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On best rank one approximation of tensors

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Abstract

In this paper we suggest a new algorithm for the computation of a best rank one approximation of tensors, called *alternating singular value decomposition*. This method is based on the computation of maximal singular values and the corresponding singular vectors of matrices. We also introduce a modification for this method and the alternating least squares method, which ensures that alternating iterations will always converge to a semi-maximal point. Finally, we introduce a new simple Newton-type method for speeding up the convergence of alternating methods near the optimum. We present several numerical examples that illustrate the computational performance of the new method in comparison to the alternating least square method.

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Key words. Singular value decomposition, rank one approximation, alternating least squares, Newton's method.

1 Introduction

In this paper we consider the best rank one approximation to real *d-mode tensors* $\mathcal{T} = [t_{i_1,\ldots,i_d}] \in \mathbb{R}^{m_1 \times \ldots \times m_d}$, i. e., d-dimensional arrays with real entries.

As usual when studying tensors, it is necessary to introduce some notation. Setting $[m] = \{1, \ldots, m\}$ for a positive integer m, for two d-mode tensors $\mathcal{T}, \mathcal{S} \in \mathbb{R}^{m_1 \times \ldots \times m_d}$ we denote by

$$\langle \mathcal{T}, \mathcal{S} \rangle := \sum_{i_j \in [m_j], j \in [d]} t_{i_1,\ldots,i_d} s_{i_1,\ldots,i_d}$$

the standard inner product of $\mathcal{T}, \mathcal{S}$, viewed as vectors in $\mathbb{R}^{m_1 \cdot m_2 \cdot \ldots \cdot m_d}$. For an integer $p \leq d$ and for $\mathbf{x}_{j_r} \in \mathbb{R}^{m_{j_r}}, r \in [p]$ we use the notation $\otimes_{j_r, r \in [p]} \mathbf{x}_{j_r} := \mathbf{x}_{j_1} \otimes \ldots \otimes \mathbf{x}_{j_p}$.

For a subset $P = \{j_1, \ldots, j_p\} \subseteq [d]$ of cardinality $p = |P|$, consider a p-mode tensor $\mathcal{X} = [x_{i_{j_1},\ldots,i_{j_p}}] \in \otimes_{j_r, r \in [p]} \mathbb{R}^{m_{j_r}}$, where $j_1 < \ldots < j_p$. Then we have that $\mathcal{T} \times$

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$\mathcal{X} := \sum_{i_{j_r} \in [m_{j_r}], r \in [p]} t_{i_1,\ldots,i_d} x_{i_{j_1},\ldots,i_{j_p}}$ is a $(d-p)$-mode tensor obtained by contraction on the indices $i_{j_1}, \ldots, i_{j_p}$ and hence for $\mathcal{T}, \mathcal{S} \in \mathbb{R}^{m_1 \times \ldots \times m_d}$, we have $\langle \mathcal{T}, \mathcal{S} \rangle = \mathcal{T} \times \mathcal{S}$.

For $\mathbf{x} \in \mathbb{R}^n$ we denote by $\|\mathbf{x}\|$ the Euclidian norm and for $A \in \mathbb{R}^{m \times n}$ by $\|A\| = \max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|$ the associated operator norm. Then it is well-known, see e. g. [5], that the best rank one approximation of A is given by $\sigma_1 \mathbf{u}_1 \mathbf{v}_1^T$, where $\sigma_1 = \|A\|$ is the largest singular value of A, and $\mathbf{u}_1, \mathbf{v}_1$ are the associated left and right singular vectors. Since the singular vectors have Euclidian norm 1, we have that the spectral norm of the best rank one approximation is equal to $\sigma_1 = \|A\|$.

To extend this property to tensors, let us for simplicity of exposition restrict ourselves in this introduction to the case of 3-mode tensors $\mathcal{T} \in \mathbb{R}^{m \times n \times l}$. Denote by $\mathrm{S}^{m-1} := \{\mathbf{x} \in \mathbb{R}^m, \ \|\mathbf{x}\| = 1\}$ the unit sphere in $\mathbb{R}^m$, by $\mathrm{S}(m,n,l)$ the set $\mathrm{S}^{m-1} \times \mathrm{S}^{n-1} \times \mathrm{S}^{l-1}$, and introduce for $(\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathrm{S}(m,n,l)$ the function $f(\mathbf{x}, \mathbf{y}, \mathbf{z}) := \langle \mathcal{T}, \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z} \rangle$. Then computing the best rank one approximation to $\mathcal{T}$ is equivalent to finding

$$\max_{(\mathbf{x},\mathbf{y},\mathbf{z}) \in \mathrm{S}(m,n,l)} f(\mathbf{x}, \mathbf{y}, \mathbf{z}) = f(\mathbf{x}^\star, \mathbf{y}^\star, \mathbf{z}^\star). \tag{1.1}$$

The tensor version of the singular value relationship takes the form, see [9],

$$\mathcal{T} \times (\mathbf{y} \otimes \mathbf{z}) = \lambda \mathbf{x}, \ \mathcal{T} \times (\mathbf{x} \otimes \mathbf{z}) = \lambda \mathbf{y}, \ \mathcal{T} \times (\mathbf{x} \otimes \mathbf{y}) = \lambda \mathbf{z}, \tag{1.2}$$

where $\|\mathbf{x}\| = \|\mathbf{y}\| = \|\mathbf{z}\| = 1$ and λ is a singular value of $\mathcal{T}$.

Let us introduce for $p \in \{1, 2\}$ the concept of a *p-semi-maximum of* f restricted to $\mathrm{S}(m,n,l)$. For $p = 1$, the p-semi-maximal points $\mathbf{x}_*, \mathbf{y}_*, \mathbf{z}_*$ of f are the global maxima for the three functions $f(\mathbf{x}, \mathbf{y}_*, \mathbf{z}_*)$, $f(\mathbf{x}_*, \mathbf{y}, \mathbf{z}_*)$, $f(\mathbf{x}_*, \mathbf{y}_*, \mathbf{z})$ restricted to S^{m-1}, S^{n-1}, S^{l-1}, respectively. For $p = 2$, the p-semi maximal points are the pairs $(\mathbf{y}_*, \mathbf{z}_*)$, $(\mathbf{x}_*, \mathbf{z}_*)$, $(\mathbf{x}_*, \mathbf{y}_*)$ that are global maxima of the functions $f(\mathbf{x}_*, \mathbf{y}, \mathbf{z})$, $f(\mathbf{x}, \mathbf{y}_*, \mathbf{z})$, $f(\mathbf{x}, \mathbf{y}, \mathbf{z}_*)$ on $\mathrm{S}^{n-1} \times \mathrm{S}^{l-1}$, $\mathrm{S}^{m-1} \times \mathrm{S}^{l-1}$, $\mathrm{S}^{m-1} \times \mathrm{S}^{n-1}$, respectively. We call $(\mathbf{x}_*, \mathbf{y}_*, \mathbf{z}_*)$ a semi-maximum if it is a p-semi-maximum for $p = 1$ or $p = 2$, and it is clear how this concept of p-semi-maxima extends to arbitrary d-mode tensors with $p = 1, 2, \ldots, d-1$.

Many approaches for finding the maximum in (1.1) have been studied in the literature, see e. g. [8]. An important method, the standard *alternating least square* (ALS) method, is an iterative procedure that starts with $\mathbf{x}_0 \in \mathrm{S}^{m-1}, \mathbf{y}_0 \in \mathrm{S}^{n-1}, \mathbf{z}_0 \in \mathrm{S}^{l-1}$, where $f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \neq 0$ and then defines the iterates $\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i$ via

$$\mathbf{x}_i = \frac{\mathcal{T} \times (\mathbf{y}_{i-1} \otimes \mathbf{z}_{i-1})}{\|\mathcal{T} \times (\mathbf{y}_{i-1} \otimes \mathbf{z}_{i-1})\|}, \ \mathbf{y}_i = \frac{\mathcal{T} \times (\mathbf{x}_i \otimes \mathbf{z}_{i-1})}{\|\mathcal{T} \times (\mathbf{x}_i \otimes \mathbf{z}_{i-1})\|}, \ \mathbf{z}_i = \frac{\mathcal{T} \times (\mathbf{x}_i \otimes \mathbf{y}_i)}{\|\mathcal{T} \times (\mathbf{x}_i \otimes \mathbf{y}_i)\|}, \tag{1.3}$$

for $i = 1, 2, \ldots, .$

Note that for all $i \in \mathbb{N}$ we have

$$f(\mathbf{x}_{i-1}, \mathbf{y}_{i-1}, \mathbf{z}_{i-1}) \leq f(\mathbf{x}_i, \mathbf{y}_{i-1}, \mathbf{z}_{i-1}) \leq f(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_{i-1}) \leq f(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i),$$

i. e., $f(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i)$ is monotonically increasing and thus converges to a limit, since f is bounded. Typically, $(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i)$ will converge to a semi-maximum $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ that satisfies (1.2), however this is not clear in general [8]. To overcome this deficiency of the ALS and related methods is one of the results of this paper.

We first discuss an alternative to the ALS algorithm for finding the maximum (1.1), where each time we fix only one variable and maximize on the other two.

Such a maximization is equivalent to finding the maximal singular value and the corresponding left and right singular vectors of a suitable matrix, which is a well-established computational procedure, [5]. We call this method the *alternating singular value decomposition* (ASVD).

Then we introduce modifications of both ALS and ASVD, that are computationally more expensive, but for which it is guaranteed that they will always converge to a semi-maximum of f.

Finally, as alternative to the Newton method suggested in [12], we also suggest a new Newton-type method for best rank one approximation that is based on a simple observation mentioned in [3], that any triple of singular vectors $(\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathrm{S}(m, n, l)$ corresponding to a nonzero singular value λ of a tensor $\mathcal{T}$ as in (1.2), can be easily transferred to a fixed point of the map

$$\mathbf{F}(\mathbf{u}, \mathbf{v}, \mathbf{w}) := (\mathcal{T} \times (\mathbf{v} \otimes \mathbf{w}), \mathcal{T} \times (\mathbf{u} \otimes \mathbf{w}), \mathcal{T} \times (\mathbf{u} \otimes \mathbf{v})). \tag{1.4}$$

from $\mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^l$ to itself. Indeed, (1.2) is equivalent to

$$\mathbf{F}(\mathbf{u}, \mathbf{v}, \mathbf{w}) - (\mathbf{u}, \mathbf{v}, \mathbf{w}) = \mathbf{0}, \tag{1.5}$$

where $(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \frac{1}{\lambda}(\mathbf{x}, \mathbf{y}, \mathbf{z})$. (This observation holds for any d-tensor for $d > 2$ but not for matrices!)

The content of the paper is as follows. In section 2 we recall some basic facts about tensors and best rank one approximations. In section 3 we recall the ALS method and introduce the ASVD procedure. The modification of these methods to guarantee convergence to a semi-maximum is introduced in section 4 and the modification of the Newton iteration in section 5. The performance of the new methods is illustrated in section 6. We finish with some conclusions.

2 Basic facts on best rank one approximations of d-mode tensors

In this section we present further notation and recall some known results about best rank one approximations.

For a d-mode tensor $\mathcal{T} = [t_{i_1,\ldots,i_d}] \in \mathbb{R}^{m_1 \times \ldots \times m_d}$, denote by $\|\mathcal{T}\| := \sqrt{\langle \mathcal{T}, \mathcal{T} \rangle}$ the Hilbert-Schmidt norm. Denote by $\mathrm{S}(\mathbf{m})$ the d-product of the sub-spheres $\mathrm{S}^{m_1-1} \times \ldots \times \mathrm{S}^{m_d-1}$, let $(\mathbf{x}_1, \ldots, \mathbf{x}_d) \in \mathrm{S}(\mathbf{m})$ and associate with $(\mathbf{x}_1, \ldots, \mathbf{x}_d)$ the d one dimensional subspaces $\mathbf{U}_i = \mathrm{span}(\mathbf{x}_i)$, $i \in [d]$. Note that

$$\| \otimes_{i \in [d]} \mathbf{x}_i \| = \prod_{i \in [d]} \|\mathbf{x}_i\| = 1.$$

The projection $P_{\otimes_{i \in [d]} \mathbf{U}_i}(\mathcal{T})$ of $\mathcal{T}$ onto the one dimensional subspace $\mathbf{U} := \otimes_{i \in [d]} \mathbf{U}_i \subset \otimes_{i \in [d]} \mathbb{R}^{m_i}$, is given by

$$f(\mathbf{x}_1, \ldots, \mathbf{x}_d) \otimes_{i \in [d]} \mathbf{x}_i, \quad f(\mathbf{x}_1, \ldots, \mathbf{x}_d) := \langle \mathcal{T}, \otimes_{i \in [d]} \mathbf{x}_i \rangle, \ (\mathbf{x}_1, \ldots, \mathbf{x}_d) \in \mathrm{S}(\mathbf{m}). \tag{2.1}$$

Denoting by $P_{(\otimes_{i \in [d]} \mathbf{U}_i)^\perp}(\mathcal{T})$ the orthogonal projection of $\mathcal{T}$ onto the orthogonal complement of $\otimes_{i \in [d]} \mathbf{U}_i$, the Pythagoras identity yields that

$$\|\mathcal{T}\|^2 = \|P_{\otimes_{i \in [d]} \mathbf{U}_i}(\mathcal{T})\|^2 + \|P_{(\otimes_{i \in [d]} \mathbf{U}_i)^\perp}(\mathcal{T})\|^2. \tag{2.2}$$

With this notation, the best rank one approximation of $\mathcal{T}$ from $\mathrm{S}(\mathbf{m})$ is given by

$$\min_{(\mathbf{x}_1,\ldots,\mathbf{x}_d)\in \mathrm{S}(\mathbf{m})} \min_{a\in\mathbb{R}} \|\mathcal{T} - a\otimes_{i\in[d]} \mathbf{x}_i\|.$$

Observing that

$$\min_{a\in\mathbb{R}} \|\mathcal{T} - a\otimes_{i\in[d]} \mathbf{x}_i\| = \|\mathcal{T} - P_{\otimes_{i\in[d]}\mathbf{U}_i}(\mathcal{T})\| = \|P_{(\otimes_{i\in[d]}\mathbf{U}_i)^\perp}(\mathcal{T})\|,$$

it follows that the best rank one approximation is obtained by the minimization of $\|P_{(\otimes_{i\in[d]}\mathbf{U}_i)^\perp}(\mathcal{T})\|$. In view of (2.2) we deduce that best rank one approximation is obtained by the maximization of $\|P_{\otimes_{i\in[d]}\mathbf{U}_i}(\mathcal{T})\|$ and finally, using (2.1), it follows that the best rank one approximation is given by

$$\sigma_1(\mathcal{T}) := \max_{(\mathbf{x}_1,\ldots,\mathbf{x}_d)\in \mathrm{S}(\mathbf{m})} f(\mathbf{x}_1,\ldots,\mathbf{x}_d). \tag{2.3}$$

Following the matrix case, in [6] $\sigma_1(\mathcal{T})$ is called the *spectral norm* and it is also shown that the computation of $\sigma_1(\mathcal{T})$ in general is NP-hard for $d > 2$.

We will make use of the following result of [9], where we present the proof for completeness.

Lemma 1 *For $\mathcal{T} \in \mathbb{R}^{m_1\times\ldots\times m_d}$, the critical points of $f|_{\mathrm{S}(\mathbf{m})}$, defined in* (2.1)*, satisfy the equations*

$$\mathcal{T}\times(\otimes_{j\in[d]\setminus\{i\}}\mathbf{x}_j) = \lambda\mathbf{x}_i \quad \textit{for all } i\in[d],\ (\mathbf{x}_1,\ldots,\mathbf{x}_d)\in \mathrm{S}(\mathbf{m}). \tag{2.4}$$

Proof. We need to find the critical points of $\langle\mathcal{T}, \otimes_{j\in[d]}\mathbf{x}_j\rangle$ where $(\mathbf{x}_1,\ldots,\mathbf{x}_d)\in \mathrm{S}(\mathbf{m})$. Using Lagrange multipliers we consider the auxiliary function

$$g(\mathbf{x}_1,\ldots,\mathbf{x}_d) := \langle\mathcal{T}, \otimes_{j\in[d]}\mathbf{x}_j\rangle - \sum_{j\in[d]} \lambda_j \mathbf{x}_j^\top\mathbf{x}_j.$$

The critical points of g then satisfy

$$\mathcal{T}\times(\otimes_{j\in[d]\setminus\{i\}}\mathbf{x}_j) = \lambda_j\mathbf{x}_i, \quad i\in[d],$$

and hence $\langle\mathcal{T}, \otimes_{j\in[d]}\mathbf{x}_j\rangle = \lambda_i\mathbf{x}_i^\top\mathbf{x}_i = \lambda_i$ for all $i\in[d]$ which implies (2.4). □

Observe next that $(\mathbf{x}_1,\ldots,\mathbf{x}_d)$ satisfies (2.4) iff the vectors $(\pm\mathbf{x}_1,\ldots,\pm\mathbf{x}_d)$ satisfy (2.4). In particular, we could choose the signs in $(\pm\mathbf{x}_1,\ldots,\pm\mathbf{x}_d)$ such that each corresponding λ is nonnegative and then these λ can be interpreted as the singular values of $\mathcal{T}$. The maximal singular value of $\mathcal{T}$ is denoted by $\sigma_1(\mathcal{T})$ and is given by (2.3). Note that to each nonnegative singular value there are at least 2^{d-1} singular vectors of the form $(\pm\mathbf{x}_1,\ldots,\pm\mathbf{x}_d)$. So it is more natural to view the singular vectors as one dimensional subspaces $\mathbf{U}_i = \mathrm{span}(\mathbf{x}_i)$, $i\in[d]$.

As observed in [3] for tensors, i. e., for $d > 2$, there is a one-to-one correspondence between the singular vectors corresponding to positive singular values of $\mathcal{T}$ and the fixed points of an induced multilinear map of degree $d-1$.

Lemma 2 *Let $d > 2$ and assume that $\mathcal{T} \in \mathbb{R}^{m_1 \times \ldots \times m_d}$. Associate with $\mathcal{T}$ the map $\mathbf{F}$ from $\mathbb{R}(\mathbf{m}) := \mathbb{R}^{m_1} \times \ldots \times \mathbb{R}^{m_d}$ to itself, where*

$$\mathbf{F} := (F_1, \ldots, F_d),\ F_i(\mathbf{u}_1, \ldots, \mathbf{u}_d) := \mathcal{T} \times (\otimes_{j \in [d] \setminus \{i\}} \mathbf{u}_j),\ i \in [d].$$

Then there is a one-to-one correspondence between the critical points of $f|_{\mathrm{S}(\mathbf{m})}$ corresponding to positive singular values λ and the nonzero fixed points of

$$\mathbf{F}(\mathbf{u}) = \mathbf{u}. \tag{2.5}$$

Namely, each $(\mathbf{x}_1, \ldots, \mathbf{x}_d) \in \mathrm{S}(\mathbf{m})$ satisfying (2.4) with $\lambda > 0$ induces a fixed point of $\mathbf{F}$ of the form

$$(\mathbf{u}_1, \ldots, \mathbf{u}_d) = \lambda^{\frac{-1}{d-2}} (\mathbf{x}_1, \ldots, \mathbf{x}_d).$$

Conversely, any nonzero fixed point satisfying (2.5) induces a d-set of singular vectors $(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \frac{1}{\|\mathbf{u}_1\|}(\mathbf{u}_1, \ldots, \mathbf{u}_d) \in \mathrm{S}(\mathbf{m})$ corresponding to $\lambda = \|\mathbf{u}_1\|^{-(d-2)}$. In particular, the spectral norm $\sigma_1(\mathcal{T})$ corresponds to a nonzero fixed point of $\mathbf{F}$ closest to the origin.

Proof. Assume that (2.4) holds for $\lambda > 0$. Dividing both sides of (2.4) by $\lambda^{\frac{d-1}{d-2}}$ we obtain that $(\mathbf{u}_1, \ldots, \mathbf{u}_d) = \lambda^{\frac{-1}{d-2}} (\mathbf{x}_1, \ldots, \mathbf{x}_d)$ is a nonzero fixed point of $\mathbf{F}$.

For the converse, assume that $(\mathbf{u}_1, \ldots, \mathbf{u}_d)$ is a nonzero fixed point of $\mathbf{F}$. Clearly $\mathbf{u}_i^\top \mathbf{u}_i = \langle \mathcal{T}, \times_{j \in [d]} \mathbf{u}_j \rangle$ for $i \in [d]$. Hence, $\|\mathbf{u}_1\| = \ldots = \|\mathbf{u}_d\| > 0$ and $(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \frac{1}{\|\mathbf{u}_1\|}(\mathbf{u}_1, \ldots, \mathbf{u}_d) \in \mathrm{S}(\mathbf{m})$ satisfies (2.4) with $\lambda = \|\mathbf{u}_1\|^{-(d-2)}$.

The largest positive singular value of $\mathcal{T}$ corresponds to the nonzero fixed point $(\mathbf{u}_1, \ldots, \mathbf{u}_d)$, where $\sum_{i \in [d]} \|\mathbf{u}_i\|^2 = d\|\mathbf{u}_1\|^2$ is the smallest. □

We also have that the trivial fixed point is isolated.

Proposition 3 *The origin $\mathbf{0} \in \mathbb{R}(\mathbf{m})$ is an isolated simple fixed point of $\mathbf{F}$.*

Proof. A fixed point of $\mathbf{F}$ satisfies

$$\mathbf{u} - \mathbf{F}(\mathbf{u}) = \mathbf{0} \tag{2.6}$$

and clearly, $\mathbf{u} = \mathbf{0}$ satisfies this system. Observe that the Jacobian matrix $D(\mathbf{u} - \mathbf{F}(\mathbf{u}))(\mathbf{0})$ is the identity matrix. Hence the implicit function theorem yields that $\mathbf{0}$ is a simple isolated solution of (2.5). □

It has been conjectured in [3] that for a generic tensor $\mathcal{T} \in \mathbb{C}^{m_1 \times \ldots \times m_d}$ the corresponding map $\mathbf{F}$ has a finite number of fixed points. This conjecture is still open. If true, it would imply that for a generic $\mathcal{T} \in \mathbb{R}^{m_1 \times \ldots \times m_d}$ the best rank one approximation is unique.

3 The ALS and the ASVD method

In this section we briefly recall the alternating least squares (ALS) method and suggest an analogous alternating singular value decomposition (ASVD) method.

Consider $\mathcal{T} \in \mathbb{R}^{m_1 \times \ldots \times m_d} \setminus \{0\}$ and choose an initial point $(\mathbf{x}_{1,0}, \ldots, \mathbf{x}_{d,0}) \in \mathrm{S}(\mathbf{m})$ such that $f(\mathbf{x}_{1,0}, \ldots, \mathbf{x}_{d,0}) \neq 0$. This can be done in different ways. One possibility is

to choose $(\mathbf{x}_{1,0},\dots,\mathbf{x}_{d,0}) \in \mathrm{S}(\mathbf{m})$ at random. This will ensure that with probability one we have $f(\mathbf{x}_{1,0},\dots,\mathbf{x}_{d,0}) \neq 0$. Another, more expensive way to obtain such an initial point $(\mathbf{x}_{1,0},\dots,\mathbf{x}_{d,0})$ is to use the higher order singular value decomposition (HOSVD) [1]. To choose $\mathbf{x}_{i,0}$ view $\mathcal{T}$ as an $m_i \times \frac{m_1\times\ldots\times m_d}{m_i}$ matrix A_i, by unfolding in direction i. Then $\mathbf{x}_i$ is the left singular vector corresponding to $\sigma_1(A_i)$ for $i \in [d]$. The use of the HOSVD is expensive, but may result in a better choice of the initial point.

Given $(\mathbf{x}_{1,p},\dots,\mathbf{x}_{d,p}) \in \mathrm{S}(\mathbf{m})$ for an integer $p \geq 0$, the points $\mathbf{x}_{i,p+1} \in \mathrm{S}^{m_i-1}$ are then computed recursively via

$$\mathbf{x}_{i,p+1} = \frac{1}{\|\mathcal{T} \times (\otimes_{j=1}^{i-1}\mathbf{x}_{j,p+1} \otimes (\otimes_{j=i+1}^{d}\mathbf{x}_{j,p}))\|}\mathcal{T} \times ((\otimes_{j=1}^{i-1}\mathbf{x}_{j,p+1}) \otimes (\otimes_{j=i+1}^{d}\mathbf{x}_{j,p})),$$

for $i \in [d]$ and $p \geq 0$. Clearly, we have the inequality

$$f(\mathbf{x}_{1,p+1},\dots,\mathbf{x}_{i-1,p+1},\mathbf{x}_{i,p},\dots,\mathbf{x}_{d,p}) \leq f(\mathbf{x}_{1,p+1},\dots,\mathbf{x}_{i,p+1},\mathbf{x}_{i+1,p},\dots,\mathbf{x}_{d,p}),$$

for $i \in [d]$ and $p \geq 0$, and the sequence $f(\mathbf{x}_{1,p},\dots,\mathbf{x}_{d,p}), p = 0,1,\dots$ is a nondecreasing sequence bounded by $\sigma_1(\mathcal{T})$, and hence it converges.

Recall that a point $(\mathbf{x}_{1,*},\dots,\mathbf{x}_{d,*}) \in \mathrm{S}(\mathbf{m})$ is called a 1-semi maximum, if $\mathbf{x}_{i,*}$ is a maximum for the function $f(\mathbf{x}_{1,*},\dots,\mathbf{x}_{i-1,*},\mathbf{x}_i,\mathbf{x}_{i+1,*},\dots,\mathbf{x}_{d,*})$ restricted to S^{m_i-1} for each $i \in [d]$. Thus, clearly any 1-semi maximum point of f is a critical point of f. In many cases the sequence $(\mathbf{x}_{1,p},\dots,\mathbf{x}_{d,p}), p = 0,1,\dots$ does converge to a 1-semi maximum point of f, however, this is not always guaranteed [8].

An alternative to the ALS method is the alternating singular value decomposition (ASVD). To introduce this method, denote for $A \in \mathbb{R}^{m\times\ell}$ by $\mathbf{u}(A) \in \mathrm{S}^{m-1}, \mathbf{v}(A) \in \mathrm{S}^{\ell-1}$ the left and the right singular vectors of A corresponding to the maximal singular value $\sigma_1(A)$, i. e.,

$$\mathbf{u}(A)^\top A = \sigma_1(A)\mathbf{v}(A)^\top, A\mathbf{v}(A) = \sigma_1(A)\mathbf{u}(A).$$

Since for $d = 2$ the singular value decomposition directly gives the best rank one approximation, we only consider the case $d \geq 3$. Let $\mathcal{T} = [t_{i_1,\dots,i_d}] \in \mathbb{R}^{m_1\times\ldots\times m_d}$ and $X := (\mathbf{x}_1,\dots,\mathbf{x}_d) \in \mathrm{S}(\mathbf{m})$ be such that $f(\mathbf{x}_1,\dots,\mathbf{x}_d) \neq 0$. Fix an index pair (i,j) with $1 \leq i < j \leq d$ and denote by $\mathcal{X}_{i,j}$ the $d-2$ tensor $\otimes_{k\in[d]\setminus\{i,j\}}\mathbf{x}_k$. Then $\mathcal{T} \times \mathcal{X}_{i,j}$ is an $m_i \times m_j$ matrix.

The basic step in the ASVD method is the substitution

$$(\mathbf{x}_i,\mathbf{x}_j) \mapsto (\mathbf{u}(\mathcal{T} \times \mathcal{X}_{i,j}), \mathbf{v}(\mathcal{T} \times \mathcal{X}_{i,j})). \tag{3.1}$$

For example, if $d = 3$ then the ASVD method is given by repeating iteratively the substitution (3.1) in the order

$$(2,3), \quad (1,3), \quad (1,2).$$

For $d > 3$, one goes consecutively through all $\binom{d}{2}$ pairs in an "evenly distributed way". For example, if $d = 4$ then one could choose the order

$$(1,2), \quad (3,4), \quad (1,3), \quad (2,4), \quad (1,4), \quad (2,3).$$

The procedure to compute the largest singular value of a large scale matrix is based on the Lanczos algorithm [5] implemented in the partial singular value

decomposition. Despite the fact that this procedure is very efficient, for tensors each iteration of ALS is still much cheaper to perform than one iteration of (3.1). However, it is not really necessary to iterate the partial SVD algorithm to full convergence of the largest singular value. Since the Lanczos algorithm converges rapidly [5], a few steps (giving only a rough approximation) may be enough to get an improvement in the outer iteration. In this case, the ASVD method may even be faster than the ALS method, however, a complete analysis of such an inner-outer iteration is an open problem. As in the ALS method, it may happen that a step of the ASVD will not decrease the value of the function f but in many cases the algorithm will converge to a semi-maximum of f. However, as in the case of the ALS method, we do not have a complete understanding when this will happen. For this reason, in the next section we suggest a modification of both ALS and ASVD method, which will guarantee convergence.

4 Modified ALS and ASVD

The aim of this section is to introduce *modified* ALS and ASVD methods, abbreviated here as MALS and MASVD. These modified algorithms ensure that every accumulation point of these algorithms is a semi-maximum point of $f|_{\mathrm{S}(\mathbf{m})}$. For simplicity of the exposition we describe the concept for the case $d = 3$, i. e., we assume that we have a tensor $\mathcal{T} \in \mathbb{R}^{m\times n\times l}$.

We first discuss the MALS. For given $(\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathrm{S}(m, n, l)$ with $f(\mathbf{x}, \mathbf{y}, \mathbf{z}) \neq 0$, the procedure requires to compute the three values

$$\begin{aligned} f_1(\mathbf{x}, \mathbf{y}, \mathbf{z}) &:= f(\frac{\mathcal{T} \times (\mathbf{y} \otimes \mathbf{z})}{\|\mathcal{T} \times (\mathbf{y} \otimes \mathbf{z})\|}, \mathbf{y}, \mathbf{z}), \\ f_2(\mathbf{x}, \mathbf{y}, \mathbf{z}) &:= f(\mathbf{x}, \frac{\mathcal{T} \times (\mathbf{x} \otimes \mathbf{z})}{\|\mathcal{T} \times (\mathbf{x} \otimes \mathbf{z})\|}, \mathbf{z}), \\ f_3(\mathbf{x}, \mathbf{y}, \mathbf{z}) &:= f(\mathbf{x}, \mathbf{y}, \frac{\mathcal{T} \times (\mathbf{x} \otimes \mathbf{y})}{\|\mathcal{T} \times (\mathbf{x} \otimes \mathbf{y})\|}). \end{aligned}$$

and to choose the maximum value. This needs 3 evaluations of f.

The modified ALS procedure then is as follows. Let $(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \in \mathrm{S}(m, n, l)$ and $f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \neq 0$. Consider the maximum value of $f_i(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)$ for $i = 1, 2, 3$. Assume for example that this value is achieved for $i = 2$. Let $\mathbf{y}_1 := \frac{\mathcal{T}\times(\mathbf{x}_0\otimes\mathbf{z}_0)}{\|\mathcal{T}\times(\mathbf{x}_0\otimes\mathbf{z}_0)\|}$. Then we replace the point $(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)$ with the new point $(\mathbf{x}_0, \mathbf{y}_1, \mathbf{z}_0)$ and consider the maximum value of $f_i(\mathbf{x}_0, \mathbf{y}_1, \mathbf{z}_0)$ for $i = 1, 2, 3$. This needs only two f evaluations, since $f_2(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) = f_2(\mathbf{x}_0, \mathbf{y}_1, \mathbf{z}_0)$. Suppose that this maximum is achieved for $i = 1$. We then replace the point in the triple $(\mathbf{x}_0, \mathbf{y}_1, \mathbf{z}_0)$ with $(\mathbf{x}_1, \mathbf{y}_1, \mathbf{z}_0)$ where $\mathbf{x}_1 = \frac{\mathcal{T}\times(\mathbf{y}_1\otimes\mathbf{z}_0)}{\|\mathcal{T}\times(\mathbf{y}_1\otimes\mathbf{z}_0)\|}$ and then as the last step we optimize the missing mode, which is in this example $i = 3$. In case that the convergence criterion is not yet satisfied, we continue iteratively in the same manner. The cost of this algorithm is about twice as much as of ALS.

For the modified ASVD we have a similar algorithm. For $(\mathbf{x}, \mathbf{y}, \mathbf{z}) \in \mathrm{S}(m, n, l)$,

$f(\mathbf{x},\mathbf{y},\mathbf{z}) \neq 0$ let

$$\begin{aligned} g_1(\mathbf{x},\mathbf{y},\mathbf{z}) &:= f(\mathbf{x},\mathbf{u}(\mathcal{T}\times\mathbf{x}),\mathbf{v}(\mathcal{T}\times\mathbf{x})),\\ g_2(\mathbf{x},\mathbf{y},\mathbf{z}) &:= f(\mathbf{u}(\mathcal{T}\times\mathbf{y}),\mathbf{y},\mathbf{v}(\mathcal{T}\times\mathbf{y})),\\ g_3(\mathbf{x},\mathbf{y},\mathbf{z}) &:= f(\mathbf{u}(\mathcal{T}\times\mathbf{z}),\mathbf{v}(\mathcal{T}\times\mathbf{z}),\mathbf{z}), \end{aligned}$$

which requires three evaluations of f. Let $(\mathbf{x}_0,\mathbf{y}_0,\mathbf{z}_0) \in \mathrm{S}(m,n,l)$ and $f(\mathbf{x}_0,\mathbf{y}_0,\mathbf{z}_0) \neq 0$ and consider the maximal value of $g_i(\mathbf{x}_0,\mathbf{y}_0,\mathbf{z}_0)$ for $i = 1,2,3$. Assume for example that this value is achieved for $i = 2$. Let $\mathbf{x}_1 := \mathbf{u}(\mathcal{T}\times\mathbf{y}_0), \mathbf{z}_1 := \mathbf{v}(\mathcal{T}\times\mathbf{y}_0)$. Then we replace the point $(\mathbf{x}_0,\mathbf{y}_0,\mathbf{z}_0)$ with the new point $(\mathbf{x}_1,\mathbf{y}_0,\mathbf{z}_1)$ and determine the maximal value of $g_i(\mathbf{x}_1,\mathbf{y}_0,\mathbf{z}_1)$ for $i = 1,2,3$. Suppose that this maximum is achieved for $i = 1$. We then replace the point in the triple $(\mathbf{x}_1,\mathbf{y}_0,\mathbf{z}_1)$ with $(\mathbf{x}_1,\mathbf{y}_1,\mathbf{z}_2)$ where $\mathbf{y}_1 = \mathbf{u}(\mathcal{T}\times\mathbf{x}_1), \mathbf{z}_2 = \mathbf{v}(\mathcal{T}\times\mathbf{x}_1)$ and if the convergence criterion is not met then we continue in the same manner. This algorithm is about twice as expensive as the ASVD method. For $d = 3$, we then have the following theorem.

Theorem 4 *Let $\mathcal{T} \in \mathbb{R}^{m\times n\times l}$ be a given tensor and consider the sequence*

$$(\mathbf{x}_i,\mathbf{y}_i,\mathbf{z}_i) \in \mathrm{S}(m,n,l) \text{ for } i = 0,1,\ldots, \tag{4.1}$$

generated either by MALS or MASVD, where $f(\mathbf{x}_0,\mathbf{y}_0,\mathbf{z}_0) \neq 0$. If $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) \in \mathrm{S}(m,n,l)$ is an accumulation point of this sequence, then $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) \in \mathrm{S}(m,n,l)$ is a 1-semi maximum if (4.1) is given by MALS and a 2-semi maximum if (4.1) is given by MASVD.

Proof. Let $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) \in \mathrm{S}(m,n,l)$ be an accumulation point of the sequence (4.1), i. e., there exists a subsequence $1 \leq n_1 < n_2 < n_3 < \ldots$ such that $\lim_{j\to\infty}(\mathbf{x}_{n_j},\mathbf{y}_{n_j},\mathbf{z}_{n_j}) = (\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$. Since the sequence $f(\mathbf{x}_i,\mathbf{y}_i,\mathbf{z}_i)$ is nondecreasing, we deduce that $\lim_{i\to\infty} f(\mathbf{x}_i,\mathbf{y}_i,\mathbf{z}_i) = f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) > 0$. Assume first that the sequence (4.1) is obtained by $MALS$. Clearly

$$\max_{\mathbf{x}\in\mathrm{S}^{m-1}} f(\mathbf{x},\mathbf{y}_*,\mathbf{z}_*) = f_1(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) \geq f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*).$$

For any $\varepsilon > 0$, since $f_1(\mathbf{x},\mathbf{y},\mathbf{z})$ is a continuous function on $\mathrm{S}(m,n,l)$, it follows that for a sufficiently large integer j that $f_1(\mathbf{x}_{n_j},\mathbf{y}_{n_j},\mathbf{z}_{n_j}) > f_1(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) - \varepsilon$. Hence

$$f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) \geq f(\mathbf{x}_{n_j+1},\mathbf{y}_{n_j+1},\mathbf{y}_{n_j+1}) \geq f_1(\mathbf{x}_{n_j},\mathbf{y}_{n_j},\mathbf{z}_{n_j}) \geq f_1(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) - \varepsilon.$$

Since $\varepsilon > 0$ can be chosen arbitrarily small, we deduce $f_1(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) = f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$. Similarly we deduce that $f_k(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) = f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$ for $k = 2,3$. Hence $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$ is 1-semi maximum.

Similar arguments show that if the sequence (4.1) is obtained by MASVD then $g_k(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*) = f(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$ for $k \in [3]$. Hence $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$ is a 2-semi maximum. □

The following questions remain open. Suppose that the assumptions of Theorem 4 hold. Assume further, that one accumulation point $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$ of the sequence (4.1) is an isolated critical point of $f|_{\mathrm{S}(m,n,l)}$. Is it true that for the MALS method that the sequence (4.1) converges to $(\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*)$, where we identify $-\mathbf{x}_*,-\mathbf{y}_*,-\mathbf{z}_*$ with $\mathbf{x}_*,\mathbf{y}_*,\mathbf{z}_*$ respectively? Is the same claim true for the MASVD method assuming the additional condition

$$\sigma_1(\mathcal{T}\times\mathbf{x}_*) > \sigma_2(\mathcal{T}\times\mathbf{x}_*),\ \sigma_1(\mathcal{T}\times\mathbf{y}_*) > \sigma_2(\mathcal{T}\times\mathbf{y}_*),\ \sigma_1(\mathcal{T}\times\mathbf{z}_*) > \sigma_2(\mathcal{T}\times\mathbf{z}_*)?$$

5 A Newton algorithm

To derive an associated Newton method, as in section 2, we replace the problem of finding a solution to (1.2), with $\lambda > 0$ to the solution of (2.6). Considering again the case $d = 3$ for ease of notation, if we had an approximation $(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)$ to a solution of (1.2), we need to obtain an approximation of a solution of (2.6) by considering $(\mathbf{u}_0, \mathbf{v}_0, \mathbf{w}_0) = (f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0))^{-\frac{1}{2}}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)$. System (2.6) can be written as $\mathbf{G}(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \mathbf{0}$, where

$$\mathbf{G}(\mathbf{u}, \mathbf{v}, \mathbf{w}) = (\mathbf{u} - \mathcal{T} \times (\mathbf{v} \otimes \mathbf{w}), \mathbf{v} - \mathcal{T} \times (\mathbf{u} \otimes \mathbf{w}), \mathbf{w} - \mathcal{T} \times (\mathbf{u} \otimes \mathbf{v})).$$

Then $D\mathbf{G}(\mathbf{u}, \mathbf{v}, \mathbf{w}) \in \mathbb{C}^{(m+n+l)\times(m+n+l)}$, the Jacobian of $\mathbf{G}$ at $(\mathbf{u}, \mathbf{v}, \mathbf{w})$, has the form

$$D\mathbf{G}(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \begin{bmatrix} I_m & -\mathcal{T} \times \mathbf{w} & -\mathcal{T} \times \mathbf{v} \\ -(\mathcal{T} \times \mathbf{w})^\top & I_n & -(\mathcal{T} \times \mathbf{u})^\top \\ -(\mathcal{T} \times \mathbf{v})^\top & -(\mathcal{T} \times \mathbf{u})^\top & I_l \end{bmatrix}. \tag{5.1}$$

Hence the Newton iteration is given by the formula

$$(\mathbf{u}_{i+1}, \mathbf{v}_{i+1}, \mathbf{w}_{i+1}) = (\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i) - (D\mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i))^{-1}\mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i),$$

for $i = 0, 1, \ldots,$. Here we abuse notation by viewing $(\mathbf{u}, \mathbf{v}, \mathbf{w})$ as a column vector $(\mathbf{u}^\top, \mathbf{v}^\top, \mathbf{w}^\top)^\top \in \mathbb{C}^{m+n+l}$.

Numerically, to find $(D\mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i))^{-1}\mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i)$ one solves the linear system

$$(D\mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i))(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \mathbf{G}(\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i).$$

The final vector $(\mathbf{u}_j, \mathbf{v}_j, \mathbf{w}_j)$ of the above Newton iterations is followed by a scaling to vectors of unit length $\mathbf{x}_j = \frac{\mathbf{u}_j}{\|\mathbf{u}_j\|}, \mathbf{y}_j = \frac{\mathbf{v}_j}{\|\mathbf{v}_j\|}, \mathbf{z}_j = \frac{w_j}{\|\mathbf{w}_j\|}$.

6 Numerical results

We have implemented a C++ library supporting the rank one tensor decomposition using vmmlib [11], LAPACK and BLAS in order to test the performance of the different best rank one approximation algorithms. The performance was measured via the actual CPU-time (seconds) needed to compute the approximate best rank one decomposition, by the number of optimization calls needed, and whether a stationary point was found. All performance tests have been carried out on a 2.8 GHz Quad-Core Intel Xeon Macintosh computer with 16GB RAM.

The performance results are discussed for synthetic and real data sets of third-order tensors. In particular, we worked with three different data sets: (1) a real computer tomography (CT) data set called MELANIX (an Osirix data set), (2) a symmetric random data set, where all indices are symmetric, and (3) a random data set. The CT data set has a 16bit, the random data set an 8bit value range. All our third-order tensor data sets are initially of size $512 \times 512 \times 512$, which we gradually reduced by a factor of 2, with the smallest data sets being of size $4 \times 4 \times 4$. The synthetic random data sets were generated for every resolution and in every run; the real data set was averaged (subsampled) for every coarser resolution.

Our simulation results are averaged over different decomposition runs of the various algorithms. In each decomposition run, we changed the initial guess, i. e., we

generated new random start vectors. We always initialized the algorithms by random start vectors, since this is cheaper than the initialization via HOSVD. Additionally, we generated for each decomposition run new random data sets. The presented timings are averages over 10 different runs of the algorithms.

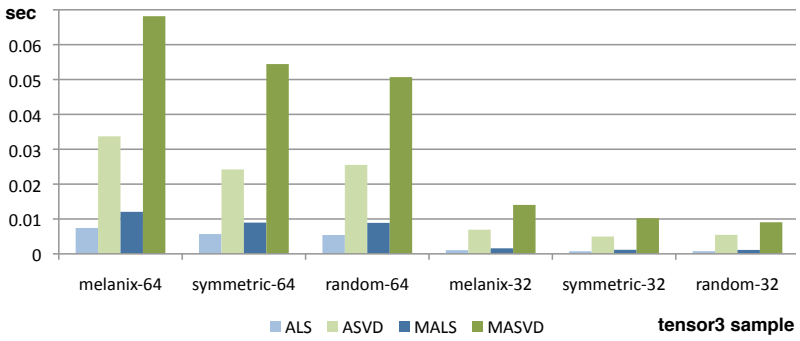
All the best rank one approximation algorithms are alternating algorithms, and based on the same convergence criterion, where convergence is achieved if one of the two following conditions: $iterations \leq 10$; $fitchange < 0.0001$ is met. The number of optimization calls within one iteration is fixed for the ALS and ASVD method. During one iteration, the ALS optimizes every mode once, while the ASVD optimizes every mode twice. The number of optimization calls can vary widely during each iteration of the modified algorithms. This results from the fact that multiple optimizations are performed in parallel, while only the best one is kept and the others are rejected.

The partial SVD is implemented by applying a symmetric eigenvalue decomposition (LAPACK DSYEVX) to the product AA^T (BLAS DGEMM) as suggested by the ARPACK package.

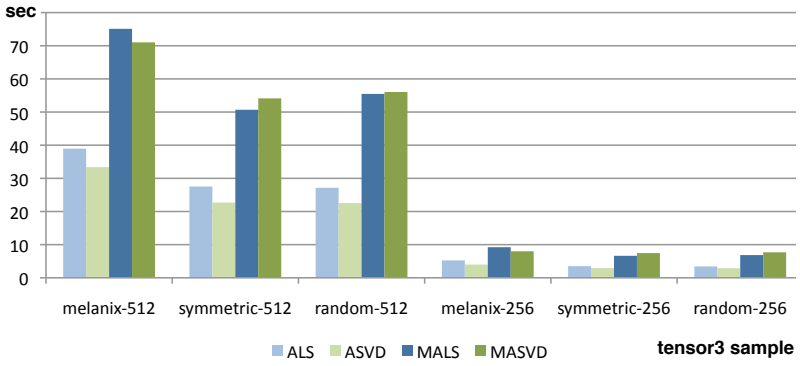
The first observation regarding the average timings is that third-order tensors (tensor3s) of size 64^3 or smaller took less than one second for the decomposition, which represents a time range, where we do not need to optimize further. On the contrary, the larger the third-order tensor gets, the more critical the differences in the decomposition times are. As shown in Figure 1, the modified versions of the algorithms took about twice as much CPU-time as the standard versions. For the large data sets, the ALS and ASVD take generally less time than the MALS and MASVD. The ASVD was fastest for large data sets, but compared to (M)ALS slow for small data sets. For larger data sets, the timings of the basic and modified algorithm versions came closer to each other.

We also compared the number of optimization calls needed for the algorithms of ALS, ASVD, MALS, and MASVD, recalling that for the ALS and the MALS, one mode is optimized per optimization call, while for ASVD and MASVD, two modes are optimized per optimization call. Figure 2 demonstrates the relationships of the four algorithms on three different data sets (color and marker encoded). As can be seen, the ASVD has the smallest number of optimization calls followed by the ALS, the MASVD and the MALS. One notices as well that the number of optimization calls for the two random data sets are close to each other for the respective algorithms. The real data set takes most optimization calls, even though it probably profits from more potential correlations. However, the larger number of optimization calls may also result from the different precision of one element of the third-order tensor (16bit vs. 8bit values). Another explanation might be that it was difficult to find good rank-one bases for a real data set (the error is approx. 70% for the 512^3 tensor). For random data, the error stays around 63%, probably due to a good distribution of the random values. Otherwise, the number of optimization calls followed the same relationships as already seen in the timings measured for the rank-one approximation algorithm.

It is not only important to check how fast the different algorithms perform, but also what quality they achieve. This was measured by checking the Frobenius norm of the resulting decompositions, which serves as a measure for the quality of the approximation. In general, we can say that the higher the Frobenius norm, the more likely it is that we find a global maximum. Accordingly, we compared



(a) CPU time (s) for medium 3-mode tensor samples



(b) CPU time (s) for larger 3-mode tensor samples

Figure 1: Average CPU times for best rank one approximations per algorithm and per data set taken over 10 different initial random guesses.

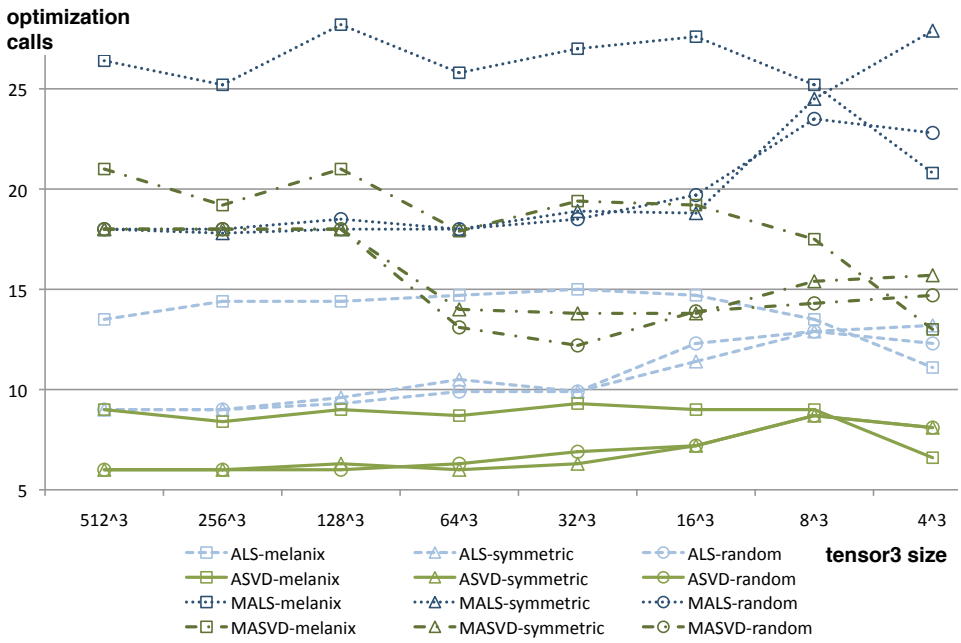


Figure 2: Average number of optimization calls needed per algorithm and per data set taken over 10 different initial random guesses.

the Frobenius norms in order to say whether the different algorithms converged to the same stationary point. In Table 1, we show the average Frobenius norm of the input tensor3 and compare it to the Frobenius norms of the approximations by ALS, ASVD, MALS, and MASVD. We observed that all the algorithms reach the same stationary point for the smaller and medium data sets. The computed Frobenius norms have the same value except for the ASVD result of the symmetric $4\times4\times4$ data set, where the final Frobenius norm is much higher. However, for the larger data sets ($\geq 128^3$) the stationary points differ slightly. We suspect that either the same stationary point was not achieved, or the precision requirement of the convergence criterion was too high. That means that the algorithms stopped earlier, since the results are not changing that much anymore in the case that precision tolerance for convergence is 0.0001.

The results of best rank one approximation for symmetric tensors using ALS, MALS, ASVD and MASVD show that the best rank one approximation is also symmetric, i. e. is of the form $a\mathbf{u}\otimes\mathbf{v}\otimes\mathbf{w}$, where $\mathbf{u}\approx\mathbf{v}\approx\mathbf{w}\in \mathrm{S}^{m-1}$. This confirms an observation made by Paul Van Dooren, (private communication), and the main result in [3], which claims that the best rank one approximation of a symmetric tensor can be always chosen symmetric. The results of ASVD an MASVD give a better symmetric rank one approximation, i. e. $\mathbf{u}-\mathbf{v}, \mathbf{u}-\mathbf{w}$ in ASVD and MASVD are smaller than in ALS and MALS.

	Input	ALS	ASVD	MALS	MASVD
melanix-512	4038720	2845680	2839270	2845680	2840890
melanix-256	1416420	1006170	1004060	1006160	1004360
melanix-128	490619	355487	353809	355487	355360
melanix-64	167341	125566	125566	125566	125566
melanix-32	56415	44066	44066	44066	44066
melanix-16	18667	15393	15393	15393	15393
melanix-8	5925	5261	5261	5261	5261
melanix-4	1674	1619	1619	1619	1619
symmetric-512	1700600	1471290	1435540	1471290	1438110
symmetric-256	601363	520329	507681	520329	508588
symmetric-128	212602	183949	179476	183949	179797
symmetric-64	75077	64969	64969	64969	64969
symmetric-32	26619	23068	23068	23068	23068
symmetric-16	9417	8184	8184	8184	8184
symmetric-8	3198	2759	2759	2759	2759
symmetric-4	1133	876	945	880	945
random-512	1700610	1471340	1435570	1471370	1438140
random-256	601277	520217	507576	520218	508487
random-128	212581	183926	179459	183926	179783
random-64	75170	65056	65056	65056	65056
random-32	26608	23045	23045	23045	23045
random-16	9423	8173	8173	8173	8173
random-8	3330	2895	2895	2895	2895
random-4	1156	1017	1017	1017	1017

Table 1: Average Frobenius norms: Initial Frobenius norm vs. the Frobenius norm of the approximations per algorithm and per data set (average taken over 10 different initial random guesses).

7 Conclusions

We have presented a new alternating algorithm for the computation of the best rank one approximation to a d-mode tensor. In contrast to the alternating least squares method, this method uses a singular value decomposition in each step. In order to achieve guaranteed convergence to a semi-maximal point, we have modified both algorithms and also presented a new Newton type method.

We have run extensive numerical tests to show the performance and convergence behavior of the new methods.

Acknowledgements

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