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# Perturbation of higher-order singular values 

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#### Abstract

The higher-order singular values for a tensor of order $d$ are defined as the singular values of the $d$ different matricizations associated with the multilinear rank. When $d \geq 3$, the singular values are generally different for different matricizations but not completely independent. Characterizing the set of feasible singular values turns out to be difficult. In this work, we contribute to this question by investigating which first-order perturbations of the singular values for a given tensor are possible. We prove that, except for trivial restrictions, any perturbation of the singular values can be achieved for almost every tensor with identical mode sizes. This settles a conjecture from [Hackbusch and Uschmajew, 2016] for the case of identical mode sizes. Our theoretical results are used to develop and analyze a variant of the Newton method for constructing a tensor with specified higher-order singular values or, more generally, with specified Gramians for the matricizations. We establish local quadratic convergence and demonstrate the robust convergence behavior with numerical experiments.


Keywords: Tensors • higher-order singular value decomposition • Newton method

## 1 Introduction

Various types of matricizations (or flattenings) of a higher-order tensor $\mathbf{X}$ are connected with subspace-based decompositions for representing and compressing $\mathbf{X}$, such as the Tucker, the hierarchical Tucker, and the tensor train decompositions; see [1,6,7,9] for surveys. In particular, the singular values of matricizations allow for quantifying the error committed when approximating $\mathbf{X}$ by such decompositions of lower rank. In this work, we continue our study [8] of the singular values for matricizations associated with the Tucker decomposition. In particular, we address the question whether these singular values can be moved in arbitrary directions by small perturbations of $\mathbf{X}$.

### 1.1 Notation

Let us briefly recall the notation from [8]. Let $\mathbf{X} \in \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \cong \mathbb{R}^{n_{1}} \otimes \cdots \otimes \mathbb{R}^{n_{d}}$ be a real tensor of order $d$ with mode sizes $n_{1}, \ldots, n_{d}$. There are $d$ principal matricizations (flattenings)

$$
M_{\mathbf{X}}^{(j)} \in \mathbb{R}^{n_{1} \times n_{j}^{c}} \cong \mathbb{R}^{n_{j}} \otimes\left(\bigotimes_{i \neq j} \mathbb{R}^{n_{i}}\right)
$$

[^0]where we have set $n_{j}^{c}=\prod_{i \neq j} n_{i}$. The $k$ th row of $M_{\mathbf{X}}^{(j)}$ contains a vectorization (in some prespecified ordering) of the slice $\mathbf{X}(\cdots, k, \cdots)$ with $k$ fixed at position $j$.

We denote with

- $\sigma_{\mathbf{X}}^{(j)} \in \mathbb{R}^{n_{j}}$ the vector of singular values of $M_{\mathbf{X}}^{(j)}$ (arranged, e.g., in decreasing order);
- $\Sigma_{\mathbf{X}}=\left(\sigma_{\mathbf{X}}^{(1)}, \ldots, \sigma_{\mathbf{X}}^{(d)}\right) \in \mathbb{R}^{n_{1}} \times \cdots \times \mathbb{R}^{n_{d}}$ the tuple of higher-order singular values of $\mathbf{X} ;$
- $G_{\mathbf{X}}^{(j)}=M_{\mathbf{X}}^{(j)}\left(M_{\mathbf{X}}^{(j)}\right)^{T}$ the Gram matrix of the $j$ th matricization;
- $\mathscr{S}=\left\{\mathbf{X} \in \mathbb{R}^{n_{1} \times \cdots \times n_{d}}:\|\mathbf{X}\|_{F}=1\right\}$ the unit sphere in $\mathbb{R}^{n_{1} \times \cdots \times n_{d}}$;
- $S^{(j)}=\left\{x \in \mathbb{R}^{n_{j}}:\|x\|_{2}=1\right\}$ the unit sphere in $\mathbb{R}^{n_{j}}$;
- $\mathfrak{S}=S^{(1)} \times \cdots \times S^{(d)}$ the Cartesian product of unit spheres;
- $\mathbb{R}_{\text {sym }}^{n \times n}$ the space of real symmetric $n \times n$ matrices.

Further notation will be introduced in the text.

## 2 Problem statement

The singular values $\sigma_{\mathbf{X}}^{(j)}$ of the matricizations $M_{\mathbf{X}}^{(j)}$ are not unrelated for different $j$. For example, if $\mathbf{X} \in \mathscr{S}$ then $\sigma_{\mathbf{X}}^{(j)} \in S^{(j)}$ for all $j$. Beyond this simple fact, it is, however, not trivial to describe the relations between $\sigma_{\mathbf{X}}^{(j)}$. For instance, it is not clear which combinations of singular values can actually occur. This amounts to the study of the following set (here $S_{n}$ is the group of $n \times n$ permutation matrices).

Definition 2.1. The set

$$
\mathfrak{F}=\mathfrak{F}\left(n_{1}, \ldots, n_{d}\right):=\left\{\left(\pi^{(1)} \sigma_{\mathbf{X}}^{(1)}, \ldots, \pi^{(d)} \sigma_{\mathbf{X}}^{(d)}\right): \mathbf{X} \in \mathscr{S}, \pi^{(j)} \in \mathrm{S}_{n_{j}} \text { for } j=1, \ldots, d\right\}
$$

is called the set of normalized feasible configurations.
By the discussion above, $\mathfrak{F}$ is a subset of $\mathfrak{S}$, actually a subset of nonnegative tuples in $\mathfrak{S}$. An interesting, but apparently hard problem is to decide for a given $\Sigma \in \mathfrak{S}$ whether $\Sigma \in \mathfrak{F}$, e.g., by constructing a tensor $\mathbf{X} \in \mathscr{S}$ with $\Sigma_{\mathbf{X}}=\Sigma$ (possibly up to sorting). Numerically, this can be tested using the alternating projection method from [8] or the Newton method introduced in Sec. 5.

In this work, we focus on a different question regarding feasible configurations, namely whether $\mathfrak{F}$ contains interior points (relative to $\mathfrak{S}$ ).

Problem 2.2. Does $\mathfrak{F}$ contain interior points (relative to $\mathfrak{S}$ )? For which $\mathbf{X} \in \mathscr{S}$ is $\Sigma_{\mathbf{X}}$ an interior point?

An interesting point about this question is that if $\Sigma_{\mathbf{X}}$ is an interior point of $\mathfrak{F}$, then the higherorder singular values of $\mathbf{X}$ are locally independent in the sense that for small, but otherwise arbitrary perturbations $\tilde{\Sigma}=\Sigma+O(\varepsilon) \in \mathfrak{S}$, there exists a tensor $\tilde{\mathbf{X}}$ with $\Sigma_{\tilde{\mathbf{X}}}=\tilde{\Sigma}$ (up to sorting). For instance it is then possible to perturb only the singular values in one direction $j$ while keeping the others fixed. Of course, this cannot hold for matrices (tensors of order $d=2$ ), since a matrix and its transpose have identical singular values. In fact, $\mathfrak{F}\left(n_{1}, n_{2}\right)$ is the closure of a $\min \left(n_{1}-1, n_{2}-1\right)$-dimensional
submanifold of $\mathfrak{S}\left(n_{1}, n_{2}\right)$ (which itself is of dimension $n_{1}+n_{2}-2$ ), and hence contains no interior point (unless $n_{1}=n_{2}=1$ ). Also, we need to exclude tensors with $n_{j}>n_{j}^{c}$ because the size $n_{j} \times n_{j}^{c}$ of the matricization $M_{\mathbf{X}}^{(j)}$ would then imply that some of the singular values are always zero. This leads us to the following conjecture from [8, Conjecture 3.5].

Conjecture 2.3. For $d \geq 3$, let $n_{1}, \ldots, n_{d}$ satisfy the compatibility condition $n_{j} \leq n_{j}^{c}$ for $j=1, \ldots, d$. Then for almost all $\mathbf{X} \in \mathscr{S}$ the higher-order singular value tuple $\Sigma_{\mathbf{X}}$ is an interior point of $\mathfrak{F}\left(n_{1}, \ldots, n_{d}\right)$ with respect to the standard Lebesgue surface measure on $\mathscr{S}$.

The main theoretical result of this paper is a rigorous proof of this conjecture for $n \times \cdots \times n$ tensors.

Theorem 2.4. Conjecture 2.3 is true for $n \times \cdots \times n$ tensors of order $d \geq 3$ and size $n \geq 2$.

### 2.1 Equivalent formulation using Gram matrices

Our proof of Theorem 2.4 follows the strategy sketched in [8, Remark 3.6]. The main role is played by the map

$$
\Phi: \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \rightarrow \mathbb{R}_{\text {sym }}^{n_{1} \times n_{1}} \times \cdots \times \mathbb{R}_{\text {sym }}^{n_{d} \times n_{d}}, \quad \mathbf{X} \mapsto\left(G_{\mathbf{X}}^{(1)}, \ldots, G_{\mathbf{X}}^{(d)}\right),
$$

which takes a tensor to the collection of Gram matrices of its principal matricizations. Compared to the mapping $\mathbf{X} \mapsto \Sigma_{\mathbf{X}}$, the function $\Phi$ is much simpler to study since it is quadratic. Note that $\Phi$ is also homogeneous of degree two, that is,

$$
\begin{equation*}
\Phi(t \mathbf{X})=t^{2} \Phi(\mathbf{X}) \tag{2.1}
\end{equation*}
$$

for all $t \in \mathbb{R}$.
For $K \in \mathbb{R}$, let us define

$$
\mathscr{P}_{K}=\left\{\left(G^{(1)}, \ldots, G^{(d)}\right) \in \mathbb{R}_{\mathrm{sym}}^{n_{1} \times n_{1}} \times \cdots \times \mathbb{R}_{\mathrm{sym}}^{n_{d} \times n_{d}}: \operatorname{tr}\left(G^{(j)}\right)=K \text { for } j=1, \ldots, d\right\} .
$$

This set is a product of affine hyperplanes in $\mathbb{R}_{\text {sym }}^{n_{j} \times n_{j}}$, and therefore

$$
\operatorname{dim}\left(\mathscr{P}_{K}\right)=-d+\frac{1}{2} \sum_{j=1}^{d} n_{j}\left(n_{j}+1\right) .
$$

Further, we consider the linear space

$$
\begin{align*}
\mathscr{P} & =\mathbb{R} \cdot \mathscr{P}_{1}  \tag{2.2}\\
& =\left\{\left(G^{(1)}, \ldots, G^{(d)}\right) \in \mathbb{R}_{\mathrm{sym}}^{n_{1} \times n_{1}} \times \cdots \times \mathbb{R}_{\mathrm{sym}}^{n_{d} \times n_{d}}: \operatorname{tr}\left(G^{(i)}\right)=\operatorname{tr}\left(G^{(j)}\right) \text { for } i, j=1, \ldots, d\right\},
\end{align*}
$$

which is of dimension

$$
\operatorname{dim}(\mathscr{P})=\operatorname{dim}\left(\mathscr{P}_{K}\right)+1 .
$$

A simple but crucial observation is that $\Phi$ maps into $\mathscr{P}$ :

$$
\begin{equation*}
\Phi\left(\mathbb{R}^{n_{1} \times \cdots \times n_{d}}\right) \subseteq \mathscr{P}, \tag{2.3}
\end{equation*}
$$

whereas the Euclidean unit sphere $\mathscr{S}$ is mapped into the affine plane $\mathscr{P}_{1}$ :

$$
\begin{equation*}
\Phi(\mathscr{S}) \subseteq \mathscr{P}_{1} \tag{2.4}
\end{equation*}
$$

It turns out that Problem 2.2 admits an equivalent formulation in terms of the map $\Phi$.

Proposition 2.5. Let $\mathbf{X} \in \mathscr{S}$. Then $\Sigma_{\mathbf{X}}$ is an interior point of $\mathfrak{F}$ relative to $\mathfrak{S}$, if and only if $\Phi(\mathbf{X})$ is an interior point of $\Phi(\mathscr{S})$ relative to $\mathscr{P}_{1}$.

Remark 1. Therefore, if Conjecture 2.3 is true, it means that the Gram matrices of tensor matricizations are generically locally independent, that is, they can be moved in arbitrary directions within $\mathscr{P}$. The simplicity of the map $\Phi$ compared to $\mathbf{X} \mapsto \Sigma_{\mathbf{X}}$ also provides a convenient starting point for a Newton method to be discussed in Sec. 5.

Proof of Proposition 2.5. Consider the spectral decomposition

$$
G_{\mathbf{X}}^{(j)}=U_{\mathbf{X}}^{(j)} \Lambda_{\mathbf{X}}^{(j)}\left(U_{\mathbf{X}}^{(j)}\right)^{T}
$$

with $\Lambda_{\mathbf{X}}^{(j)}=\operatorname{diag}\left(\sigma_{\mathbf{X}}^{(j)}\right)^{2}$. Knowing that $\Sigma_{\mathbf{X}}$ or $\Phi(\mathbf{X})$ is an interior point implies $\sigma_{\mathbf{X}}^{(j)}>0($ for $\Phi(\mathbf{X})$ note that $\Phi(\mathscr{S})$ contains only tuples of positive semidefinite matrices).

Now suppose that $\left(G_{\mathbf{X}}^{(1)}, \ldots, G_{\mathbf{X}}^{(d)}\right)=\Phi(\mathbf{X})$ is an interior point of $\Phi(\mathscr{S})$. If $\sigma^{(j)} \in S^{(j)}$ is a positive vector sufficiently close to $\sigma_{\mathbf{X}}^{(j)}$ then the symmetric matrix $G^{(j)}=U_{\mathbf{X}}^{(j)} \operatorname{diag}\left(\sigma^{(j)}\right)^{2}\left(U_{\mathbf{X}}^{(j)}\right)^{T} \in$ $\mathscr{P}_{1}$ is in a prescribed neighborhood of $G_{\mathbf{X}}^{(j)}$. Since $\Phi(\mathbf{X})$ is an interior point, there exists a tensor $\mathbf{Y}$ such that $G_{\mathbf{Y}}^{(j)}=G^{(j)}$ for $j=1, \ldots, d$. In particular, $\mathbf{Y}$ has the higher-order singular values $\left(\sigma^{(1)}, \ldots, \sigma^{(d)}\right)$. It follows that $\Sigma_{\mathbf{X}}$ is a relative interior point of $\mathfrak{F}$.

To prove the reverse implication, let $\Sigma_{\mathbf{X}}$ be an interior point of $\mathfrak{F}$. Consider $\left(G^{(1)}, \ldots, G^{(d)}\right) \in \mathscr{P}_{1}$ sufficiently close to $\Phi(\mathbf{X})$ so that each $G^{(j)}$ is positive definite and therefore admits a spectral decomposition $G^{(j)}=V^{(j)} \Lambda^{(j)}\left(V^{(j)}\right)^{T}$ with $\Lambda^{(j)}=\operatorname{diag}\left(\sigma^{(j)}\right)^{2}$ for some positive vector $\sigma^{(j)}$. By continuity of eigenvalues, $\sigma^{(j)}$ is close to $\sigma_{\mathbf{X}}^{(j)}$. Since $\Sigma_{\mathbf{X}}$ is an interior point of $\mathfrak{F}$, this implies that there is a tensor $\mathbf{Y}$ with higher-order singular values $\left(\sigma^{(1)}, \ldots, \sigma^{(d)}\right)$. Denoting by $V_{\mathbf{Y}}^{(j)}$ the matrix of eigenvectors for $G_{\mathbf{Y}}^{(j)}$, we apply the orthogonal transformation

$$
\left(V^{(1)}\left(V_{\mathbf{Y}}^{(1)}\right)^{T} \otimes \cdots \otimes V^{(d)}\left(V_{\mathbf{Y}}^{(d)}\right)^{T}\right) \cdot \mathbf{Y}
$$

Here, the application of the tensor product operator is in the usual sense. ${ }^{1}$ In particular, the $j$ th Gram matrix of this tensor is given by

$$
V^{(j)}\left(V_{\mathbf{Y}}^{(j)}\right)^{T} M_{\mathbf{Y}}^{(j)}\left(M_{\mathbf{Y}}^{(j)}\right)^{T} V_{\mathbf{Y}}^{(j)}\left(V^{(j)}\right)^{T}=V^{(j)} \Lambda^{(j)}\left(V^{(j)}\right)^{T}=G^{(j)}
$$

which completes the proof.

### 2.2 Sufficient conditions

Due to (2.4), $\Phi(\mathbf{X})$ will be an interior point of $\mathscr{P}_{1}$, if its derivative

$$
\Phi^{\prime}(\mathbf{X}): \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \rightarrow \mathbb{R}_{\text {sym }}^{n_{1} \times n_{1}} \times \cdots \times \mathbb{R}_{\text {sym }}^{n_{d} \times n_{d}}
$$

has rank $\operatorname{dim}\left(\mathscr{P}_{1}\right)$ on the tangent space $T_{\mathscr{S}}(\mathbf{X})$ of $\mathscr{S}$ at $\mathbf{X}$, because this implies that the restriction $\left.\Phi\right|_{\mathscr{S}}$ as a map to $\mathscr{P}_{1}$ is a submersion at $\mathbf{X}$ and hence maps an open neighborhood of $\mathbf{X}_{0}$ in $\mathscr{S}$ to an open neighborhood of $\Phi\left(\mathbf{X}_{0}\right)$ in $\mathscr{P}_{1}$; see, e.g., [4, § 16.7.5]. Note that $\Phi^{\prime}(\mathbf{X})$ maps $T_{\mathscr{S}}(\mathbf{X})$ on the linear space $\mathscr{P}_{0}$. Since $\Phi$ is homogenous, the total rank of $\Phi^{\prime}(\mathbf{X})$ is one larger than its restriction to that tangent space.

Hence we obtain the following sufficient conditions.

[^1]Proposition 2.6. If $\mathbf{X} \in \mathscr{S}$ satisfies

$$
\begin{equation*}
\operatorname{rank}\left(\Phi^{\prime}(\mathbf{X})\right)=\operatorname{dim}(\mathscr{P}) \tag{2.5}
\end{equation*}
$$

or, equivalently,

$$
\begin{equation*}
\Phi^{\prime}(\mathbf{X})\left[T_{\mathscr{S}}(\mathbf{X})\right]=\mathscr{P}_{0}, \tag{2.6}
\end{equation*}
$$

then $\Phi(\mathbf{X})$ is an interior point of $\mathscr{P}_{1}$.
In fact, since $\Phi^{\prime}(\mathbf{X})$ depends polynomially on the entries of $\mathbf{X}$, we can state a little more.
Proposition 2.7. If there exists a single tensor $\mathbf{X}_{0} \in \mathbb{R}^{n_{1} \times \cdots \times n_{d}}$ satisfying (2.5), then almost all $\mathbf{X} \in \mathbb{R}^{n_{1} \times \cdots \times n_{d}}$ satisfy (2.5). In particular, (2.5) holds for almost all $\mathbf{X} \in \mathscr{S}$ with respect to the standard Lebesgue surface measure and Conjecture 2.3 is true for $n_{1} \times \cdots \times n_{d}$ tensors.

Proof. The genericity claim follows from a standard logic. Set $r:=\operatorname{dim}(\mathscr{P})$ for brevity and assume $\operatorname{rank}\left(\Phi^{\prime}\left(\mathbf{X}_{0}\right)\right)=r$. Since, by (2.3), the rank of $\Phi^{\prime}(\mathbf{X})$ cannot be larger than $r$, it suffices to prove that it takes at least this value for all $\mathbf{X} \in \mathbb{R}^{n_{1} \times \cdots \times n_{d}}$. This property can be encoded as $p(\mathbf{X}) \neq 0$, where $p$ is a polynomial in the entries of $\mathbf{X}$ (for instance one may use the sum of squares of all $r \times r$ minors of a matrix representation of $\Phi^{\prime}(\mathbf{X})$ ). Hence it either holds $p(\mathbf{X}) \neq 0$ for almost all $\mathbf{X}$, or $p \equiv 0$. By assumption, the latter is not the case.

To prove that the property (2.5) is generic with respect to the surface measure on $\mathscr{S}$ as well, we could apply the same argument by using real-analytic charts of $\mathscr{S}$ (the set of zeros of a non-zero real-analytic function is of measure zero). However, it also follows from what we have already proved. Namely, by $(2.1), \operatorname{rank}\left(\Phi^{\prime}(t \mathbf{X})\right)=\operatorname{rank}\left(\Phi^{\prime}(\mathbf{X})\right)$ for all $t \neq 0$. This implies that the set of $\mathbf{X} \in \mathscr{S}$ with $\operatorname{rank}\left(\Phi^{\prime}(\mathbf{X})\right) \leq \operatorname{dim}\left(\mathscr{P}_{1}\right)=\operatorname{dim}(\mathscr{P})-1$ must be of surface measure zero, since otherwise there is a set of positive volume with $\operatorname{rank}\left(\Phi^{\prime}(\mathbf{X})\right) \leq \operatorname{dim}(\mathscr{P})-1$, which in light of the previous considerations is not possible.

## 3 Proof of Theorem 2.4 (Conjecture $\mathbf{2 . 3}$ for $n \times \cdots \times n$ tensors)

By Proposition 2.7, Theorem 2.4 is proven via the construction of an $n \times \cdots \times n$ tensor $\mathbf{X}_{0}$ for each $d \geq 3$ and $n \geq 2$ such that $\Phi^{\prime}\left(\mathbf{X}_{0}\right)$ has rank $d n(n+1) / 2-d+1$. By the definition of $\Phi$, we have

$$
\begin{equation*}
\Phi^{\prime}(\mathbf{X})[\mathbf{H}]=\left(M_{\mathbf{X}}^{(1)}\left(M_{\mathbf{H}}^{(1)}\right)^{T}+M_{\mathbf{H}}^{(1)}\left(M_{\mathbf{X}}^{(1)}\right)^{T}, \ldots, M_{\mathbf{X}}^{(d)}\left(M_{\mathbf{H}}^{(d)}\right)^{T}+M_{\mathbf{H}}^{(d)}\left(M_{\mathbf{X}}^{(d)}\right)^{T}\right) . \tag{3.1}
\end{equation*}
$$

We first discuss the case $d=3, n=2$ separately and then give a general construction that is valid for all other cases.

Case $d=3, n=2$. Consider a general $2 \times 2 \times 2$ tensor $\mathbf{X}$ with its matricization

$$
M_{\mathbf{X}}^{(1)}=\mathbf{X}=\left(\begin{array}{ll|ll}
a & c & e & g \\
b & d & f & h
\end{array}\right) .
$$

A matrix representation of $\Phi^{\prime}(\mathbf{X}): \mathbb{R}^{2 \times 2 \times 2} \rightarrow \mathbb{R}_{\mathrm{sym}}^{2 \times 2} \times \mathbb{R}_{\mathrm{sym}}^{2 \times 2} \times \mathbb{R}_{\mathrm{sym}}^{2 \times 2}$ can be directly computed from (3.1):

$$
\Phi^{\prime}(\mathbf{X})=\left(\begin{array}{cccccccc}
2 a & 0 & 2 c & 0 & 2 e & 0 & 2 g & 0 \\
b & a & d & c & f & e & h & g \\
0 & 2 b & 0 & 2 d & 0 & 2 f & 0 & 2 h \\
\hline 2 a & 2 b & 0 & 0 & 2 e & 2 f & 0 & 0 \\
c & d & a & b & g & h & e & f \\
0 & 0 & 2 c & 2 d & 0 & 0 & 2 g & 2 h \\
\hline 2 a & 2 b & 2 c & 2 d & 0 & 0 & 0 & 0 \\
e & f & g & h & a & b & c & d \\
0 & 0 & 0 & 0 & 2 e & 2 f & 2 g & 2 h
\end{array}\right) .
$$

We know that $\operatorname{rank}\left(\Phi^{\prime}(\mathbf{X})\right) \leq 7$ for all $\mathbf{X}$. Choosing the particular tensor $\mathbf{X}_{0}$ given by the matricization

$$
M_{\mathbf{X}_{0}}^{(1)}=\left(\begin{array}{ll|ll}
1 & 1 & 0 & 0 \\
1 & 0 & 0 & 1
\end{array}\right)
$$

we have

$$
\Phi^{\prime}\left(\mathbf{X}_{0}\right)=\left(\begin{array}{cccccccc}
2 & 0 & 2 & 0 & 0 & 0 & 0 & 0  \tag{3.2}\\
1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 \\
2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 \\
2 & 2 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2
\end{array}\right), \quad Z=\left(\begin{array}{ccccccc}
1 & 1 & 0 & 0 & 0 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 2 \\
1 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 2 \\
2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2
\end{array}\right) .
$$

The $7 \times 7$ matrix $Z$ is obtained by omitting rows 1,4 and column 4 from $\Phi^{\prime}\left(\mathbf{X}_{0}\right)$. One calculates that $\operatorname{det} Z=16$, which implies that $\operatorname{rank} \Phi^{\prime}\left(\mathbf{X}_{0}\right)=7=d n(n+1) / 2-d+1$.

General construction. Let $\mathbf{X}_{0}$ be the $n \times \cdots \times n$ tensor of order $d$ that has all entries zeros except for

$$
\mathbf{X}_{0}(k, \ldots, k)=1, \quad k=1, \ldots, n
$$

and

$$
\begin{gathered}
\mathbf{X}_{0}(k, 1,1, \ldots, 1)=1, \quad k=1, \ldots, n \\
\mathbf{X}_{0}(1, k, 1, \ldots, 1)=1, \quad k=1, \ldots, n \\
\vdots \\
\mathbf{X}_{0}(1, \ldots, 1,1, k)=1, \quad k=1, \ldots, n
\end{gathered}
$$

In other words, $\mathbf{X}_{0}$ has ones on its diagonal, and in all fibers intersecting with $(1, \ldots, 1)$. For example, when $d=3$ and $n=4$, this results in a matricization

$$
M_{\mathbf{X}_{0}}^{(1)}=\left(\begin{array}{llll|llll|llll|llll}
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0  \tag{3.3}\\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{array}\right)
$$

Note that $\mathbf{X}_{0}$ is super-symmetric and hence all matricizations are essentially the same.
Theorem 3.1. For all $d, n$ satisfying $d=3, n \geq 3$ or $d \geq 4, n \geq 2$, the tensor $\mathbf{X}_{0}$ constructed above satisfies (2.5).

The rest of this section is concerned with the proof of Theorem 3.1.

### 3.1 Theorem 3.1 for $d=3, n=3$

This case is treated explicitly, in analogy to the case $d=3, n=2$ discussed above. As the involved matrices are quite large, we refrain from displaying them and only describe the construction. We first construct the $18 \times 27$ matrix representation of $\Phi^{\prime}\left(\mathbf{X}_{0}\right)$ analogous to (3.2). After omitting rows 1,7 and columns $4,6,7,8,9,11,13,15,17,21,23$, the resulting $16 \times 16$ matrix has determinant 384 . Thus, $\operatorname{rank}\left(\Phi^{\prime}\left(\mathbf{X}_{0}\right)\right)=16=d n(n+1) / 2-d+1$.

### 3.2 Theorem 3.1 for remaining cases

To prove Theorem 3.1 for the remaining cases we show (2.6) by constructing elements $\mathbf{H}$ from the tangent space $T_{\mathscr{L}}\left(\mathbf{X}_{0}\right)$ (that is, $\mathbf{H}$ is orthogonal to $\left.\mathbf{X}_{0}\right)$ such that $\Phi^{\prime}\left(\mathbf{X}_{0}\right)$ applied to these elements yields a basis of the space $\mathscr{P}_{0}$. Using (3.1), it is easy to verify that such a basis is obtained from the following two lemmas by sweeping through all combinations of $j, k$ and $\ell$ as indicated. In particular, note that the diagonal vectors appearing in Lemma 3.2 (i) form a basis of the subspace of all vectors in $\mathbb{R}^{n}$ whose entries sum up to zero.
Lemma 3.2 (Diagonal entries). For any $1 \leq j \leq d$ and $2 \leq k \leq n$ there exists $\mathbf{H} \in T_{\mathscr{S}}\left(\mathbf{X}_{0}\right)$ such that
(i) the diagonal of $M_{\mathbf{X}_{0}}^{(j)}\left(M_{\mathbf{H}}^{(j)}\right)^{T}$ is the vector $(1,0, \ldots, 0,-1,0, \ldots, 0)$ with -1 at position $k$;
(ii) the diagonal of $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}$ is zero for $i \neq j$.

Lemma 3.3 (Off-diagonal entries). For any $1 \leq j \leq d$ and $1 \leq \ell<k \leq n$ there exists $\mathbf{H} \in T_{\mathscr{L}}\left(\mathbf{X}_{0}\right)$ such that
(i) the only nonzero of $M_{\mathbf{X}_{0}}^{(j)}\left(M_{\mathbf{H}}^{(j)}\right)^{T}$ is at position ( $\left.k, \ell\right)$;
(ii) $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}=0$ for all $i \neq j$.

Proof of Lemma 3.2 Because $\mathbf{X}_{0}$ is super-symmetric, it suffices to treat $j=1$. For fixed $2 \leq k \leq n$ consider $\mathbf{H}$ with all entries zeros except for an entry 1 at position $(1, \ldots, 1)$ and an entry -1 at position $(k, 1, \ldots, 1)$. The $p$ th diagonal entry of $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}$ is the Frobenius inner product of the slices $\mathbf{X}_{0}(\cdots, p, \cdots)$ and $\mathbf{H}(\cdots, p, \cdots)$ with $p$ at position $i$.

When $i \neq j=1$, the slice $\mathbf{H}(\cdots, p, \cdots)$ contains non-zero entries only when $p=1$, namely an entry 1 at $(1, \ldots,[1], \ldots, 1)$ and an entry -1 at $(k, 1, \ldots,[1], \ldots, 1)$. (To simplify notation, we use square brackets to indicate the fixed index of slices.) Since the entries of $\mathbf{X}_{0}$ are 1 at both of these positions, the slices are orthogonal for $p=1$ as well. In turn, we have proved that $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}$ has a zero diagonal when $i \neq 1$.

When $i=j=1$, the slices $\mathbf{H}(p, \cdots)$ are non-zero only if $p=1$ or $p=k$. In both cases they contain a single non-zero entry at $([1], 1 \ldots, 1)$ resp. $([k], 1, \ldots, 1)$, which will be multiplied with a 1 at the corresponding position of $\mathbf{X}_{0}(p, \cdots)$ when forming the inner product. Hence, the diagonal entries of $M_{\mathbf{X}_{0}}^{(1)}\left(M_{\mathbf{H}}^{(1)}\right)^{T}$ are as asserted.

Proof of Lemma 3.3 Again, it suffices to consider $j=1$. Three cases will be distinguished.

Case $d \geq 4, n \geq 2$
This case is simpler than the case $d=3$ and we therefore treat it first. Given $1 \leq \ell<k \leq n$, we consider the tensor $\mathbf{H}$ that contains only zeros except for a nonzero at position $(\ell, k, \ldots, k)$.

The $(p, q)$ entry of $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}$ is the Frobenius inner products of the slices $\mathbf{X}_{0}(\cdots, p, \cdots)$ and $\mathbf{H}(\cdots, q, \cdots)$ with $p, q$ at positions $i$. When $i \neq 1$, this slice of $\mathbf{H}$ is nonzero only if $q=k$, in which case the nonzero entry is at $(\ell, k, \ldots,[k], \ldots, k)$. The nonzero entries of $\mathbf{X}_{0}$ are at multi-indices where either all indices are the same, or contain $d-1$ indices equal to one. Since $1 \leq \ell<k$ and $d \geq 4$, it follows that $\mathbf{X}_{0}(\ell, k, \ldots, k, p, k, \ldots, k)=0$ for any $p$ and hence none of the slices $\mathbf{X}_{0}(\cdots, p, \cdots)$ has a nonzero matching the one at $(\ell, k, \ldots,[k], \ldots, k)$. We conclude $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}=0$ for $i \neq 1$.

When $i=1$, we note that the slice $\mathbf{H}(q, \cdots)$ has a nonzero entry only if $q=\ell$, namely at $([\ell], k, \ldots, k)$. Since $k>1$, a slice $\mathbf{X}_{0}(p, \cdots)$ has a nonzero at the same place only if $p=k$. Hence the only nonzero entry of $M_{\mathbf{X}_{0}}^{(1)}\left(M_{\mathbf{H}}^{(1)}\right)^{T}$ is at $(p, q)=(k, \ell)$.

Case $d=3,2 \leq \ell<k \leq n$.
In this case, we again consider the tensor $\mathbf{H}$ which contains only zeros except at entry $(\ell, k, k)$.
For $i=2$, the $(p, q)$ entry of $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}$ is the Frobenius inner product of the slices $\mathbf{X}_{0}(\cdot, p, \cdot)$ and $\mathbf{H}(\cdot, q, \cdot)$. This slice of $\mathbf{H}$ is non-zero only if $q=k$, in which case the nonzero entry is at $(\ell,[k], k)$. The slice $\mathbf{X}_{0}(\cdot, p, \cdot)$ on the other hand has possibly nonzeros at $(p,[p], p)$ and $(\alpha,[p], \beta)$ where either $\alpha$ or $\beta$ (or both if $p=1$ ) are equal to one. Since $2 \leq \ell<k$, it is not possible that $\alpha=\ell, \beta=k$ and, hence, $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}=0$. The argument for $i=3$ is analogous.

Considering $i=1$, we note that the slice $\mathbf{H}(q, \cdot, \cdot)$ is zero unless $q=\ell$, in which case it has a single nonzero entry at $([\ell], k, k)$. Since $k>\ell \geq 1$, the slice $\mathbf{X}_{0}(p, \cdot, \cdot)$ has a nonzero at the same place only if $p=k$. The only nonzero entry of $M_{\mathbf{X}_{0}}^{(1)}\left(M_{\mathbf{H}}^{(1)}\right)^{T}$ is therefore at $(p, q)=(k, \ell)$.

Case $d=3, n \geq 4,1=\ell<k \leq n$.
Let us first assume $2<k<n$. Then we consider the tensor $\mathbf{H}$ which contains only zero entries, except that the slice $\mathbf{H}(1, \cdot, \cdot)$ contains the submatrix

$$
\mathbf{H}([1], k-1: k+1, k-1: k+1)=\left(\begin{array}{ccc}
0 & -\frac{1}{2} & \frac{1}{2} \\
-\frac{1}{2} & 1 & -\frac{1}{2} \\
\frac{1}{2} & -\frac{1}{2} & 0
\end{array}\right) .
$$

For example, when $n=4, k=3$, the resulting tensor has the matricization

$$
M_{\mathbf{H}}^{(1)}=\left(\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} & 0  \tag{3.4}\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
$$

A comparison with (3.3) immediately shows that $M_{\mathbf{X}_{0}}^{(1)}\left(M_{\mathbf{H}}^{(1)}\right)^{T}$ has a single nonzero entry at $(k, 1)$. One also easily checks that $M_{\mathbf{X}_{0}}^{(i)}\left(M_{\mathbf{H}}^{(i)}\right)^{T}=0$ for $i=2,3$. For instance, for $i=3$ this can be seen from the fact that the 'frontal' slices of $\mathbf{X}_{0}$ depicted in (3.3) are pair-wise orthogonal in the Frobenius inner product to the 'frontal' slices of $\mathbf{H}$ given in (3.4). This reasoning remains valid for larger $n$, as $\mathbf{H}$ will only have additional zero blocks.

When $k=2$, one considers the submatrix

$$
\mathbf{H}([1], 2: 4,2: 4)=\left(\begin{array}{ccc}
1 & -\frac{1}{2} & -\frac{1}{2} \\
-\frac{1}{2} & 0 & \frac{1}{2} \\
-\frac{1}{2} & \frac{1}{2} & 0
\end{array}\right),
$$

whereas for $k=n$ one chooses

$$
\mathbf{H}([1], n-2: n, n-2: n)=\left(\begin{array}{ccc}
0 & \frac{1}{2} & -\frac{1}{2} \\
-\frac{1}{2} & 0 & -\frac{1}{2} \\
-\frac{1}{2} & -\frac{1}{2} & 1
\end{array}\right) .
$$

This completes the proof of Lemma 3.3.

## 4 Numerical evidence for unequal mode sizes

The construction of the tensor $\mathbf{X}_{0}$ from Section 3 does not extend to cases where the mode sizes $n_{1}, \ldots, n_{d}$ are not identical. At this point, we are not aware of a construction that admits analytic verification of the condition of Proposition 2.7 for general $n_{1}, \ldots, n_{d}$. For a specific choice of $n_{1}, \ldots, n_{d}$, it is certainly possible to extend the technique from Section 3.1. In the following, we use a simpler approach to provide strong numerical evidence for $d=3$ and a range of (small) mode sizes.

We used Matlab with Tensor Toolbox [2] to construct the matrix representation of $\Phi^{\prime}(\mathbf{X})$ with the range restricted to $\mathbb{R}_{\text {sym }}^{n_{1} \times n_{1}} \times \cdots \times \mathbb{R}_{\text {sym }}^{n_{d} \times n_{d}}$; see (3.2) for an example. This matrix has size $N \times\left(n_{1} \cdots n_{d}\right)$ with $N=\frac{1}{2} \sum_{j=1}^{d} n_{j}\left(n_{j}+1\right)$ and, by Proposition 2.7, Conjecture 2.3 holds if $\Phi^{\prime}(\mathbf{X})$ has rank $N-d+1$ for some $\mathbf{X}$. To verify this condition numerically we have computed $\sigma_{N-d+1}\left(\Phi^{\prime}(\mathbf{X})\right) / \sigma_{1}\left(\Phi^{\prime}(\mathbf{X})\right)$ for random $\mathbf{X}$, where $\sigma_{k}(\cdot)$ denotes the $k$ th largest singular value of a matrix. If this ratio is sufficiently larger than $10^{-16}$ in double precision then Conjecture 2.3 is likely to hold, because singular values are perfectly well conditioned [5]. Table 1 displays the results obtained for tensors constructed by typing

```
rand('seed',0); X = rand(n1,n2,n3);
```

in Matlab. The condition of Proposition 2.7 is confirmed for all mode sizes tested, with the notable exceptions $\left(n_{1}, n_{2}, n_{3}\right)=(2,2,5)$ and $\left(n_{1}, n_{2}, n_{3}\right)=(2,5,2)$, for which the compatibility condition $n_{j} \leq n_{j}^{c}$ of Conjecture 2.3 is not satisfied.

## 5 A fast iterative method for assigning higher-order singular values

In [8], an alternating projection method for prescribing higher-order singular values was proposed. This method was observed to converge linearly to a feasible set of singular values, but no theoretical analysis was provided. Based on the results of the present paper, we develop a variant of the Newton method for which local quadratic convergence can be proven.

### 5.1 Newton method

Given a collection of symmetric, positive definite matrices $\left(G^{(1)}, \ldots, G^{(d)}\right)$, we aim at finding a tensor $\mathbf{X}$ such that

$$
\begin{equation*}
\Phi(\mathbf{X})=\left(G^{(1)}, \ldots, G^{(d)}\right) \tag{5.1}
\end{equation*}
$$

Table 1: Computed values of $\sigma_{N-d+1}\left(\Phi^{\prime}(\mathbf{X})\right) / \sigma_{1}\left(\Phi^{\prime}(\mathbf{X})\right)$ for random $n_{1} \times n_{2} \times n_{3}$ tensors $\mathbf{X}$.

| $n_{1}=2$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $n_{3}=2$ | $n_{3}=3$ | $n_{3}=4$ | $n_{3}=5$ |
| $n_{2}=2$ | 0.034 | 0.027 | 0.016 | $6 \times 10^{-17}$ |
| $n_{2}=3$ | 0.035 | 0.046 | 0.013 | 0.011 |
| $n_{2}=4$ | 0.012 | 0.028 | 0.032 | 0.033 |
| $n_{2}=5$ | $7 \times 10^{-17}$ | 0.030 | 0.034 | 0.028 |
| $n_{1}=4$ |  |  |  |  |
| $n_{3}=4$ |  |  |  |  |
| $n_{3}=5$ | $n_{3}=6$ | $n_{3}=7$ |  |  |
| $n_{2}=4$ | 0.059 | 0.055 | 0.053 | 0.048 |
| $n_{2}=5$ | 0.059 | 0.067 | 0.059 | 0.057 |
| $n_{2}=6$ | 0.043 | 0.059 | 0.059 | 0.057 |
| $n_{2}=7$ | 0.055 | 0.057 | 0.057 | 0.053 |


| $n_{1}=3$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $n_{3}=3$ | $n_{3}=4$ | $n_{3}=5$ | $n_{3}=6$ |
| $n_{2}=3$ | 0.060 | 0.071 | 0.053 | 0.045 |
| $n_{2}=4$ | 0.060 | 0.061 | 0.053 | 0.040 |
| $n_{2}=5$ | 0.054 | 0.055 | 0.060 | 0.051 |
| $n_{2}=6$ | 0.034 | 0.046 | 0.052 | 0.050 |
| $n_{1}=5$ |  |  |  |  |
| $n_{3}=5$ |  |  |  |  |
| $n_{3}=6$ | $n_{3}=7$ | $n_{3}=8$ |  |  |
| $n_{2}=5$ | 0.066 | 0.062 | 0.059 | 0.046 |
| $n_{2}=6$ | 0.061 | 0.062 | 0.056 | 0.053 |
| $n_{2}=7$ | 0.057 | 0.054 | 0.055 | 0.056 |
| $n_{2}=8$ | 0.047 | 0.054 | 0.056 | 0.054 |

Our method and the analysis simplify if we do not impose a normalization on $\|\mathbf{X}\|_{F}$. We only assume that the right-hand side of (5.1) is contained in the linear space $\mathscr{P}$ from (2.2), that is, the traces of all $G^{(j)}$ are equal. For the rest of this section, we restrict the co-domain of $\Phi$ to $\mathscr{P}$, that is, $\Phi: \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \rightarrow \mathscr{P}$.

If we are only interested in perturbing singular values, we compute the spectral decomposition of the Gram matrices for an initial tensor $\mathbf{X}_{0}$,

$$
G_{\mathbf{X}_{0}}^{(j)}=U_{\mathbf{X}_{0}}^{(j)} \Lambda_{\mathbf{X}_{0}}^{(j)}\left(U_{\mathbf{X}_{0}}^{(j)}\right)^{T}
$$

and set

$$
G^{(j)}=U_{\mathbf{X}_{0}}^{(j)} \Lambda^{(j)}\left(U_{\mathbf{X}_{0}}^{(j)}\right)^{T}
$$

with

$$
\Lambda^{(j)}=\Lambda_{\mathbf{X}_{0}}^{(j)}+O(\varepsilon)
$$

After a suitable normalization, $\left(G^{(1)}, \ldots, G^{(d)}\right) \in \mathscr{P}$. In view of our results, (5.1) is likely to have at least one solution for sufficiently small $\varepsilon$.

Applying the Newton method to (5.1) requires solving an equation of the form

$$
\begin{equation*}
\Phi^{\prime}\left(\mathbf{X}_{n}\right)\left[\mathbf{H}_{n}\right]=\Phi\left(\mathbf{X}_{n}\right)-\left(G^{(1)}, \ldots, G^{(d)}\right) \tag{5.2}
\end{equation*}
$$

Because $\mathscr{P}$ is linear, the right-hand side is contained in $\mathscr{P}$.
Suppose that $\Phi^{\prime}\left(\mathbf{X}_{n}\right): \mathbb{R}^{n_{1} \times \cdots \times n_{d}} \rightarrow \mathscr{P}$ satisfies the full rank condition (2.5) of Proposition 2.7. Then $\Phi^{\prime}\left(\mathbf{X}_{n}\right)$ has full row rank, in other words, (5.2) is consistent. Following [3, Sec. 4.4], we choose the solution of smallest norm:

$$
\begin{equation*}
\mathbf{H}_{n}=\Phi^{\prime}\left(\mathbf{X}_{n}\right)^{+}\left(\Phi\left(\mathbf{X}_{n}\right)-\left(G^{(1)}, \ldots, G^{(d)}\right)\right) \tag{5.3}
\end{equation*}
$$

where $\Phi^{\prime}\left(\mathbf{X}_{n}\right)^{+}: \mathscr{P} \rightarrow \mathbb{R}^{n_{1} \times \cdots \times n_{d}}$ denotes the Moore-Penrose pseudoinverse of $\Phi^{\prime}\left(\mathbf{X}_{n}\right)$. The next iterate is

$$
\begin{equation*}
\mathbf{X}_{n+1}=\mathbf{X}_{n}-\mathbf{H}_{n} \tag{5.4}
\end{equation*}
$$

### 5.2 Convergence analysis

In the following, we study the convergence of (5.3)-(5.4). For this purpose, we need to choose a norm on $\mathscr{P}$. Given $\tilde{G}=\left(\tilde{G}^{(1)}, \ldots, \tilde{G}^{(d)}\right) \in \mathscr{P}$, we let $\|\tilde{G}\|$ be the norm obtained by taking the Euclidean norm of the vector containing all entries in the upper triangular parts of the symmetric matrices $\tilde{G}^{(j)}$. Based on this norm, we define

$$
\begin{equation*}
\kappa(\mathbf{X}):=1 / \sup \left\{\left\|\Phi^{\prime}(\mathbf{X})^{+} \tilde{G}\right\|_{F}: \tilde{G} \in \mathscr{P},\|\tilde{G}\|=1\right\}=\sigma_{\operatorname{dim}(\mathscr{P})}\left(\Phi^{\prime}(\mathbf{X})\right), \tag{5.5}
\end{equation*}
$$

which is positive for any $\mathbf{X}$ satisfying (2.5).
Theorem 5.1. Assume that $\mathbf{X}_{0}$ satisfies (2.5) and

$$
\begin{equation*}
\left\|\Phi\left(\mathbf{X}_{0}\right)-\left(G^{(1)}, \ldots, G^{(d)}\right)\right\| \leq \frac{\kappa\left(\mathbf{X}_{0}\right)^{2}}{6 \sqrt{d}} \tag{5.6}
\end{equation*}
$$

for $\left(G^{(1)}, \ldots, G^{(d)}\right) \in \mathscr{P}$. Then all iterates $\mathbf{X}_{n}$ defined by (5.3)-(5.4) satisfy (2.5) and converge to a solution of (5.1). Moreover,

$$
\left\|\mathbf{X}_{n+1}-\mathbf{X}_{n}\right\|_{F} \leq \frac{1}{2} \omega\left\|\mathbf{X}_{n}-\mathbf{X}_{n-1}\right\|_{F}^{2}
$$

holds with $\omega=6 \sqrt{d} / \kappa\left(\mathbf{X}_{0}\right)$.
Proof. Let us first note that $\Phi^{\prime}(\mathbf{Y})$ is linear in $\mathbf{Y}$ and (3.1) implies the bound

$$
\left\|\Phi^{\prime}(\mathbf{Y})[\mathbf{H}]\right\|^{2} \leq \sum_{j=1}^{d}\left\|M_{\mathbf{Y}}^{(j)}\left(M_{\mathbf{H}}^{(j)}\right)^{T}+M_{\mathbf{H}}^{(j)}\left(M_{\mathbf{Y}}^{(j)}\right)^{T}\right\|_{F}^{2} \leq 4 d\|\mathbf{Y}\|_{F}^{2}\|\mathbf{H}\|_{F}^{2} .
$$

Hence, the induced operator norm of $\Phi^{\prime}(\mathbf{Y})$ satisfies $\left\|\Phi^{\prime}(\mathbf{Y})\right\| \leq 2 \sqrt{d}\|\mathbf{Y}\|_{F}$.
Now, let $F(\mathbf{X}):=\Phi(\mathbf{X})-\left(G^{(1)}, \ldots, G^{(d)}\right)$. By (5.6),

$$
\left\|F^{\prime}\left(\mathbf{X}_{0}\right)^{+} F\left(\mathbf{X}_{0}\right)\right\|_{F}=\left\|\Phi^{\prime}\left(\mathbf{X}_{0}\right)^{+} F\left(\mathbf{X}_{0}\right)\right\|_{F} \leq \frac{\kappa\left(\mathbf{X}_{0}\right)}{6 \sqrt{d}}=: \delta .
$$

Set $\rho:=2 \delta=\kappa\left(\mathbf{X}_{0}\right) /(3 \sqrt{d})$. Then for every $\mathbf{X}$ such that $\left\|\mathbf{X}-\mathbf{X}_{0}\right\| \leq \rho$ it holds that

$$
\kappa(\mathbf{X}) \geq \kappa\left(\mathbf{X}_{0}\right)-\left\|\Phi^{\prime}\left(\mathbf{X}_{0}-\mathbf{X}\right)\right\| \geq \kappa\left(\mathbf{X}_{0}\right)-2 \sqrt{d} \rho=\kappa\left(\mathbf{X}_{0}\right) / 3>0 .
$$

This implies that $\mathbf{X}$ satisfies (2.5) and

$$
\begin{aligned}
\left\|\Phi^{\prime}(\mathbf{X})^{+}\left(\Phi^{\prime}(\mathbf{Y})-\Phi^{\prime}(\mathbf{X})\right)[\mathbf{Y}-\mathbf{X}]\right\|_{F} & \leq \frac{3}{\kappa\left(\mathbf{X}_{0}\right)}\left\|\left(\Phi^{\prime}(\mathbf{Y}-\mathbf{X})\right)[\mathbf{Y}-\mathbf{X}]\right\| \\
& \leq \frac{6 \sqrt{d}}{\kappa\left(\mathbf{X}_{0}\right)}\|\mathbf{Y}-\mathbf{X}\|_{F}^{2}=\omega\|\mathbf{Y}-\mathbf{X}\|_{F}^{2}
\end{aligned}
$$

Because of $\delta \omega \leq 1$, all conditions of a Newton-Kantorovich-like theorem for underdetermined systems are satisfied and the claim of the theorem follows from [3, Thm. 4.19].

### 5.3 Numerical examples

Numerically, we observed rather robust convergence of the Newton method (5.3)-(5.4). In the following, we report on two examples that are representative for our observations.

Example 5.2. We created a random $10 \times 10 \times 10$ tensor $\mathbf{X}_{0}$, computed the Gram matrices and perturbed every Gram matrix by a random perturbation of norm $\varepsilon$. If a perturbed matrix happens to be indefinite, it is shifted by the smallest eigenvalue to become positive semidefinite. All Gram matrices are normalized to have trace 1. The Newton method has been applied with starting tensor $\mathbf{X}_{0}$ to match the perturbed Gram matrices. Figure 1 shows the obtained results for $\varepsilon \in$ $\left\{10^{-1}, 10^{-2}, 10^{-3}\right\}$. For $\varepsilon=10^{-2}$ and $\varepsilon=10^{-3}$, we clearly observe local quadratic convergence. For $\varepsilon=10^{-1}$, one of the Gram matrices has a zero eigenvalue. Clearly, such perturbed Gram matrices cannot represent an interior point in the image of $\Phi$, and we can therefore not expect local quadratic convergence. It turns out that the Newton method still converges but it deteriorates to linear convergence.


Figure 1: Error $\left\|\Phi\left(\mathbf{X}_{n}\right)-\left(G^{(1)}, \ldots, G^{(d)}\right)\right\|$ vs. iteration number $n$ for Example 5.2.

Example 5.3. We use the same tensor $\mathbf{X}_{0}$ as in Example 5.2 as a starting point, but now prescribe, rather arbitrarily, diagonal Gram matrices

$$
\begin{equation*}
G^{(1)}=G^{(2)}=G^{(3)}=\frac{1}{10} \operatorname{diag}(1,2, \ldots, 10) \tag{5.7}
\end{equation*}
$$

The Newton method still converges quadratically; see Figure 2. Having diagonal Gram matrices, the resulting tensor is an HOSVD tensor as defined in [8]. Despite the fact that the Gram matrices are actually all equal, the resulting tensor is not diagonal. In fact, a diagonal tensor never satisfies condition (2.5).

We now modify the last Gram matrix as follows:

$$
\begin{equation*}
G^{(1)}=G^{(2)}=\frac{1}{10} \operatorname{diag}(1,2, \ldots, 10), \quad G^{(3)}=\operatorname{diag}(1,0, \ldots, 0) \tag{5.8}
\end{equation*}
$$

This is not a feasible configuration and, not surprisingly, the Newton method does not converge for this example.


Figure 2: Error $\left\|\Phi\left(\mathbf{X}_{n}\right)-\left(G^{(1)}, \ldots, G^{(d)}\right)\right\|$ vs. iteration number $n$ for Example 5.3, using the diagonal Gram matrices (5.7) (diagonal I) and (5.8) (diagonal II)

## 6 Conclusions and open problems

In this work, we have shown that the higher-order singular values can be moved in arbitrary directions for almost every tensor with identical mode sizes. Numerical evidence suggests that this property also holds for tensors with unequal, compatible mode sizes. While our results reveal insights into the independence of the higher-order singular values, a complete characterization of the set of feasible higher-order singular values remains an open problem. Also, it would be interesting to extend our results to other subspace-based tensor decompositions, such as the tensor train and hierarchical Tucker decompositions, for which one has to investigate more complicated systems of tensor matricizations.

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[^1]:    ${ }^{1}$ Using the $j$-mode matrix product $\times_{j}$ [9], the formula becomes $\mathbf{Y} \times{ }_{1}\left(V_{\mathbf{Y}}^{(1)}\right)^{T} V^{(1)} \times \times_{2} \cdots \times_{d}\left(V_{\mathbf{Y}}^{(d)}\right)^{T} V^{(d)}$.

