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Uniqueness of Nonnegative Tensor Approximations

Yang Qi*, Pierre Comon* Fellow, IEEE, and Lek-Heng Lim[‡]

Abstract

We show that a best nonnegative rank-r approximation of a nonnegative tensor is almost always unique and that nonnegative tensors with nonunique best nonnegative rank-r approximation form a semialgebraic set contained in an algebraic hypersurface. We then establish a singular vector variant of the Perron–Frobenius Theorem for positive tensors and apply it to show that a best nonnegative rank-r approximation of a positive tensor can almost never be obtained by deflation. We show the subset of real tensors which admit more than one best rank one approximations is a hypersurface, and give a polynomial equation to ensure a tensor without satisfying this equation to have a unique best rank one approximation.

I. INTRODUCTION

Nonnegative tensor decomposition, *i.e.*, a decomposition of a tensor with nonnegative entries (with respect to a fixed choice of bases) into a sum of tensor products of nonnegative vectors, arises in a wide range of applications. These include hyperspectral imaging, spectroscopy, statistics, phylogenetics, data mining, pattern recognition, among other areas; see [25], [29], [31], [36] and the references therein. One important reason for its prevalence is that such a decomposition shows how a joint distribution of discrete random variables decomposes when they are independent conditional on a discrete latent random variable [25], [37] — a ubiquitous model that underlies many applications. This is in fact one of the simplest Bayesian network [14], [18], [19], a local expression of the joint distribution of a set of random variables x_i as

$$p(x_1, \dots, x_d) = \int \prod_{i=1}^d p(x_i \mid \theta) \, d\mu_\theta \tag{I.1}$$

where θ is some unknown latent random variable. The relation expressed in (I.1) is often called the *naive Bayes hypothesis*. In the case when both the random variables x_1, \ldots, x_d and the latent variable θ take only a finite number of values, the decomposition becomes one of the form

$$t_{i_1,\dots,i_d} = \sum_{p=1}^r \lambda_r u_{i_1,p} \cdots u_{i_d,p}.$$
 (I.2)

One can show [25] that *any* decomposition of a nonnegative tensor of the form in (I.2) may, upon normalization by a suitable constant, be regarded as (I.1), a marginal decomposition of joint probability mass function into conditional probabilities under the naive Bayes hypothesis. In the event when the latent variable θ is not discrete or finite, one may argue that (I.2) becomes an approximation with ' \approx ' in place of '='.

In this article, we investigate several questions regarding nonnegative tensor decompositions and approximations, focusing in particular on uniqueness issues. We first define nonnegative tensors in a way that parallels the usual abstract definition of tensors in algebra. We will view them as elements in a tensor product of cones, *i.e.*, tensors in $C_1 \otimes \cdots \otimes C_d$ where C_1, \ldots, C_d are cones and the tensor product is that of \mathbb{R}_+ -semimodules (we write $\mathbb{R}_+ := [0, \infty)$) for the nonnegative reals). The special case $C_1 = \mathbb{R}_+^{n_1}, \ldots, C_d = \mathbb{R}_+^{n_d}$ then reduces to nonnegative tensors.

It has been established in [25] that every nonnegative tensor has a best nonnegative rank-r approximation. Here we will show that this best approximation is almost always unique. Furthermore, the set of nonnegative tensors of nonnegative rank > rthat do not have a unique best rank-r approximation form a semialgebraic set contained in some hypersurface. By exploring normalized singular pairs and eigenpairs we then show that the tensors that admit non-unique best rank-1 approximations form a hypersurface, and find a polynomial equation such that any real tensor which does not satisfy this equation has a best rank one approximation. Lastly we show that one cannot in general obtain a best nonnegative rank-r approximation by 'deflation', *i.e.*, by finding r successive best nonnegative rank-1 approximations.

II. NONNEGATIVE TENSORS

A tensor of order d (d-tensor for short) may be represented as a d-dimensional hypermatrix, *i.e.*, a d-way array of (usually) real or complex values. This is a higher-order generalization of the fact that a 2-tensor, *i.e.*, a linear operator, a bilinear form, or a dyad, can always be represented as a matrix. Such a coordinate representation sometimes hides intrinsic properties — in particular, this array of coordinates is meaningful only if the bases of underlying vector spaces have been specified in the first place. With this in mind, we prefer to define tensors properly rather than simply regarding them as d-way arrays of numbers.

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The following is the standard definition of tensors. We will see later how we may obtain an analogous definition for nonnegative tensors.

Definition 1. Let V_i be a vector space of finite dimension n_i over a field \mathbb{K} , i = 1, ..., d, and let $V_1 \times \cdots \times V_d$ be the set of d-tuples of vectors. Then the *tensor product* $V = V_1 \otimes \cdots \otimes V_d$ is the free linear space spanned by $V_1 \times \cdots \times V_d$ quotient by an equivalence relation that imposes the two properties below for every $\alpha_i, \beta_i \in \mathbb{K}$:

$$(\alpha_1 u_1, \alpha_2 u_2, \dots, \alpha_d u_d) \equiv \left(\prod_{i=1}^d \alpha_i\right) (u_1, u_2, \dots, u_d), \tag{II.1}$$

$$(u_1, \dots, \alpha_i u_i, \dots, u_d) + (u_1, \dots, \beta_i v_i, \dots, u_d) \equiv (u_1, \dots, \alpha_i u_i + \beta_i v_i, \dots, u_d).$$
(II.2)

A *tensor* is any element of $V_1 \otimes \cdots \otimes V_d$.

More details on the definition of tensor spaces may be found in [7], [16], [21], [23].

Definition 2. A decomposable tensor is one of the form $u_1 \otimes \cdots \otimes u_d$, $u_i \in V_i$, $i = 1, \ldots, d$. It represents the equivalence class of tuples up to scaling as in (II.1), *i.e.*, $u_1 \otimes \cdots \otimes u_d = \{(\alpha_1 u_1, \ldots, \alpha_d u_d) : \prod_{i=1}^d \alpha_i = 1\}$.

By the above definition, it is clear that a decomposable tensor cannot in general be uniquely represented by a *d*-tuple of vectors, what is often called a "scaling indeterminacy" in the engineering literature. When we use the term 'unique' in this article, it is implicit that the uniqueness is only up to scaling of this nature.

From the way a tensor is defined in Definition 1, it is immediate that a non-zero tensor can always be expressed as a finite sum of nonzero decomposable tensors. When the number of summands is minimal, this decomposition is called a *rank decomposition* (the term "canonical polyadic" or CP is often also used) and the number of summands in such a decomposition is called the *rank* of the tensor. In other words, we have the following:

Definition 3 (Rank decomposition). For every $T \in V_1 \otimes \cdots \otimes V_d$, there exist $u_{i,p} \in V_i$, $i = 1, \dots, d$, $p = 1, \dots, \operatorname{rank}(T)$, such that

$$T = \sum_{p=1}^{\operatorname{rank}(T)} u_{1,p} \otimes \dots \otimes u_{d,p}.$$
(II.3)

We present the above material, which is largely standard knowledge, to motivate an analogous construction for real nonnegative tensors. We will first define nonnegative tensors in a coordinate-dependent manner (*i.e.*, depending on a choice of bases on V_1, \ldots, V_d), and then in a coordinate-independent manner.

For each i = 1, ..., d, let V_i be a real vector space with dim $V_i = n_i$. For any fixed choice of basis $\{v_{i,1}, ..., v_{i,n_i}\}$ for V_i , we denote by V_i^+ the subset of vectors with nonnegative coefficients in V_i , *i.e.*,

$$V_i^+ = \left\{ \sum_{p=1}^{n_i} \alpha_p v_{i,p} \in V_i : \alpha_1, \dots, \alpha_{n_i} \in \mathbb{R}_+ \right\}$$

We will call an element in $V := V_1 \otimes \cdots \otimes V_d$ of the form $u_1 \otimes \cdots \otimes u_d$ where $u_i \in V_i^+$ for i = 1, ..., d, a nonnegatively decomposable tensor. The set of nonnegative tensors V^+ is then the subset of V defined by

$$V^{+} = \left\{ \sum_{p=1}^{r} u_{1,p} \otimes \dots \otimes u_{d,p} \in V : u_{i,p} \in V_{i}^{+}, \ i = 1, \dots, d, \ p = 1, \dots, r, \ r \in \mathbb{N} \right\}.$$

By its definition, every element of V^+ has a representation as a finite sum of nonnegatively decomposable tensors. A decomposition of minimal length then yields the notions of *nonnegative tensor rank*, denoted by $\operatorname{rank}_+(T)$, and nonnegative tensor rank decomposition. For every $T \in V^+$, there exist $u_{i,p} \in V_i^+$, $i = 1, \ldots, d$, $p = 1, \ldots, r$, such that

$$T = \sum_{p=1}^{\operatorname{rank}_{+}(T)} u_{1,p} \otimes \dots \otimes u_{d,p}.$$
(II.4)

We will call the nonnegative tensor rank the *nonnegative rank* and the decomposition above a *nonnegative decomposition* of the nonnegative tensor T, for short. An obvious property is that $rank_+(T) \ge rank(T)$ for any $T \in V^+$.

We now examine an alternative coordinate-free approach for defining nonnegative tensors and nonnegative rank. This approach is also more general, yielding a notion of *conic rank* for a tensor product of any convex cones. We first recall the definition of a tensor product of semimodules. See [2] for details on the existence and a construction of such a tensor product.

Definition 4. Let R be a commutative semiring and M, N be R-semimodules. A *tensor product* $M \otimes_R N$ of M and N is an R-semimodule satisfying the universal property: There is an R-bilinear map $\varphi : M \times N \to M \otimes_R N$ such that given any other R-semimodule S together with an R-bilinear map $h : M \times N \to S$, there is a unique R-linear map $\tilde{h} : M \otimes_R N \to S$ satisfying $h = \tilde{h} \circ \varphi$.

Definition 5. A *convex cone* C is a subset of a vector space over an ordered field that is closed under linear combinations with nonnegative coefficients, *i.e.*, $\alpha x + \beta y$ belongs to C for all $x, y \in C$ and any nonnegative scalars α, β .

Since any convex cone $C_i \subset V_i$ is a semimodule over the semiring \mathbb{R}_+ , we have the unique tensor product of these convex cones $C_1 \otimes \cdots \otimes C_d$ as an \mathbb{R}_+ -semimodule up to isomorphism. More precisely, the *tensor product of cones* $C_1 \otimes \cdots \otimes C_d$ is the quotient monoid $F(C_1, \ldots, C_d) / \sim$, where $F(C_1, \ldots, C_d)$ is the free monoid generated by all *n*-tuples $(v_1, \ldots, v_d) \in C_1 \times \cdots \times C_d$, and \sim is the equivalence relation on $F(C_1, \ldots, C_d)$ generated by

$$(v_1,\ldots,\alpha v_i+\beta v'_i,\ldots,v_d)\sim \alpha(v_1,\ldots,v_i,\ldots,v_d)+\beta(v_1,\ldots,v'_i,\ldots,v_d)$$

for all $v_i, v'_i \in C_i$, $\alpha, \beta \in \mathbb{R}_+$, and i = 1, ..., d. The commutative monoid $C_1 \otimes \cdots \otimes C_d$ is an \mathbb{R}_+ -semimodule. We write $v_1 \otimes \cdots \otimes v_d$ for the equivalence class representing $(v_1, ..., v_d)$ in $F(C_1, ..., C_d) / \sim$.

A multiconic map from $C_1 \times \cdots \times C_d$ to a convex cone C is a map $\varphi : C_1 \times C_2 \times \cdots \times C_d \to C$ with the property

$$\varphi(u_1,\ldots,\alpha v_i+\beta w_i,\ldots,u_d)=\alpha\varphi(u_1,\ldots,v_i,\ldots,u_d)+\beta\varphi(u_1,\ldots,w_i,\ldots,u_d),\quad \alpha,\beta\in\mathbb{R}_+,$$

for all $i = 1, \ldots, d$.

The tensor product space $C_1 \otimes \cdots \otimes C_d$ with $\nu : C_1 \times \cdots \times C_m \to C_1 \otimes \cdots \otimes C_d$ defined by

$$\nu(v_1,\ldots,v_d) = v_1 \otimes \cdots \otimes v_d \in F(C_1,\ldots,C_d) / \sim$$

and extended nonnegative linearly satisfies the Universal Factorization Property often used to define tensor product spaces: If φ is a multiconic map from $C_1 \times \cdots \times C_d$ into a convex cone C, then there exists a unique \mathbb{R}_+ -linear map ψ from $C_1 \otimes \cdots \otimes C_d$ into C, that makes the following diagram commutative:



i.e., $\psi \nu = \varphi$. Strictly speaking we should have written $C_1 \otimes_{\mathbb{R}_+} \cdots \otimes_{\mathbb{R}_+} C_d$ to indicate that the tensor product is one of \mathbb{R}_+ -semimodules but this is obvious from context. Note that Definition 4 is consistent with our earlier definition of nonnegative tensors since $V^+ = V_1^+ \otimes \cdots \otimes V_d^+$ as tensor product of cones over \mathbb{R}_+ .

In [34], Velasco defines the tensor product of C_1, \ldots, C_d to be the convex cone in $V_1 \otimes \cdots \otimes V_d$ formed by $v_1 \otimes \cdots \otimes v_d \in V_1 \otimes \cdots \otimes V_d$, where $v_i \in C_i$, and shows this tensor product satisfies the above Universal Factorization Property. By the uniqueness of the \mathbb{R}_+ -semimodule satisfying the universal property, the two constructions are equivalent.

If $C_1 = \mathbb{R}^{n_1}_+, \ldots, C_d = \mathbb{R}^{n_d}_+$, we may identify

$$\mathbb{R}^{n_1}_{+} \otimes \cdots \otimes \mathbb{R}^{n_d}_{+} = \mathbb{R}^{n_1 \times \cdots \times n_d}_{+}$$

through the interpretation of the tensor product of vectors as a hypermatrix via the Segre outer product

$$[a_1,\ldots,a_l]^\mathsf{T}\otimes[b_1,\ldots,b_m]^\mathsf{T}\otimes[c_1,\ldots,c_n]^\mathsf{T}=[a_ib_jc_k]_{i,j,k=1}^{l,m,n}$$

We note that one may easily extend the notion of nonnegative rank and nonnegative rank decomposition to tensor product of other cones.

Definition 6. A tensor $T \in C_1 \otimes \cdots \otimes C_d$ is said to be *decomposable* if T is of the form $u_1 \otimes \cdots \otimes u_d$, where $u_i \in C_i$. For $T \in C_1 \otimes \cdots \otimes C_d$, the *conic rank* of T, denoted by $\operatorname{rank}_+(T)$, is the minimal value of r such that $T = \sum_{p=1}^r u_{1,p} \otimes \cdots \otimes u_{d,p}$, where $u_{i,p} \in C_i$, *i.e.*, T is contained in the convex cone generated by $u_{1,1} \otimes \cdots \otimes u_{d,1}, \ldots, u_{1,r} \otimes \cdots \otimes u_{d,r}$. Such a decomposition will be called a *conic rank decomposition*.

In the remainder of this paper, we focus our attention on the case $V^+ = V_1^+ \otimes \cdots \otimes V_d^+$, the convex cone of nonnegative *d*-tensors although we will point out whenever a result holds more generally for arbitrary cones. For any given positive integer *r*, we let

$$D_r^+ = \{ X \in V_1^+ \otimes \dots \otimes V_d^+ : \operatorname{rank}_+(X) \le r \}$$

denote the set of tensors of nonnegative rank not more than r.

III. UNIQUENESS OF RANK DECOMPOSITIONS

From the standpoints of both identifiability and well-posedness, an important issue is whether a rank decomposition of the form (II.3) is unique. It is clear that such decompositions can never be unique when d = 2, *i.e.*, for matrices. But when d > 2, rank decompositions are often unique, which is probably the strongest reason for their utility in applications. There are well-known sufficient conditions ensuring uniqueness of rank decomposition [20], [30], [3], [6], notably the two following results.

Theorem 7 (Kruskal). The rank decomposition of a d-tensor T is unique if

$$\operatorname{rank}(T) \le \frac{1 + \sum_{i=1}^{d} (\kappa_i - 1)}{2}$$

where κ_i denote the Kruskal rank of the factors $u_{i,1}, \ldots, u_{i, \operatorname{rank}(T)}$, which is generically equal to the dimension n_i when $n_i \leq \operatorname{rank}(T)$.

Theorem 8 (Bocci–Chiantini–Ottaviani). The rank decomposition of a generic d-tensor T of rank-r is unique when

$$r \le \frac{\prod_{i=1}^{d} n_i - (n_1 + n_2 + n_3 - 2) \prod_{i=3}^{d} n_i}{1 + \sum_{i=1}^{d} (n_i - 1)},$$

Theorem 9 (Chiantini–Ottaviani–Vannieuwenhoven). The rank decomposition of a generic d-tensor T of rank-r is unique when

$$r < \left| \frac{\prod_{i=1}^{d} n_i}{1 + \sum_{i=1}^{d} (n_i - 1)} \right|.$$

if $\prod_{i=1}^{d} n_i \leq 15000$ except for some exceptional cases.

The authors of [6] also strengthened the above result by a prior compression of tensor T. The consequence is that the dimensions n_i in Theorem 9 may be replaced by the multilinear rank of T, which allows significant tightening of the upper bound for low multilinear rank tensors.

Nevertheless these results do not apply to *nonnegative* decompositions over \mathbb{R}_+ (as opposed to decompositions over \mathbb{C}) nor to rank-*r* approximations (as opposed to rank-*r* decompositions). The purpose of this paper is to provide some of the first results in these directions. In particular, it will be necessary to distinguish between an *exact* nonnegative rank-*r* decomposition and a best nonnegative rank-*r* approximation. Note that when a best nonnegative rank-*r* approximation to a nonnegative tensor *T* is unique, it means that

$$\min_{\operatorname{ank}_+(X) \le r} \|T - X\|$$

has a unique minimizer X^* . The nonnegative rank-r decomposition of X^* may not however be unique.

A nonnegative rank decomposition $X = \sum_{p=1}^{r} u_{1,p} \otimes \cdots \otimes u_{d,p} \in V_1^+ \otimes \cdots \otimes V_d^+$ is said to be *unique* if for any other nonnegative rank decomposition $X = \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p}$, there is a permutation σ of $\{1, \ldots, d\}$ such that $u_{1,p} \otimes \cdots \otimes u_{d,p} = v_{1,\sigma(p)} \otimes \cdots \otimes v_{d,\sigma(p)}$ for all $p = 1, \ldots, r$.

IV. EXISTENCE AND GENERIC UNIQUENESS OF RANK-r APPROXIMATIONS

Given a nonnegative tensor $T \in V^+$, we consider the best nonnegative rank-*r* approximations of *T*, where *r* is less than the nonnegative rank of *T*. We will assume that each V_i has a given inner product, which induces an inner product $\langle \cdot, \cdot \rangle$ on $V_1 \otimes \cdots \otimes V_d$ that restricts to $C_1 \otimes \cdots \otimes C_d$. We let

$$\delta(T) = \inf_{X \in D_r^+} \|T - X\| = \inf_{\operatorname{rank}_+(X) \le r} \|T - X\|,$$

where $\|\cdot\|$ is the *Hilbert–Schmidt norm*, *i.e.*, the l^2 -norm given by the inner product. Henceforth any unlabelled norm $\|\cdot\|$ on $V_1 \otimes \cdots \otimes V_d$ will always denote the Hilbert–Schmidt norm with respect to some fixed choices of orthonormal bases on V_1, \ldots, V_d (which induces an orthonormal basis on $V_1 \otimes \cdots \otimes V_d$). When d = 2, the Hilbert–Schmidt norm reduces to the Frobenius norm of matrices and when d = 1, it reduces to the Euclidean norm of vectors.

Proposition 10. $D_r^+ = \{X \in C_1 \otimes \cdots \otimes C_d : \operatorname{rank}_+(X) \leq r\}$ is a closed semialgebraic set if each $C_i \subseteq V_i^+$ is a closed semialgebraic cone.

Proof. The closedness follows from [25], and the fact that it is semialgebraic follows from Tarski–Seidenberg Theorem [9].

By the closedness of D_r^+ , for any $T \notin D_r^+$, there is some $T^* \in D_r^+$ such that $||T - T^*|| = \delta(T)$. The following result is an analogue of [12, Theorem 27] for nonnegative tensors based on [12, Corollary 18].

Proposition 11. Almost every $T \in V^+$ with nonnegative rank > r has a unique best nonnegative rank-r approximation.

Proof. For any $T, T' \in V_1 \otimes \cdots \otimes V_d$, $|\delta(T) - \delta(T')| \le ||T - T'||$, *i.e.*, δ is Lipschitz and thus differentiable almost everywhere in $V = V_1 \otimes \cdots \otimes V_d$ by Rademacher Theorem.

Consider a general $T \in V^+$. Then in particular T lies in the interior of V^+ and there is an open neighborhood $B(T, \delta)$ of T contained in V^+ . So δ is differentiable almost everywhere in V^+ as well. Suppose δ is differentiable at $T \in V^+$. For any $U \in V$, let $\partial \delta_T^2(U)$ be the differential of δ^2 at T along the direction U. Since $||T - T^*|| = \delta(T)$ we obtain

$$\begin{split} \delta^2(T+tU) &= \delta^2(T) + t\partial \delta^2_T(U) + O(t^2) \\ &\leq \|T+tU-T^*\|^2 = \delta^2(T) + 2t\langle U, T-T^*\rangle + t^2 \|U\|^2 \,. \end{split}$$

Therefore, for any t, we have $t\partial \delta_T^2(U) \leq 2t \langle U, T - T^* \rangle$, which implies that

$$\partial \delta_T^2(U) = 2 \langle U, T - T^* \rangle$$

If T' is another best nonnegative rank-r approximation of T, then

$$2\langle U, T - T^* \rangle = \partial \delta_T^2(U) = 2\langle U, T - T' \rangle,$$

from which it follows that $\langle T' - T^*, U \rangle = 0$ for any U, *i.e.*, $T' = T^*$.

We note that Proposition 11 holds more generally for arbitrary closed cones C_1, \ldots, C_d in place of V_1^+, \ldots, V_d^+ .

Proposition 12. The nonnegative tensors which have nonnegative rank > r and do not have a unique best rank-r approximation form a semialgebraic set which does not contain an open set and is contained in some hypersurface.

Proof. Observe that D_r^+ is the image of the polynomial map

$$\phi_r \colon (V_1^+ \times \cdots \times V_d^+)^r \to V^+,$$

$$(u_{1,1}, \dots, u_{d,1}, \dots, u_{1,r}, \dots, u_{d,r}) \mapsto \sum_{j=1}^r u_{1,j} \otimes \cdots \otimes u_{d,j}$$

Hence D_r^+ is semialgebraic by the Tarski–Seidenberg Theorem [9] and the required result follows from [13, Theorem 3.4].

Proposition 12 remains true for arbitrary closed semialgebraic cones C_1, \ldots, C_d .

Now we examine a useful necessary condition for $\sum_{p=1}^{r} T_p$ to be a best rank-*r* approximation of $T \in V_1 \otimes \cdots \otimes V_d$. We will borrow a standard notation from algebraic topology where a hat over a quantity means that quantity is omitted. So for example,

$$\widehat{u_1} \otimes u_2 \otimes u_3 = u_2 \otimes u_3, \quad u_1 \otimes \widehat{u_2} \otimes u_3 = u_1 \otimes u_3, \quad u_1 \otimes u_2 \otimes \widehat{u_3} = u_1 \otimes u_2, \\ u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d = u_1 \otimes \cdots \otimes u_{i-1} \otimes u_{i+1} \otimes \cdots \otimes u_d.$$

The notation $\langle T, X \rangle$ denotes tensor contraction in all possible indices [23]. When T and X are of the same order, $\langle T, X \rangle$ reduces to inner product and our notation is consistent with the inner product notation. When T is a d-tensor and X is a (d-1)-tensor, $\langle T, X \rangle$ is a vector — this is the only other case that will arise in our discussions below.

Lemma 13. Let $\operatorname{rank}(T) > r$ and $\lambda \sum_{p=1}^{r} T_p$ be a best rank-r approximation, where $T_p = u_{1,p} \otimes \cdots \otimes u_{d,p}$ and $\left\|\sum_{p=1}^{r} T_p\right\| = 1$. If $\left<\sum_{p=1}^{r} T_p, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p}\right> \neq 0$ for some $i \in \{1, \ldots, d\}$, then

$$\langle T, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p} \rangle = \lambda \left\langle \sum_{p=1}^{r} T_p, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p} \right\rangle,$$
 (IV.1)

with $\lambda = \langle T, \sum_{p=1}^{r} T_p \rangle$.

Proof. Let L denote the line in $V_1 \otimes \cdots \otimes V_d$ spanned by $\sum_{p=1}^r v_{1,p} \otimes \cdots \otimes v_{d,p}$, and L^{\perp} denote the orthogonal complement of L. Denote the orthogonal projection of T onto L by $\operatorname{Proj}_L(T)$. Then

$$\|T\|^{2} = \|\operatorname{Proj}_{L}(T)\|^{2} + \|\operatorname{Proj}_{L^{\perp}}(T)\|^{2},$$
$$\min_{\alpha \ge 0} \left\|T - \alpha \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p}\right\|^{2} = \|T - \operatorname{Proj}_{L}(T)\|^{2} = \|\operatorname{Proj}_{L^{\perp}}(T)\|^{2} = \|T\|^{2} - \|\operatorname{Proj}_{L}(T)\|^{2}.$$

So computing

$$\min_{v_{1,1},\ldots,v_{d,r}}\min_{\alpha\geq 0}\left\|T-\alpha\sum_{p=1}^r v_{1,p}\otimes\cdots\otimes v_{d,p}\right\|$$

is equivalent to computing

$$\max_{v_{1,1},\ldots,v_{d,r}} \operatorname{Proj}_{L}(T) = \max_{v_{1,1},\ldots,v_{d,r}} \left\langle T, \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p} \right\rangle$$

If at least one $\langle \sum_{p=1}^{r} T_p, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p} \rangle$ is nonzero, then the Jacobian matrix of the hypersurface defined by $\left\| \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p} \right\| = 1$ around $(u_{1,1}, \ldots, u_{d,1}, \ldots, u_{1,r}, \ldots, u_{d,r})$ has constant rank 1, *i.e.*, this real hypersurface is smooth at the point $(u_{1,1}, \ldots, u_{d,1}, \ldots, u_{d,r})$, so we can consider the Lagrangian

$$\mathcal{L} = \left\langle T, \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p} \right\rangle - \lambda \left(\left\| \sum_{p=1}^{r} v_{1,p} \otimes \cdots \otimes v_{d,p} \right\| - 1 \right).$$
(IV.2)

Then $\partial \mathcal{L} / \partial v_{i,p} = 0$ at the point $(u_{1,1}, \ldots, u_{d,1}, \ldots, u_{1,r}, \ldots, u_{d,r})$ gives

$$\langle T, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p} \rangle = \lambda \left\langle \sum_{p=1}^{r} T_p, u_{1,p} \otimes \cdots \otimes \widehat{u_{i,p}} \otimes \cdots \otimes u_{d,p} \right\rangle$$
(IV.3)

with $\lambda = \langle T, \sum_{p=1}^{r} T_p \rangle$ for all $i = 1, \dots, d$, and $p = 1, \dots, r$.

V. RANK-ONE APPROXIMATIONS FOR NONNEGATIVE TENSORS

We have established in Section IV that the best nonnegative rank-r approximation of a nonnegative tensor is generically unique. In this section we focus on the case r = 1, where we could say more. In particular, we will investigate some sufficient conditions under which a nonnegative tensor has a unique best nonnegative rank-1 approximation.

We begin with the following simple but useful observation: for a nonnegative tensor, a best rank-1 approximation can always be chosen to be a best nonnegative rank-1 approximation.

Lemma 14. Given $T \in V^+$. Let $u_1 \otimes \cdots \otimes u_d \in V_1 \otimes \cdots \otimes V_d$ be a best rank-1 approximation of T, then u_1, \ldots, u_d can be chosen to so that $u_1 \in V_1^+, \ldots, u_d \in V_d^+$.

Proof. Let $T = (T_{i_1,...,i_d})$ and $u_i = (u_j(1),...,u_i(n_j))$, where we have denoted the *j*th coordinate of a vector $u_i \in V_i$ by $u_i(j), j = 1, ..., n_i$. Then

$$\|T - u_1 \otimes \cdots \otimes u_d\|^2 = \sum_{i_1, \dots, i_d=1}^{n_1, \dots, n_d} (T_{i_1, \dots, i_d} - u_1(i_1) \cdots u_d(i_d))^2 \ge \sum_{i_1, \dots, i_d=1}^{n_1, \dots, n_d} (T_{i_1, \dots, i_d} - |u_1(i_1)| \cdots |u_d(i_d)|)^2.$$

Since $u_1 \otimes \cdots \otimes u_d$ is a best rank-1 approximation, then we can choose $u_i(j_i) = |u_i(j_i)|$, *i.e.*, $u_1 \otimes \cdots \otimes u_d \in V^+$.

Motivated partly by the notion of singular pairs of a tensor [24] and partly by Lemma 13, we propose the following definition.

Definition 15. Let V_1, \ldots, V_d be vector spaces over K of dimensions n_1, \ldots, n_d , for $T \in V_1 \otimes \cdots \otimes V_d$, $(\lambda, u_1, \ldots, u_d)$ is called a *normalized singular pair* of T if

$$\begin{cases} \langle T, u_1 \otimes \dots \otimes \widehat{u_i} \otimes \dots \otimes u_d \rangle = \lambda u_i \\ \langle u_i, u_i \rangle = 1 \end{cases}$$
(V.1)

for $i = 1, \ldots, d$. λ is called a normalized singular value, and (u_1, \ldots, u_d) is called a normalized singular vector tuple corresponding to λ . If $\mathbb{K} = \mathbb{R}$, $\lambda \ge 0$ and $u_i \in V_i^+$, $(\lambda, u_1, \dots, u_d)$ is called a *nonnegative normalized singular pair* of T.

In Definition 15 we require $\langle u_i, u_i \rangle = 1$ instead of $||u_i|| = 1$ because $\langle u_i, u_i \rangle = 1$ is an algebraic condition, but this requirement does not allow singular vector tuples with $\langle u_i, u_i \rangle = 0$ for some i. In this sense the following definition introduced in [12] is useful.

Definition 16 ([12]). For $T \in V_1 \otimes \cdots \otimes V_d$, $([u_1], \dots, [u_d]) \in \mathbb{P}V_1 \times \cdots \times \mathbb{P}V_d$ is called a *singular vector tuple* if

$$\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle = \lambda_i u_i$$

for some $\lambda_i \in \mathbb{C}$, i = 1, ..., d, and $\prod \lambda_i$ corresponds to a singular value.

It is shown in [12, Corollary 10] that for a singular vector tuple $([u_1], \ldots, [u_d])$ of T corresponding to a nonzero singular value, either $\langle u_i, u_i \rangle = 0$ for all i, or $\langle u_i, u_i \rangle \neq 0$ for all i. Inspired by [4], we can also propose the following definition to describe singular vector tuples in a weighted projective space, and give a well defined description of singular values.

Definition 17. For $T \in V_1 \otimes \cdots \otimes V_d$, $([u_1, \ldots, u_d, \prod \lambda_i])$ in the weighted projective space $\mathbb{P}(1, \ldots, 1, d^2 - 2d)$ is called a projective singular pair if

 $\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle = \lambda_i u_i$

for some $\lambda_i \in \mathbb{C}$, i = 1, ..., d. In $\mathbb{P}(1, ..., 1, d^2 - 2d)$, $([u_1, ..., u_d, \prod \lambda_i])$ and $([v_1, ..., v_d, \prod \mu_i])$ are equivalent if and only if $u_i = tv_i$ and $\prod \lambda_i = t^{d^2 - 2d} \cdot \prod \mu_i$ for some $t \neq 0$, and $\prod \lambda_i$ is called a *projective singular value* corresponding to the singular vector tuple (u_1, \ldots, u_d) .

In [12], it is shown a generic T does not have a zero singular value, and does not have a singular vector tuple $([u_1], \ldots, [u_d])$ such that $\langle u_i, u_i \rangle = 0$ for some *i*. Thus, for a generic T, all the above definitions are equivalent. We will use different definitions of singular vector tuples in different situations to make problems easier. In this paper, we mainly consider normalized singular pairs of a tensor.

The next three lemmas give an analogue of the tensorial Perron–Frobenius Theorem ([5], [11], [24], [35]) for nonnegative normalized singular pairs (as opposed to nonnegative eigenpairs [24]).

Lemma 18 (Existence). A nonnegative tensor T has at least one nonnegative normalized singular pair.

Proof. Let $D = \{(u_1, \ldots, u_d) \in V_1^+ \times \cdots \times V_d^+ : \sum_{i=1}^d ||u_i||_1 = 1\}$. Then D is a compact convex set. If $\sum_{i=1}^d ||\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle||_1 = 0$ for some (u_1, \ldots, u_d) , then $\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle = 0$ for all i, which implies that $\lambda = 0$. On the other hand, if $\sum_{i=1}^d ||\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle||_1 > 0$, define the map $\phi: D \to D$ by

$$\phi(u_1,\ldots,u_d) = \frac{1}{\sum_{i=1}^d \|\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle\|_1} \left(\langle T, u_2 \otimes \cdots \otimes u_d \rangle, \ldots, \langle T, u_1 \otimes \cdots \otimes u_{d-1} \rangle \right).$$

Note that each term $\langle T, u_1 \otimes \cdots \otimes \hat{u_i} \otimes \cdots \otimes u_d \rangle$ in the denominator is a the contraction of a d-tensor with a (d-1)-tensor and therefore the result is a vector. We then normalize by the sum of the l^1 -norms of these vectors so that $\|\phi\|_1 = 1$.

By Brouwer's Fixed Point Theorem, there is some $u_1 \otimes \cdots \otimes u_d$ such that $\langle T, u_1 \otimes \cdots \otimes \hat{u_i} \otimes \cdots \otimes u_d \rangle = \lambda u_i$, where $\lambda = \sum_{i=1}^{d} \|\langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle\|_1.$ Since $\langle T, u_1 \otimes \cdots \otimes u_d \rangle = \lambda \|u_i\|^2$ for $i = 1, \ldots, d$, $\|u_1\| = \cdots = \|u_d\|$. Let $\widetilde{u_i} = \frac{u_i}{\|u_i\|}$, and $\widetilde{\lambda} = \langle T, \widetilde{u_1} \otimes \cdots \otimes \widetilde{u_d} \rangle$, then $(\lambda, \widetilde{u_1}, \ldots, \widetilde{u_d})$ is a nonnegative normalized singular pair.

Lemma 19 (Positivity). If T is positive, T has a positive normalized singular pair $(\lambda, u_1, \ldots, u_d)$ with $\lambda > 0$.

Proof. By Lemma 18, T has a nonnegative normalized singular pair $(\lambda, u_1, \ldots, u_d)$. We assume that a choice of bases has been fixed for V_1, \ldots, V_d . We denote the *j*th coordinate of a vector $v_i \in V_i$ by $v_i(j), j = 1, \ldots, n_i$. Let $I_i = \{j : u_i(j) \neq 0\}$ be the support of u_i and set $\alpha = \min\{u_i(j) : i = 1, \dots, d, j \in I_i\}$. For any i and j,

$$\lambda u_i(j) = \langle T, u_1 \otimes \cdots \otimes \widehat{u_i} \otimes \cdots \otimes u_d \rangle(j) \ge \alpha^{d-1} \sum_{l_j \in I_j} T_{l_1 \dots l_{i-1} j l_{i+1} \dots l_d} > 0$$

which means λ and each coordinate of u_i is positive.

Definition 20. [17] For $T \in V_1 \otimes \cdots \otimes V_d$ over \mathbb{R} , let $\rho(T) = \max\{|\langle T, u_1 \otimes \cdots \otimes u_d \rangle| : ||u_1|| = \cdots = ||u_d|| = 1\}$, and call $\rho(T)$ the spectral norm of T.

It is shown in [17] that it is *NP-hard* to compute and approximate the spectral norm of a tensor.

Lemma 21 (Generic Uniqueness). A general real tensor T has a unique normalized singular pair $(\lambda, u_1, \ldots, u_d)$ with $\lambda =$ $\rho(T)$.

Proof. By [12, Theorem 20] and Lemma 13.

VI. UNIQUENESS OF SYMMETRIC RANK-ONE APPROXIMATIONS FOR SYMMETRIC TENSORS

Not every tensor has a unique best rank one approximation [32, Proposition 1]. For example, the symmetric 3-tensor $x \otimes x \otimes x + y \otimes y \otimes y$, where x and y are orthonormal, has two best rank-1 approximations: $x \otimes x \otimes x$ and $y \otimes y \otimes y$. It is known that a best rank-1 approximation of a symmetric tensor can be chosen to be symmetric over \mathbb{R} and \mathbb{C} [1], [10]. We give below some description of the subset of symmetric tensors whose elements do not have unique symmetric best rank one approximations.

For any group G acting on W over \mathbb{C} , G acts naturally on S^dW and S^dW^* , where W^* is the dual space of W, such that $\langle S,T\rangle = \langle g \cdot S, g \cdot T \rangle$ for $g \in G, T \in S^d W$ and $S \in S^d W^*$. In particular, after fixing a metric on a real vector space V of dimension n, V is self dual, $V \cong V^*$, and $\langle T, S \rangle$ is invariant under the orthogonal group O(n) for $T, S \in S^d V$.

Let \mathbb{S}^{n-1} denote the unit sphere in V. The subset $A_0 = \{u \in \mathbb{S}^{n-1} : \langle T, u^d \rangle = \rho(T)\}$ is non-empty and closed in \mathbb{S}^{n-1} and invariant under O(n). Denote also $\rho(T)$ by $\sigma_1(T)$, the maximal or minimal spectrum of T.

Definition 22 ([24], [27], [4]). For $T \in S^d W$ over \mathbb{C} , (λ, u) is called a normalized eigenpair of T if $\langle T, u^{d-1} \rangle = \lambda u$ and $\langle u, u \rangle = 1$. Two normalized eigenpairs (λ, u) and (μ, v) of T are called equivalent if $(\lambda, u) = (\mu, v)$, or $(-1)^{d-2} \cdot \lambda = \mu$ and u = -v. For $T \in S^d V$ over \mathbb{R} , normalized eigenpairs are invariant under the orthogonal group.

Definition 23 ([28]). For $T \in S^d W$ and d = 2l, let $\psi_T(\lambda)$ be the resultant of the equation $\langle T, u^{d-1} \rangle - \lambda \langle u, u \rangle^{l-1} u = 0$. For d odd, let $\psi_T(\lambda)$ be the resultant of the equations

$$\begin{cases} \langle T, u^{d-1} \rangle - \lambda x^{d-2} u = 0 \\ x^2 - \langle u, u \rangle = 0 \end{cases}$$

 $\psi_T(\lambda)$ is called the *E*-characteristic polynomial of *T*.

Proposition 24. The subset $H_{\sigma_1} \subset S^d V$ over \mathbb{R} consisting of symmetric tensors which have non-unique equivalence classes of normalized eigenpairs corresponding to their spectral norms is an algebraic hypersurface in $S^{d}V$.

Proof. For convenience of notation, we let d = 3. Assume there exist $u_1 \neq v \in V$ such that $||u_1|| = ||v|| = 1$, $\langle T, u_1^2 \rangle = 0$ $\sigma_1(T)u_1$, and $\langle T, v^2 \rangle = \sigma_1(T)v$. Fix an orthonormal basis $\{u_1, \ldots, u_n\}$ for V, and by an action of the orthogonal group O(n)on V, we can assume $v = \cos \theta u_1 + \sin \theta u_2$ for some $\theta \neq 0, \pi$. Denote $\langle T, u_i u_j u_k \rangle$ by T_{ijk} . Thus

$$T_{111} = \sigma_1(T) \tag{VI.1}$$

$$T_{i11} = 0 \tag{VI.2}$$

$$\begin{cases} T_{i11} = 0 & (VI.2) \\ T_{111} \cos^2 \theta + T_{122} \sin^2 \theta = T_{111} \cos \theta & (VI.3) \\ 2T_{122} \sin \theta \cos \theta + T_{222} \sin^2 \theta = T_{111} \sin \theta & (VI.4) \end{cases}$$

$$2T_{122}\sin\theta\cos\theta + T_{222}\sin^2\theta = T_{111}\sin\theta \tag{VI.4}$$

 $\int \frac{2T_{i12}\cos\theta + T_{i22}\sin\theta}{2T_{i12}\cos\theta + T_{i22}\sin\theta} = 0$ (VI.5)

for $i \neq 1$ and j > 2. By eliminating the parameter θ we can obtain the equations that T_{ijk} need satisfy.

For example, Equation VI.3 implies $\cos \theta = 1$ or $(T_{111} - T_{122}) \cos \theta = T_{122}$, and Equation VI.4 implies $\sin \theta = 0$ or $2T_{122} \cos \theta + T_{222} \sin \theta = T_{111}$. By using the identity $\sin^2 \theta + \cos^2 \theta = 1$ and $\theta \neq 0, \pi$, we have

$$\begin{cases} [T_{111}(T_{111} - T_{122}) - 2T_{122}^2]^2 + T_{222}^2 T_{122}^2 &= T_{222}^2 (T_{111} - T_{122})^2 \\ (T_{111}T_{122} + 2T_{122}^2 - T_{111}^2) T_{j22} &= 2T_{j12}T_{222} (T_{111} - T_{122}) \end{cases}$$
(VI.6)

Define

$$I = \{(T, [u_1, \dots, u_n]) \in S^3 V \times O(n) : T_{ijk} \text{ satisfies } VI.6\}$$

$$S^3 V \xrightarrow{\pi_1} O(n)$$
(VI.7)

by $\pi_1(T, [u_1, \ldots, u_n]) = T$ and $\pi_2(T, [u_1, \ldots, u_n]) = [u_1, \ldots, u_n]$. By [28], $\sigma_1(T)$ is a root of the *E*-characteristic polynomial $\psi_T(\lambda)$ of *T*, so $\sigma_1(T)$ and any corresponding eigenvector depends algebraically on *T*. Hence *I* is a variety, and *T* has more than one eigenvectors corresponding to $\sigma_1(T)$ if and only if *T* is in the image of π_1 , i.e. $H_{\sigma_1} = \pi_1(I)$.

than one eigenvectors corresponding to $\sigma_1(T)$ if and only if T is in the image of π_1 , i.e. $H_{\sigma_1} = \pi_1(I)$. Define $T' \in S^3V$ by $T'_{111} = 1, T'_{122} = 2\sqrt{3} - 3, T'_{222} = 6\sqrt{3} - 10$, and other terms $T'_{ijk} = 0$, then T' has two eigenvectors corresponding to the maximal eigenvalue 1, so $T' \in \pi_1(I)$. T' has a finite number of eigenvectors, hence by semicontinuity a generic $T \in \pi_1(I)$ has a finite number of eigenvectors, i.e. $\dim \pi_1^{-1}(T) = \dim O(n-2)$ for a generic $T \in \pi_1(I)$. So $\dim H_{\sigma_1} = \dim \pi_1(I) = \dim I - \dim O(n-2) = \dim I - \frac{(n-2)(n-3)}{2}$.

Since π_2 is a dominant morphism, and the dimension of a generic fiber $\pi_2^{-1}([u_1, \ldots, u_n])$ is dim $S^3V - 2(n-1)$, then dim $I = \dim S^3V - 2(n-1) + \dim O(n)$. Therefore dim $H = \dim S^3V - 1$, i.e. H_{σ_1} is a hypersurface.

Corollary 25. Given a positive $T \in S^3V$ over \mathbb{R} , assume $\langle T, u^3 \rangle = \sigma_1(T)$. Let $\sigma_2 = \min_v \{|\langle T, uv^2 \rangle| : v \perp u, ||v|| = 1\}$. If $\sigma_2 \geq \frac{1}{2}\sigma_1(T)$, then T has a unique symmetric nonnegative best rank one approximation.

Proof. By Lemma 13, assume there exists $v \neq u$ such that ||v|| = 1, $v \perp u$, and $\langle T, (\cos \theta u + \sin \theta v)^3 \rangle = \sigma_1(T)$ for some $0 < \theta \leq \pi$, then by Lemma 19, $0 < \theta < \frac{\pi}{2}$. By Equation VI.3, $\langle T, uv^2 \rangle = \frac{\cos \theta}{1 + \cos \theta} \sigma_1(T)$. Since $0 < \frac{\cos \theta}{1 + \cos \theta} < \frac{1}{2}$ on $0 < \theta < \frac{\pi}{2}$, then $0 < \langle T, uv^2 \rangle < \frac{1}{2} \sigma_1(T)$, which contradicts the assumption.

Let V be a real vector space of dimension n, and $W = V \otimes_{\mathbb{R}} \mathbb{C}$. A generic $T \in S^d W$ has distinct eigenvalues [4], so the resultant of the equations $\psi_T(\lambda) = \psi'_T(\lambda) = 0$, denoted by $\tilde{\chi}(T)$, is a nonzero polynomial on $S^d W$. $\tilde{\chi}(T) = 0$ defines the complex hypersurface H consisting of tensors $T \in S^d W$ which admit multiple equivalence classes of normalized eigenpairs. For $T \in S^d V$, H_{σ_1} forms some components of the real points of the complex hypersurface H. In fact, if we replace $\sigma_1(T)$ by any real normalized eigenvalue λ of T in the proof of Proposition 24, we can show that the subset of symmetric tensors which admits multiple equivalence classes of normalized eigenvectors corresponding to λ is a real algebraic hypersurface, which forms some components of the real points of H. Therefore

Proposition 26. For $T \in S^d V$, $\tilde{\chi}(T) = 0$ is a defining equation of the hypersurface H formed by symmetric tensors which have multiple equivalence classes of normalized eigenvalues. Assume $\tilde{\chi}(T) \neq 0$. Over \mathbb{R} , when d is odd, there is a unique eigenvector v_{λ} corresponding to each eigenvalue λ of T. When d is even, there are two eigenvectors $\pm v_{\lambda}$ corresponding to each eigenvalue λ of T. When d is even, there are two eigenvectors $\pm v_{\lambda}$ corresponding to each eigenvalue λ of T. So for a real $T \in S^d V$, if $\tilde{\chi}(T) \neq 0$, T has a unique symmetric best rank one approximation.

Example 27. For $T = [T_{ijk}] \in S^3 \mathbb{R}^2$, $\psi_T(\lambda)$ is the resultant of the following equations:

$$\begin{cases} F_0 = T_{111}x^2 + 2T_{112}xy + T_{122}y^2 - \lambda xz \\ F_1 = T_{112}x^2 + 2T_{122}xy + T_{222}y^2 - \lambda yz \\ F_2 = x^2 + y^2 - z^2 \end{cases}$$

Denote the Jacobian determinant of F_0, F_1, F_2 by J, then

$$\begin{split} J &= \det \begin{pmatrix} \frac{\partial F_0}{\partial x} & \frac{\partial F_0}{\partial y} & \frac{\partial F_0}{\partial z} \\ \frac{\partial F_1}{\partial x} & \frac{\partial F_1}{\partial y} & \frac{\partial F_1}{\partial z} \\ \frac{\partial F_2}{\partial x} & \frac{\partial F_2}{\partial y} & \frac{\partial F_2}{\partial z} \end{pmatrix} \\ &= (8T_{112}^2 - 8T_{111}T_{122} - 2\lambda^2)x^2z + 4T_{112}\lambda y^3 + (8T_{122}^2 - 8T_{222}T_{112} - 2\lambda^2)y^2z + 4T_{122}\lambda x^3 + (4T_{111}\lambda - 8T_{122}\lambda)xy^2 \\ &+ (4T_{122}\lambda + 4T_{111}\lambda)xz^2 - 2\lambda^2 z^3 + (4T_{222}\lambda - 8T_{112}\lambda)x^2y + (4T_{112}\lambda + 4T_{222}\lambda)yz^2 + (8T_{112}T_{122} - 8T_{111}T_{222})xyz. \end{split}$$

$$\begin{split} \frac{\partial J}{\partial x} &= 12T_{122}\lambda x^2 + (4T_{111}\lambda - 8T_{122}\lambda)y^2 + (4T_{111}\lambda + 4T_{122}\lambda)z^2 \\ &+ (8T_{222}\lambda - 16T_{112}\lambda)xy + (16T_{112}^2 - 4\lambda^2 - 16T_{111}T_{122})xz + (8T_{112}T_{122} - 8T_{111}T_{222})yz \\ \frac{\partial J}{\partial y} &= (4T_{222}\lambda - 8T_{112}\lambda)x^2 + 12T_{112}\lambda y^2 + (4T_{112}\lambda + 4T_{222}\lambda)z^2 \\ &+ (8T_{111}\lambda - 16T_{122}\lambda)xy + (8T_{112}T_{122} - 8T_{111}T_{222})xz + (16T_{122}^2 - 4\lambda^2 - 16T_{112}T_{222})yz \\ \frac{\partial J}{\partial z} &= (8T_{112}^2 - 8T_{111}T_{122} - 2\lambda^2)x^2 + (8T_{122}^2 - 8T_{222}T_{112} - 2\lambda^2)y^2 - 6\lambda^2 z^2 \\ &+ (8T_{112}T_{122} - 8T_{111}T_{222})xy + (8T_{122}\lambda + 8T_{111}\lambda)xz + (8T_{112}\lambda + 8T_{222}\lambda)yz \end{split}$$

By a formula of Salmon [8], $\psi_T(\lambda) = \frac{1}{512} \det(G)$, where G is defined by

$$G = \begin{pmatrix} T_{111} & T_{122} & 0 & 2T_{112} & -\lambda & 0 \\ T_{112} & T_{222} & 0 & 2T_{122} & 0 & -\lambda \\ 1 & 1 & -1 & 0 & 0 & 0 \\ 12T_{122} & 4T_{111}\lambda - 8T_{122}\lambda & 4T_{111}\lambda + 4T_{122}\lambda & 8T_{222}\lambda - 16T_{112}\lambda & 16T_{112}^2 - 4\lambda^2 - 16T_{111}T_{122} & 8T_{112}T_{122} - 8T_{111}T_{222} \\ 4T_{222}\lambda - 8T_{112}\lambda & 12T_{112}\lambda & 4T_{112}\lambda + 4T_{222}\lambda & 8T_{111}\lambda - 16T_{122}\lambda & 8T_{112}T_{122} - 8T_{111}T_{222} & 16T_{122}^2 - 4\lambda^2 - 16T_{112}T_{222} \\ 8T_{112}^2 - 8T_{111}T_{122} - 2\lambda^2 & 8T_{122}^2 - 8T_{222}T_{112} - 2\lambda^2 & -6\lambda^2 & 8T_{112}T_{122} - 8T_{111}T_{222} & 8T_{122}\lambda + 8T_{111}\lambda & 8T_{112}\lambda + 8T_{222}\lambda \end{pmatrix}$$

Thus $\psi_T(\lambda) = c_2\lambda^6 + c_4\lambda^4 + c_6\lambda^2 + c_8$ for some homogeneous polynomials c_i of degree *i* in T_{jkl} , see also [4], [22]. Then $\tilde{\chi}(T)$ is the determinant of some 11×11 matrix in T_{jkl} . For a generic T, $\psi_T(\lambda) = c(\lambda^2 - \gamma_1)(\lambda^2 - \gamma_2)(\lambda^2 - \gamma_3)$ for some $c \in \mathbb{C}$ and distinct $\gamma_i \in \mathbb{C}$, and $\tilde{\chi}(T) \neq 0$. For $T \in H$, $\psi_T(\lambda)$ has multiple roots. For example, let T' by $T'_{111} = T'_{222} = 1$ and other terms $T'_{ijk} = 0$, then $\tilde{\chi}(T) = 0$ implies T' has multiple eigenpairs. In fact, $\psi_{T'}(\lambda) = (\lambda + 1)^2(\lambda - 1)^2(2\lambda^2 - 1)$, there are two eigenvectors (1, 0) and (0, 1) corresponding to the eigenvalue 1, and two eigenvectors (-1, 0) and (0, -1) corresponding to the eigenvalue -1.

VII. UNIQUENESS OF BEST RANK-ONE APPROXIMATIONS FOR REAL TENSORS

Definition 28. Let W_1, \ldots, W_d be complex vector spaces, for $T \in W_1^* \otimes \cdots \otimes W_d^*$, $u_i \in W_i$, and $\alpha_i \in \mathbb{C}$, denote by $\phi_T(\lambda)$ the resultant of the following homogeneous equations

$$\begin{cases} \alpha_i \langle T, u_1 \otimes \dots \otimes \widehat{u_i} \otimes \dots \otimes u_d \rangle = \lambda(\prod_{j \neq i} \alpha_j) u_i \\ \langle u_i, u_i \rangle = \alpha_i^2 \end{cases}$$
(VII.1)

By the resultant theory ([8], [15]), $\phi_T(\lambda)$ vanishes if and only if Equations VII.1 has a nontrivial solution, i.e. $\phi_T(\lambda) = 0$ if and only if $(\lambda, u_1, \dots, u_d)$ is a normalized singular pair of T. $\phi_T(\lambda)$ is called the *singular characteristic polynomial* of T, whose roots λ are normalized singular values of T.

Definition 29. Two normalized singular pairs $(\lambda, u_1, \ldots, u_d)$ and (μ, v_1, \ldots, v_d) of T are called equivalent if $(\lambda, u_1, \ldots, u_d) = (\mu, v_1, \ldots, v_d)$, or $(-1)^{d-2}\lambda = \mu$ and $u_i = -v_i$. For $T \in V_1 \otimes \cdots \otimes V_d$ over \mathbb{R} , normalized singular pairs are invariant under the product of orthogonal groups $O(n_1) \times \cdots \times O(n_d)$.

Proposition 30. The subset $X_{\sigma_1} \subset V_1^* \otimes \cdots \otimes V_d^*$ consisting of tensors which have non-unique best rank one approximations forms an algebraic hypersurface.

Proof. By Lemma 13, X_{σ_1} is the subset consisting of T which admits more than one equivalence classes of normalized singular pairs corresponding to $\rho(T)$. For convenience of notation, assume d = 3, and there exist $u_{i,1} \neq v_i \in V_i$ such that $||u_{i,1}|| = ||v_i|| = 1$, $\langle T, u_{1,1} \otimes u_{2,1} \otimes u_{3,1} \rangle = \rho(T) = \langle T, v_1 \otimes v_2 \otimes v_3 \rangle$. Choose an orthonormal basis $\{u_{i,1}, \ldots, u_{i,n_i}\}$ for each V_i , and by an action of the product of orthogonal groups $O(n_1) \times O(n_2) \times O(n_3)$ on $V_1 \otimes V_2 \otimes V_3$, we can assume $v_i = \cos \theta_i u_{i,1} + \sin \theta_i u_{i,2}$. Denote $\langle T, u_{1,i} \otimes u_{2,j} \otimes u_{3,k} \rangle$ by T_{ijk} . Thus

$$\begin{cases} T_{111} = \rho(T) \\ T_{i11} = T_{1i1} = T_{11i} = 0 \\ T_{111} \cos \theta_2 \cos \theta_3 + T_{122} \sin \theta_2 \sin \theta_3 = T_{111} \cos \theta_1 \\ T_{212} \cos \theta_2 \sin \theta_3 + T_{221} \sin \theta_2 \cos \theta_3 + T_{222} \sin \theta_2 \sin \theta_3 = T_{111} \sin \theta_1 \\ T_{j12} \cos \theta_2 \sin \theta_3 + T_{j21} \sin \theta_2 \cos \theta_3 + T_{j22} \sin \theta_2 \sin \theta_3 = 0 \\ T_{111} \cos \theta_1 \cos \theta_3 + T_{212} \sin \theta_1 \sin \theta_3 = T_{111} \cos \theta_2 \\ T_{122} \cos \theta_1 \sin \theta_3 + T_{221} \sin \theta_1 \cos \theta_3 + T_{222} \sin \theta_1 \sin \theta_3 = T_{111} \sin \theta_2 \\ T_{1j2} \cos \theta_1 \sin \theta_3 + T_{2j1} \sin \theta_1 \cos \theta_3 + T_{2j2} \sin \theta_1 \sin \theta_3 = 0 \\ T_{111} \cos \theta_1 \cos \theta_2 + T_{221} \sin \theta_1 \sin \theta_2 = T_{111} \cos \theta_3 \\ T_{122} \cos \theta_1 \sin \theta_2 + T_{212} \sin \theta_1 \cos \theta_2 + T_{222} \sin \theta_1 \sin \theta_2 = T_{111} \sin \theta_3 \\ T_{122} \cos \theta_1 \sin \theta_2 + T_{212} \sin \theta_1 \cos \theta_2 + T_{222} \sin \theta_1 \sin \theta_2 = 0 \end{cases}$$

for $i \neq 1$ and j > 2. By eliminating the parameter θ we can obtain the equations that T_{ijk} need satisfy.

Let I be the incidence variety in $V_1^* \otimes V_2^* \otimes V_3^* \times O(n_1) \times O(n_2) \times O(n_3)$ such that for each $(T, g_1, g_2, g_3) \in I$, where $g_i = [u_{i,1}, \ldots, u_{i,n_i}]$, there is some $(\theta_1, \theta_2, \theta_3)$ such that all T_{ijk} satisfy VII.2. Define

$$V_{1}^{*} \otimes V_{2}^{*} \otimes V_{3}^{*} \qquad O(n_{1}) \times O(n_{2}) \times O(n_{3})$$
(VII.3)

by $\pi_1((T, g_1, g_2, g_3)) = T$ and $\pi_2((T, g_1, g_2, g_3)) = (g_1, g_2, g_3)$. $\rho(T)$ is a root of $\phi_T(\lambda)$, T has more than one singular vector tuples corresponding to $\rho(T)$ if and only if T is in the image of π_1 , i.e. $X_{\sigma_1} = \pi_1(I)$.

Define T' by $T'_{111} = T'_{222} = 1$ and other terms $T'_{ijk} = 0$. T' has two singular vector tuples corresponding to its maximal singular value, so $T' \in \pi_1(I)$. Since T' has a finite number of singular pairs, then a generic $T \in \pi_1(I)$ has a finite number of singular pairs. So dim $\pi_1^{-1}(T) = \dim O(n_1 - 2) + \dim O(n_2 - 2) + \dim O(n_3 - 2)$ for a generic $T \in \pi_1(I)$, and dim $X_{\sigma_1} = \dim \pi_1(I) = \dim I - \dim O(n_1 - 2) - \dim O(n_2 - 2) - \dim O(n_3 - 2)$.

Since π_2 is a dominant morphism, and the dimension of a generic fiber $\pi_2^{-1}(g_1, g_2, g_3)$ is $\dim V_1^* \otimes V_2^* \otimes V_3^* - 2(n_1 + n_2 + n_3) + 8$, then $\dim I = \dim V_1^* \otimes V_2^* \otimes V_3^* - 2(n_1 + n_2 + n_3) + 8 + \dim O(n_1) + \dim O(n_2) + \dim O(n_3)$. Therefore the codimension of X_{σ_1} is 1.

The following property of singular vector tuples is probably known to experts, and we give it a proof here based on the method introduced by Friedland and Ottaviani in [12]. For more details of this method, please see [12].

Proposition 31. A generic $T \in W_1 \otimes \cdots \otimes W_d$ over \mathbb{C} has distinct equivalence classes of normalized singular pairs.

The proof is based on the following "Bertini-type" theorem introduced in [12].

Theorem 32. [12] Let E be a vector bundle on a smooth variety M, and $S \subset H^0(M, E)$ generate E. If $\operatorname{rank}(E) > \dim M$, then the zero locus of a generic $\zeta \in S$ is empty.

To simplify the argument we will just consider some open subset of an affine smooth variety based on the following lemma.

Lemma 33. For a generic $T \in W_1 \otimes \cdots \otimes W_d$, if (u_1, \ldots, u_d) is a singular vector tuple of T, then $(u_1, \ldots, u_{d-1}, v_d)$ is not a singular vector tuple of T if v_d is not parallel to u_d .

Proof. Assume $\lambda u_d = \langle T, u_1 \otimes \cdots \otimes u_{d-1} \rangle = \mu v_d$ for some v_d not parallel with u_d , then 0 is a singular value of T, which contradicts with the genericness of T by [12, Theorem 1].

For convenience of notation we consider the case d = 3. Let $C_i = \{u_i \in W_i : \langle u_i, u_i \rangle = 1\}$, F_i be the trivial vector bundle on C_i with fibre isomorphic to W_i , T_i be the tautological line bundle on C_i , and Q_i be the quotient bundle F_i/T_i on C_i . Let $\widetilde{M_i} = C_1 \times C_2 \times C_3$ for i = 1, 2, and define $\pi_{i,j} : \widetilde{M_i} \to C_j$ be the natural projection. Let $p_i : \widetilde{M_1} \times \widetilde{M_2} \to \widetilde{M_i}$ be the projection, and $\widetilde{E} = \bigoplus_{j=1}^{3} p_1^* \pi_{1,j}^*(Q_j) \oplus p_2^* \pi_{2,1}^*(F_1) \oplus \bigoplus_{j=2}^{3} p_2^* \pi_{2,j}^*(Q_j)$ on $\widetilde{M_1} \times \widetilde{M_2}$. Let $X_i = \{(v_1, v_2, v_3, u_1, u_2, u_3) \in \widetilde{M_1} \times \widetilde{M_2} : u_j = v_j$ for all $j \neq i\}$, $M = \widetilde{M_1} \times \widetilde{M_2} \setminus (X_1 \cup X_2 \cup X_3)$, and $E = \widetilde{E}|_M$.

Lemma 34. Given $u_i, v_i, x_i \in W_i$ such that $\langle u_i, u_i \rangle = \langle v_i, v_i \rangle = 1$ for all $1 \le i \le 3$, and $u_j = v_j$ for at most one j, $1 \le j \le 3$, then

1) the system of linear equations

$$\begin{cases} \langle T, u_2 \otimes u_3 \rangle = \langle T, v_1 \otimes v_2 \otimes v_3 \rangle u_1 + x_1 \\ \langle T, u_1 \otimes u_3 \rangle = x_2 \\ \langle T, u_1 \otimes u_2 \rangle = x_3 \end{cases}$$
(VII.4)

is solvable for $T \in W_1 \otimes W_2 \otimes W_3$ if and only if $\langle u_2, x_2 \rangle = \langle u_3, x_3 \rangle$.

2) the system of linear equations

$$\begin{cases} \langle T, u_2 \otimes u_3 \rangle = \langle T, v_1 \otimes v_2 \otimes v_3 \rangle u_1 + x_1 \\ [\langle T, u_1 \otimes u_3 \rangle] = [x_2] \\ [\langle T, u_1 \otimes u_2 \rangle] = [x_3] \end{cases}$$
(VII.5)

is always solvable, where $[x_i]$ denotes the corresponding element in the quotient space $W_i/\langle x_i \rangle$.

Proof. 1) Let U denote the coefficient matrix of T_{ijk} in the system of linear equations VII.4, and [U|x] denote the augmented matrix. The system VII.4 is solvable if and only if U and [U|x] have the same rank, i.e. if there is some $a_i \in W_i$ such that $a_1 \otimes u_2 \otimes u_3 + u_1 \otimes a_2 \otimes u_3 + u_1 \otimes u_2 \otimes a_3 - \langle a_1, u_1 \rangle \cdot v_1 \otimes v_2 \otimes v_3 = 0$ then $\langle a_1, x_1 \rangle + \langle a_2, x_2 \rangle + \langle a_3, x_3 \rangle = 0$. Since

 $a_1 \otimes u_2 \otimes u_3 + u_1 \otimes a_2 \otimes u_3 + u_1 \otimes u_2 \otimes a_3 - \langle a_1, u_1 \rangle \cdot v_1 \otimes v_2 \otimes v_3 = 0$ if and only if $a_1 = 0$, $a_2 = \alpha u_2$, $a_3 = -\alpha u_3$ or $a_1 = 0$, $a_2 = -\alpha u_2$, $a_3 = \alpha u_3$ for some α , then the system VII.4 is solvable if and only if $\langle u_2, x_2 \rangle = \langle u_3, x_3 \rangle$.

2) The system VII.5 is solvable if and only if $\langle u_2, x_2 + t_2 u_2 \rangle = \langle u_3, x_3 + t_3 u_3 \rangle$ for some $t_2, t_3 \in \mathbb{C}$. Let $t_3 - t_2 = \langle u_2, x_2 \rangle - \langle u_3, x_3 \rangle$, then the system is always solvable.

Proof of Proposition 31. Define $S = \{s \in H^0(M, E) : s(v_1, v_2, v_3, u_1, u_2, u_3) = ([\langle T, v_2 \otimes v_3 \rangle], [\langle T, v_1 \otimes v_3 \rangle], [\langle T, v_1 \otimes v_2 \rangle], \langle T, u_2 \otimes u_3 \rangle - \langle T, v_1 \otimes v_2 \otimes v_3 \rangle u_1, [\langle T, u_1 \otimes u_3 \rangle], [\langle T, u_1 \otimes u_2 \rangle])\}$, By Lemma 34 and [12, Lemma 8], S generates E. By Theorem 32, a generic section of E does not vanish on M, i.e. there is a unique normalized singular vector tuple up to sign corresponding to each normalized singular value of a generic tensor T.

Since for a generic T has distinct equivalence classes of normalized singular pairs, $\phi_T(\lambda)$ has simple roots, then the resultant of the polynomials $\phi_T(\lambda)$ and $\phi'_T(\lambda)$, denoted by $\chi(T)$, does not vanish. Therefore

Theorem 35. The subset M formed by any tensor whose singular characteristic polynomial has multiple roots is a hypersurface, which is defined by $\chi(T) = 0$. X_{σ_1} forms some components of the real points of M. Any real tensor T with $\chi(T) \neq 0$ has a unique best rank one approximation. If this T is symmetric, then its unique best rank one approximation is also symmetric.

VIII. DEFLATABILITY

The relation between best rank-r and best rank-1 approximations of a matrix over \mathbb{R} or \mathbb{C} is well-known: A best rank-r approximation can be obtained from r successive best rank-1 approximations — a consequence of the Eckart–Young Theorem. It has been shown in [32] that this 'deflation procedure' does not work for real or complex d-tensors of order d > 2. In fact, more recently, it has been shown in [33] that the property almost never holds when d > 2.

We will see here that the 'deflatability' property does not hold for nonnegative tensor rank either.

Proposition 36. Let $r \ge 1$. For almost every positive tensor T of nonnegative rank > r + 1, a best nonnegative rank-(r + 1) approximation of T cannot be obtained from a best nonnegative rank-1 approximation of $T - T_{(r)}$, where $T_{(r)}$ is a best nonnegative rank-r approximation of T.

Proof. We will proceed by contradiction. Suppose T_p and T_p , $p = 1, \ldots, r+1$, are of rank 1 and satisfy

$$\left\| T - \lambda \sum_{p=1}^{r} T_{p} \right\| = \min_{X \in D_{r}^{+}} \left\| T - X \right\|,$$
$$\left\| T - \mu \sum_{p=1}^{r+1} \widetilde{T}_{p} \right\| = \min_{X \in D_{r+1}^{+}} \left\| T - X \right\|,$$

where $\left\|\sum_{p=1}^{r} T_{p}\right\| = \left\|\sum_{p=1}^{r+1} \widetilde{T}_{p}\right\| = 1$, and $\lambda \sum_{p=1}^{r} T_{p} = \mu \sum_{p=1}^{r} \widetilde{T}_{p}$. Hence we can assume $\widetilde{T}_{p} = \alpha T_{p}$ and $T_{p} = u_{1,p} \otimes \cdots \otimes u_{d,p}$ for each $p \in \{1, \ldots, r\}$, where $\alpha \mu = \lambda$, and $\widetilde{T}_{r+1} = \alpha u_{1,r+1} \otimes \cdots \otimes u_{d,r+1}$.

By Lemma 13, we have for every j = 1, ..., r, and $\ell = 1, ..., r + 1$,

$$\left\langle T - \lambda \sum_{p=1}^{r} u_{1,p} \otimes \cdots \otimes u_{d,p}, u_{1,j} \otimes \cdots \otimes \widehat{u_{i,j}} \otimes \cdots \otimes u_{d,j} \right\rangle = 0,$$
(VIII.1)

$$\left\langle T - \mu \sum_{p=1}^{r+1} \alpha u_{1,p} \otimes \cdots \otimes u_{d,p}, \, \alpha u_{1,\ell} \otimes \cdots \otimes \widehat{u_{i,\ell}} \otimes \cdots \otimes u_{d,\ell} \right\rangle = 0.$$
 (VIII.2)

We may simplify (VIII.2) to get

$$\left\langle T - \lambda \sum_{p=1}^{r+1} u_{1,p} \otimes \cdots \otimes u_{d,p}, u_{1,\ell} \otimes \cdots \otimes \widehat{u_{i,\ell}} \otimes \cdots \otimes u_{d,\ell} \right\rangle = 0.$$
 (VIII.3)

For $\ell = j$, we subtract (VIII.1) from (VIII.3) to get

 $\langle u_{1,r+1} \otimes \cdots \otimes u_{d,r+1}, u_{1,j} \otimes \cdots \otimes \widehat{u_{i,j}} \otimes \cdots \otimes u_{d,j} \rangle = 0$

for i = 1, ..., d, and j = 1, ..., r. By the nonnegativity of the vector $u_{i,r+1}$,

$$\prod_{k \neq i} \langle u_{k,r+1}, u_{k,j} \rangle = 0, \qquad (\text{VIII.4})$$

and

$$\langle T, u_{1,r+1} \otimes \cdots \otimes \widehat{u_{i,r+1}} \otimes \cdots \otimes u_{d,r+1} \rangle = \langle \lambda \sum_{p=1}^{r+1} u_{1,p} \otimes \cdots \otimes u_{d,p}, u_{1,r+1} \otimes \cdots \otimes \widehat{u_{i,r+1}} \otimes \cdots \otimes u_{d,r+1} \rangle$$
$$= \lambda \prod_{k \neq i} \|u_{k,r+1}\|^2 \cdot u_{i,r+1}.$$

In other words,

$$\left(\lambda \prod_{k=1}^{d} \|u_{k,r+1}\|, \frac{u_{1,r+1}}{\|u_{1,r+1}\|} \otimes \cdots \otimes \frac{u_{d,r+1}}{\|u_{d,r+1}\|}\right)$$

is a singular pair of T. So by Lemma 19, $u_{k,r+1} > 0$ for all k = 1, ..., d, which contradicts (VIII.4).

Following [33], we say that a tensor $T \in V^+$ with nonnegative rank *s* admits a *Schmidt–Eckart–Young decomposition* if it can be written as a linear combination of nonnegatively decomposable tensors $T = \sum_{p=1}^{s} u_{1,p} \otimes \cdots \otimes u_{d,p}$, and such that $\sum_{p=1}^{r} u_{1,p} \otimes \cdots \otimes u_{d,p}$ is a best nonnegative rank-*r* approximation of *T* for all $r = 1, \ldots, s$. Proposition 36 shows that a general nonnegative tensor does not admit a Schmidt–Eckart–Young decomposition.

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