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SUBTRACTING A BEST RANK-1 APPROXIMATION MAY INCREASE TENSOR RANK

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ABSTRACT
Is has been shown that a best rank-\(R\) approximation of an order-\(k\) tensor may not exist when \(R \geq 2\) and \(k \geq 3\). This poses a serious problem to data analysts using Can-decomp/Parafac and related models. It has been observed numerically that, generally, this issue cannot be solved by consecutively computing and subtracting best rank-1 approximations. The reason for this is that subtracting a best rank-1 approximation generally does not decrease tensor rank. In this paper, we provide a mathematical treatment of this phenomenon. We assume throughout the following notation: bold italic up-sors are usually assimilated with their array representation. We consider tensors of order \(d\) defined on the outer product of \(d\)-way arrays. For simplicity, tensors play a wider and wider role in numerous application areas including blind techniques for Telecommunications, Data Analysis, Arithmetic Complexity, and keeping other indices fixed.

Usefulness. Tensors play a wider and wider role in numerous application areas including blind techniques for Telecommunications, Data Analysis, Arithmetic Complexity, and keeping other indices fixed.

Matrix algebra is insufficient. The manipulation of tensors remains difficult, because of major differences between their properties when we go from second order to higher. Several of these differences have already been underlined in the past \(8\), e.g. i) tensor rank often exceeds dimensions, ii) tensor rank can be different in real and complex fields, iii) maximal tensor rank is not generic, and is still unknown in general, (iv) computing the rank of a tensor is very difficult, (v) a tensor may not have a best low-rank approximate \(23\)\(22\)\(23\)\(23\)\(23\)\(23\)\(23\). It has been observed numerically in \(17\) section 7 that a best or ”good” rank-\(R\) approximation cannot be obtained by consecutively computing and subtracting \(R\) best rank-1 approximations (which always exist). The reason for this is that subtracting a best rank-1 approximation generally does not decrease tensor rank. Hence, the deflation technique practiced for matrices (via the Singular Value Decomposition)
cannot generally be extended to higher-order tensors. A special case where this deflation technique works is when the tensor is diagonalizable by orthonormal multilinear transformation; see [12], section 7.

In this paper, we provide a mathematical treatment of the (in)validity of a rank-1 deflation procedure for higher-order tensors. We consider $2 \times 2 \times 2$ tensors over the real field, with symmetric tensors as a special case. First, however, we discuss the problem of finding a best rank-1 approximate to a 3rd order tensor. The proofs of our results will be available in a forthcoming full-length version of this paper.

## 2. BEST RANK-1 APPROXIMATION

Finding the best rank-1 approximate consists of minimizing the criterion

$$\Psi = \frac{1}{2} \|X - a \otimes b \otimes c\|^2 \quad (3)$$

with respect to vectors $a$, $b$, and $c$. The solution will likely depend on the norm, and we shall restrict to the Frobenius norm: $\|X\|^2 = \sum_{ijk} |X_{ijk}|^2$. Obviously there is a scale indeterminacy in this problem, and we could impose two of these three vectors to be unit norm. We shall not do that here because the presentation would be slightly longer. Let $\otimes$ denote the summation over the $t$th index (that is the contraction operator in the $t$th space). For instance, the product $AB^T$ between two matrices can be written as $A \otimes B^T$ if $X$ is a 3rd order tensor, $X \otimes a$ is a matrix, and $X \otimes a \otimes b$ is a vector. And let us rewrite criterion (3) as:

$$\Psi = \frac{1}{2} \|X\|^2 - X \otimes a \otimes b \otimes c + \frac{1}{2} \|a\|^2 \|b\|^2 \|c\|^2. \quad (4)$$

Proceeding as in [3], gradients with respect to the three vectors can be obtained:

$$d\Psi_a = -X \otimes b \otimes c + a\|b\|^2 \|c\|^2$$

$$d\Psi_b = -X \otimes a \otimes c + b\|a\|^2 \|c\|^2$$

$$d\Psi_c = -X \otimes a \otimes b + c\|a\|^2 \|b\|^2.$$

Concerning the uniqueness of a best rank-1 approximate, one may ask the following question: are there tensors for which the solution defined by $a = ||b||^{-2}||c||^{-2}X \otimes b \otimes c$ and $d\Psi_b = d\Psi_c = 0$ is not unique up to scale? We exhibit in this section a family of such tensors.

If we plug the expression of $a$ back in the equation of stationary values of $b$, we get that $(X \otimes c) \otimes 1 (X \otimes c) \otimes b = \lambda b$, where $\lambda = ||a||^2 \|b\|^2 \|c\|^2$, which means that $b$ is an eigenvector of the matrix $(X \otimes c) \otimes 1 (X \otimes c)$. If the latter matrix is proportional to the identity for any $c$, then any $b$ is an eigenvector. Analogously, substituting the expression for $a$ into $d\Psi_b$, we get that $(X \otimes b) \otimes 1 (X \otimes b) \otimes c = \mu c$, where $\mu = ||a||^2 \|b\|^2 \|c\|^2$. If $(X \otimes b) \otimes 1 (X \otimes b)$ is also proportional to the identity for any $c$, then it follows that any $(a, b, c)$ with a given by $d\Psi_b = 0$ is a stationary point. Substituting the expression of $a$ into the criterion (3) then yields a criterion function in $(b, c)$ for which any $(b, c)$ is a stationary point. Hence, the function is constant and any $(b, c)$ is a minimizer. This yields the following proposition

**Proposition 1** If a tensor $X$ is such that the matrix $(X \otimes 1 c)$ is orthogonal for any vector $c$, and $(X \otimes b)$ is orthogonal for any vector $b$, then $X$ has infinitely many best rank-1 approximates.

In accordance with the usual practice, we shall represent a $p \times p \times 2$ tensor $X$ with two $p \times p$ matrix slices, $X_1$ and $X_2$, as $[X_1 \ | \ X_2]$.

**Example 1.** Let $X = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$. Then for any choice of non zero vector $c$, the matrix $(X \otimes 1 c)$, obtained by linear combination of the above two matrix slices, is orthogonal. Also, for any non zero vector $b$, the matrix $(X \otimes b)$ is orthogonal. Hence $X$ has infinitely many rank-1 approximates.

Most tensors have multiple locally best rank-1 approximates, with one of them being better than the others (i.e., a unique best rank-1 approximate), as pointed out in Section 3. Examples will illustrate this fact.

**Remark.** The tensor in Example 1 has rank 3. Ten Berge et al. [29] showed that $X$ has no best rank-2 approximation, the infimum of $\|X - Y\|^2$ over $Y$ of rank at most 2 being 1. A more general result was obtained by De Silva and Lim [12] who showed that no $2 \times 2 \times 2$ tensor of rank 3 has a best rank-2 approximation. Stegeman [23] showed that any sequence of rank-2 approximations $Y^{(n)}$ for which $\|X - Y^{(n)}\|^2$ converges to the infimum of 1, features diverging components. It is shown in [11] that the stationary points of the $2 \times 2 \times 2$ symmetric best rank-1 approximation problem are obtained as the roots of a 3rd degree polynomial.

## 3. BEST RANK-1 SUBTRACTION

From now on, we restrict our discussion to tensors in the real field. De Silva and Lim [12], Section 7] showed that $2 \times 2 \times 2$ tensors (over the real field) can be transformed by invertible multilinear matrix multiplications into eight distinct canonical forms. This partitions the space $\mathbb{R}^{2 \times 2 \times 2}$ into eight distinct orbits under the action of invertible transformations in each of the 3 modes. Table 1 lists the canonical forms for each orbit as well as their rank and multilinear rank. These quantities are invariant under the transformations defining an orbit. This kind of classification is better known for symmetric tensors or multivariate polynomials [6]. Recall the following result stated by De Silva and Lim [12]:

**Lemma 2** Let $X$ be a $2 \times 2 \times 2$ tensor with matrix slices $X_1$ and $X_2$.

(i) If $X_2 X_1^{-1}$ or $X_1 X_2^{-1}$ has real eigenvalues and is diagonalizable, then $X$ is in orbit $G_2$. 

(ii) If $X_2 X_1^{-1}$ or $X_1 X_2^{-1}$ has two identical real eigenvalues with only one associated eigenvector, then $X$ is in orbit $D_3$. 

(iii) If $X_2 X_1^{-1}$ has complex eigenvalues, then $X$ is in orbit $G_3$.

We shall use this lemma to verify the orbit of 2-dimensional 3rd order tensors.

**Example 2.** Consider the tensor

$$X = \begin{bmatrix} 1 & 0 & 0 & -2 \\ 0 & 1 & 1 & 0 \end{bmatrix}. \quad (5)$$

Since $X_2 X_1^{-1}$ has complex eigenvalues, $X$ is in orbit $G_3$. It can be verified that $X$ has a unique best rank-1 approximation

$$Y = \begin{bmatrix} 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (6)$$
When $Y$ is subtracted from $X$ we end up in orbit $D_3$, since
\begin{equation}
Z = X - Y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix},
\end{equation}
can be transformed to the canonical form of orbit $D_3$ by swapping rows within each slice.

<table>
<thead>
<tr>
<th>Canonical form</th>
<th>Tensor rank</th>
<th>Multilinear rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_0$:</td>
<td>0</td>
<td>(0, 0, 0)</td>
</tr>
<tr>
<td>$D_1$:</td>
<td>1</td>
<td>(1, 1, 1)</td>
</tr>
<tr>
<td>$D_2$:</td>
<td>2</td>
<td>(2, 2, 1)</td>
</tr>
<tr>
<td>$D_1'$:</td>
<td>2</td>
<td>(1, 2, 2)</td>
</tr>
<tr>
<td>$D_2'$:</td>
<td>2</td>
<td>(2, 2, 2)</td>
</tr>
<tr>
<td>$G_2$:</td>
<td>2</td>
<td>(2, 2, 2)</td>
</tr>
<tr>
<td>$D_3$:</td>
<td>3</td>
<td>(2, 2, 2)</td>
</tr>
<tr>
<td>$G_3$:</td>
<td>3</td>
<td>(2, 2, 2)</td>
</tr>
</tbody>
</table>

Table 1: Canonical forms of $2 \times 2 \times 2$ tensors for the eight orbits under the action of invertible multilinear matrix multiplications over the real field. The letters $D$ and $G$ stand for “degenerate” (zero volume set in the 8-dimensional space of $2 \times 2 \times 2$ tensors) and “typical” (positive volume set), respectively.

For tensors $X$ in the orbits of Table 1, we would like to know in which orbit $X - Y$ is contained, where $Y$ is a best rank-1 approximation of $X$. We have the following result for the degenerate orbits of ranks 1 and 2.

**Proposition 3** Let $X$ be a $2 \times 2 \times 2$ tensor, and let $Y$ be a best rank-1 approximation of $X$.

(i) If $X$ is in orbit $D_1$, then $X - Y$ is in orbit $D_0$.

(ii) If $X$ is in orbit $D_2$, $D_1'$, or $D_2'$, then $X - Y$ is in orbit $D_1$.

For $X$ in orbit $G_2$ or $D_3$, the tensor $X - Y$ is not restricted to a single orbit.

**Example 3.** For the canonical tensor $X$ of orbit $G_2$ in Table 1 it can be seen that $X - Y$ is in $D_1$. On the other hand, consider
\begin{equation}
X = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.
\end{equation}

For this tensor, $X_3X_{11}^{-1}$ has two distinct real eigenvalues. Hence, by Lemma 3, the tensor is in $G_2$. It can be shown that $X$ has a unique best rank-1 approximation $Y$ such that $X - Y$ equals the canonical tensor of orbit $D_3$ in Table 1.

**Example 4.** Next, consider tensors in orbit $D_3$:
\begin{equation}
\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 2 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.
\end{equation}

Subtracting the best rank-1 approximation $Y$ from these tensors amounts to replacing the element 2 by zero. Hence, $X - Y$ is in orbit $D_3$, $D_1'$, and $D_2'$, respectively.

On the other hand, it can be verified numerically or analytically that for $X$ equal to the canonical tensor of orbit $D_1$ in Table 1, $X - Y$ is also in orbit $D_3$. Moreover, numerical experiments show that for a generic $X$ in orbit $D_3$, we have $X - Y$ in orbit $D_3$ as well. This suggests the following

**Conjecture 4** If $X$ is in $D_3$ and $Y$ is the best rank-1 approximation of $X$, then almost all tensors $X - Y$ are in $D_3$.

Tensors given in Examples 1 or 2 were both in orbit $G_3$, and we have seen that $X - Y$ is in orbit $D_3$ in Example 3. For Example 4, this can be proven for any of the infinite best rank-1 approximates $Y$ of $X$. Numerically and analytically, we have not found any $X$ in orbit $G_3$ for which $X - Y$ is not in orbit $D_3$.

We have no deterministic result for tensors in orbits $D_2$ and $G_3$, but we still have the following result, verified almost everywhere (hence the word “generic”):

**Proposition 5** Let $X$ be a generic $2 \times 2 \times 2$ tensor, and $Y$ be a best rank-1 approximation of $X$. Then almost all tensors $X - Y$ are in orbit $D_3$.

Hence, for typical tensors in orbit $G_2$, subtracting a best rank-1 approximate increases the rank to 3. For typical tensors in orbit $G_3$, subtracting a best rank-1 approximate does not affect the rank.

However, some non typical tensors of rank 2 may have a different behavior, as now shown.

**Proposition 6** Let $X$ be a $2 \times 2 \times 2$ rank-2 tensor with diagonal slices, and let $Y$ be a best rank-1 approximation of $X$. Then $X - Y$ is in orbit $D_1$.

**Example 5.** Let $X = \begin{bmatrix} a & 0 & 0 \\ 0 & d & 0 \\ 0 & 0 & h \end{bmatrix}$. Then
\begin{equation}
X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} a \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} d \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} e \\ h \end{bmatrix}.
\end{equation}

Then it can be seen that $X = (1, 1, T) \cdot I$, where $I$ denotes the identity matrix and $T$ the diagonal tensor tensor with ones on its diagonal:
\begin{equation}
I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{and} \quad T = \begin{bmatrix} a & d \\ e & h \end{bmatrix}.
\end{equation}

This shows that $X$ is in orbit $G_2$, and Proposition 5 implies that this is an exception to Proposition 3.

**Example 6** states that such exceptions form a set of null measure.

### 4. Symmetric Tensors

A tensor is symmetric if its entries are invariant under arbitrary permutations of its indices. There is a bijection between the space of symmetric $I \times I \times I$ tensors and the space of homogeneous polynomials of degree 3 in $I$ variables. A symmetric $I \times I \times I$ tensor $X$ can be associated with the polynomial
\begin{equation}
p(s_1, \ldots, s_I) = \sum_{i,j,k} x_{ijk} s_is_js_k.
\end{equation}
The symmetric rank of an order-3 symmetric tensor $X$ is the minimal number $R$ such that \[ X = \sum_{i=1}^{R} a_i \otimes a_i \otimes a_i. \] (10)

The orbits of symmetric $2 \times 2 \times 2$ tensors are given in Table 2.

<table>
<thead>
<tr>
<th>canonical form</th>
<th>polynomial</th>
<th>sym. rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>$D_1$</td>
<td>$s_1^3$</td>
<td>$1$</td>
</tr>
<tr>
<td>$G_2$</td>
<td>$s_1^3 + s_2^3$</td>
<td>$2$</td>
</tr>
<tr>
<td>$D_3$</td>
<td>$3s_1^2s_2$</td>
<td>$3$</td>
</tr>
<tr>
<td>$G_3$</td>
<td>$-s_1^3 + 3s_1s_2^2 + s_2^3$</td>
<td>$3$</td>
</tr>
</tbody>
</table>

Table 2: Canonical forms of symmetric $2 \times 2 \times 2$ tensors and associated polynomials, for the three orbits under the action of invertible multilinear transformations over the real field. The letters $D$ and $G$ stand for “degenerate” (zero volume set in the 4-dimensional space of symmetric $2 \times 2 \times 2$ tensors) and “typical” (positive volume set), respectively.

The symmetric rank of symmetric tensors of dimension 2 can be obtained from the Sylvester Theorem, at any order. This Theorem is formulated below in the case of third order tensors.

**Theorem 7 (Sylvester)** A symmetric $2 \times 2 \times 2$ tensor with associated polynomial
\[ p(s_1, s_2) = \gamma_0 s_1^3 + 3 \gamma_2 s_1^2 s_2 + 3 \gamma_1 s_1 s_2^2 + \gamma_6 s_2^3, \] (11)
has a symmetric rank-$R$ decomposition (10) if and only if there exists a vector $g = (g_0, \ldots, g_R)^T$ such that
\[
\begin{pmatrix}
\gamma_0 & \cdots & \gamma_R \\
\gamma_1 & \cdots & \gamma_{R+1} \\
\vdots & \ddots & \vdots \\
\gamma_{R-R} & \cdots & \gamma_R
\end{pmatrix}
g = 0,
\] (12)
and if the polynomial $q(s_1, s_2) = g_R s_1^R + g_{R-1} s_1^{R-1} s_2 + \cdots + g_1 s_1 s_2^{R-1} + g_0 s_2^R$ has $R$ distinct real roots.

**Example 6.** Using Sylvester’s Theorem, one can obtain the following decomposition for the representative of orbit $D_1$ given in Table 2:
\[ 6s_1^2s_2 = (s_1 + s_2)^3 + (-s_1 + s_2)^3 - 2s_2^3. \] (13)

In other words, the associated tensor can be written $X = a^3 + b^3 - 2c^3$, where $a = [1, 1]^T$, $b = [-1, 1]^T$ and $c = [0, 1]^T$.

We have the following analogue of Lemma 3 to verify the orbit of symmetric tensors of dimension 2.

**Lemma 8** Let $X$ be a symmetric $2 \times 2 \times 2$ tensor with matrix slices $X_1$ and $X_2$.
(i) If $X_2X_1^{-1}$ or $X_1X_2^{-1}$ has distinct real eigenvalues, then $X$ is in orbit $G_2$.
(ii) If $X_2X_1^{-1}$ or $X_1X_2^{-1}$ has two identical real eigenvalues, then $X$ is in orbit $D_3$.
(iii) If $X_2X_1^{-1}$ has complex eigenvalues, then $X$ is in orbit $G_3$.

Next, we present an example of a symmetric $2 \times 2 \times 2$ tensor in orbit $G_3$, that has a unique best symmetric rank-1 approximation $Y$, such that $X = Y$ is in orbit $D_3$.

**Example 7.** Let
\[
X = \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 0
\end{bmatrix},
\] (14)
we have
\[
X_2X_1^{-1} = \begin{bmatrix}
-1 & 1 \\
-1 & 1
\end{bmatrix},
\] (15)
which has complex eigenvalues. Hence, by Lemma (iii) the tensor is in orbit $G_3$.

Next, we compute the best symmetric rank-1 approximation $Y$ to $X$, which has the form
\[
Y = \begin{bmatrix}
x_1^3 & x_1^2 x_2 & x_1 x_2^2 & x_2^3
\end{bmatrix}.
\] (16)
After some manipulations, it can be shown that the minimum of $\|X - Y\|^2$ is obtained for $x_1^3 = x_2^3 = 3/4$, that is
\[
Y = \frac{1}{4} \begin{bmatrix}
3 & 3 & 3 & 3
\end{bmatrix}.
\] (17)

By subtraction, we obtain
\[
Z = X - Y = \begin{bmatrix}
-3 & 1 & 1 & 1 \\
1 & 1 & 1 & -3
\end{bmatrix},
\] (18)
and $Z_1Z_1^{-1} = \begin{bmatrix}
0 & 1 \\
-1 & -2
\end{bmatrix},$ (19)
which has a double eigenvalue $-1$. Hence, by Lemma (ii) the tensor $Z$ is in orbit $D_1$.

In our next example, the symmetric $2 \times 2 \times 2$ tensor is in orbit $G_2$, and has a unique best symmetric rank-1 approximation $Y$, such that $X = Y$ is in orbit $D_3$.

**Example 8.** Let
\[
X = \begin{bmatrix}
3 & 1 & 1 & 1 \\
1 & 1 & 1 & 3
\end{bmatrix},
\] (20)
we have
\[
X_2X_1^{-1} = \begin{bmatrix}
0 & 1 \\
-1 & 4
\end{bmatrix},
\] (21)
which has real and distinct eigenvalues. Hence, by Lemma (i) the tensor is in orbit $G_2$.

Next, we compute the best symmetric rank-1 approximation $Y$ to $X$. It can be shown that the minimum of $\|X - Y\|^2$ is obtained for
\[
Y = \frac{3}{2} \begin{bmatrix}
1 & 1 & 1 & 1
\end{bmatrix}.
\] (22)
By subtraction, we obtain
\[
Z = X - Y = \frac{1}{2} \begin{bmatrix}
1 & -1 & -1 & -1 \\
-1 & 1 & -1 & -1 \\
-1 & -1 & 1 & -1 \\
-1 & -1 & -1 & 1
\end{bmatrix},
\] (23)
and
\[
Z_2 Z_1^T = \begin{bmatrix}
0 & 1 \\
-1 & -2
\end{bmatrix},
\] (24)
which has a double eigenvalue \(-1\). Hence, by Lemma 8 (ii) the tensor \(Z\) is in orbit \(D_3\).

Finally, we have the following analogue of Proposition 5.

**Proposition 9** Let \(X\) be a generic symmetric \(2 \times 2 \times 2\) tensor, and \(Y\) be a best rank-1 approximation of \(X\). Then almost all tensors \(X - Y\) are in orbit \(D_3\).

Hence, for typical symmetric \(2 \times 2 \times 2\) tensors with symmetric rank 2, subtracting a best rank-1 approximate increases the symmetric rank to 3. For typical symmetric tensors with symmetric rank 3, subtracting a best rank-1 approximate does not affect the symmetric rank.

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