatorname{Span}\left\{\mathbf{w}, \mathbf{w}^{\prime}\right\}$ is possible only if either $\mathbf{z}$ is collinear to $\mathbf{w}$ or if the third entry of $\mathbf{w}^{\prime}$ is null. In the latter case, it means that $\chi_{q}=\pi / 2$, and then that $\chi_{p}=\pi / 2$ and $\theta_{p}=\theta_{q}$. In the former case, it can be seen that $\sin \theta_{p}=\sin \theta_{q}$, and finally that $\chi_{p}=\chi_{q}$.

The last step is to rewrite $\gamma$ and $\eta$ as a function of angle $\theta_{p}-\theta_{q}$, using trigonometric relations: $\gamma=\cos \left(\theta_{p}-\theta_{q}\right)(1+$ $\left.\sin \chi_{p} \sin \chi_{q}\right)+\cos \chi_{p} \cos \chi_{q}$ and $\eta=\sin \left(\theta_{p}-\theta_{q}\right)\left(\sin \chi_{p}+\right.$ $\sin \chi_{q}$ ). This eventually shows that $\gamma=1$ and $\eta=0$. As a consequence, $\left|\mathbf{v}_{p}^{\mathrm{H}} \mathbf{v}_{q}\right|=1$ only if $\mathbf{B}_{p}^{\top} \mathbf{B}_{q}=\mathbf{I}$, and the proposition follows by applying the lemma.

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We thank Ignat Domanov for pointing out that in Proposition 25, the factor on the right hand side may be improved from $r$ to $r-1$, and that the improvement is sharp. Sections VIII-D and VIII-E came from an enlightening series of lectures Vladimir Temlyakov gave at the IMA in Minneapolis and the useful pointers he graciously provided afterwards. We also gratefully acknowledge Tom Luo, Nikos Sidiropoulos, and Yuan Yao, for their very helpful discussions.

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[^1]:    ${ }^{1}$ Point values of $L^{p}$-functions are undefined in general. So equations like these are taken to implicitly mean almost everywhere. Anyway all functions that arise in our applications will at least be continuous and so this is really not a point of great concern.

[^2]:    ${ }^{2}$ We clarify our terminologies: A multipartite function is one for which the arguments $\mathbf{x}_{1}, \ldots, \mathbf{x}_{d}$ can come from any $X_{1}, \ldots, X_{d}$ but a multivariate function, in the usual sense of the word, is one where $X_{1}, \ldots, X_{d}$ are (measurable) subsets of $\mathbb{R}$. So the former is a more general notion.

[^3]:    ${ }^{3}$ Also called the greatest convex minorant, in this case also equivalent to the Legendre-Frenchel biconjugate or convex biconjugate.

[^4]:    ${ }^{4}$ A dictionary is any set $\Phi \subseteq \mathbb{H}$ whose linear span is dense in the Hilbert space $\mathbb{H}$.

