

# Subtracting a best rank-1 approximation may increase tensor rank<sup>1</sup>

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## Abstract

It 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 tensor decompositions. 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 property for real-valued  $2 \times 2 \times 2$  tensors, with symmetric tensors as a special case. Regardless of the symmetry, we show that for generic  $2 \times 2 \times 2$  tensors (which have rank 2 or 3), subtracting a best rank-1 approximation results in a tensor that has rank 3 and lies on the boundary between the rank-2 and rank-3 sets. Hence, for a typical tensor of rank 2, subtracting a best rank-1 approximation *increases* the tensor rank.

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# 1 Introduction

Tensors of order  $d$  are defined on the outer product of  $d$  linear spaces,  $\mathcal{S}_\ell$ ,  $1 \leq \ell \leq d$ . Once bases of spaces  $\mathcal{S}_\ell$  are fixed, they can be represented by  $d$ -way arrays. For simplicity, tensors are usually assimilated with their array representation. We assume throughout the following notation: underscored bold uppercase for tensors e.g.  $\underline{\mathbf{X}}$ , bold uppercase for matrices e.g.  $\mathbf{T}$ , bold lowercase for vectors e.g.  $\mathbf{a}$ , calligraphic for sets e.g.  $\mathcal{S}$ , and plain font for scalars e.g.  $X_{ijk}$ ,  $T_{ij}$  or  $a_i$ . In this paper, we consider only 3rd order tensors. The three spaces of a 3rd order tensor are also referred to as the three “modes”.

Let  $\underline{\mathbf{X}}$  be a 3rd order tensor defined on the tensor product  $\mathcal{S}_1 \otimes \mathcal{S}_2 \otimes \mathcal{S}_3$ . If a change of bases is performed in the spaces  $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3$  by invertible matrices  $\mathbf{S}, \mathbf{T}, \mathbf{U}$ , then the tensor representation  $\underline{\mathbf{X}}$  is transformed into

$$\tilde{\underline{\mathbf{X}}} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \underline{\mathbf{X}}, \quad (1.1)$$

whose coordinates are given by  $\tilde{X}_{ijk} = \sum_{pqr} S_{ip} T_{jq} U_{kr} X_{pqr}$ . This is known as the *multilinearity property* enjoyed by tensors. Matrices, which can be associated with linear operators, are tensors of order 2. The multilinear transformation (1.1) is also denoted as

$$\tilde{\underline{\mathbf{X}}} = \underline{\mathbf{X}} \bullet_1 \mathbf{S} \bullet_2 \mathbf{T} \bullet_3 \mathbf{U}, \quad (1.2)$$

where  $\bullet_\ell$  denotes the multiplication (or contraction) operator in the  $\ell$ th mode of  $\underline{\mathbf{X}}$ , and  $\mathbf{S}, \mathbf{T}, \mathbf{U}$  are contracted in their second index. Note that the matrix multiplication  $\mathbf{STU}^T$  can be denoted as  $\mathbf{T} \bullet_1 \mathbf{S} \bullet_2 \mathbf{U} = \mathbf{T} \bullet_2 \mathbf{U} \bullet_1 \mathbf{S}$ . For two contractions with matrices in the same mode, we have the rule  $\underline{\mathbf{X}} \bullet_\ell \mathbf{T} \bullet_\ell \mathbf{S} = \underline{\mathbf{X}} \bullet_\ell (\mathbf{ST})$ , see e.g. [9, section 2].

The rank of a tensor  $\underline{\mathbf{X}}$  is defined as the smallest number of outer product tensors whose sum equals  $\underline{\mathbf{X}}$ , i.e. the smallest  $R$  such that

$$\underline{\mathbf{X}} = \sum_{r=1}^R \mathbf{a}_r \otimes \mathbf{b}_r \otimes \mathbf{c}_r. \quad (1.3)$$

Hence a rank-1 tensor  $\underline{\mathbf{X}}$  is the outer product of vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  and has entries  $X_{ijk} = a_i b_j c_k$ . The decomposition of a tensor into a sum of outer products of vectors and the corresponding notion of tensor rank were first introduced and studied by [14] [15].

Tensors play a wider and wider role in numerous application areas including blind source separation techniques for Telecommunications [26] [27] [6] [11] [8], Arithmetic Complexity [21] [34] [1] [32], or Data Analysis [13] [2] [28] [20]. In some applications, tensors may be symmetric only in some modes, or may not be symmetric nor have equal dimensions. In most applications, the decomposition of a tensor into a sum of rank-1 terms is relevant, since tensors entering the models

to fit have a reduced rank. For example, such a tensor decomposition describes the basic structure of fourth-order cumulants of multivariate data on which a lot of algebraic methods for Independent Component Analysis are based [3] [10]. For an overview of applications of tensor decompositions, refer to [18].

An important advantage of using tensor decompositions of order 3 and higher, is that the decomposition is rotationally unique under mild conditions [21] [32]. This is not the case for most matrix decompositions, e.g. Principal Component Analysis. However, the manipulation of tensors remains difficult, because of major differences between their properties when we go from second order to higher orders. We mention the following: (i) tensor rank often exceeds dimensions, (ii) tensor rank can be different over the real and complex fields, (iii) maximal tensor rank is not generic, and is still unknown in general, (iv) generic tensor rank may not have a single value over the real field, (v) computing the rank of a tensor is very difficult, (vi) a tensor may not have a best rank- $R$  approximation for  $R \geq 2$ . For (i)-(v), see e.g. [22] [12] [7]. For (iv), see e.g. [36] [37]. For (vi), see e.g. [29] [30] [31] [12] [19] [33]. A discussion specifically focussed on symmetric tensors can be found in [7].

In [12] it is shown that (vi) holds on a set of positive measure. It is recalled in [7] and [12] that any tensor has a best rank-1 approximation. However, 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. 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 [17, 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. For such a tensor  $\underline{\mathbf{X}}$ , let the frontal slabs be denoted as  $\mathbf{X}_1$  and  $\mathbf{X}_2$ . Our main result is for generic tensors  $\underline{\mathbf{X}}$ , which have rank 2 if  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has distinct real eigenvalues, and rank 3 if  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has complex eigenvalues. We show that for generic  $\underline{\mathbf{X}}$ , subtraction of a best rank-1 approximation  $\underline{\mathbf{Y}}$  yields a tensor  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$  of rank 3. Hence, for a typical  $\underline{\mathbf{X}}$  of rank 3 this does not affect the rank, and for a typical  $\underline{\mathbf{X}}$  of rank 2 this has *increased* the rank. In fact, we show that  $\underline{\mathbf{Z}}$  lies on the boundary between the rank-2 and rank-3 sets, i.e.  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  has identical real eigenvalues. The result that subtraction of a best rank-1 approximation yields identical eigenvalues is new and expands the knowledge of the topology of tensor rank. Also, we show that the same result holds for symmetric  $2 \times 2 \times 2$  tensors. Based on numerical experiments we conjecture that the results can be extended

to  $p \times p \times 2$  tensors over the real field.

The above contributions are new to the literature on best rank-1 approximation of higher-order tensors. The latter includes best rank-1 approximation algorithms [9] [38] [17], conditions under which the best rank-1 approximation is equal to the best symmetric rank-1 approximation [24], and a relation between the best symmetric rank-1 approximation and the notions of eigenvalues and eigenvectors of a symmetric tensor [5] [25].

This paper is organized as follows. In Section 2, we introduce the best rank-1 approximation problem for 3rd order tensors, and state first order conditions for the optimal solution. Next, we consider  $2 \times 2 \times 2$  tensors. Section 3 contains rank criteria and orbits for  $2 \times 2 \times 2$  tensors. In Section 4, we present examples and general results for subtraction of a best rank-1 approximation from a  $2 \times 2 \times 2$  tensor. In Section 5, 6 and 7, we discuss the special case of symmetric tensors. Section 5 provides first order conditions for the best symmetric rank-1 approximation of a symmetric 3rd order tensor. Section 6 contains rank criteria and orbits of symmetric  $2 \times 2 \times 2$  tensors. These results are used in Section 7, when studying the subtraction of a best symmetric rank-1 approximation from a symmetric  $2 \times 2 \times 2$  tensor. Section 8 contains a discussion of our results. The proofs of our main results are contained in appendices.

## 2 Best rank-1 approximation

We consider the problem of finding a best rank-1 approximation to a given 3rd order tensor  $\underline{\mathbf{X}} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ , i.e.

$$\min_{\mathbf{x} \in \mathbb{R}^{d_1}, \mathbf{y} \in \mathbb{R}^{d_2}, \mathbf{z} \in \mathbb{R}^{d_3}} \|\underline{\mathbf{X}} - \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}\|^2, \quad (2.1)$$

where  $\|\cdot\|$  denotes the Frobenius norm, i.e.  $\|\underline{\mathbf{X}}\|^2 = \sum_{ijk} |X_{ijk}|^2$ . Since the set of rank-1 tensors is closed, problem (2.1) is guaranteed to have an optimal solution [12, proposition 4.2]. Note that the vectors  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  of the rank-1 tensor ( $\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$ ) are determined up to scaling. One could impose two of the vectors to be unit norm.

Let  $\Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \|\underline{\mathbf{X}} - \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}\|^2$ . Then  $\Psi$  can be written as

$$\Psi = \|\underline{\mathbf{X}}\|^2 - 2 \underline{\mathbf{X}} \bullet_1 \mathbf{x}^T \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T + \|\mathbf{x}\|^2 \|\mathbf{y}\|^2 \|\mathbf{z}\|^2. \quad (2.2)$$

Hence, the minimization problem (2.1) is equivalent to minimizing (2.2). Using this fact, and setting the gradients of  $\Psi$  with respect to the vectors  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  equal to zero, we obtain the following equations:

$$\mathbf{x} = \frac{\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T}{\|\mathbf{y}\|^2 \|\mathbf{z}\|^2}, \quad \mathbf{y} = \frac{\underline{\mathbf{X}} \bullet_1 \mathbf{x}^T \bullet_3 \mathbf{z}^T}{\|\mathbf{x}\|^2 \|\mathbf{z}\|^2}, \quad \mathbf{z} = \frac{\underline{\mathbf{X}} \bullet_1 \mathbf{x}^T \bullet_2 \mathbf{y}^T}{\|\mathbf{x}\|^2 \|\mathbf{y}\|^2}. \quad (2.3)$$

Substituting

$$\mathbf{x} = \frac{\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T}{\|\mathbf{y}\|^2 \|\mathbf{z}\|^2}, \quad (2.4)$$

into the last two equations of (2.3), we obtain

$$(\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T) \bullet_2 \mathbf{y}^T = \lambda \mathbf{y}, \quad (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T) \bullet_3 \mathbf{z}^T = \mu \mathbf{z}, \quad (2.5)$$

where  $\lambda = \|\mathbf{x}\|^2 \|\mathbf{y}\|^2 \|\mathbf{z}\|^4$  and  $\mu = \|\mathbf{x}\|^2 \|\mathbf{y}\|^4 \|\mathbf{z}\|^2$ . Hence,  $\mathbf{y}$  is an eigenvector of the matrix  $(\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T)$  and  $\mathbf{z}$  is an eigenvector of the matrix  $(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T)$ .

Substituting (2.4) into (2.2) yields

$$\Psi = \|\underline{\mathbf{X}}\|^2 - \frac{(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T)}{\|\mathbf{y}\|^2 \|\mathbf{z}\|^2} = \|\underline{\mathbf{X}}\|^2 - \frac{\|\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T\|^2}{\|\mathbf{y}\|^2 \|\mathbf{z}\|^2}. \quad (2.6)$$

Hence, a best rank-1 approximation  $(\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z})$  of  $\underline{\mathbf{X}}$  is found by minimizing (2.6) over  $(\mathbf{y}, \mathbf{z})$  and obtaining  $\mathbf{x}$  as (2.4). The stationary points  $(\mathbf{y}, \mathbf{z})$  are given by (2.5), which can also be written as

$$(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T) = \frac{\|\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T\|^2}{\|\mathbf{y}\|^2} \mathbf{y}, \quad (2.7)$$

$$(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T) = \frac{\|\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{z}^T\|^2}{\|\mathbf{z}\|^2} \mathbf{z}. \quad (2.8)$$

Next, we consider transformations of the best rank-1 approximation. The following well-known result states that a best rank-1 approximation is preserved under orthonormal multilinear transformation.

**Lemma 2.1** *Let  $\mathbf{S}, \mathbf{T}, \mathbf{U}$  be orthonormal matrices. If a tensor  $\underline{\mathbf{X}}$  admits  $\underline{\mathbf{Y}}$  as a best rank-1 approximation, then  $(\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \underline{\mathbf{Y}}$  is a best rank-1 approximation of  $(\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \underline{\mathbf{X}}$ .*

**Proof.** Let  $\underline{\mathbf{Y}} = \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$  be a best rank-1 approximation of  $\underline{\mathbf{X}}$ , and let  $\tilde{\underline{\mathbf{X}}} = (\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \underline{\mathbf{X}}$ . Since orthonormal transforms leave the Frobenius norm invariant, we obtain the following analogue of (2.2):

$$\begin{aligned} \|\tilde{\underline{\mathbf{X}}} - \tilde{\mathbf{x}} \otimes \tilde{\mathbf{y}} \otimes \tilde{\mathbf{z}}\|^2 &= \|\tilde{\underline{\mathbf{X}}}\|^2 - 2\tilde{\underline{\mathbf{X}}} \bullet_1 \tilde{\mathbf{x}}^T \bullet_2 \tilde{\mathbf{y}}^T \bullet_3 \tilde{\mathbf{z}}^T + \|\tilde{\mathbf{x}}\|^2 \|\tilde{\mathbf{y}}\|^2 \|\tilde{\mathbf{z}}\|^2 \\ &= \|\underline{\mathbf{X}}\|^2 - 2\underline{\mathbf{X}} \bullet_1 (\tilde{\mathbf{x}}^T \mathbf{S}) \bullet_2 (\tilde{\mathbf{y}}^T \mathbf{T}) \bullet_3 (\tilde{\mathbf{z}}^T \mathbf{U}) + \|\mathbf{S}^T \tilde{\mathbf{x}}\|^2 \|\mathbf{T}^T \tilde{\mathbf{y}}\|^2 \|\mathbf{U}^T \tilde{\mathbf{z}}\|^2. \end{aligned} \quad (2.9)$$

Hence, since  $(\mathbf{x}, \mathbf{y}, \mathbf{z})$  is a minimizer of (2.2), it follows that  $(\mathbf{S}\mathbf{x}, \mathbf{T}\mathbf{y}, \mathbf{U}\mathbf{z})$  is a minimizer of (2.9). In other words, a best rank-1 approximation of  $\tilde{\underline{\mathbf{X}}}$  is given by  $(\mathbf{S}\mathbf{x} \otimes \mathbf{T}\mathbf{y} \otimes \mathbf{U}\mathbf{z})$ . This completes the proof.  $\square$

As we will see later, most tensors have multiple locally best rank-1 approximations, with one of them being better than the others (i.e., a unique global best rank-1 approximation). Our final

result in this section states a condition under which there exist infinitely many best (global) rank-1 approximations.

**Proposition 2.2** *Let  $\underline{\mathbf{X}}$  be such that the matrix  $(\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T)$  is orthogonal for any nonzero vector  $\mathbf{z}$ , and  $(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T)$  is orthogonal for any nonzero vector  $\mathbf{y}$ . Then  $\underline{\mathbf{X}}$  has infinitely many best rank-1 approximations.*

**Proof.** The proof follows from equation (2.5) for the stationary points  $(\mathbf{y}, \mathbf{z})$ . The conditions of the proposition imply that the matrices  $(\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T)$  and  $(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T) \bullet_1 (\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T)$  are proportional to the identity matrix for any nonzero  $\mathbf{y}$  and  $\mathbf{z}$ . Therefore, any vector is an eigenvector of these matrices, and (2.5) holds for any nonzero  $\mathbf{y}$  and  $\mathbf{z}$ .

Since any  $(\mathbf{y}, \mathbf{z})$  (with nonzero  $\mathbf{y}$  and  $\mathbf{z}$ ) is a stationary point of minimizing (2.6), it follows that the latter is constant. We conclude that any  $(\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z})$  with  $\mathbf{x}$  as in (2.4), is a best rank-1 approximation of  $\underline{\mathbf{X}}$ .  $\square$

Below is a  $2 \times 2 \times 2$  example satisfying the conditions of Proposition 2.2. We denote a tensor  $\underline{\mathbf{X}}$  with two slabs  $\mathbf{X}_1$  and  $\mathbf{X}_2$  as  $[\mathbf{X}_1 | \mathbf{X}_2]$ .

**Example 2.3** Let

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \end{array} \right]. \quad (2.10)$$

Then for any choice of nonzero vector  $\mathbf{z}$ , the matrix  $(\underline{\mathbf{X}} \bullet_3 \mathbf{z}^T)$ , obtained by linear combination of the above two matrix slices, is orthogonal. Also, for any nonzero vector  $\mathbf{y}$ , the matrix  $(\underline{\mathbf{X}} \bullet_2 \mathbf{y}^T)$  is orthogonal. Hence,  $\underline{\mathbf{X}}$  has infinitely many rank-1 approximations. One can verify that each rank-1 approximation  $(\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z})$  with  $\mathbf{x}$  as in (2.4), satisfies  $\|\underline{\mathbf{X}} - \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}\|^2 = 3$ .  $\square$

The tensor (2.10) has rank 3 and is studied in [35] where it is shown that it has no best rank-2 approximation, the infimum of  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\|^2$  over  $\underline{\mathbf{Y}}$  of rank at most 2 being 1. A more general result is obtained in [12] where it is shown that no  $2 \times 2 \times 2$  tensor of rank 3 has a best rank-2 approximation. In [29] it is shown that any sequence of rank-2 approximations  $\underline{\mathbf{Y}}^{(n)}$  for which  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}^{(n)}\|^2$  converges to the infimum of 1, features diverging components.

### 3 Rank criteria and orbits of $2 \times 2 \times 2$ tensors

It was shown in [12, section 7] that  $2 \times 2 \times 2$  tensors (over the real field) can be transformed by invertible multilinear multiplications (1.1) 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 of a tensor “from the three sides”.

Before the eight orbits are introduced, we define some concepts. A mode- $n$  vector of a  $d_1 \times d_2 \times d_3$  tensor is an  $d_n \times 1$  vector obtained from the tensor by varying the  $n$ -th index and keeping the other indices fixed. The mode- $n$  rank is defined as the dimension of the subspace spanned by the mode- $n$  vectors of the tensor. The *multilinear rank* of the tensor is the triplet (mode-1 rank, mode-2 rank, mode-3 rank). The mode- $n$  rank generalizes the row and column rank of matrices. Note that a tensor with multilinear rank  $(1, 1, 1)$  has rank 1 and vice versa. The multilinear rank is invariant under invertible multilinear transformation [12, section 2].

Related to the orbits of  $2 \times 2 \times 2$  tensors is the *hyperdeterminant*. Slab operations on  $[\mathbf{X}_1 | \mathbf{X}_2]$  generate new slabs of the form  $\lambda_1 \mathbf{X}_1 + \lambda_2 \mathbf{X}_2$ . There holds

$$\det(\lambda_1 \mathbf{X}_1 + \lambda_2 \mathbf{X}_2) = \lambda_1^2 \det(\mathbf{X}_1) + \lambda_1 \lambda_2 \frac{\det(\mathbf{X}_1 + \mathbf{X}_2) - \det(\mathbf{X}_1 - \mathbf{X}_2)}{2} + \lambda_2^2 \det(\mathbf{X}_2). \quad (3.1)$$

The hyperdeterminant of  $\underline{\mathbf{X}}$ , denoted as  $\Delta(\underline{\mathbf{X}})$ , is defined as the discriminant of the quadratic polynomial (3.1):

$$\Delta(\underline{\mathbf{X}}) = \left[ \frac{\det(\mathbf{X}_1 + \mathbf{X}_2) - \det(\mathbf{X}_1 - \mathbf{X}_2)}{2} \right]^2 - 4 \det(\mathbf{X}_1) \det(\mathbf{X}_2). \quad (3.2)$$

Hence, if  $\Delta(\underline{\mathbf{X}})$  is nonnegative, then a real slabmix exists that is singular. If  $\Delta(\underline{\mathbf{X}})$  is positive, then two real and linearly independent singular slabmixes exist. It follows from (3.1)-(3.2) that the hyperdeterminant is equal to the discriminant of the characteristic polynomial of  $\det(\mathbf{X}_1)\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\det(\mathbf{X}_2)\mathbf{X}_1\mathbf{X}_2^{-1}$ . The sign of the hyperdeterminant is invariant under invertible multilinear transformation [12, section 5].

Table 1 lists the canonical forms for each orbit as well as their rank, multilinear rank and hyperdeterminant sign. Generic  $2 \times 2 \times 2$  tensors have rank 2 or 3 over the real field, both on a set of positive measure [22] [36].

canonical form	tensor rank	multilinear rank	sign $\Delta$
$D_0 : \left[ \begin{array}{cc cc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	0	(0, 0, 0)	0
$D_1 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	1	(1, 1, 1)	0
$D_2 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array} \right]$	2	(2, 2, 1)	0
$D'_2 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{array} \right]$	2	(1, 2, 2)	0
$D''_2 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right]$	2	(2, 1, 2)	0
$G_2 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right]$	2	(2, 2, 2)	+
$D_3 : \left[ \begin{array}{cc cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right]$	3	(2, 2, 2)	0
$G_3 : \left[ \begin{array}{cc cc} -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array} \right]$	3	(2, 2, 2)	-

Table 1: Orbits of  $2 \times 2 \times 2$  tensors under the action of invertible multilinear transformation  $(\mathbf{S}, \mathbf{T}, \mathbf{U})$  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 later use, we state the following rank and orbit criteria. The rank criteria have been proven for  $p \times p \times 2$  tensors in [16]. The  $2 \times 2 \times 2$  orbits can be found in [12, section 7]. In the sequel, we will use this result to verify the orbit of a  $2 \times 2 \times 2$  tensor.

**Lemma 3.1** *Let  $\underline{\mathbf{X}}$  be a  $2 \times 2 \times 2$  tensor with slabs  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , of which at least one is nonsingular.*

- (i) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has real eigenvalues and is diagonalizable, then  $\underline{\mathbf{X}}$  is in orbit  $G_2$ .*
- (ii) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has two identical real eigenvalues with only one associated eigenvector, then  $\underline{\mathbf{X}}$  is in orbit  $D_3$ .*
- (iii) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has complex eigenvalues, then  $\underline{\mathbf{X}}$  is in orbit  $G_3$ .*

□

## 4 Best rank-1 subtraction for $2 \times 2 \times 2$ tensors

For  $2 \times 2 \times 2$  tensors  $\underline{\mathbf{X}}$  in the orbits of Table 1, we would like to know in which orbit  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is contained, where  $\underline{\mathbf{Y}}$  is a best rank-1 approximation of  $\underline{\mathbf{X}}$ . In this section, we present both examples and general results. We begin by formulating our main result. It is not a deterministic result, but involves generic  $2 \times 2 \times 2$  tensors, which are in orbits  $G_2$  and  $G_3$ . Any tensor randomly generated from a continuous distribution can be considered to be typical. The full proof of Theorem 4.1 is contained in Appendix A.

**Theorem 4.1** *For almost all  $2 \times 2 \times 2$  tensors  $\underline{\mathbf{X}}$ , and all best rank-1 approximations  $\underline{\mathbf{Y}}$  of  $\underline{\mathbf{X}}$ , the tensor  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ .*

**Proof sketch.** We proceed as in the first part of Section 2. We show that there are eight stationary points  $(\mathbf{y}, \mathbf{z})$  satisfying (2.7)-(2.8), and that these can be obtained as roots of an 8th degree polynomial. There are two stationary points that yield  $\mathbf{x} = \mathbf{0}$  in (2.4), and do not correspond to the minimum of (2.2). For the other six stationary points, we have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ , where  $\underline{\mathbf{Y}}$  is the corresponding rank-1 tensor. Finally, we show that the multilinear rank of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  equals  $(2, 2, 2)$  for these six rank-1 tensors  $\underline{\mathbf{Y}}$ . Hence, it follows that the best rank-1 approximation  $\underline{\mathbf{Y}}$  satisfies  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$  and that the multilinear rank of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is equal to  $(2, 2, 2)$ . From Table 1 it then follows that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ . □

Hence, for typical tensors in orbit  $G_2$ , subtracting a best rank-1 approximation *increases* the rank to 3. For typical tensors in orbit  $G_3$ , subtracting a best rank-1 approximation does not affect the rank. This is completely different from matrix analysis.

In the proof of Theorem 4.1 in Appendix A, it is shown that the slabs of  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$  are non-singular almost everywhere. From Lemma 3.1 it follows that  $\underline{\mathbf{Z}}_2 \underline{\mathbf{Z}}_1^{-1}$  has identical real eigenvalues and is not diagonalizable, while  $\underline{\mathbf{X}}_2 \underline{\mathbf{X}}_1^{-1}$  has either distinct real eigenvalues or complex eigenvalues. Hence, the subtraction of a best rank-1 approximation yields identical real eigenvalues.

Next, we consider  $\underline{\mathbf{X}}$  in other orbits, and present deterministic results. We have the following result for the degenerate orbits of ranks 1 and 2.

**Proposition 4.2** *Let  $\underline{\mathbf{X}}$  be a  $2 \times 2 \times 2$  tensor, and let  $\underline{\mathbf{Y}}$  be a best rank-1 approximation of  $\underline{\mathbf{X}}$ .*

(i) *If  $\underline{\mathbf{X}}$  is in orbit  $D_1$ , then  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_0$ .*

(ii) *If  $\underline{\mathbf{X}}$  is in orbit  $D_2$ ,  $D'_2$ , or  $D''_2$ , then  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_1$ .*

**Proof.** For  $\underline{\mathbf{X}}$  in orbit  $D_1$  it is obvious that  $\underline{\mathbf{Y}} = \underline{\mathbf{X}}$  is the unique best rank-1 approximation. Then  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_0$ .

Next, let  $\underline{\mathbf{X}}$  be in orbit  $D_2$ . Then there exist orthonormal  $\mathbf{S}, \mathbf{T}, \mathbf{U}$  such that

$$(\mathbf{S}, \mathbf{T}, \mathbf{U}) \cdot \underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} \lambda & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 \end{array} \right], \quad (4.1)$$

see [12, proof of lemma 8.2]. Subtracting a best rank-1 approximation from this tensor results in  $\lambda$  or  $\mu$  being set to zero (whichever has the largest absolute value; for  $\lambda = \mu$  there are two best rank-1 approximations). Hence, the result is a rank-1 tensor. From Lemma 2.1 it follows that the same is true for subtracting a best rank-1 approximation from  $\underline{\mathbf{X}}$ . For  $\underline{\mathbf{X}}$  in orbits  $D'_2$  and  $D''_2$  the proof is analogous.  $\square$

For  $\underline{\mathbf{X}}$  in orbit  $G_2$  or  $D_3$ , the tensor  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is not restricted to a single orbit. The following examples illustrate this fact.

**Example 4.3** Let

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right], \quad (4.2)$$

which is the canonical tensor of orbit  $G_2$  in Table 1. It can be seen that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in  $D_1$  (the only nonzero entry of  $\underline{\mathbf{Y}}$  is either  $Y_{111}$  or  $Y_{222}$ ).

On the other hand, consider

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 2 \end{array} \right]. \quad (4.3)$$

For this tensor,  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has two distinct real eigenvalues. Hence, by Lemma 3.1, the tensor is in orbit  $G_2$ . It can be shown that  $\underline{\mathbf{X}}$  has a unique best rank-1 approximation  $\underline{\mathbf{Y}}$  and that

$$\underline{\mathbf{X}} - \underline{\mathbf{Y}} = \left[ \begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right], \quad (4.4)$$

which is the canonical tensor of orbit  $D_3$  in Table 1.  $\square$

**Example 4.4** It follows from Lemma 3.1 that the following tensors are in orbit  $D_3$ :

$$\left[ \begin{array}{cc|cc} 2 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right], \quad \left[ \begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 0 & 2 & 0 \end{array} \right], \quad \left[ \begin{array}{cc|cc} 1 & 0 & 0 & 2 \\ 0 & 0 & 1 & 0 \end{array} \right]. \quad (4.5)$$

Subtracting the best rank-1 approximation  $\underline{\mathbf{Y}}$  from these tensors amounts to replacing the element 2 by zero. Hence,  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_2$ ,  $D'_2$ , and  $D''_2$ , respectively.  $\square$

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

**Conjecture 4.5** *For almost all tensors  $\underline{\mathbf{X}}$  in orbit  $D_3$ , and all best rank-1 approximations  $\underline{\mathbf{Y}}$  of  $\underline{\mathbf{X}}$ , the tensor  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in  $D_3$ .*  $\square$

The tensor  $\underline{\mathbf{X}}$  in Example 2.3 is in orbit  $G_3$  by Lemma 3.1. It can be shown that any of the infinitely many best rank-1 approximations of  $\underline{\mathbf{X}}$  yields  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_3$  (proof available on request). The example below yields the same result for another  $\underline{\mathbf{X}}$  in orbit  $G_3$ . Numerically and analytically, we have not found any  $\underline{\mathbf{X}}$  in orbit  $G_3$  for which  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is not in orbit  $D_3$ .

**Example 4.6** Let

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 1 & 0 & 0 & -2 \\ 0 & 1 & 1 & 0 \end{array} \right]. \quad (4.6)$$

Since  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has complex eigenvalues,  $\underline{\mathbf{X}}$  is in orbit  $G_3$  by Lemma 3.1. It can be verified that  $\underline{\mathbf{X}}$  has a unique best rank-1 approximation such that

$$\underline{\mathbf{X}} - \underline{\mathbf{Y}} = \left[ \begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{array} \right]. \quad (4.7)$$

The latter tensor can be transformed to the canonical form of orbit  $D_3$  by swapping rows within each slab (i.e., by applying a permutation in the first mode).  $\square$

Our next result concerns tensors with diagonal slabs, i.e.

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} a & 0 & e & 0 \\ 0 & d & 0 & h \end{array} \right]. \quad (4.8)$$

Then  $\underline{\mathbf{X}}$  has rank at most 2, since

$$\underline{\mathbf{X}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} a \\ e \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} d \\ h \end{pmatrix}. \quad (4.9)$$

Also, if  $ah \neq de$ , then  $\underline{\mathbf{X}} = (\mathbf{I}_2, \mathbf{I}_2, \mathbf{U}) \cdot \tilde{\underline{\mathbf{X}}}$ , where  $\tilde{\underline{\mathbf{X}}}$  is the canonical tensor of orbit  $G_2$  in Table 1, and

$$\mathbf{U} = \begin{bmatrix} a & d \\ e & h \end{bmatrix}. \quad (4.10)$$

Hence, in this case  $\underline{\mathbf{X}}$  is in orbit  $G_2$ .

We show that, for  $2 \times 2 \times 2$  tensors with diagonal slabs, we have  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_1$ . Naturally, the same holds for  $\underline{\mathbf{X}}$  that can be transformed to a tensor with diagonal slabs by orthonormal multilinear transformation (see Lemma 2.1). Note that tensors with diagonal slabs in orbit  $G_2$  form an exception to the result of Theorem 4.1, as does the canonical tensor of orbit  $G_2$  (see Example 4.3). However, Theorem 4.1 states that these exceptions form a set of measure zero.

**Proposition 4.7** *Let  $\underline{\mathbf{X}}$  be a  $2 \times 2 \times 2$  tensor with diagonal slabs and rank 2, and let  $\underline{\mathbf{Y}}$  be a best rank-1 approximation of  $\underline{\mathbf{X}}$ . Then  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_1$ .*

**Proof.** We use the first part of Section 2. Let  $\underline{\mathbf{X}}$  be as in (4.8). First, we assume  $a^2 + e^2 < d^2 + h^2$ . For

$$\underline{\mathbf{Y}} = \left[ \begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 0 & d & 0 & h \end{array} \right], \quad (4.11)$$

we have  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\|^2 = a^2 + e^2$  and  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_1$ . Next, we show that (4.11) is the unique best rank-1 approximation of  $\underline{\mathbf{X}}$ . Using (2.6), the equation  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\|^2 \leq a^2 + e^2$  can be written as

$$(d^2 + h^2)(y_1^2 + y_2^2)(z_1^2 + z_2^2) \leq (ay_1z_1 + ey_1z_2)^2 + (dy_2z_1 + hy_2z_2)^2, \quad (4.12)$$

which can be rewritten as

$$(d^2 + h^2 - a^2 - e^2)y_1^2(z_1^2 + z_2^2) + (ez_1 - az_2)^2y_1^2 + (hz_1 - dz_2)^2y_2^2 \leq 0. \quad (4.13)$$

Since  $(d^2 + h^2 - a^2 - e^2)$  is positive by assumption, and  $\mathbf{y}$  nor  $\mathbf{z}$  can be all-zero, it follows that (4.13) can only hold with equality, that is, for  $y_1 = 0$  and  $hz_1 = dz_2$ . Using (2.4), it then follows

that the  $\underline{\mathbf{Y}}$  for which we have equality in (4.13) is given by (4.11). This shows that (4.11) is the unique best rank-1 approximation of  $\underline{\mathbf{X}}$ .

Next, we consider the case  $a^2 + e^2 > d^2 + h^2$ . Analogous to the first part of the proof, it can be shown that

$$\underline{\mathbf{Y}} = \left[ \begin{array}{cc|cc} a & 0 & e & 0 \\ 0 & 0 & 0 & 0 \end{array} \right], \quad (4.14)$$

is the unique best rank-1 approximation of  $\underline{\mathbf{X}}$ . This implies that  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\|^2 = d^2 + h^2$  and  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_1$ .

Finally, we consider the case  $a^2 + e^2 = d^2 + h^2$ . Here, we have multiple best rank-1 approximations. Setting  $y_1 = 0$  in (4.13) yields (4.11) as a best rank-1 approximation. Setting  $y_2 = 0$  yields (4.14) as a best rank-1 approximation. If  $ah = de$ , then (4.13) can also be satisfied by setting  $ez_1 = az_2$  and  $hz_1 = dz_2$ . This yields

$$\underline{\mathbf{Y}} = (y_1^2 + y_2^2)^{-1} \left[ \begin{array}{cc|cc} y_1^2 a & y_1 y_2 a & y_1^2 e & y_1 y_2 e \\ y_1 y_2 d & y_2^2 d & y_1 y_2 h & y_2^2 h \end{array} \right]. \quad (4.15)$$

It can be verified that for  $\underline{\mathbf{Y}}$  in (4.15) we have  $\|\underline{\mathbf{X}} - \underline{\mathbf{Y}}\|^2 = d^2 + h^2 = a^2 + e^2$  and  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_1$ . This completes the proof.  $\square$

## 5 Best rank-1 approximation for symmetric tensors

Here, we consider the best rank-1 approximation problem for a 3rd order tensor  $\underline{\mathbf{X}} \in \mathbb{R}^{d \times d \times d}$  that is symmetric in all modes, i.e.  $X_{ijk} = X_{jik} = X_{kji} = X_{ikj} = X_{jki} = X_{kij}$ . We assume the same for the rank-1 approximation, which yields the problem

$$\min_{\mathbf{y} \in \mathbb{R}^d} \|\underline{\mathbf{X}} - \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{y}\|^2. \quad (5.1)$$

An adaption of [12, proposition 4.2] shows that problem (5.1) always has an optimal solution.

Let  $\Psi_2(\mathbf{y}) = \|\underline{\mathbf{X}} - \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{y}\|^2$ . Analogous to the first part of Section 2,  $\Psi_2$  can be written as

$$\Psi_2 = \|\underline{\mathbf{X}}\|^2 - 2 \underline{\mathbf{X}} \bullet_1 \mathbf{y}^T \bullet_2 \mathbf{y}^T \bullet_3 \mathbf{y}^T + \|\mathbf{y}\|^6. \quad (5.2)$$

Hence, the minimization problem (5.1) is equivalent to minimizing (5.2). Using this fact, and setting the gradient of  $\Psi_2$  with respect to  $\mathbf{y}$  equal to zero, we obtain

$$\mathbf{y} = \frac{\underline{\mathbf{X}} \bullet_1 \mathbf{y}^T \bullet_2 \mathbf{y}^T}{\|\mathbf{y}\|^4}. \quad (5.3)$$

Substituting (5.3) into (5.2) yields

$$\Psi_2 = \|\underline{\mathbf{X}}\|^2 - \frac{\|\underline{\mathbf{X}} \bullet_1 \mathbf{y}^T \bullet_2 \mathbf{y}^T\|^2}{\|\mathbf{y}\|^4}. \quad (5.4)$$

Hence, a best symmetric rank-1 approximation ( $\mathbf{y} \otimes \mathbf{y} \otimes \mathbf{y}$ ) of  $\underline{\mathbf{X}}$  is found by minimizing (5.2) or (5.4) over  $\mathbf{y}$ . The stationary points  $\mathbf{y}$  are given by (5.3); this was already noticed in [5, section 2.3].

One may wonder whether the restriction to symmetry of the rank-1 approximation in (5.1) is necessary. That is, if we solve the unrestricted problem (2.1) for symmetric  $\underline{\mathbf{X}}$ , will the best rank-1 approximation be symmetric? Numerical experiments with random symmetric  $\underline{\mathbf{X}}$  yield the following conjecture.

**Conjecture 5.1** *For almost all symmetric  $2 \times 2 \times 2$  tensors  $\underline{\mathbf{X}}$ , the best rank-1 approximation  $\underline{\mathbf{Y}}$  of  $\underline{\mathbf{X}}$  is unique and symmetric.*  $\square$

However, for

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array} \right], \quad (5.5)$$

Proposition 2.2 holds, and infinitely many best rank-1 approximations  $\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$  exist. Taking  $\mathbf{y} \neq \mathbf{z}$  and  $\mathbf{x}$  as in (2.4), then yields infinitely many asymmetric best rank-1 approximations. As in Example 2.3, one can verify that  $\|\underline{\mathbf{X}} - \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}\|^2 = 3$  for any best rank-1 approximation. Note that also the symmetric rank-1 tensor with  $\mathbf{x} = \mathbf{y} = \mathbf{z} = (-1 \ 0)^T$  is a best rank-1 approximation of  $\underline{\mathbf{X}}$ .

## 6 Rank criteria and orbits of symmetric $2 \times 2 \times 2$ tensors

Here, we consider real symmetric  $2 \times 2 \times 2$  tensors. We establish their ranks and orbits under invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$ . These transformations preserve the symmetry. The *symmetric tensor rank* [7, section 4] is defined as the smallest  $R$  such that

$$\underline{\mathbf{X}} = \sum_{r=1}^R \mathbf{a}_r \otimes \mathbf{a}_r \otimes \mathbf{a}_r. \quad (6.1)$$

There is a bijection between symmetric  $d \times d \times d$  tensors and homogeneous polynomials of degree 3 in  $d$  variables. A symmetric  $d \times d \times d$  tensor  $\underline{\mathbf{X}}$  is associated with the polynomial

$$p(u_1, \dots, u_d) = \sum_{ijk} x_{ijk} u_i u_j u_k. \quad (6.2)$$

A multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$  is equivalent to a change of variables  $\mathbf{v} = \mathbf{S}\mathbf{u}$  in the associated polynomial.

The symmetric rank of symmetric  $2 \times 2 \times \dots \times 2$  tensors can be obtained from the well-known Sylvester Theorem, which makes use of the polynomial representation [23, section 5] [4]. For generic symmetric  $2 \times 2 \times \dots \times 2$  tensors, [4] show that the Sylvester Theorem defines an algorithm to compute a symmetric decomposition (6.1) with  $R$  equal to the symmetric rank. Below, the Sylvester Theorem for symmetric  $2 \times 2 \times 2$  tensors is formulated.

**Theorem 6.1 (Sylvester)** *A real symmetric  $2 \times 2 \times 2$  tensor with associated polynomial*

$$p(u_1, u_2) = \gamma_3 u_1^3 + 3\gamma_2 u_1^2 u_2 + 3\gamma_1 u_1 u_2^2 + \gamma_0 u_2^3, \quad (6.3)$$

*has a symmetric decomposition (6.1) into  $R$  rank-1 terms if and only if there exists a vector  $\mathbf{g} = (g_0, \dots, g_R)^T$  with*

$$\begin{bmatrix} \gamma_0 & \dots & \gamma_R \\ \gamma_1 & \dots & \gamma_{R+1} \\ \vdots & & \vdots \\ \gamma_{3-R} & \dots & \gamma_3 \end{bmatrix} \mathbf{g} = \mathbf{0}, \quad (6.4)$$

*and if the polynomial  $q(u_1, u_2) = g_R u_1^R + \dots + g_1 u_1 u_2^{R-1} + g_0 u_2^R$  has  $R$  distinct real roots.*  $\square$

For our purposes, we make use of a symmetric rank criterion similar to Lemma 3.1, formulated as Lemma 6.2 below. The link between this rank criterion and the Sylvester Theorem will be explained at the end of this section.

Let the entries of a symmetric  $2 \times 2 \times 2$  tensor be denoted as

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} a & b & b & c \\ b & c & c & d \end{array} \right]. \quad (6.5)$$

For later use, we mention that the hyperdeterminant (3.2) of  $\underline{\mathbf{X}}$  in (6.5) is given by

$$\Delta(\underline{\mathbf{X}}) = (bc - ad)^2 - 4(bd - c^2)(ac - b^2). \quad (6.6)$$

As in the asymmetric case, the sign of the hyperdeterminant is invariant under invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$ .

**Lemma 6.2** *Let  $\underline{\mathbf{X}}$  be a real symmetric  $2 \times 2 \times 2$  tensor with slabs  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , of which at least one is nonsingular.*

(i) If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has distinct real eigenvalues, then  $\underline{\mathbf{X}}$  has symmetric rank 2.

(ii) If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has identical real eigenvalues, then  $\underline{\mathbf{X}}$  has symmetric rank at least 3.

(iii) If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has complex eigenvalues, then  $\underline{\mathbf{X}}$  has symmetric rank at least 3.

**Proof.** First, we prove (i). We consider  $\mathbf{X}_2\mathbf{X}_1^{-1}$ . The proof for  $\mathbf{X}_1\mathbf{X}_2^{-1}$  is completely analogous. Note that since  $\mathbf{X}_1$  is nonsingular, the symmetric rank of  $\underline{\mathbf{X}}$  is at least 2. Let  $\mathbf{X}_2\mathbf{X}_1^{-1}$  have distinct real eigenvalues  $\lambda_1$  and  $\lambda_2$ . Using (6.5), we have

$$\mathbf{X}_2\mathbf{X}_1^{-1} = \begin{bmatrix} 0 & 1 \\ x & y \end{bmatrix}, \quad x = \frac{c^2 - bd}{ac - b^2}, \quad y = \frac{ad - bc}{ac - b^2}, \quad (6.7)$$

which has eigenvalues

$$\lambda_1 = \frac{y + \sqrt{y^2 + 4x}}{2}, \quad \lambda_2 = \frac{y - \sqrt{y^2 + 4x}}{2}. \quad (6.8)$$

It can be verified that the eigenvectors of  $\mathbf{X}_2\mathbf{X}_1^{-1}$  are  $\alpha(1 \ \lambda_1)^T$  and  $\beta(1 \ \lambda_2)^T$ , respectively. Next, we show that appropriate choices of  $\alpha$  and  $\beta$  yield a symmetric rank-2 decomposition (6.1) for  $\underline{\mathbf{X}}$ .

Let  $\mathbf{A}$  contain the eigenvectors of  $\mathbf{X}_2\mathbf{X}_1^{-1}$ , i.e.

$$\mathbf{A} = \begin{bmatrix} \alpha & \beta \\ \alpha\lambda_1 & \beta\lambda_2 \end{bmatrix}. \quad (6.9)$$

Note that a symmetric rank-2 decomposition (6.1) can be denoted as  $\mathbf{X}_k = \mathbf{A} \mathbf{A}_k \mathbf{A}^T$ , with  $\mathbf{A}_k = \text{diag}(a_{k1}, a_{k2})$ ,  $k = 1, 2$ . The eigendecomposition of  $\mathbf{X}_2\mathbf{X}_1^{-1}$  is then given by  $\mathbf{A} \mathbf{A}_2 \mathbf{A}_1^{-1} \mathbf{A}^{-1}$ , which is consistent with (6.9) since  $\mathbf{A}_2 \mathbf{A}_1^{-1} = \text{diag}(\lambda_1, \lambda_2)$ . To obtain a symmetric rank-2 decomposition, it remains to solve the equations

$$\mathbf{A}^{-1} \mathbf{X}_1 = \mathbf{A}_1 \mathbf{A}^T = \begin{bmatrix} \alpha^3 & \alpha^3 \lambda_1 \\ \beta^3 & \beta^3 \lambda_2 \end{bmatrix}, \quad \mathbf{A}^{-1} \mathbf{X}_2 = \mathbf{A}_2 \mathbf{A}^T = \begin{bmatrix} \alpha^3 \lambda_1 & \alpha^3 \lambda_1^2 \\ \beta^3 \lambda_2 & \beta^3 \lambda_2^2 \end{bmatrix}. \quad (6.10)$$

By writing out the entries of  $\mathbf{A}^{-1} \mathbf{X}_1$  and  $\mathbf{A}^{-1} \mathbf{X}_2$ , it can be seen that a solution  $(\alpha, \beta)$  exists if and only if

$$a \lambda_1 \lambda_2 - b(\lambda_1 + \lambda_2) + c = 0, \quad b \lambda_1 \lambda_2 - c(\lambda_1 + \lambda_2) + d = 0. \quad (6.11)$$

Using (6.8), we have  $\lambda_1 \lambda_2 = -x$  and  $\lambda_1 + \lambda_2 = y$ . Combined with the expressions for  $x$  and  $y$  in (6.7), this verifies (6.11). This completes the proof of (i).

As shown in the proof of (i), if  $\underline{\mathbf{X}}$  has one slab nonsingular, say  $\mathbf{X}_1$ , and symmetric rank 2, then  $\mathbf{X}_2\mathbf{X}_1^{-1}$  is diagonalizable. As also shown in the proof of (i), when  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has identical real eigenvalues it does not have two linearly independent eigenvectors and, hence, is not diagonalizable.



Therefore, in case (ii) the symmetric rank of  $\underline{\mathbf{X}}$  is at least 3. The same holds in case (iii). This completes the proof.  $\square$

**Proposition 6.3** *The orbits of real symmetric  $2 \times 2 \times 2$  tensors  $\underline{\mathbf{X}}$  under the action of invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$ , are as given in Table 2.*

**Proof.** Let  $\mathbf{e}_1$  and  $\mathbf{e}_2$  denote the first and second column of  $\mathbf{I}_2$ . Orbit  $D_0$  corresponds to the all-zero tensor. For  $\underline{\mathbf{X}}$  with symmetric rank 1, we have  $\underline{\mathbf{X}} = \mathbf{a} \otimes \mathbf{a} \otimes \mathbf{a}$ . There exists a nonsingular  $\mathbf{S}$  with  $\mathbf{S}\mathbf{a} = \mathbf{e}_1$ . Then  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$  equals the canonical form of orbit  $D_1$  in Table 2, which has multilinear rank  $(1, 1, 1)$ . Analogously, for  $\underline{\mathbf{X}}$  with symmetric rank 2, we have  $\underline{\mathbf{X}} = \mathbf{a}_1 \otimes \mathbf{a}_1 \otimes \mathbf{a}_1 + \mathbf{a}_2 \otimes \mathbf{a}_2 \otimes \mathbf{a}_2$ , with  $\mathbf{a}_1$  and  $\mathbf{a}_2$  linearly independent. There exists a nonsingular  $\mathbf{S}$  with  $\mathbf{S}[\mathbf{a}_1 \ \mathbf{a}_2] = [\mathbf{e}_1 \ \mathbf{e}_2]$ . Then  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$  equals the canonical form of orbit  $G_2$  in Table 2, which has positive hyperdeterminant (6.6) and multilinear rank  $(2, 2, 2)$ .

Next, let  $\underline{\mathbf{X}}$  have symmetric rank 3 and decomposition (6.1) with  $\mathbf{A} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \mathbf{a}_3]$ . No two columns of  $\mathbf{A}$  are proportional, since otherwise a symmetric rank-2 decomposition is possible. It follows that there exists a nonsingular  $\mathbf{S}$  with

$$\mathbf{S}\mathbf{A} = \begin{bmatrix} \alpha & 0 & 1 \\ 0 & \beta & 1 \end{bmatrix}. \quad (6.12)$$

This yields

$$(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} a & 1 & 1 & 1 \\ 1 & 1 & 1 & d \end{array} \right], \quad (6.13)$$

with  $a = 1 + \alpha^3$  and  $d = 1 + \beta^3$ . We define orbits  $D_3$  and  $G_3$  according to whether the hyperdeterminant  $\Delta$  is zero or negative, respectively. Note that  $\Delta > 0$  is associated with orbit  $G_2$ .

In Appendix C, we show that any tensor  $\underline{\mathbf{X}}$  in orbit  $D_3$  or  $G_3$  is related to the canonical form  $\underline{\mathbf{Y}}$  of the orbit by an invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{Y}} = \underline{\mathbf{X}}$ .

We conclude our proof by showing that the symmetric rank of real symmetric  $2 \times 2 \times 2$  tensors is at most 3. Let  $\underline{\mathbf{X}}$  be as in (6.5). Suppose  $b \neq 0$  and  $c \neq 0$ . Then  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{X}}$  is of the form (6.13) for  $\mathbf{S} = \text{diag}(\mu, \eta)$  with  $\mu^3 = c/b^2$  and  $\eta^3 = b/c^2$ . Since (6.13) has the symmetric rank-3 decomposition (6.12), the tensor  $\underline{\mathbf{X}}$  has at most symmetric rank 3.

Next, suppose  $b = 0$  and  $c \neq 0$ . We subtract a symmetric rank-1 tensor  $\mathbf{a} \otimes \mathbf{a} \otimes \mathbf{a}$  with  $\mathbf{a} = \gamma \mathbf{e}_1$  from  $\underline{\mathbf{X}}$  such that  $(a - \gamma^3)c > 0$ . Denote the resulting tensor by  $\underline{\mathbf{Z}}$ . It can be verified that  $\mathbf{Z}_2 \mathbf{Z}_1^{-1}$  has distinct real eigenvalues. By Lemma 6.2 (i) it has symmetric rank 2. Combined with the subtracted rank-1 tensor, this implies a symmetric rank-3 decomposition of  $\underline{\mathbf{X}}$ .

The case  $c = 0$  and  $b \neq 0$  can be dealt with analogously. When  $b = c = 0$ , a symmetric rank-2 decomposition is immediate. Hence, the symmetric rank is at most 3.  $\square$

canonical form	symmetric rank	multilinear rank	sign $\Delta$
$D_0 : \left[ \begin{array}{cc cc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	0	(0, 0, 0)	0
$D_1 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	1	(1, 1, 1)	0
$G_2 : \left[ \begin{array}{cc cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right]$	2	(2, 2, 2)	+
$D_3 : \left[ \begin{array}{cc cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right]$	3	(2, 2, 2)	0
$G_3 : \left[ \begin{array}{cc cc} -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array} \right]$	3	(2, 2, 2)	-

Table 2: Orbits of symmetric  $2 \times 2 \times 2$  tensors under the action of invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S})$  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 following corollary follows from Lemma 6.2 and Proposition 6.3. It is the full analogue of Lemma 3.1.

**Corollary 6.4** *Let  $\underline{\mathbf{X}}$  be a real symmetric  $2 \times 2 \times 2$  tensor with slabs  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , of which at least one is nonsingular.*

- (i) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has distinct real eigenvalues, then  $\underline{\mathbf{X}}$  is in orbit  $G_2$ .*
- (ii) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has identical real eigenvalues, then  $\underline{\mathbf{X}}$  is in orbit  $D_3$ .*
- (iii) *If  $\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\mathbf{X}_1\mathbf{X}_2^{-1}$  has complex eigenvalues, then  $\underline{\mathbf{X}}$  is in orbit  $G_3$ .*

**Proof.** Since there is only one orbit with symmetric rank 2, the proof of (i) is the proof of Lemma 6.2 (i). Since the symmetric rank is at most 3, cases (ii) and (iii) have symmetric rank 3. As in the asymmetric case, the hyperdeterminant (6.6) is equal to the discriminant of the characteristic polynomial of  $\det(\mathbf{X}_1)\mathbf{X}_2\mathbf{X}_1^{-1}$  or  $\det(\mathbf{X}_2)\mathbf{X}_1\mathbf{X}_2^{-1}$ . Hence, case (ii) has  $\Delta = 0$  and corresponds to orbit  $D_3$ , and case (iii) has  $\Delta < 0$  and corresponds to orbit  $G_3$ .  $\square$

The hyperdeterminant (6.6) is equal to the discriminant of the polynomial  $q(u_1, u_2)$  in the Sylvester Theorem (Theorem 6.1) for  $\underline{\mathbf{X}}$  in (6.5) and  $R = 2$ . Indeed, we have  $\gamma_3 = a$ ,  $\gamma_2 = b$ ,  $\gamma_1 = c$  and  $\gamma_0 = d$ . The vector  $\mathbf{g} = (g_0, g_1, g_2)^T$  should satisfy

$$\begin{bmatrix} d & c & b \\ c & b & a \end{bmatrix} \mathbf{g} = \mathbf{0}, \quad (6.14)$$

which implies

$$g_0 = ac - b^2, \quad g_1 = bc - ad, \quad g_2 = bd - c^2. \quad (6.15)$$

The discriminant of  $q(u_1, u_2)$  is given by  $g_1^2 - 4g_0g_2$  which is equal to the hyperdeterminant (6.6). This establishes the equivalence between the Sylvester Theorem with  $R = 2$  and the symmetric rank criteria of Lemma 6.2.

## 7 Best rank-1 subtraction for symmetric $2 \times 2 \times 2$ tensors

Here, we consider the problem of determining the rank and orbit of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$ , where  $\underline{\mathbf{X}}$  is a symmetric  $2 \times 2 \times 2$  tensor and  $\underline{\mathbf{Y}}$  is a best symmetric rank-1 approximation of  $\underline{\mathbf{X}}$ . Obviously, if  $\underline{\mathbf{X}}$  is in orbit  $D_1$ , then  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_0$ . Next, we present our main result in Theorem 7.1, which is the analogue of Theorem 4.1. It concerns generic symmetric  $2 \times 2 \times 2$  tensors, which are in orbits  $G_2$  and  $G_3$ . The full proof of Theorem 7.1 is contained in Appendix B.

**Theorem 7.1** *For almost all symmetric  $2 \times 2 \times 2$  tensors  $\underline{\mathbf{X}}$ , and all best symmetric rank-1 approximations  $\underline{\mathbf{Y}}$  of  $\underline{\mathbf{X}}$ , the tensor  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ .*

**Proof sketch.** We proceed as in Section 5. It is shown in [9, section 3.5] that there are three stationary points  $\mathbf{y}$  satisfying (5.3), and that these can be obtained as roots of a 3rd degree polynomial. We show that, for all three stationary points, we have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ , where  $\underline{\mathbf{Y}}$  is the corresponding rank-1 tensor. Finally, we show that the multilinear rank of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  equals  $(2, 2, 2)$  for these three rank-1 tensors  $\underline{\mathbf{Y}}$ . This suffices to conclude that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ .  $\square$

Hence, as in the asymmetric  $2 \times 2 \times 2$  case, for typical symmetric tensors in orbit  $G_2$ , subtracting a best symmetric rank-1 approximation *increases* the symmetric rank to 3. For typical symmetric tensors in orbit  $G_3$ , subtracting a best symmetric rank-1 approximation does not affect the symmetric rank.

In the proof of Theorem 7.1 in Appendix B, it is shown that the slabs of  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$  are non-singular almost everywhere. From Lemma 6.2 it follows that  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  has identical real eigenvalues, while  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has either distinct real eigenvalues or complex eigenvalues. Hence, also for symmetric  $2 \times 2 \times 2$  tensors, the subtraction of a best rank-1 approximation yields identical real eigenvalues.

We conclude this section with examples of  $\underline{\mathbf{X}}$  in orbits  $G_2$  and  $G_3$  such that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ . These examples illustrate Theorem 7.1, and are the symmetric analogues of Examples 4.3 and 4.6.

**Example 7.2** Let

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{array} \right], \quad \mathbf{X}_2\mathbf{X}_1^{-1} = \left[ \begin{array}{cc} 0 & 1 \\ -1 & 1 \end{array} \right]. \quad (7.1)$$

Since the latter has complex eigenvalues, Lemma 6.2 shows that  $\underline{\mathbf{X}}$  is in orbit  $G_3$ .

Next, we compute the best symmetric rank-1 approximation  $\underline{\mathbf{Y}}$  to  $\underline{\mathbf{X}}$ , which has the form

$$\underline{\mathbf{Y}} = \left[ \begin{array}{cc|cc} y_1^3 & y_1^2 y_2 & y_1^2 y_2 & y_1 y_2^2 \\ y_1^2 y_2 & y_1 y_2^2 & y_1 y_2^2 & y_2^3 \end{array} \right]. \quad (7.2)$$

The stationary points (5.3) are given by

$$6 y_1^5 + 12 y_1^3 y_2^2 + 6 y_1 y_2^4 - 12 y_1 y_2 - 6 y_2^2 = 0, \quad (7.3)$$

$$6 y_2^5 + 12 y_1^2 y_2^3 + 6 y_1^4 y_2 - 12 y_1 y_2 - 6 y_1^2 = 0. \quad (7.4)$$

It follows that  $y_1 \neq 0$  and  $y_2 \neq 0$  (if one of them equals zero, then both are zero and  $\underline{\mathbf{Y}}$  is all-zero).

Multiplying (7.4) by  $y_1$  and subtracting (7.3) multiplied by  $y_2$  yields

$$6 (y_2 - y_1) \left( y_2 - \frac{-3 + \sqrt{5}}{2} y_1 \right) \left( y_2 - \frac{-3 - \sqrt{5}}{2} y_1 \right) = 0. \quad (7.5)$$

Hence,  $y_2 = y_1$  or  $y_2 = (-3/2 \pm \sqrt{5}/2) y_1$ . However, it can be verified that the latter is in contradiction with (7.3)-(7.4). Therefore,  $y_2 = y_1$  and it follows from (7.3)-(7.4) that  $y_1^3 = y_2^3 = 3/4$ .

This yields  $\Psi = 3/2$  and

$$\underline{\mathbf{Y}} = \frac{1}{4} \left[ \begin{array}{cc|cc} 3 & 3 & 3 & 3 \\ 3 & 3 & 3 & 3 \end{array} \right], \quad \underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}} = \frac{1}{4} \left[ \begin{array}{cc|cc} -3 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 \end{array} \right]. \quad (7.6)$$

Hence,

$$\mathbf{Z}_2\mathbf{Z}_1^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & -2 \end{bmatrix}, \quad (7.7)$$

which has a double eigenvalue  $-1$ . Hence,  $\underline{\mathbf{Z}}$  is in orbit  $D_3$  by Lemma 6.2.  $\square$

**Example 7.3** Let

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 3 \end{array} \right], \quad \mathbf{X}_2\mathbf{X}_1^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & 4 \end{bmatrix}. \quad (7.8)$$

Since the latter has real and distinct eigenvalues, Lemma 6.2 shows that  $\underline{\mathbf{X}}$  is in orbit  $G_2$ .

Analogous to Example 7.2, it can be shown that the best symmetric rank-1 approximation of  $\underline{\mathbf{X}}$  is given by

$$\underline{\mathbf{Y}} = \frac{3}{2} \left[ \begin{array}{cc|cc} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{array} \right]. \quad (7.9)$$

We obtain

$$\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}} = \frac{1}{2} \left[ \begin{array}{cc|cc} 3 & -1 & -1 & -1 \\ -1 & -1 & -1 & 3 \end{array} \right], \quad \mathbf{Z}_2\mathbf{Z}_1^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & -2 \end{bmatrix}. \quad (7.10)$$

The latter has a double eigenvalue  $-1$ . Hence,  $\underline{\mathbf{Z}}$  is in orbit  $D_3$  by Lemma 6.2.  $\square$

## 8 Discussion

It is now rather well known that consecutively subtracting a best rank-1 approximation from a higher-order tensor generally does not either reveal tensor rank nor yield a “good” low-rank approximation. A numerical example and discussion is provided in [17, section 7]. Hence, a rank-1 deflation procedure as is available for matrices, generally does not exist for higher-order tensors. We have given a mathematical treatment of this property for real  $2 \times 2 \times 2$  tensors. In Theorem 4.1, we showed that subtracting a best rank-1 approximation from a generic  $2 \times 2 \times 2$  tensor (which has rank 2 or 3) results in a rank-3 tensor located on the boundary between the sets of rank-2 and rank-3 tensors. Hence, for typical tensors of rank 2, subtracting a best rank-1 approximation *increases* the rank to 3.

A generic  $2 \times 2 \times 2$  tensor  $\underline{\mathbf{X}}$  has rank 2 if  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has distinct real eigenvalues, and rank 3 if  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has complex eigenvalues; see Lemma 3.1. If  $\underline{\mathbf{Y}}$  is a best rank-1 approximation of  $\underline{\mathbf{X}}$ , then  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$  has rank 3 and lies on the boundary between the rank-2 and rank-3 sets, i.e.  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  has

identical real eigenvalues. The rank-2 and rank-3 orbits  $G_2$  and  $G_3$  are characterized by positive and negative hyperdeterminant  $\Delta$ , respectively, while on the boundary we have  $\Delta = 0$ . The result that subtraction of a best rank-1 approximation yields identical real eigenvalues for  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  is new and expands the knowledge of the topology of tensor rank.

Numerical experiments yield the conjecture that for a generic real-valued  $p \times p \times 2$  tensor  $\underline{\mathbf{X}}$ , subtracting its best rank-1 approximation  $\underline{\mathbf{Y}}$  results in  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$  with  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  having one pair of identical real eigenvalues with only one associated eigenvector. Moreover, if the number of pairs of complex eigenvalues of  $\mathbf{X}_2\mathbf{X}_1^{-1}$  equals  $n$ , then  $\mathbf{Z}_2\mathbf{Z}_1^{-1}$  has  $\max(0, n-1)$  pairs of complex eigenvalues. For  $n = 0$ , this implies that  $\underline{\mathbf{X}}$  has rank  $p$  and  $\underline{\mathbf{Z}}$  has rank  $p+1$  [16] [33, lemma 2.2].

We also considered real symmetric  $2 \times 2 \times 2$  tensors. In Lemma 6.2, we provided a symmetric rank criterion via the eigenvalues of  $\mathbf{X}_2\mathbf{X}_1^{-1}$ , which is similar to the asymmetric case. Symmetric tensors have rank 2 and 3 on sets of positive volume, and  $\mathbf{X}_2\mathbf{X}_1^{-1}$  with distinct real eigenvalues implies  $\Delta > 0$  and orbit  $G_2$ , while  $\mathbf{X}_2\mathbf{X}_1^{-1}$  with complex eigenvalues implies  $\Delta < 0$  and orbit  $G_3$ . When  $\mathbf{X}_2\mathbf{X}_1^{-1}$  has identical real eigenvalues, it has  $\Delta = 0$  and symmetric rank 3 (orbit  $D_3$ ). The rank criteria of Lemma 6.2 are equivalent to the well-known Sylvester Theorem for symmetric rank 2. In Theorem 7.1, we showed that subtracting a best symmetric rank-1 approximation from a typical symmetric tensor yields a tensor in orbit  $D_3$ , i.e. it has symmetric rank 3 and  $\Delta = 0$ . This result is completely analogous to the asymmetric  $2 \times 2 \times 2$  case.

A third case not reported here is that of  $2 \times 2 \times 2$  tensors with symmetric slabs, i.e.  $X_{12k} = X_{21k}$ ,  $k = 1, 2$ . The rank-1 approximation problem is then

$$\min_{\mathbf{y} \in \mathbb{R}^2, \mathbf{z} \in \mathbb{R}^2} \|\underline{\mathbf{X}} - \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{z}\|^2. \quad (8.1)$$

We can define a *symmetric slab rank* analogous to the symmetric rank and propose a rank criterion similar to Lemma 3.1 and Lemma 6.2. Generic  $2 \times 2 \times 2$  tensors with symmetric slabs have *symmetric slab ranks* 2 and 3 on sets of positive volume. Moreover, a result analogous to Theorem 4.1 and Theorem 7.1 can be proven in this case.

## Appendix A: Proof of Theorem 4.1

We make use of the first part of Section 2. Let  $\underline{\mathbf{X}}$  be a generic  $2 \times 2 \times 2$  tensor with entries

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} a & b & e & f \\ c & d & g & h \end{array} \right]. \quad (\text{A.1})$$

We consider the rank-1 approximation problem (2.1). It is our goal to show that, for the optimal solution  $\underline{\mathbf{Y}} = \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$ , we have  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_3$ . From the list of orbits in Table 1, it follows that it suffices to show  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$  and  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  has multilinear rank  $(2, 2, 2)$ . We will do this by considering the stationary points of the rank-1 approximation problem. For later use, we mention that the hyperdeterminant (3.2) of  $\underline{\mathbf{X}}$  in (A.1) is given by

$$\Delta(\underline{\mathbf{X}}) = (ah - bg + de - cf)^2 - 4(ad - bc)(eh - fg). \quad (\text{A.2})$$

We begin our proof by showing that for the best rank-1 approximation of  $\underline{\mathbf{X}}$  we have  $x_1 \neq 0$ ,  $x_2 \neq 0$ ,  $y_1 \neq 0$ ,  $y_2 \neq 0$ ,  $z_1 \neq 0$  and  $z_2 \neq 0$  almost everywhere. Due to the scaling indeterminacy in  $(\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z})$ , this implies that we may set  $y_1 = z_1 = 1$  without loss of generality.

**Lemma A.1** *Let  $\underline{\mathbf{X}}$  be a generic  $2 \times 2 \times 2$  tensor with a best rank-1 approximation  $\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$ . Then  $x_1 \neq 0$ ,  $x_2 \neq 0$ ,  $y_1 \neq 0$ ,  $y_2 \neq 0$ ,  $z_1 \neq 0$ ,  $z_2 \neq 0$  almost everywhere.*

**Proof.** We show that  $z_1 \neq 0$  almost everywhere. The proofs for  $y_1$ ,  $y_2$  and  $z_2$  are analogous. The proofs for  $x_1$  and  $x_2$  follow by interchanging the roles of  $\mathbf{x}$  and  $\mathbf{y}$ .

Let  $\Psi$  be as in (2.6) and let  $\Psi_0$  denote (2.6) with  $z_1 = 0$ . Then  $\Psi < \Psi_0$  is equivalent to

$$\begin{aligned} & [(ay_1z_1 + by_2z_1 + ey_1z_2 + fy_2z_2)^2 + (cy_1z_1 + dy_2z_1 + gy_1z_2 + hy_2z_2)^2] > \\ & (z_1^2 + z_2^2) [(ey_1 + fy_2)^2 + (gy_1 + hy_2)^2], \end{aligned} \quad (\text{A.3})$$

which, after setting  $y_1 = z_1 = 1$ , can be rewritten as

$$\begin{aligned} & (a^2 + c^2 - e^2 - g^2 + 2z_2(ae + cg)) + \\ & 2y_2(ab + cd - ef - gh + z_2(af + be + ch + dg)) + \\ & y_2^2(b^2 + d^2 - f^2 - h^2 + 2z_2(bf + dh)) > 0. \end{aligned} \quad (\text{A.4})$$

Since  $(bf + dh) \neq 0$  almost everywhere, it is possible to choose  $z_2$  such that the coefficient of  $y_2^2$  is positive. Then there is a range of values  $y_2$  for which (A.4) holds. This shows that, almost everywhere, we can find a better rank-1 approximation than setting  $z_1 = 0$ . This completes the

proof of  $z_1 \neq 0$ . □

As mentioned above Lemma A.1, we set  $y_1 = z_1 = 1$  without loss of generality. Since the optimal  $\mathbf{x}$  is given by (2.4), the problem of finding a best rank-1 approximation of  $\mathbf{X}$  is now a problem in the variables  $y_2$  and  $z_2$  only.

Next, we rewrite equations (2.7) and (2.8) specifying the stationary points  $(y_2, z_2)$  as

$$\begin{aligned} & z_2^2 [(ef + gh) y_2^2 + (e^2 + g^2 - f^2 - h^2) y_2 - (ef + gh)] + \\ z_2 & [(af + be + ch + dg) y_2^2 + 2(ae + cg - bf - dh) y_2 - (af + be + ch + dg)] + \\ & [(ab + cd) y_2^2 + (a^2 + c^2 - b^2 - d^2) y_2 - (ab + cd)] = 0, \end{aligned} \quad (\text{A.5})$$

and

$$\begin{aligned} & z_2^2 [(bf + dh) y_2^2 + (af + be + ch + dg) y_2 + (ae + cg)] + \\ z_2 & [(b^2 + d^2 - f^2 - h^2) y_2^2 + 2(ab + cd - ef - gh) y_2 + (a^2 + c^2 - e^2 - g^2)] + \\ & [-(bf + dh) y_2^2 - (af + be + ch + dg) y_2 - (ae + cg)] = 0. \end{aligned} \quad (\text{A.6})$$

Using the expression (2.4) for  $\mathbf{x}$ , also the hyperdeterminant (3.2) of  $\mathbf{X} - \mathbf{Y}$  can be written as a function of  $(y_2, z_2)$  only. After some manipulations, we obtain

$$\begin{aligned} (1 + y_2^2)^2 (1 + z_2^2)^2 \Delta(\mathbf{X} - \mathbf{Y}) &= [z_2^2 [(bg - de) y_2^2 + (ag - bh - ce + df) y_2 + (cf - ah)] + \\ & z_2 [(bc - ad + eh - fg) y_2^2 + (bc - ad + eh - fg)] + \\ & [(ah - cf) y_2^2 + (ag - bh - ce + df) y_2 + (de - bg)]]^2. \end{aligned} \quad (\text{A.7})$$

Equations (A.5) and (A.6) specifying the stationary points  $(y_2, z_2)$ , and the hyperdeterminant (A.7) without the square, are of the same form: a polynomial of degree 4 in  $y_2$  and  $z_2$  that is quadratic in both  $y_2$  and  $z_2$ . We use the result of the following lemma to compare the stationary points satisfying (A.5) and (A.6) to the roots of (A.7).

**Lemma A.2** *Let  $f(u) = \alpha u^2 + \beta u + \gamma$  and  $g(u) = \delta u^2 + \epsilon u + \nu$  be second degree polynomials. Then  $f$  and  $g$  have a common root if and only if*

$$(\alpha\epsilon - \beta\delta)(\beta\nu - \epsilon\gamma) = (\gamma\delta - \alpha\nu)^2. \quad (\text{A.8})$$

Moreover, if  $(\gamma\delta - \alpha\nu)$  and  $(\alpha\epsilon - \beta\delta)$  are nonzero, the common root is given by

$$\frac{(\beta\nu - \epsilon\gamma)}{(\gamma\delta - \alpha\nu)} = \frac{(\gamma\delta - \alpha\nu)}{(\alpha\epsilon - \beta\delta)}. \quad (\text{A.9})$$



**Proof.** First, suppose  $f$  and  $g$  have a common root  $r$ . Then  $f(u) = \alpha(u - r)(u - r_1)$  and  $g(u) = \delta(u - r)(u - r_2)$  for some  $r_1$  and  $r_2$ . It follows that

$$\beta = -\alpha(r + r_1) \quad \epsilon = -\delta(r + r_2) \quad \gamma = \alpha r r_1 \quad \nu = \delta r r_2. \quad (\text{A.10})$$

Using these expressions, it can be verified that (A.8) holds, and  $r$  equals the expressions in (A.9).

Next, suppose (A.8) holds. Let  $f(u) = \alpha(u - r_1)(u - r_2)$  and  $g(u) = \delta(u - r_3)(u - r_4)$  for some  $r_1, r_2, r_3, r_4$ . It follows that

$$\beta = -\alpha(r_1 + r_2) \quad \epsilon = -\delta(r_3 + r_4) \quad \gamma = \alpha r_1 r_2 \quad \nu = \delta r_3 r_4. \quad (\text{A.11})$$

Substituting these expressions into (A.8) and dividing both sides by  $\alpha^2 \delta^2$  yields

$$(r_1 + r_2 - r_3 - r_4)(r_1 r_2 (r_3 + r_4) - r_3 r_4 (r_1 + r_2)) = (r_1 r_2 - r_3 r_4)^2. \quad (\text{A.12})$$

This can be rewritten as

$$(r_1 - r_3)(r_1 - r_4)(r_2 - r_3)(r_2 - r_4) = 0, \quad (\text{A.13})$$

which implies that  $f$  and  $g$  must have a common root. As above, we have the expressions (A.9) for the common root.  $\square$

Using Lemma A.2, the stationary points  $(y_2, z_2)$  are found as follows. Equations (A.5)-(A.6) represent two quadratic polynomials in  $y_2$  that have a common root. Lemma A.2 states that (A.8) must hold, where all coefficients are second degree polynomials in  $z_2$ . We rewrite this equation as  $P_z^{\text{stat}}(z_2) = 0$ , where  $P_z^{\text{stat}}$  is a polynomial of degree 8. The 8 roots of  $P_z^{\text{stat}}$  are the  $z_2$  corresponding to stationary points. For each  $z_2$ , the corresponding  $y_2$  is the common root given by (A.9). Hence, there are 8 stationary points  $(y_2, z_2)$ , and some of these may be complex.

Instead of interpreting (A.5)-(A.6) as polynomials in  $y_2$ , we may interpret them as polynomials in  $z_2$  with coefficients depending on  $y_2$ . As above, the  $y_2$  of the stationary points are then found by finding the roots of an 8th degree polynomial  $P_y^{\text{stat}}(y_2)$  that is defined by (A.8). For each  $y_2$ , the corresponding  $z_2$  is the common root given by (A.9). Both ways of obtaining the stationary points necessarily yield the same result.

Analogously, we may determine the points  $(y_2, z_2)$  satisfying (A.5) and having  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$  in (A.7). The same approach yields the points satisfying (A.6) that are roots of (A.7). We denote the 8th degree polynomials corresponding to (A.5) and the roots of (A.7) as  $P_y^{\text{eig}1}$  and  $P_z^{\text{eig}1}$ . We denote the 8th degree polynomials corresponding to (A.6) and the roots of (A.7) as  $P_y^{\text{eig}2}$  and  $P_z^{\text{eig}2}$ . Using this approach, we obtain the following relation between the stationary points and the roots of (A.7).

(A.5) and (A.6)	$y^{(1)}$	$y^{(2)}$	$y^{(3)}$	$y^{(4)}$	$y^{(5)}$	$y^{(6)}$	$y^{(7)}$	$y^{(8)}$
	$z^{(1)}$	$z^{(2)}$	$z^{(3)}$	$z^{(4)}$	$z^{(5)}$	$z^{(6)}$	$z^{(7)}$	$z^{(8)}$
(A.5) and root of (A.7)	$y^{(1)}$	$y^{(2)}$	$y^{(3)}$	$y^{(4)}$	$y^{(5)}$	$y^{(6)}$	$y^{(9)}$	$y^{(10)}$
	$z^{(1)}$	$z^{(2)}$	$z^{(3)}$	$z^{(4)}$	$z^{(5)}$	$z^{(6)}$	$z^{(7)}$	$z^{(8)}$
(A.6) and root of (A.7)	$y^{(1)}$	$y^{(2)}$	$y^{(3)}$	$y^{(4)}$	$y^{(5)}$	$y^{(6)}$	$y^{(7)}$	$y^{(8)}$
	$z^{(1)}$	$z^{(2)}$	$z^{(3)}$	$z^{(4)}$	$z^{(5)}$	$z^{(6)}$	$z^{(9)}$	$z^{(10)}$

Table 3: Schedule of points  $(y_2, z_2)$  satisfying each pair of the equations (A.5), (A.6), root of (A.7). Equations (A.5)-(A.6) describe stationary points, while the roots of (A.7) have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ . As can be seen, the points  $(y^{(i)}, z^{(i)})$ ,  $i = 1, \dots, 6$ , satisfy all three equations.

**Lemma A.3** *The points  $(y_2, z_2)$  satisfying two of the three equations (A.5), (A.6), root of (A.7), are related as specified in Table 3. In particular, 6 of the 8 stationary points are roots of (A.7).*

**Proof.** After some tedious analysis (or by using symbolic computation software), it can be verified that

$$\frac{P_z^{\text{stat}}(z_2)}{P_z^{\text{eig}1}(z_2)} = 1, \quad \frac{P_z^{\text{stat}}(z_2)}{P_z^{\text{eig}2}(z_2)} = \frac{(eh - fg)z_2^2 + (ah - bg + de - cf)z_2 + (ad - bc)}{(ad - bc)z_2^2 - (ah - bg + de - cf)z_2 + (eh - fg)}, \quad (\text{A.14})$$

$$\frac{P_y^{\text{stat}}(y_2)}{P_y^{\text{eig}2}(y_2)} = 1, \quad \frac{P_y^{\text{stat}}(y_2)}{P_y^{\text{eig}1}(y_2)} = \frac{(df - bh)y_2^2 - (ah + bg - de - cf)y_2 + (ce - ag)}{(ce - ag)y_2^2 + (ah + bg - de - cf)y_2 + (df - bh)}. \quad (\text{A.15})$$

Hence, the roots  $z_2$  of  $P_z^{\text{stat}}$  and  $P_z^{\text{eig}1}$  are identical, and so are the roots  $y_2$  of  $P_y^{\text{stat}}$  and  $P_y^{\text{eig}2}$ . Also,  $P_z^{\text{stat}}$  and  $P_z^{\text{eig}2}$  have 6 of the 8 roots in common, as do  $P_y^{\text{stat}}$  and  $P_y^{\text{eig}1}$ . This implies that the  $z_2$ -values of the stationary points coincide with the  $z_2$ -values of the points satisfying (A.5) that are roots of (A.7). Analogously, the  $y_2$ -values of the stationary points coincide with the  $y_2$ -values of the points satisfying (A.6) that are roots of (A.7). Also, 6 of the  $z_2$ -values of the stationary points coincide with the  $z_2$ -values of the points satisfying (A.6) that are roots of (A.7). And 6 of the  $y_2$ -values of the stationary points coincide with the  $y_2$ -values of the points satisfying (A.5) that are roots of (A.7).

In order to prove the relations in Table 3, it remains to show that the 6 common  $y_2$ -values and the 6 common  $z_2$ -values form 6 common points  $(y_2, z_2)$ . Let  $z_2$  be a root of  $P_z^{\text{stat}}$  and, hence, of  $P_z^{\text{eig}1}$ . The corresponding  $y_2$  of the stationary point is the common root given by (A.9). The corresponding  $y_2$  of the point satisfying (A.5) that is a root of (A.7) is given by an analogous expression. Equating these two expressions for  $y_2$  yields an 8th degree polynomial in  $z_2$  analogous

to (A.8). We denote this polynomial as  $P_z^{\text{com}}$ . After some tedious analysis (or by using symbolic computation software), it can be verified that

$$\frac{P_z^{\text{stat}}(z_2)}{P_z^{\text{com}}(z_2)} = \frac{(eh - fg)z_2^2 + (ah - bg + de - cf)z_2 + (ad - bc)}{(ef + gh)z_2^2 + (af + be + ch + dg)z_2 + (ab + cd)}. \quad (\text{A.16})$$

Hence,  $P_z^{\text{stat}}$  and  $P_z^{\text{com}}$  have 6 common roots. This implies that 6 stationary points  $(y_2, z_2)$  are also roots of (A.7). This completes the proof of the relations in Table 3.  $\square$

So far, we have shown that 6 of the 8 stationary points in the rank-1 approximation problem satisfy  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ . In Lemma A.4 below, we show that the two other stationary points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$  correspond to  $\mathbf{x} = \mathbf{0}$  in (2.4), which is not a best rank-1 approximation. The global minimum of the rank-1 approximation problem is thus attained in one of the stationary points  $(y^{(i)}, z^{(i)})$ ,  $i = 1, \dots, 6$ . In Lemma A.5 the proof of Theorem 4.1 is completed by showing that the multilinear rank of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  equals  $(2, 2, 2)$  for these stationary points. Together with  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ , this implies that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  is in orbit  $D_3$ .

Next, we consider the two stationary points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$ . Note that  $y^{(7)}$  and  $y^{(8)}$  are the roots of the numerator of (A.15),  $y^{(9)}$  and  $y^{(10)}$  are the roots of the denominator of (A.15),  $z^{(7)}$  and  $z^{(8)}$  are the roots of the numerator of (A.14), and  $z^{(9)}$  and  $z^{(10)}$  are the roots of the denominator of (A.14). Moreover, these four polynomials of degree 2 have identical discriminant that is equal to the hyperdeterminant of  $\underline{\mathbf{X}}$  as given in (A.2).

Hence, if  $\Delta(\underline{\mathbf{X}}) < 0$ , i.e.  $\underline{\mathbf{X}}$  is in orbit  $G_3$ , then the stationary points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$  are complex. Since we only consider real-valued rank-1 approximations, we discard these two stationary points. If  $\Delta(\underline{\mathbf{X}}) > 0$ , i.e.  $\underline{\mathbf{X}}$  is in orbit  $G_2$ , we resort to Lemma A.4.

**Lemma A.4** *Suppose  $\Delta(\underline{\mathbf{X}}) > 0$ . Then the stationary points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$  in Table 3 yield  $\mathbf{x} = \mathbf{0}$  in (2.4), and do not correspond to the global minimum almost everywhere.*

**Proof.** It can be verified that  $y^{(7)}$  and  $y^{(8)}$  are given by

$$\frac{(ah + bg - de - cf) \pm \sqrt{(ah + bg - de - cf)^2 - 4(df - bh)(ce - ag)}}{2(df - bh)}, \quad (\text{A.17})$$

and  $z^{(7)}$  and  $z^{(8)}$  are given by

$$\frac{-(ah - bg + de - cf) \pm \sqrt{(ah - bg + de - cf)^2 - 4(eh - fg)(ad - bc)}}{2(eh - fg)}, \quad (\text{A.18})$$

where  $\pm$  is  $+$  in one stationary point and  $-$  in the other. After some tedious analysis (or by using symbolic computation software), it can be verified that the expression for  $\mathbf{x}$  in (2.4) is all-zero for

$(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$ . Hence, both stationary points yield the all-zero solution. This is not the global minimum since the solution

$$\mathbf{x} = \begin{pmatrix} a \\ 0 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{z} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (\text{A.19})$$

yields a lower  $\Psi$  in (2.2) when  $a \neq 0$ . This completes the proof.  $\square$

**Lemma A.5** *For the stationary points  $(y^{(i)}, z^{(i)})$ ,  $i = 1, \dots, 6$ , in Table 3 the multilinear rank of  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  equals  $(2, 2, 2)$  almost everywhere.*

**Proof.** Let  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}} = \underline{\mathbf{X}} - \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$ , where  $\mathbf{x}$  is given by (2.4),  $y_1 = z_1 = 1$ , and  $(y_2, z_2)$  is a stationary point. If one of the frontal slabs  $\mathbf{Z}_1$  and  $\mathbf{Z}_2$  of  $\underline{\mathbf{Z}}$  is nonsingular, then the mode-1 and mode-2 ranks of  $\underline{\mathbf{Z}}$  are equal to 2. Next, we show that  $\det(\mathbf{Z}_1) = \det(\mathbf{Z}_2) = 0$  corresponds to a set of measure zero. It can be verified that

$$\det(\mathbf{Z}_1) = \frac{z_2 [-(de - bg) - (ag - bh - ce + df) y_2 - (ah - cf) y_2^2 + (ad - bc)(1 + y_2^2) z_2]}{(1 + y_2^2)(1 + z_2^2)}, \quad (\text{A.20})$$

and

$$\det(\mathbf{Z}_2) = \frac{(eh - fg)(1 + y_2^2) + z_2 [-(ah - cf) + (ag - bh - ce + df) y_2 - (de - bg) y_2^2]}{(1 + y_2^2)(1 + z_2^2)}. \quad (\text{A.21})$$

Suppose  $\det(\mathbf{Z}_1) = \det(\mathbf{Z}_2) = 0$ , i.e. the numerators of the above expressions are zero. Since  $z_2 \neq 0$  almost everywhere (see Lemma A.1), we divide the numerator of  $\det(\mathbf{Z}_1)$  by  $z_2$ . We then obtain two equations of the form  $z_2 = s(y_2)/t(y_2)$ . Equating both expressions for  $z_2$  yields a fourth degree polynomial in  $y_2$  that can be written as

$$[(ag - ce) y_2^2 - (ah + bg - cf - de) y_2 + (bh - df)] [(df - bh) y_2^2 - (ah + bg - cf - de) y_2 + (ce - ag)] = 0. \quad (\text{A.22})$$

These two second degree polynomials are the numerator (times  $-1$ ) and denominator of (A.15). As explained above, the roots of these polynomials are complex if  $\Delta(\underline{\mathbf{X}}) < 0$ . In this case, it is not possible to choose  $y_2$  and  $z_2$  such that  $\det(\mathbf{Z}_1) = \det(\mathbf{Z}_2) = 0$ . When  $\Delta(\underline{\mathbf{X}}) > 0$ , the sought values of  $y_2$  are  $y^{(7)}$ ,  $y^{(8)}$ ,  $y^{(9)}$  and  $y^{(10)}$ . Therefore, in this case we may conclude that the points  $(y_2, z_2)$  for which  $\det(\mathbf{Z}_1) = \det(\mathbf{Z}_2) = 0$  are not among the first 6 stationary points in Table 3 almost everywhere.

Hence, the multilinear rank of  $\underline{\mathbf{Z}}$  equals  $(2, 2, *)$ . If one of the top and bottom slabs of  $\underline{\mathbf{Z}}$  is nonsingular, then also its mode-3 rank equals 2. A proof of this can be obtained analogous as above by interchanging the roles of  $\mathbf{x}$  and  $\mathbf{z}$ . This completes the proof.  $\square$

## Numerical examples

Here, we illustrate the proof of Theorem 4.1 by means of two examples. We take two random  $\underline{\mathbf{X}}$ , one that has  $\Delta(\underline{\mathbf{X}}) > 0$  (orbit  $G_2$ ) and one that has  $\Delta(\underline{\mathbf{X}}) < 0$  (orbit  $G_3$ ).

Our first example is

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} -0.4326 & 0.1253 & -1.1465 & 1.1892 \\ -1.6656 & 0.2877 & 1.1909 & -0.0376 \end{array} \right]. \quad (\text{A.23})$$

We have  $\Delta(\underline{\mathbf{X}}) = 2.7668$ . In the table below, we list the stationary points  $(y_2, z_2)$ , their values of  $\Psi$  in (2.6), their values of  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$ , and state whether their Hessian matrix is positive definite or not. Two of the stationary points  $(y^{(i)}, z^{(i)})$ ,  $i = 1, \dots, 6$ , are complex. The remaining four points are the first four points in the table, and have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$  close to zero. The second point corresponds to the global minimum and is also found when computing a best rank-1 approximation to  $\underline{\mathbf{X}}$  via an alternating least squares algorithm. For  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$ , the matrix  $\mathbf{Z}_2 \mathbf{Z}_1^{-1}$  has a double eigenvalue 0.9185 with only one associated eigenvector. Lemma 3.1 implies that  $\underline{\mathbf{Z}}$  is in orbit  $D_3$ . The last two points in the table are the stationary points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$ . From Lemma A.4 it follows that they have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = \Delta(\underline{\mathbf{X}})$  and  $\Psi = \|\underline{\mathbf{X}}\|^2$ .

$y_2$	$z_2$	$\Psi$	$\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$	Hessian PD
-0.592958	0.621735	5.1164	1.4166e-12	no
-0.229249	-1.08855	2.6863	9.6802e-13	yes
2.22613	0.452035	7.1313	2.1210e-12	no
2.42488	-2.88759	6.5289	1.2999e-14	no
1.17156	1.15843	7.2081	2.7668	no
5.96728	-0.05296	7.2081	2.7668	no

Our second example is

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} -1.6041 & -1.0565 & 0.8156 & 1.2902 \\ 0.2573 & 1.4151 & 0.7119 & 0.6686 \end{array} \right]. \quad (\text{A.24})$$

We have  $\Delta(\underline{\mathbf{X}}) = -2.7309$ . In the table below, we list the stationary points  $(y_2, z_2)$  in the same way as in the first example. Two of the stationary points  $(y^{(i)}, z^{(i)})$ ,  $i = 1, \dots, 6$ , are complex. Since  $\Delta(\underline{\mathbf{X}}) < 0$ , the points  $(y^{(7)}, z^{(7)})$  and  $(y^{(8)}, z^{(8)})$  are also complex. Hence, four real stationary

points are left, that all have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$  close to zero. The first point in the table corresponds to the global minimum and is also found when computing a best rank-1 approximation to  $\underline{\mathbf{X}}$  via an alternating least squares algorithm. For  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$ , the matrix  $\mathbf{Z}_2 \mathbf{Z}_1^{-1}$  has a double eigenvalue 1.6712 with only one associated eigenvector. Lemma 3.1 implies that  $\underline{\mathbf{Z}}$  is in orbit  $D_3$ .

$y_2$	$z_2$	$\Psi$	$\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$	Hessian PD
0.995675	-0.598339	3.1185	1.3801e-11	yes
-0.865475	0.0601889	8.2319	1.5479e-13	no
2.06437	1.78102	6.6050	1.6050e-13	no
-0.675154	9.24487	9.0028	2.6216e-13	no

## Appendix B: Proof of Theorem 7.1

We make use of the derivations in Section 5. Let  $\underline{\mathbf{X}}$  be a generic symmetric  $2 \times 2 \times 2$  tensor (6.5). We consider the symmetric rank-1 approximation problem (5.1). It is our goal to show that, for the optimal solution  $\underline{\mathbf{Y}} = \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{y}$ , we have  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  in orbit  $D_3$ . From the list of orbits in Table 2, it follows that it suffices to show  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$  and  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  has multilinear rank  $(2, 2, 2)$ . We will do this by considering the stationary points of the symmetric rank-1 approximation problem.

Let  $\underline{\mathbf{Y}}$  be as in (7.2). The stationary points are given by (5.3), which can be written as

$$y_1^5 + y_1 y_2^4 + 2 y_1^3 y_2^2 - 2 b y_1 y_2 - a y_1^2 - c y_2^2 = 0, \quad (\text{B.1})$$

$$y_2^5 + y_1^4 y_2 + 2 y_1^2 y_2^3 - 2 c y_1 y_2 - d y_2^2 - b y_1^2 = 0. \quad (\text{B.2})$$

Note that the entries  $a, b, c, d$  are nonzero almost everywhere. If one of  $y_1$  and  $y_2$  is zero, it follows that both are zero almost everywhere. Since this corresponds to an all-zero  $\underline{\mathbf{Y}}$ , which is not the optimal solution, we may assume that  $y_1 \neq 0$  and  $y_2 \neq 0$  almost everywhere.

Multiplying (B.2) by  $y_1$  and subtracting  $y_2$  times (B.1) yields

$$-b y_1^3 + (a - 2c) y_1^2 y_2 + (2b - d) y_1 y_2^2 + c y_2^3 = 0. \quad (\text{B.3})$$

Defining  $z = y_1/y_2$  and dividing (B.3) by  $y_2^3$ , we obtain

$$-b z^3 + (a - 2c) z^2 + (2b - d) z + c = 0. \quad (\text{B.4})$$

This yields three solutions for  $z = y_1/y_2$ , two of which may be complex. For each solution  $z$ , the corresponding stationary point  $(y_1, y_2)$  satisfying (B.1)-(B.2) is given by

$$y_1 = z y_2, \quad y_2^3 = \frac{a z^2 + 2 b z + c}{z^5 + 2 z^3 + z} = \frac{b z^2 + 2 c z + d}{z^4 + 2 z^2 + 1}, \quad (\text{B.5})$$

where the latter equality is equivalent to (B.4). The polynomial (B.4) determining the stationary points is also reported by [9, section 3.5].

Next, we consider the hyperdeterminant  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}})$ . For  $y_1 = z y_2$ , we have

$$\underline{\mathbf{X}} - \underline{\mathbf{Y}} = \begin{bmatrix} a - z^3 y_2^3 & b - z^2 y_2^3 & b - z^2 y_2^3 & c - z y_2^3 \\ b - z^2 y_2^3 & c - z y_2^3 & c - z y_2^3 & d - y_2^3 \end{bmatrix}. \quad (\text{B.6})$$

Using (6.6), we obtain

$$\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = \Delta(\underline{\mathbf{X}}) + f(z) y_2^3 + (a - 3 b z + 3 c z^2 - d z^3)^2 y_2^6, \quad (\text{B.7})$$

with

$$f(z) = [-4 b^3 + 6 a b c - 2 a^2 d] + z [6 b^2 c - 12 a c^2 + 6 a b d] + z^2 [6 b c^2 - 12 b^2 d + 6 a c d] + z^3 [6 b c d - 2 a d^2]. \quad (\text{B.8})$$

We substitute the second expression for  $y_2^3$  in (B.5) into (B.7) and multiply by  $(z^4 + 2 z^2 + 1)^2$ . After some tedious analysis (or by using symbolic computation software), it can be verified that this yields

$$(-b z^3 + (a - 2c) z^2 + (2b - d) z + c) P(z), \quad (\text{B.9})$$

where  $P(z)$  is a 7th degree polynomial in  $z$ . By (B.4), the expression (B.9) is identical to zero. Hence, for all three stationary points  $(y_1, y_2)$ , we have  $\Delta(\underline{\mathbf{X}} - \underline{\mathbf{Y}}) = 0$ .

In the final part of the proof, we show that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  has multilinear rank  $(2, 2, 2)$  almost everywhere. Since the mode- $n$  ranks of symmetric tensors are equal for each mode, it suffices to show that the two slabs of (B.6) are nonsingular almost everywhere. Let  $\underline{\mathbf{Z}} = \underline{\mathbf{X}} - \underline{\mathbf{Y}}$ . We have

$$\det(\mathbf{Z}_1) = (ac - b^2) + y_2^3 (-c z^3 + 2 b z^2 - a z), \quad (\text{B.10})$$

$$\det(\mathbf{Z}_2) = (bd - c^2) + y_2^3 (-d z^2 + 2 c z - b). \quad (\text{B.11})$$

Hence,  $\det(\mathbf{Z}_1) = \det(\mathbf{Z}_2) = 0$  implies

$$(bd - c^2)(c z^3 - 2 b z^2 + a z) + (ac - b^2)(d z^2 - 2 c z + b) = 0, \quad (\text{B.12})$$

which can be written as

$$z^3 [bcd - c^3] + z^2 [2 b c^2 + a c d - 3 b^2 d] + z [2 b^2 c + a b d - 3 a c^2] + [a b c - b^3] = 0. \quad (\text{B.13})$$

Since the 3rd degree polynomials (B.4) and (B.13) do not have generically common roots, it follows that at least one of the slabs  $\mathbf{Z}_1$  and  $\mathbf{Z}_2$  is nonsingular almost everywhere. As explained above, this implies that  $\underline{\mathbf{X}} - \underline{\mathbf{Y}}$  has multilinear rank  $(2, 2, 2)$  almost everywhere. This completes the proof of Theorem 7.1.

## Appendix C: Orbits $D_3$ and $G_3$ of real symmetric $2 \times 2 \times 2$ tensors

Here, we show that any real symmetric  $2 \times 2 \times 2$  tensor  $\underline{\mathbf{X}}$  in orbit  $D_3$  or  $G_3$  is related to the canonical form  $\underline{\mathbf{Y}}$  of the orbit by an invertible multilinear transformation  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{Y}} = \underline{\mathbf{X}}$ .

First, we consider orbit  $D_3$ , which is defined by symmetric rank 3, multilinear rank  $(2, 2, 2)$ , and hyperdeterminant  $\Delta = 0$ . It follows from the proof of Proposition 6.3 that we may assume without loss of generality that  $\underline{\mathbf{X}}$  in orbit  $D_3$  has the form

$$\underline{\mathbf{X}} = \left[ \begin{array}{cc|cc} a & 1 & 1 & 1 \\ 1 & 1 & 1 & d \end{array} \right], \quad (\text{C.1})$$

with

$$\Delta(\underline{\mathbf{X}}) = a^2 d^2 - 6ad + 4a + 4d - 3 = 0. \quad (\text{C.2})$$

Our goal is to find a nonsingular

$$\mathbf{S} = \begin{bmatrix} s_1 & s_2 \\ s_3 & s_4 \end{bmatrix}, \quad (\text{C.3})$$

such that  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{Y}} = \underline{\mathbf{X}}$ , where the canonical form  $\underline{\mathbf{Y}}$  of orbit  $D_3$  is given in Table 2, i.e.

$$(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \left[ \begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right] = \left[ \begin{array}{cc|cc} a & 1 & 1 & 1 \\ 1 & 1 & 1 & d \end{array} \right]. \quad (\text{C.4})$$

This yields the following four equations:

$$3s_1^2 s_2 = a, \quad 3s_3^2 s_4 = d, \quad (\text{C.5})$$

$$s_1^2 s_4 + 2s_1 s_2 s_3 = 1, \quad s_2 s_3^2 + 2s_1 s_3 s_4 = 1. \quad (\text{C.6})$$

Note that the case  $a = d = 1$  has  $\Delta = 0$  but yields multilinear rank  $(1, 1, 1)$  and, hence, is not included in orbit  $D_3$ . The case  $a = 0, d = 3/4$  is in orbit  $D_3$  and its solution of (C.5)-(C.6) is

$$\mathbf{S} = \begin{bmatrix} 1 & 0 \\ 1/2 & 1 \end{bmatrix}. \quad (\text{C.7})$$



The case  $a = 3/4$ ,  $d = 0$  can be treated analogously. In the remaining part of the proof we assume  $a \neq 0$  and  $d \neq 0$ . This implies that all entries of  $\mathbf{S}$  are nonzero. From (C.2) it follows that

$$d = \frac{3a - 2 \pm 2(1-a)\sqrt{1-a}}{a^2}. \quad (\text{C.8})$$

Hence, we must have  $a < 1$ . Since (C.2) is symmetric in  $a$  and  $d$ , also  $d < 1$  must hold.

Next, we solve the system (C.5)-(C.6). From (C.5) we get  $s_2 = a/(3s_1^2)$  and  $s_4 = d/(3s_3^2)$ . Substituting this into (C.6) yields, after rewriting,

$$\frac{d}{3} \left( \frac{s_1}{s_3} \right)^3 = \left( \frac{s_1}{s_3} \right) - \frac{2a}{3}, \quad \frac{d}{3} \left( \frac{s_1}{s_3} \right)^3 = \frac{1}{2} \left( \frac{s_1}{s_3} \right)^2 - \frac{a}{6}. \quad (\text{C.9})$$

We equate the right-hand sides of (C.9), which yields

$$\left( \frac{s_1}{s_3} \right) = 1 \pm \sqrt{1-a}. \quad (\text{C.10})$$

Substituting this into one equation of (C.9) gives us

$$d = \frac{3 - 2a \pm 3\sqrt{1-a}}{(1 \pm \sqrt{1-a})^3}. \quad (\text{C.11})$$

It can be verified that this expression for  $d$  is identical to (C.8). Hence, equation (C.10), together with  $s_2 = a/(3s_1^2)$  and  $s_4 = d/(3s_3^2)$ , solves the system (C.5)-(C.6). Note that since both tensors in (C.4) have multilinear rank  $(2, 2, 2)$ , it follows that  $\mathbf{S}$  is nonsingular. Hence, we have shown that for any  $\underline{\mathbf{X}}$  in orbit  $D_3$  there exists a nonsingular  $\mathbf{S}$  such that  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{Y}} = \underline{\mathbf{X}}$ , where  $\underline{\mathbf{Y}}$  is the canonical form of orbit  $D_3$ .

Next, we consider orbit  $G_3$ , which is defined by symmetric rank 3, multilinear rank  $(2, 2, 2)$ , and hyperdeterminant  $\Delta < 0$ . As above, we may assume that  $\underline{\mathbf{X}}$  in  $G_3$  has the form (C.1) with

$$\Delta(\underline{\mathbf{X}}) = a^2d^2 - 6ad + 4a + 4d - 3 < 0. \quad (\text{C.12})$$

It is our goal to find nonsingular  $\mathbf{S}$  in (C.7) such that

$$(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \left[ \begin{array}{cc|cc} -1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array} \right] = \left[ \begin{array}{cc|cc} a & 1 & 1 & 1 \\ 1 & 1 & 1 & d \end{array} \right], \quad (\text{C.13})$$

where the former tensor is the canonical form of orbit  $G_3$  as given in Table 2. This yields the following four equations:

$$-s_1^3 + 3s_1s_2^2 = a, \quad -s_3^3 + 3s_3s_4^2 = d, \quad (\text{C.14})$$

$$-s_1^2s_3 + 2s_1s_2s_4 + s_2^2s_3 = 1, \quad -s_1s_3^2 + 2s_2s_3s_4 + s_1s_4^2 = 1. \quad (\text{C.15})$$

The case  $a = 0$ ,  $d < 3/4$  has solution  $s_1 = 0$ ,  $s_3^3 = 3/4 - d > 0$ ,  $s_2^2 = 1/s_3$ ,  $s_4^2 = 1/(4s_3)$ , with  $\det(\mathbf{S}) = -\sqrt{s_3} < 0$ . The case  $a < 3/4$ ,  $d = 0$  can be treated analogously. In the remaining part of the proof we assume  $a \neq 0$  and  $d \neq 0$ . This implies that  $s_1$  and  $s_3$  are nonzero. Note that  $a = 1$  implies  $\Delta = (d - 1)^2$ , which is not in orbit  $G_3$ . Analogously,  $d = 1$  is not in orbit  $G_3$  either. In fact,  $\Delta < 0$  implies  $a < 1$  and  $d < 1$ .

Next, we solve the system (C.14)-(C.15). Expressions for  $s_2$  and  $s_4$  are obtained from (C.14) as

$$s_2^2 = \frac{s_1^3 + a}{3s_1}, \quad s_4^2 = \frac{s_3^3 + d}{3s_3}. \quad (\text{C.16})$$

Equations (C.15) can be written as

$$2s_2s_4 = \frac{1 + s_1^2s_3 - s_2^2s_3}{s_1}, \quad 2s_2s_4 = \frac{1 + s_1s_3^2 - s_1s_4^2}{s_3}. \quad (\text{C.17})$$

Equating the right-hand sides and substituting (C.16) yields, after rewriting,

$$d \left( \frac{s_1}{s_3} \right)^3 - 3 \left( \frac{s_1}{s_3} \right)^2 + 3 \left( \frac{s_1}{s_3} \right) - a = 0. \quad (\text{C.18})$$

The discriminant of this 3rd degree polynomial equals  $-27\Delta > 0$ , which implies that (C.18) has three distinct real roots. Let  $s_1 = \alpha s_3$ , where the root  $\alpha$  satisfies

$$d\alpha^3 = 3\alpha^2 - 3\alpha + a. \quad (\text{C.19})$$

Substituting  $s_1 = \alpha s_3$  and (C.16) into the first equation of (C.15) yields

$$4s_3^3(d\alpha^4 + 2a\alpha - 3\alpha^2) = 9 - 6a/\alpha + a^2/\alpha^2 - 4ad\alpha. \quad (\text{C.20})$$

Using (C.19), this can be rewritten as

$$s_3^3 = \frac{\alpha(3 - d\alpha)^2 - 4ad}{12(\alpha^2 - 2\alpha + a)}. \quad (\text{C.21})$$

It remains to verify that the expressions (C.16) are nonnegative. Our proof is tedious and long. Below, we give a summary of it. The full proof is available on request.

Substituting (C.21) and using (C.19), it can be shown that the expressions (C.16) are nonnegative if

$$P_1(\alpha) = \alpha^2(4 - 3d) + \alpha(ad - 3) + a \geq 0, \quad P_2(\alpha) = -d\alpha^2 + \alpha(3 - ad) - a \geq 0. \quad (\text{C.22})$$

Note that  $P_1 + P_2 = 4\alpha^2(1 - d) > 0$ . Also, the leading coefficient of  $P_1$  is always positive. The roots of  $P_1$  are given by

$$r_1 = \frac{3 - ad - \sqrt{a^2d^2 + 6ad - 16a + 9}}{2(4 - 3d)}, \quad r_2 = \frac{3 - ad + \sqrt{a^2d^2 + 6ad - 16a + 9}}{2(4 - 3d)}. \quad (\text{C.23})$$

The roots of  $P_2$  are given by

$$r_3 = \frac{ad - 3 - \sqrt{a^2d^2 - 10ad + 9}}{-2d}, \quad r_4 = \frac{ad - 3 + \sqrt{a^2d^2 - 10ad + 9}}{-2d}. \quad (\text{C.24})$$

Let  $P_3(x) = dx^3 - 3x^2 + 3x - a$ . To prove (C.22), we focus on the sign of  $P_3$  in the roots  $r_1, r_2, r_3, r_4$ . When the discriminant of  $P_1$  is nonnegative, we can distinguish three cases. In these cases, the sign of  $P_3$  in the roots  $r_1$  and  $r_2$  is as follows:

$$\text{case I: } a > 0 \quad \text{and} \quad a^2d > -3a + 4a\sqrt{a} \Rightarrow P_3(r_1) \geq 0 \quad P_3(r_2) \geq 0, \quad (\text{C.25})$$

$$\text{case II: } a > 0 \quad \text{and} \quad a^2d < -3a - 4a\sqrt{a} \Rightarrow P_3(r_1) \leq 0 \quad P_3(r_2) \leq 0, \quad (\text{C.26})$$

$$\text{case III: } a < 0 \Rightarrow P_3(r_1) \geq 0 \quad P_3(r_2) \geq 0. \quad (\text{C.27})$$

When the discriminant of  $P_2$  is nonnegative, we have

$$P_3(r_4) \leq 0, \quad P_3(r_3) \begin{cases} \geq 0 & \text{if } d > 0, \\ \leq 0 & \text{if } d < 0. \end{cases} \quad (\text{C.28})$$

Suppose  $d > 0$ . Then the leading coefficient of  $P_2$  is negative and its discriminant is positive (since  $a < 1$  and  $d < 1$ ). Hence,  $P_2$  has real roots. Recall that the leading coefficient of  $P_1$  is always positive. Suppose the roots of  $P_1$  are real. Then we are in case I or case III (since case II implies  $d < 0$ ). Since  $P_1 + P_2 > 0$ , there must hold  $r_4 \leq r_1 \leq r_2 \leq r_3$ . From (C.25), (C.27), and (C.28), it follows that  $P_3$  has a root  $\alpha$  in the interval  $[r_4, r_1]$  for which (C.22) holds. If the roots of  $P_1$  are not real, then (C.28) implies that  $P_3$  has a root  $\alpha$  in the interval  $[r_4, r_3]$  for which (C.22) holds.

Suppose next that  $d < 0$ . Then the leading coefficients of  $P_1$  and  $P_2$  are positive. Suppose  $P_1$  and  $P_2$  both have real roots. Since  $P_1 + P_2 > 0$ , there must hold either  $r_3 \leq r_4 \leq r_1 \leq r_2$  or  $r_1 \leq r_2 \leq r_3 \leq r_4$ . From (C.25)-(C.28) we obtain the following. Suppose we are in case I or case III. If  $r_3 \leq r_4 \leq r_1 \leq r_2$ , then  $P_3$  has a root  $\alpha$  in the interval  $[r_4, r_1]$  for which (C.22) holds. If  $r_1 \leq r_2 \leq r_3 \leq r_4$ , then  $P_3$  has a root  $\alpha$  in the interval  $[r_2, r_3]$  for which (C.22) holds. Suppose we are in case II. Then  $P_3(r_3) \leq 0$  and  $P_3(r_1) \leq 0$ . From the shape of  $P_3$  it follows that it has a root  $\alpha \leq r_3$  if  $r_3 \leq r_4 \leq r_1 \leq r_2$ , or a root  $\alpha \leq r_1$  if  $r_1 \leq r_2 \leq r_3 \leq r_4$ . In both situations, we have (C.22) for this root  $\alpha$ .

When  $d < 0$  and  $P_1$  does not have real roots, (C.28) implies that  $P_3$  has a root  $\alpha \leq r_3$  for which (C.22) holds. When  $d < 0$  and  $P_2$  does not have real roots, (C.25)-(C.27) imply that  $P_3$  cannot have all three roots in the interval  $[r_1, r_2]$ . Hence, there exists a root  $\alpha$  for which (C.22) holds. Finally, it can be shown that  $P_1$  and  $P_2$  cannot both have complex roots when  $a < 1$  and  $d < 1$ .

Hence, we have shown that the system (C.14)-(C.15) is solved by (C.16), (C.21), and  $s_1 = \alpha s_3$ , where  $\alpha$  is a root of  $P_3$  satisfying (C.22). In numerical experiments we found that any root of  $P_3$

satisfies (C.22). Note that since both tensors in (C.13) have multilinear rank  $(2, 2, 2)$ , it follows that  $\mathbf{S}$  is nonsingular. Hence, we have shown that for any  $\underline{\mathbf{X}}$  in orbit  $G_3$  there exists a nonsingular  $\mathbf{S}$  such that  $(\mathbf{S}, \mathbf{S}, \mathbf{S}) \cdot \underline{\mathbf{Y}} = \underline{\mathbf{X}}$ , where  $\underline{\mathbf{Y}}$  is the canonical form of orbit  $G_3$ .

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