TENSOR RANK AND THE ILL-POSEDNESS OF THE BEST LOW-RANK APPROXIMATION PROBLEM*

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Abstract. There has been continued interest in seeking a theorem describing optimal low-rank approximations to tensors of order 3 or higher that parallels the Eckart–Young theorem for matrices. In this paper, we argue that the naive approach to this problem is doomed to failure because, unlike matrices, tensors of order 3 or higher can fail to have best rank-r approximations. The phenomenon is much more widespread than one might suspect: examples of this failure can be constructed over a wide range of dimensions, orders, and ranks, regardless of the choice of norm (or even Brègman divergence). Moreover, we show that in many instances these counterexamples have positive volume: they cannot be regarded as isolated phenomena. In one extreme case, we exhibit a tensor space in which no rank-3 tensor has an optimal rank-2 approximation. The notable exceptions to this misbehavior are rank-1 tensors and order-2 tensors (i.e., matrices). In a more positive spirit, we propose a natural way of overcoming the ill-posedness of the low-rank approximation problem, by using weak solutions when true solutions do not exist. For this to work, it is necessary to characterize the set of weak solutions, and we do this in the case of rank 2, order 3 (in arbitrary dimensions). In our work we emphasize the importance of closely studying concrete low-dimensional examples as a first step toward more general results. To this end, we present a detailed analysis of equivalence classes of $2 \times 2 \times 2$ tensors, and we develop methods for extending results upward to higher orders and dimensions. Finally, we link our work to existing studies of tensors from an algebraic geometric point of view. The rank of a tensor can in theory be given a semialgebraic description; in other words, it can be determined by a system of polynomial inequalities. We study some of these polynomials in cases of interest to us; in particular, we make extensive use of the hyperdeterminant Δ on $\mathbb{R}^{2\times 2\times 2}$.

Key words. numerical multilinear algebra, tensors, multidimensional arrays, multiway arrays, tensor rank, tensor decompositions, low-rank tensor approximations, hyperdeterminants, Eckart–Young theorem, principal component analysis, PARAFAC, CANDECOMP, Brègman divergence of tensors

AMS subject classifications. 14P10, 15A03, 15A21, 15A69, 15A72, 49M27, 62H25, 68P01

DOI. 10.1137/06066518X

1. Introduction. Given an order-k tensor $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$, one is often required to find a *best rank-r approximation* to A—in other words, determine vectors $\mathbf{x}_i \in \mathbb{R}^{d_1}, \mathbf{y}_i \in \mathbb{R}^{d_2}, \ldots, \mathbf{z}_i \in \mathbb{R}^{d_k}, i = 1, \ldots, r$, which minimize

$$||A - \mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \cdots \otimes \mathbf{z}_1 - \cdots - \mathbf{x}_r \otimes \mathbf{y}_r \otimes \cdots \otimes \mathbf{z}_r||;$$

or, in short,

(APPROX(A, r)) $\operatorname{argmin}_{\operatorname{rank}_{\otimes}(B) \leq r} ||A - B||.$

Here $\|\cdot\|$ denotes some choice of norm on $\mathbb{R}^{d_1 \times \cdots \times d_k}$. When k = 2, the problem is completely resolved for unitarily invariant norms on $\mathbb{R}^{m \times n}$ with the *Eckart-Young*

http://www.siam.org/journals/simax/30-3/66518.html

^{*}Received by the editors July 16, 2006; accepted for publication (in revised form) by L. De Lathauwer June 7, 2007; published electronically September 25, 2008. This work was partially supported by DARPA grant 32905 and NSF grant DMS 01-01364.

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theorem [28], which states that if

$$A = U\Sigma V = \sum_{i=1}^{\operatorname{rank}(A)} \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i, \quad \sigma_i \ge \sigma_{i+1},$$

is the singular value decomposition of $A \in \mathbb{R}^{m \times n}$, then a best rank-*r* approximation is given by the first *r* terms in the above sum [33]. The best rank-*r* approximation problem for higher order tensors is a problem of central importance in the statistical analysis of multiway data [11, 16, 20, 21, 45, 50, 38, 56, 66, 67, 75, 76].

It is therefore not surprising that there has been continued interest in finding a satisfactory "singular value decomposition" and an "Eckart–Young theorem"-like result for tensors of higher order. The view expressed in the conclusion of [46] is representative of such efforts, and we reproduce it here:

An Eckart-Young type of best rank-r approximation theorem for tensors continues to elude our investigations but can perhaps eventually be attained by using a different norm or yet other definitions of orthogonality and rank.

It will perhaps come as a surprise to the reader that the problem of finding an "Eckart–Young-type theorem" is ill-founded because of a more fundamental difficulty: the best rank-r approximation problem APPROX(A, r) has no solution in general! This paper seeks to provide an answer to this and several related questions.

1.1. Summary. Since this is a long paper, we present an "executive summary" of selected results in this section and the next. We begin with the five main objectives of this article:

- 1. APPROX(A, r) is ill-posed for many r. We will show that, regardless of the choice of norm, the problem of determining a best rank-r approximation for an order-k tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ has no solution in general for $r = 2, \ldots, \min\{d_1, \ldots, d_k\}$ and $k \geq 3$. In other words, the best low-rank approximation problem for tensors is ill-posed for all orders (higher than 2), all norms, and many ranks.
- 2. APPROX(A, r) is ill-posed for many A. We will show that the set of tensors that fail to have a best low-rank approximation has positive volume. In other words, such failures are not rare; if one randomly picks a tensor A in a suitable tensor space, then there is a nonzero probability that A will fail to have a best rank-r approximation for some $r < \operatorname{rank}_{\otimes}(A)$.
- 3. Weak solutions to APPROX(A, r). We will propose a natural way to overcome the ill-posedness of the best rank-*r* approximation problem with the introduction of "weak solutions," which we explicitly characterize in the case r = 2, k = 3.
- 4. Semialgebraic description of tensor rank. From the Tarski–Seidenberg theorem in model theory [72, 65] we will deduce the following: for any d_1, \ldots, d_k , there exists a finite number of polynomial functions, $\Delta_1, \ldots, \Delta_m$, defined on $\mathbb{R}^{d_1 \times \cdots \times d_k}$ such that the rank of any $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ is completely determined by the signs of $\Delta_1(A), \ldots, \Delta_m(A)$. We work this out in the special case $\mathbb{R}^{2 \times 2 \times 2}$.
- 5. Reduction. We will give techniques for reducing certain questions about tensors (orbits, invariants, limits) from high-dimensional tensor spaces to lowerdimensional tensor spaces. For instance, if two tensors in $\mathbb{R}^{c_1 \times \cdots \times c_k}$ lie in distinct $\operatorname{GL}_{c_1,\ldots,c_k}(\mathbb{R})$ -orbits, then they lie in distinct $\operatorname{GL}_{d_1,\ldots,d_k}(\mathbb{R})$ -orbits in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ for any $d_i \geq c_i$.

The first objective is formally stated and proved in Theorem 4.10. The two notable exceptions where APPROX(A, r) has a solution are the cases r = 1 (approximation by rank-1 tensors) and k = 2 (A is a matrix). The standard way to prove these assertions is to use brute force: show that the sets where the approximators are to be found may be defined by polynomial equations. We will provide alternative elementary proofs of these results in Propositions 4.2 and 4.3 (see also Proposition 4.4).

The second objective is proved in Theorem 8.4, which holds true on $\mathbb{R}^{d_1 \times d_2 \times d_3}$ for arbitrary $d_1, d_2, d_3 \geq 2$. Stronger results can hold in specific cases: in Theorem 8.1, we will give an instance where *every* rank-*r* tensor fails to have a best rank-(r-1) approximator.

The third objective is primarily possible because of the following theorem, which asserts that the boundary of the set of rank-2 tensors can be explicitly parameterized. The proof, and a discussion of weak solutions, is given in section 5.

THEOREM 1.1. Let $d_1, d_2, d_3 \geq 2$. Let $A_n \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ be a sequence of tensors with rank_{\otimes} $(A_n) \leq 2$ and

$$\lim_{n \to \infty} A_n = A,$$

where the limit is taken in any norm topology. If the limiting tensor A has rank higher than 2, then rank_{\otimes}(A) must be exactly 3, and there exist pairs of linearly independent vectors $\mathbf{x}_1, \mathbf{y}_1 \in \mathbb{R}^{d_1}, \mathbf{x}_2, \mathbf{y}_2 \in \mathbb{R}^{d_2}, \mathbf{x}_3, \mathbf{y}_3 \in \mathbb{R}^{d_3}$ such that

(1.1)
$$A = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3.$$

Furthermore, the above result is not vacuous since

$$A_n = n\left(\mathbf{x}_1 + \frac{1}{n}\mathbf{y}_1\right) \otimes \left(\mathbf{x}_2 + \frac{1}{n}\mathbf{y}_2\right) \otimes \left(\mathbf{x}_3 + \frac{1}{n}\mathbf{y}_3\right) - n\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3$$

is an example of a sequence that converges to A.

A few conclusions can immediately be drawn from Theorem 1.1: (i) the boundary points of all order-3 rank-2 tensors can be completely parameterized by (1.1); (ii) a sequence of order-3 rank-2 tensors cannot "jump rank" by more than 1; (iii) A in (1.1), in particular, is an example of a tensor that has no best rank-2 approximation.

The formal statements and proofs of the fourth objective appear in section 6. The fifth objective is exemplified by our approach throughout the paper; some specific technical tools are discussed in sections 5.1 and 7.5.

On top of these five objectives, we pick up the following smaller results along the way. Some of these results address frequently asked questions in tensor approximation. They are discussed in sections 4.3–4.7, respectively.

- 6. *Divergence of coefficients.* Whenever a low-rank sequence of tensors converges to a higher-rank tensor, some of the terms in the sequence must blow up. In examples of minimal rank, all the terms blow up.
- 7. Maximum rank. For $k \geq 3$, the maximum rank of an order-k tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ (where $d_i \geq 2$) always exceeds $\min(d_1, \ldots, d_k)$. In contrast, for matrices $\min(d_1, d_2)$ does bound the rank.
- 8. Tensor rank can leap large gaps. Conclusion (ii) above does not generalize to rank r > 2. We will show that a sequence of fixed rank tensors can converge to a limiting tensor of arbitrarily higher rank.
- 9. Brègman divergences do not help. If we replace the norm by any continuous measure of "nearness" (including nonmetric measures like Brègman divergences), it does not change the ill-foundedness of APPROX(A, r).

10. Leibniz tensors. We will construct a rich family of sequences of tensors with degenerate limits, labeled by partial derivative operators. The special case $L_3(1)$ is in fact the principal example (1.1) in this paper.

1.2. Relation to prior work. The existence of tensors that can fail to have a best rank-r approximation has been known to algebraic geometers as early as the 19th century, albeit in a different language—the locus of rth secant planes to a Segre variety may not define a (closed) algebraic variety. It is also known to computational complexity theorists as the phenomenon underlying the concept of *border rank* [5, 6, 12, 48, 54] and is related to (but different from) what chemometricians and psychometricians call "CANDECOMP/PARAFAC degeneracy" [49, 51, 63, 68, 69]. We do not claim to be the first to have found such an example—that honor belongs to Bini, Capovani, Lotti, and Romani, who gave an explicit example of a sequence of rank-5 tensors converging to a rank-6 tensor in 1979 [7]. The novelty of Theorem 1.1 is not in demonstrating that a tensor may be approximated arbitrarily well by tensors of strictly lower rank but in *characterizing all such tensors* in the order-3 rank-2 case.

Having said this, we would like to point out that the ill-posedness of the best rankr approximation problem for high-order tensors is not at all well known, as is evident from the paragraph quoted earlier as well as other discussions in recent publications [44, 45, 46, 47, 80]. One likely reason is that in algebraic geometry, computational complexity, chemometrics, and psychometrics, the problem is neither stated in the form nor viewed in the light of obtaining a best low-rank approximation with respect to a choice of norm (we give several equivalent formulations of APPROX(A, r) in Proposition 4.1). As such, one goal of this paper will be to debunk, once and for all, the question of finding best low-rank approximations for tensors of order 3 or higher. As we stated earlier (as our first and second objectives), our contribution will be to show that such failures (i) can and will occur for tensors of *any* order higher than 2, (ii) will occur for tensors of many different ranks, (iii) will occur regardless of the choice of norm, and (iv) will occur with nonzero probability. Formally, we have the following two theorems (which will appear as Theorems 4.10 and 8.4 subsequently).

THEOREM 1.2. Let $k \geq 3$ and $d_1, \ldots, d_k \geq 2$. For any s such that $2 \leq s \leq \min\{d_1, \ldots, d_k\}$, there exists $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ with $\operatorname{rank}_{\otimes}(A) = s$ such that A has no best rank-r approximation for some r < s. The result is independent of the choice of norms.

THEOREM 1.3. If $d_1, d_2, d_3 \ge 2$, then the set

 $\{A \in \mathbb{R}^{d_1 \times d_2 \times d_3} \mid A \text{ does not have a best rank-2 approximation}\}$

has positive volume; indeed, it contains a nonempty open set.

A few features distinguish our work in this paper from existing studies in algebraic geometry [13, 14, 54, 55, 79] and algebraic computational complexity [2, 3, 5, 6, 7, 8, 12, 70]: (i) we are interested in tensors over \mathbb{R} as opposed to tensors over \mathbb{C} (it is well known that the rank of a tensor is dependent on the underlying field; cf. (7.5) and [4]); (ii) our interest is not limited to order-3 tensors (as is often the case in algebraic computational complexity)—we would like to prove results that hold for tensors of any order $k \geq 3$; (iii) since we are interested in questions pertaining to approximations in the norm, the Euclidean (norm-induced) topology will be more relevant than the Zariski topology¹ on the tensor product spaces—note in particular that the claim that a set is not closed in the Euclidean topology is a stronger statement than the corresponding claim in Zariski topology.

Our work in this paper in general, and in section 4.2 in particular, is related to studies of "CANDECOMP/PARAFAC degeneracy" or "diverging CANDECOMP/PARAFAC components" in psychometrics and chemometrics [49, 51, 63, 68, 69]. Diverging coefficients are a necessary consequence of the ill-posedness of APPROX(A, r) (see Propositions 4.8 and 4.9). In fact, examples of "k-factor divergence" abound for arbitrary k—see sections 4.4 and 4.7 for various constructions.

Section 5.4 discusses how the nonexistence of a best rank-r approximation poses serious difficulties for multilinear statistical models based on such approximations. In particular, we will see (i) why it is meaningless to ask for a "good" rank-r approximation when a best rank-r approximation does not exist; (ii) why even a small perturbation to a rank-r tensor can result in a tensor that has no best rank-r approximation; and (iii) why the computational feasibility of finding a "good" rank-rapproximation is questionable.

1.3. Outline of the paper. Section 2 introduces the basic algebra of tensors and k-way arrays. Section 3 defines tensor rank and gives some of its known (and unknown) algebraic properties. Section 4 studies the topological properties of tensor rank and the phenomenon of rank-jumping. Section 5 characterizes the problematic tensors in $\mathbb{R}^{2\times2\times2}$ and discusses the implications for approximation problems. Section 6 gives a short exposition of the semialgebraic point of view. Section 7 classifies tensors in $\mathbb{R}^{2\times2\times2}$ by orbit type. The orbit structure of tensor spaces is studied from several different aspects. Section 8 is devoted to the result that failure of APPROX(A, 2) occurs on a set of positive volume.

2. Tensors. Even though tensors are well-studied objects in the standard graduate mathematics curriculum [1, 27, 41, 52, 64] and more specifically in multilinear algebra [9, 34, 59, 60, 62, 78], a "tensor" continues to be viewed as a mysterious object by outsiders. We feel that we should say a few words to demystify the term.

In mathematics, the question "What is a vector?" has the simple answer "A vector is an element of a vector space"—in other words, a vector is characterized by the axioms that define the algebraic operations on a vector space. In physics, however, the question "What is a vector?" often means "What kinds of physical quantities can be represented by vectors?" The criterion has to do with the change of basis theorem: an *n*-dimensional vector is an "object" that is represented by n real numbers once a basis is chosen *only* if those real numbers transform themselves as expected when one changes the basis. For exactly the same reason, the meaning of a tensor is obscured by its more restrictive use in physics. In physics (and also engineering), a tensor is an "object" represented by a k-way array of real numbers that transforms according to certain rules (cf. (2.2)) under a change of basis. In mathematics, these "transformation rules" are simply consequences of the multilinearity of the tensor product and the change of basis theorem for vectors. Today, books written primarily for a physics audience [32, 61] have increasingly adopted the mathematical definition, but a handful of recently published books continue to propagate the obsolete (and vague) definition. To add to the confusion, "tensor" is frequently used to refer to a

¹Note that the Zariski topology on \mathbb{k}^n is defined for any field \mathbb{k} (not just algebraically closed ones). It is the weakest topology such that all polynomial functions are continuous. In particularly, the closed sets are precisely the zero sets of collections of polynomials.

tensor field (e.g., metric tensor, stress tensor, Riemann curvature tensor).

For our purposes, an order-k tensor **A** is simply an element of a tensor product of k real vector spaces, $V_1 \otimes V_2 \otimes \cdots \otimes V_k$, as defined in any standard algebra textbook [1, 9, 27, 34, 41, 52, 59, 60, 62, 64, 78]. Up to a choice of bases on V_1, \ldots, V_k , such an element may be coordinatized, i.e., represented as a k-way array A of real numbers much as an element of an n-dimensional vector space may be, up to a choice of basis, represented by an n-tuple of numbers in \mathbb{R}^n . We will let $\mathbb{R}^{d_1 \times \cdots \times d_k}$ denote the vector space of k-way array of real numbers $A = [a_{j_1 \cdots j_k}]_{j_1=1,\ldots,j_k=1}^{d_1,\ldots,d_k}$ with addition and scalar multiplication defined coordinatewise:

(2.1)
$$[\![a_{j_1\cdots j_k}]\!] + [\![b_{j_1\cdots j_k}]\!] := [\![a_{j_1\cdots j_k} + b_{j_1\cdots j_k}]\!]$$
 and $\lambda[\![a_{j_1\cdots j_k}]\!] := [\![\lambda a_{j_1\cdots j_k}]\!]$

A k-way array of numbers (or k-array) is also sometimes referred to as a k-dimensional hypermatrix [30].

It may be helpful to think of a k-array as a *data structure*, convenient for representing or storing the coefficients of a tensor with respect to a set of bases. The tensor itself carries with it an *algebraic structure*, by virtue of being an element of a tensor product of vector spaces. Once bases have been chosen for these vector spaces, we may view the order-k tensor as a k-way array equipped with the algebraic operations defined in (2.1) and (2.3). Despite this correspondence, it is not wise to regard "tensor" as being synonymous with "array."

Notation. We will denote elements of abstract tensor spaces in boldface uppercase letters, whereas k-arrays will be denoted in italic uppercase letters. Thus **A** is an abstract tensor, which may be represented by an array of numbers A with respect to a basis. We will use double brackets to enclose the entries of a k-array— $A = [\![a_{j_1\cdots j_k}]\!]_{j_1=1,\ldots,j_k=1}^{d_1,\ldots,d_k}$ —and when there is no risk of confusion, we will leave out the range of the indices and simply write $A = [\![a_{j_1\cdots j_k}]\!]_{.}$

2.1. Multilinear matrix multiplication. Matrices can act on other matrices through two independent multiplication operations: left-multiplication and right-multiplication. Matrices act on order-3 tensors via *three* different multiplication operations. These can be combined into a single formula. If $A = \llbracket a_{ijk} \rrbracket \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $L = [\lambda_{pi}] \in \mathbb{R}^{c_1 \times d_1}$, $M = [\mu_{qj}] \in \mathbb{R}^{c_2 \times d_2}$, $N = [\nu_{rk}] \in \mathbb{R}^{c_3 \times d_3}$, then the array A may be transformed into an array $A' = \llbracket a'_{pqr} \rrbracket \in \mathbb{R}^{c_1 \times c_2 \times c_3}$ by the equation

(2.2)
$$a'_{pqr} = \sum_{i,j,k=1}^{d_1,d_2,d_3} \lambda_{pi} \mu_{qj} \nu_{rk} a_{ijk}.$$

We call this operation the *multiplication* of A by matrices L, M, N, which we write succinctly as

$$A' = (L, M, N) \cdot A$$

Informally, we are multiplying the 3-way array A on its three "sides" by the matrices L, M, N, respectively.

Remark. This notation is standard in mathematics—the elements of a product $G_1 \times G_2 \times G_3$ are generally grouped in the form (L, M, N), and when a set with some algebraic structure G acts on another set X, the result of $g \in G$ acting on $x \in X$ is almost universally written $g \cdot x$ [1, 9, 27, 41, 52, 64]. Here we are just looking at the case when $G = \mathbb{R}^{c_1 \times d_1} \times \mathbb{R}^{c_2 \times d_2} \times \mathbb{R}^{c_3 \times d_3}$ and $X = \mathbb{R}^{d_1 \times d_2 \times d_3}$. This is consistent with notation adopted in earlier work [42], but more recent publications such as [20, 21] have used $A \times_1 L^{\top} \times_2 M^{\top} \times_3 N^{\top}$ in place of $(L, M, N) \cdot A$.

Multilinear matrix multiplication extends in a straightforward way to arrays of arbitrary order: if $A = \llbracket a_{i_1\cdots i_k} \rrbracket \in \mathbb{R}^{d_1\times\cdots\times d_k}$ and $L_1 = [\lambda_{ij}^{(1)}] \in \mathbb{R}^{c_1\times d_1}, \ldots, L_k = [\lambda_{ij}^{(k)}] \in \mathbb{R}^{c_k\times d_k}$, then $A' = (L_1, \ldots, L_k) \cdot A$ is the array $A' = \llbracket a'_{i_1\cdots i_k} \rrbracket \in \mathbb{R}^{c_1\times\cdots\times c_k}$ given by

(2.3)
$$a'_{i_1\cdots i_k} = \sum_{i_1,\dots,i_k=1}^{d_1,\dots,d_k} \lambda_{i_1j_1}\cdots\lambda_{i_kj_k} a_{j_1\cdots j_k}$$

We will now see how a 3-way array representing a tensor in $V_1 \otimes V_2 \otimes V_3$ transforms under changes of bases of the vector spaces V_i . Suppose the 3-way array $A = [\![a_{ijk}]\!] \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ represents an order-3 tensor $\mathbf{A} \in V_1 \otimes V_2 \otimes V_3$ with respect to bases $\mathcal{B}_1 = \{\mathbf{e}_i \mid i = 1, \ldots, d_1\}$, $\mathcal{B}_2 = \{\mathbf{f}_j \mid j = 1, \ldots, d_2\}$, $\mathcal{B}_3 = \{\mathbf{g}_k \mid k = 1, \ldots, d_3\}$ on V_1, V_2, V_3 , i.e.,

(2.4)
$$\mathbf{A} = \sum_{i,j,k=1}^{d_1,d_2,d_3} a_{ijk} \mathbf{e}_i \otimes \mathbf{f}_j \otimes \mathbf{g}_k$$

Suppose we choose different bases $\mathcal{B}'_1 = \{\mathbf{e}'_i \mid i = 1, ..., d_1\}, \mathcal{B}'_2 = \{\mathbf{f}'_j \mid j = 1, ..., d_2\}, \mathcal{B}'_3 = \{\mathbf{g}'_k \mid k = 1, ..., d_3\}$ on V_1, V_2, V_3 , where

(2.5)
$$\mathbf{e}_{i} = \sum_{p=1}^{d_{1}} \lambda_{ip} \mathbf{e}'_{p}, \quad \mathbf{f}_{j} = \sum_{q=1}^{d_{2}} \mu_{jq} \mathbf{f}'_{q}, \quad \mathbf{g}_{k} = \sum_{r=1}^{d_{3}} \nu_{kr} \mathbf{g}'_{r},$$

and $L = [\lambda_{pi}] \in \mathbb{R}^{d_1 \times d_1}$, $M = [\mu_{qj}] \in \mathbb{R}^{d_2 \times d_2}$, $N = [\nu_{rk}] \in \mathbb{R}^{d_3 \times d_3}$ are the respective change-of-basis matrices. Substituting the expressions for (2.5) into (2.4), we get

$$\mathbf{A} = \sum_{p,q,r=1}^{d_1,d_2,d_3} a'_{pqr} \mathbf{e}'_p \otimes \mathbf{f}'_q \otimes \mathbf{g}'_r,$$

where

(2.6)
$$a'_{pqr} = \sum_{i,j,k=1}^{d_1,d_2,d_3} \lambda_{pi} \mu_{qj} \nu_{rk} a_{ijk}$$

or, more simply, $A' = (L, M, N) \cdot A$. Here the 3-way array $A' = \llbracket a'_{pqr} \rrbracket \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ represents **A** with respect to the new choice of bases $\mathcal{B}'_1, \mathcal{B}'_2, \mathcal{B}'_3$.

All of this extends immediately to order-k tensors and k-way arrays. Henceforth, when a choice of basis is implicit, we will not distinguish between an order-k tensor and the k-way array that represents it.

The change-of-basis matrices L, M, N in the discussion above are of course invertible; in other words they belong to their respective general linear groups. We write $\operatorname{GL}_d(\mathbb{R})$ for the group of nonsingular matrices in $\mathbb{R}^{d \times d}$. Thus $L \in \operatorname{GL}_{d_1}(\mathbb{R})$, $M \in \operatorname{GL}_{d_2}(\mathbb{R})$, and $N \in \operatorname{GL}_{d_3}(\mathbb{R})$. In addition to general linear transformations, it is natural to consider orthogonal transformations. We write $O_d(\mathbb{R})$ for the subgroup of $\operatorname{GL}_d(\mathbb{R})$ of transformations which preserve the Euclidean inner product. The following shorthand is helpful:

$$GL_{d_1,\ldots,d_k}(\mathbb{R}) := GL_{d_1}(\mathbb{R}) \times \cdots \times GL_{d_k}(\mathbb{R}),$$

$$O_{d_1,\ldots,d_k}(\mathbb{R}) := O_{d_1}(\mathbb{R}) \times \cdots \times O_{d_k}(\mathbb{R}).$$

Then $O_{d_1,\ldots,d_k}(\mathbb{R}) \leq GL_{d_1,\ldots,d_k}(\mathbb{R})$, and both groups act on $\mathbb{R}^{d_1 \times \cdots \times d_k}$ via multilinear multiplication.

DEFINITION 2.1. Two tensors $A, A' \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ are said to be GL-equivalent (or simply "equivalent") if there exists $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R})$ such that A' =

 $(L_1, \ldots, L_k) \cdot A$. More strongly, we say that A, A' are O-equivalent if such a transformation L can be found in $O_{d_1,\ldots,d_k}(\mathbb{R})$.

For example, if V_1, \ldots, V_k are vector spaces and $\dim(V_i) = d_i$, then $A, A' \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ represent the same tensor in $V_1 \otimes \cdots \otimes V_k$ with respect to two different bases if and only if A, A' are GL-equivalent.

We finish with some trivial properties of multilinear matrix multiplication: for $A, B \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $\alpha, \beta \in \mathbb{R}$,

$$(2.7) \qquad (L_1,\ldots,L_k) \cdot (\alpha A + \beta B) = \alpha(L_1,\ldots,L_k) \cdot A + \beta(L_1,\ldots,L_k) \cdot B$$

and for $L_i \in \mathbb{R}^{c_i \times d_i}$, $M_i \in \mathbb{R}^{b_i \times c_i}$, $i = 1, \dots, k$,

(2.8)
$$(M_1, \ldots, M_k) \cdot [(L_1, \ldots, L_k) \cdot A] = (M_1 L_1, \ldots, M_k L_k) \cdot A.$$

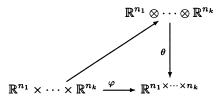
Last, the name multilinear matrix multiplication is justified since for any $M_i, N_i \in \mathbb{R}^{c_i \times d_i}, \alpha, \beta \in \mathbb{R}$,

(2.9)
$$(L_1, \dots, \alpha M_i + \beta N_i, \dots, L_k) \cdot A = \alpha(L_1, \dots, M_i, \dots, L_k) \cdot A + \beta(L_1, \dots, N_i, \dots, L_k) \cdot A.$$

2.2. Outer-product rank and outer-product decomposition of a tensor. Let $\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}$ be the tensor product of the vector spaces $\mathbb{R}^{d_1}, \ldots, \mathbb{R}^{d_k}$. Note that the Segre map

$$(2.10) \qquad \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}^{d_1 \times \cdots \times d_k}, \qquad (\mathbf{x}_1, \dots, \mathbf{x}_k) \mapsto [\![x_{j_1}^{(1)} \cdots x_{j_k}^{(k)}]\!]_{j_1, \dots, j_k=1}^{d_1, \dots, d_k}$$

is multilinear and so by the universal property of the tensor product [1, 9, 27, 34, 41, 52, 59, 60, 62, 64, 78], we have a unique linear map φ such that the following diagram commutes:



Clearly,

(2.11)
$$\varphi(\mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k) = \llbracket x_{j_1}^{(1)} \cdots x_{j_k}^{(k)} \rrbracket_{j_1, \dots, j_k=1}^{d_1, \dots, d_k}$$

and φ is a vector space isomorphism since $\dim(\mathbb{R}^{d_1 \times \cdots \times d_k}) = \dim(\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}) = d_1 \cdots d_k$. Henceforth we will not distinguish between these two spaces. The elements of $\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k} \cong \mathbb{R}^{d_1 \times \cdots \times d_k}$ will be called a tensor and we will also drop φ in (2.11) and write

(2.12)
$$\mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k = \llbracket x_{j_1}^{(1)} \cdots x_{j_k}^{(k)} \rrbracket_{j_1, \dots, j_k=1}^{d_1, \dots, d_k}$$

Note that the symbol \otimes in (2.11) denotes the formal tensor product and by dropping φ , we are using the same symbol \otimes to define the *outer product* of the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_k$ via the formula (2.12). Hence, a tensor can be represented either as a k-dimensional array or as a sum of formal tensor products of k vectors, where the equivalence between

these two objects is established by taking the formal tensor product of k vectors as defining a k-way array via (2.12).

It is clear that the map in (2.10) is not surjective—the image consists precisely of the *decomposable tensors*: a tensor $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ is said to be *decomposable* if it can be written in the form

$$A = \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k$$

with $\mathbf{x}_i \in \mathbb{R}^{d_i}$ for i = 1, ..., k. It is easy to see that multilinear matrix multiplication of decomposable tensors obeys the formula

(2.13)
$$(L_1,\ldots,L_k) \cdot (\mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k) = L_1 \mathbf{x}_1 \otimes \cdots \otimes L_k \mathbf{x}_k.$$

Remark. The outer product can be viewed as a special case of multilinear matrix multiplication. For example, a linear combination of outer products of vectors may be expressed in terms of multilinear matrix multiplication:

$$\sum_{i=1}^r \lambda_i \mathbf{x}_i \otimes \mathbf{y}_i \otimes \mathbf{z}_i = (X, Y, Z) \cdot \Lambda$$

with matrices $X = [\mathbf{x}_1, \dots, \mathbf{x}_r] \in \mathbb{R}^{l \times r}$, $Y = [\mathbf{y}_1, \dots, \mathbf{y}_r] \in \mathbb{R}^{m \times r}$, $Z = [\mathbf{z}_1, \dots, \mathbf{z}_r] \in \mathbb{R}^{n \times r}$ and a "diagonal tensor" $\Lambda = \text{diag}[\lambda_1, \dots, \lambda_r] \in \mathbb{R}^{r \times r \times r}$.

We now come to the main concept of interest in this paper.

DEFINITION 2.2. A tensor has outer-product rank r if it can be written as a sum of r decomposable tensors, but no fewer. We will write rank_{\otimes}(A) for the outer-product rank of A. So

$$\operatorname{rank}_{\otimes}(A) := \min\left\{r \mid A = \sum_{i=1}^{r} \mathbf{u}_i \otimes \mathbf{v}_i \otimes \cdots \otimes \mathbf{z}_i\right\}.$$

Note that a nonzero decomposable tensor has outer-product rank 1.

Despite several claims of originality as well as many misplaced attributions to these claims, the concepts of tensor rank and the decomposition of a tensor into a sum of outer products of vectors was the product of much earlier work by Frank L. Hitch-cock in 1927 [39, 40]. We call this the outer-product rank mainly to distinguish it from the *multilinear rank* to be defined in section 2.5 (also due to Hitchcock), but we will use the term *rank* or *tensor rank* most of the time when there is no danger of confusion.

LEMMA 2.3 (invariance of tensor rank). (1) If $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $(L_1, \ldots, L_k) \in \mathbb{R}^{c_1 \times d_1} \times \cdots \times \mathbb{R}^{c_k \times d_k}$, then

(2.14)
$$\operatorname{rank}_{\otimes}((L_1, \ldots, L_k) \cdot A) \leq \operatorname{rank}_{\otimes}(A).$$

(2) If $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R}) := \operatorname{GL}_{d_1}(\mathbb{R}) \times \cdots \times \operatorname{GL}_{d_k}(\mathbb{R})$, then

(2.15)
$$\operatorname{rank}_{\otimes}((L_1,\ldots,L_k)\cdot A) = \operatorname{rank}_{\otimes}(A).$$

Proof. Inequality (2.14) follows from (2.13) and (2.7). Indeed, if $A = \sum_{j=1}^{r} \mathbf{x}_{1}^{j} \otimes \cdots \otimes \mathbf{x}_{k}^{j}$, then $(L_{1}, \ldots, L_{k}) \cdot A = \sum_{j=1}^{r} L_{1} \mathbf{x}_{1}^{j} \otimes \cdots \otimes L_{k} \mathbf{x}_{k}^{j}$. Furthermore, if the L_{i} are invertible, then by (2.8) we get

$$A = (L_1^{-1}, \dots, L_k^{-1}) \cdot [(L_1, \dots, L_k) \cdot A],$$

and so $\operatorname{rank}_{\otimes}(A) \leq \operatorname{rank}_{\otimes}((L_1, \ldots, L_k) \cdot A)$, and hence (2.15). \Box

2.3. The outer product and direct sum operations on tensors. The outer product of vectors defined earlier is a special case of the *outer product* of two tensors. Let $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ be a tensor of order k and $B \in \mathbb{R}^{c_1 \times \cdots \times c_\ell}$ be a tensor of order ℓ ; then the outer product of A and B is the tensor $C := A \otimes B \in \mathbb{R}^{d_1 \times \cdots \times d_k \times c_1 \times \cdots \times c_\ell}$ of order $k + \ell$ defined by

$$c_{i_1\cdots i_k j_1\cdots j_l} = a_{i_1\cdots i_k} b_{j_1\cdots j_l}.$$

The direct sum of two order-k tensors $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $B \in \mathbb{R}^{c_1 \times \cdots \times c_k}$ is the order-k tensor $C := A \oplus B \in \mathbb{R}^{(c_1+d_1) \times \cdots \times (c_k+d_k)}$ defined by

$$c_{i_1,\ldots,i_k} = \begin{cases} a_{i_1,\ldots,i_k} & \text{if } 1 \le i_\alpha \le d_\alpha, \ \alpha = 1,\ldots,k; \\ b_{i_1-d_1,\ldots,i_k-d_k} & \text{if } d_\alpha + 1 \le i_\alpha \le c_\alpha + d_\alpha, \ \alpha = 1,\ldots,k; \\ 0 & \text{otherwise.} \end{cases}$$

For matrices, the direct sum of $A \in \mathbb{R}^{m_1 \times n_1}$ and $B \in \mathbb{R}^{m_2 \times n_2}$ is simply the blockdiagonal matrix

$$A \oplus B = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \in \mathbb{R}^{(m_1 + m_2) \times (n_1 + n_2)}.$$

The direct sum of two order-3 tensors $A \in \mathbb{R}^{l_1 \times m_1 \times n_1}$ and $B \in \mathbb{R}^{l_2 \times m_2 \times n_2}$ is a "block tensor" with A in the (1, 1, 1)-block and B in the (2, 2, 2)-block

$$A \oplus B = \begin{bmatrix} A & 0 & 0 & 0 \\ 0 & 0 & 0 & B \end{bmatrix} \in \mathbb{R}^{(l_1 + l_2) \times (m_1 + m_2) \times (n_1 + n_2)}.$$

In abstract terms, if U_i, V_i, W_i are vector spaces such that $W_i = U_i \oplus V_i$ for i = 1, ..., k, then tensors $A \in U_1 \otimes \cdots \otimes U_k$ and $B \in V_1 \otimes \cdots \otimes V_k$ have direct sum $A \oplus B \in W_1 \otimes \cdots \otimes W_k$.

2.4. Tensor subspaces. Whenever $c \leq d$ there is a canonical embedding $\mathbb{R}^c \subseteq \mathbb{R}^d$ given by identifying the *c* coordinates of \mathbb{R}^c with the first *c* coordinates of \mathbb{R}^d .

Let $c_i \leq d_i$ for $i = 1, \ldots, k$. Then there is a canonical embedding $\mathbb{R}^{c_1 \times \cdots \times c_k} \subset \mathbb{R}^{d_1 \times \cdots \times d_k}$, defined as the tensor product of the embeddings $\mathbb{R}^{c_i} \subseteq \mathbb{R}^{d_i}$. We say that $\mathbb{R}^{c_1 \times \cdots \times c_k}$ is a *tensor subspace* of $\mathbb{R}^{d_1 \times \cdots \times d_k}$. More generally, if U_i, V_i are vector spaces with $U_i \subset V_i$ for $i = 1, \ldots, k$, then there is an inclusion $U_1 \otimes \cdots \otimes U_k \subset V_1 \otimes \cdots \otimes V_k$ defined as the tensor product of the inclusions $U_i \subset V_i$. Again we say that $U_1 \otimes \cdots \otimes U_k$ is a tensor subspace of $V_1 \otimes \cdots \otimes V_k$.

If $B \in \mathbb{R}^{c_1 \times \cdots \times c_k}$ then its image under the canonical embedding into $\mathbb{R}^{d_1 \times \cdots d_k}$ can be written in the form $B \oplus 0$, where $0 \in \mathbb{R}^{(d_1 - c_1) \times \cdots \times (d_k - c_k)}$ is the zero tensor. A tensor $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ is said to be GL-*equivalent* (or simply "equivalent") to B if there exists $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R})$ such that $B \oplus 0 = (L_1, \ldots, L_k) \cdot A$. More strongly, we say that A is O-*equivalent* ("orthogonally equivalent") to B if such a transformation can be found in $O_{d_1, \ldots, d_k}(\mathbb{R})$.

We note that A is GL-equivalent to B if and only if there exist full-rank matrices $M_i \in \mathbb{R}^{d_i \times c_i}$ such that $A = (M_1, \ldots, M_k) \cdot B$. In one direction, M_i can be obtained as the first c_i columns of L_i^{-1} . In the other direction, L_i^{-1} can be obtained from M_i by adjoining extra columns. There is a similar statement for O-equivalence. Instead of full rank, the condition is that the matrices M_i have orthogonal columns.

An important simplifying principle in tensor algebra is that questions about a tensor—such as "What is its rank?"—can sometimes, as we shall see, be reduced to analogous questions about an equivalent tensor in a lower-dimensional tensor subspace.

2.5. Multilinear rank and multilinear decomposition of a tensor. Although we focus on outer product rank in this paper, there is a simpler notion of multilinear rank which directly generalizes the column and row ranks of a matrix to higher order tensors.

For convenience, we will consider order-3 tensors only. Let $A = \llbracket a_{ijk} \rrbracket \in \mathbb{R}^{d_1 \times d_2 \times d_3}$. For fixed values of $j \in \{1, \ldots, d_2\}$ and $k \in \{1, \ldots, d_3\}$, consider the vector $A_{\bullet jk} := [a_{ijk}]_{i=1}^{d_1} \in \mathbb{R}^{d_1}$. Likewise consider (column) vectors $A_{i\bullet k} := [a_{ijk}]_{j=1}^{d_2} \in \mathbb{R}^{d_2}$ for fixed values of i, k, and consider (row) vectors $A_{ij\bullet} := [a_{ijk}]_{k=1}^{d_3} \in \mathbb{R}^{d_3}$ for fixed values of i, j. In analogy with row rank and column rank, define

$$r_1(A) := \dim(\operatorname{span}_{\mathbb{R}} \{A_{\bullet jk} \mid 1 \le j \le d_2, 1 \le k \le d_3\}), r_2(A) := \dim(\operatorname{span}_{\mathbb{R}} \{A_{i\bullet k} \mid 1 \le i \le d_1, 1 \le k \le d_3\}), r_3(A) := \dim(\operatorname{span}_{\mathbb{R}} \{A_{ij\bullet} \mid 1 \le i \le d_1, 1 \le j \le d_2\}).$$

For another interpretation, note that $\mathbb{R}^{d_1 \times d_2 \times d_3}$ can be viewed as $\mathbb{R}^{d_1 \times d_2 d_3}$ by ignoring the multiplicative structure between the second and third factors. Then $r_1(A)$ is simply the rank of A regarded as $d_1 \times d_2 d_3$ matrix. There are similar definitions for $r_2(A)$ and $r_3(A)$.

The multilinear rank of A, denoted² rank_{\boxplus}(A), is the 3-tuple $(r_1(A), r_2(A), r_3(A))$. Again, this concept is not new but was first explored by Hitchcock in the same papers where he introduced tensor rank [39, 40]. Hitchcock introduces a very general multiplex rank, which includes tensor rank and the separate terms of our multilinear rank as special cases. A point to note is that $r_1(A)$, $r_2(A)$, $r_3(A)$, and rank_{\otimes}(A) are in general all different—a departure from the case of matrices, where the row rank, column rank, and outer product rank are always equal. Observe that we will always have

(2.16)
$$r_i(A) \le \min\{\operatorname{rank}_{\otimes}(A), d_i\}.$$

Let us verify this for r_1 : if $A = \mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{z}_1 + \cdots + \mathbf{x}_r \otimes \mathbf{y}_r \otimes \mathbf{z}_r$, then each vector $A_{\bullet jk}$ belongs to $\operatorname{span}(\mathbf{x}_1, \ldots, \mathbf{x}_r)$. This implies that $r_1 \leq \operatorname{rank}_{\otimes}(A)$, and $r_1 \leq d_1$ is immediate from the definitions. A simple but useful consequence of (2.16) is that

(2.17)
$$\operatorname{rank}_{\otimes}(A) \ge \|\operatorname{rank}_{\boxplus}(A)\|_{\infty} = \max\{r_i(A) \mid i = 1, \dots, k\}$$

If $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $\operatorname{rank}_{\boxplus}(A) = (r_1, r_2, r_3)$, then there exist subspaces $U_i \subset \mathbb{R}^{d_i}$ with $\dim(U_i) = r_i$, such that $A \in U_1 \otimes U_2 \otimes U_3$. We call these the supporting subspaces of A. The supporting subspaces are minimal in the sense that if $A \in V_1 \otimes V_2 \otimes V_3$, then $U_i \subset V_i$ for i = 1, 2, 3. This observation leads to an alternate definition:

$$r_i(A) = \min\{\dim(U_i) \mid U_1 \subset \mathbb{R}^{d_1}, U_2 \subset \mathbb{R}^{d_2}, U_3 \subset \mathbb{R}^{d_3}, A \in U_1 \otimes U_2 \otimes U_3\}$$

An immediate consequence of this characterization is that $\operatorname{rank}_{\mathbb{H}}(A)$ is invariant under the action of $\operatorname{GL}_{d_1,d_2,d_3}(\mathbb{R})$: if $A' = (L, M, N) \cdot A$, where $(L, M, N) \in$ $\operatorname{GL}_{d_1,d_2,d_3}(\mathbb{R})$, then $\operatorname{rank}_{\mathbb{H}}(A) = \operatorname{rank}_{\mathbb{H}}((L, M, N) \cdot A)$. Indeed, if U_1, U_2, U_3 are the supporting subspaces of A, then $L(U_1), M(U_2), N(U_3)$ are the supporting subspaces of $(L, M, N) \cdot A$.

More generally, we have multilinear rank equivalents of (2.14) and (2.15): if $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $(L_1, \ldots, L_k) \in \mathbb{R}^{c_1 \times d_1} \times \cdots \times \mathbb{R}^{c_k \times d_k}$, then

(2.18) $\operatorname{rank}_{\boxplus}((L_1, \dots, L_k) \cdot A) \le \operatorname{rank}_{\boxplus}(A),$

²The symbol \boxplus is meant to evoke an impression of the rows and columns in a matrix.

and if $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R})$, then

(2.19)
$$\operatorname{rank}_{\boxplus}((L_1,\ldots,L_k)\cdot A) = \operatorname{rank}_{\boxplus}(A).$$

Suppose rank_{\mathbb{H}} $(A) = (r_1, r_2, r_3)$. By applying transformations $L_i \in \operatorname{GL}_{d_i}(\mathbb{R})$ which carry U_i to \mathbb{R}^{r_i} , it follows that A is equivalent to some $B \in \mathbb{R}^{r_1 \times r_2 \times r_3}$. Alternatively there exist $B \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ and full-rank matrices $L \in \mathbb{R}^{d_1 \times r_1}$, $M \in \mathbb{R}^{d_2 \times r_2}$, $N \in \mathbb{R}^{d_3 \times r_3}$, such that

$$A = (L, M, N) \cdot B$$

The matrices L, M, N may be chosen to have orthonormal columns or to be unit lower-triangular—a fact easily deduced from applying the QR-decomposition or the LU-decomposition to the full-rank matrices L, M, N and using (2.8).

To a large extent, the study of tensors $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank_{\mathbb{H}} $(A) \leq (r_1, r_2, r_3)$ reduces to the study of tensors in $\mathbb{R}^{r_1 \times r_2 \times r_3}$. This is a useful reduction, but (unlike the matrix case) it does not even come close to giving us a full classification of tensor types.

2.6. Multilinear orthogonal projection. If U is a subspace of an innerproduct space V (for instance, $V = \mathbb{R}^n$ with the usual dot product), then there is an orthogonal projection from V onto U, which we denote π_U . We regard this as a map $V \to V$. As such, it is self-adjoint (i.e., has a symmetric matrix with respect to any orthonormal basis) and satisfies $\pi_U^2 = \pi_U$, $\operatorname{im}(\pi_U) = U$, $\operatorname{ker}(\pi_U) = U^{\perp}$. We note Pythagoras's theorem for any $\mathbf{v} \in V$:

$$\|\mathbf{v}\|^2 = \|\pi_U \mathbf{v}\|^2 + \|(1 - \pi_U)\mathbf{v}\|^2.$$

We now consider orthogonal projections for tensor spaces. If U_1, U_2, U_3 are subspaces of V_1, V_2, V_3 , respectively, then $U_1 \otimes U_2 \otimes U_3$ is a tensor subspace of $V_1 \otimes V_2 \otimes V_3$, and the multilinear map $\Pi = (\pi_{U_1}, \pi_{U_2}, \pi_{U_3})$ is a projection onto that subspace. In fact, Π is orthogonal with respect to the Frobenius norm. The easiest way to see this is to identify $U_i \subset V_i$ with $\mathbb{R}^{c_i} \subset \mathbb{R}^{d_i}$ by taking suitable orthonormal bases; then Π acts by zeroing out all the entries of a $d_1 \times d_2 \times d_3$ array outside the initial $c_1 \times c_2 \times c_3$ block. In particular we have Pythagoras's theorem for any $A \in V_1 \otimes V_2 \otimes V_3$:

(2.20)
$$||A||_F^2 = ||\Pi A||_F^2 + ||(1 - \Pi)A||_F^2.$$

Being a multilinear map, Π is nonincreasing for rank_{\otimes}, rank_{\boxplus}, as in (2.14), (2.18).

There is a useful orthogonal projection Π_A associated with any tensor $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$. Let U_1, U_2, U_3 be the supporting subspaces of A so that $A \in U_1 \otimes U_2 \otimes U_3$, and $\dim(U_i) = r_i(A)$ for i = 1, 2, 3. Define

$$\Pi_A = (\pi_1(A), \pi_2(A), \pi_3(A)) = (\pi_{U_1}, \pi_{U_2}, \pi_{U_3}).$$

PROPOSITION 2.4. $\Pi_A(A) = A$.

Proof. A belongs to $U_1 \otimes U_2 \otimes U_3$, which is fixed by Π_A .

PROPOSITION 2.5. The function $A \mapsto \prod_A$ is continuous over subsets of $\mathbb{R}^{d_1 \times d_2 \times d_3}$ on which rank_{\boxplus}(A) is constant.

Proof. We show, for example, that $\pi_1 = \pi_1(A)$ depends continuously on A. For any $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, select $r = r_1(A)$ index pairs (j, k) such that the vectors $A_{\bullet jk}$ are linearly independent. For any B near A, assemble the marked vectors as a matrix

 $X = X(B) \in \mathbb{R}^{d_i \times r}$. Then $\pi_1 = X(X^\top X)^{-1}X^\top =: P(B)$ by a well-known formula in linear algebra. The function P(B) is defined and continuous as long as the *r* selected vectors remain independent, which is true on a neighborhood of *A*. Finally, the orthogonal projection defined by P(B) maps onto the span of the *r* selected vectors. Thus, if $r_1(B) = r$, then $P(B) = \pi_1(B)$. \Box

It is clear that the results of this section apply to tensor spaces of all orders.

3. The algebra of tensor rank. We will state and prove a few basic results about the outer-product rank.

PROPOSITION 3.1. Let $A \in \mathbb{R}^{c_1 \times \cdots \times c_k} \subset \mathbb{R}^{d_1 \times \cdots \times d_k}$. The rank of A regarded as a tensor in $\mathbb{R}^{c_1 \times \cdots \times c_k}$ is the same as the rank of A regarded as a tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$.

Proof. For each *i* the identity on \mathbb{R}^{c_i} factors as a pair of maps $\mathbb{R}^{c_i} \stackrel{\iota_i}{\hookrightarrow} \mathbb{R}^{d_i} \xrightarrow{\pi_i} \mathbb{R}^{c_i}$, where ι_i is the canonical inclusion and π is the projection map given by deleting the last $d_i - c_i$ coordinates. Applying (2.14) twice, we have

$$\operatorname{rank}_{\otimes}(A) \ge \operatorname{rank}_{\otimes}((\iota_1, \dots, \iota_k) \cdot A) \ge \operatorname{rank}_{\otimes}((\pi_1, \dots, \pi_k) \cdot (\iota_1, \dots, \iota_k) \cdot A)$$
$$= \operatorname{rank}_{\otimes}((\pi_1 \iota_1, \dots, \pi_k \iota_k) \cdot A)$$
$$= \operatorname{rank}_{\otimes}(A),$$

so $A \in \mathbb{R}^{c_1 \times \cdots \times c_k}$ and its image $(\iota_1, \ldots, \iota_k) \cdot A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ must have equal tensor ranks. \Box

COROLLARY 3.2. Suppose $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and $\operatorname{rank}_{\mathbb{H}}(A) \leq (c_1, \ldots, c_k)$. Then $\operatorname{rank}_{\otimes}(A) = \operatorname{rank}_{\otimes}(B)$ for an equivalent tensor $B \in \mathbb{R}^{c_1 \times \cdots \times c_k}$.

The next corollary asserts that tensor rank is consistent under a different scenario: when order-k tensors are regarded as order-l tensors for l > k by taking the tensor product with a nonzero monomial term.

COROLLARY 3.3. Let $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ be an order-k tensor and $\mathbf{u}_{k+1} \in \mathbb{R}^{d_{k+1}}, \ldots, \mathbf{u}_{k+\ell} \in \mathbb{R}^{d_{k+\ell}}$ be nonzero vectors. Then

$$\operatorname{rank}_{\otimes}(A) = \operatorname{rank}_{\otimes}(A \otimes \mathbf{u}_{k+1} \otimes \cdots \otimes \mathbf{u}_{k+\ell})$$

Proof. Let $c_{k+1} = \cdots = c_{k+l} = 1$ and apply Proposition 3.1 to $A \in \mathbb{R}^{d_1 \times \cdots \times d_k} = \mathbb{R}^{d_1 \times \cdots \times d_k \times c_{k+1} \times \cdots \times c_{k+\ell}} \hookrightarrow \mathbb{R}^{d_1 \times \cdots \times d_k \times d_{k+1} \times \cdots \times d_{k+\ell}}$. Note that the image of the inclusion is $A \otimes \mathbf{e}_1^{(k+1)} \otimes \cdots \otimes \mathbf{e}_1^{(k+\ell)}$, where $\mathbf{e}_1^{(i)} = (1, 0, \dots, 0)^\top \in \mathbb{R}^{d_i}$. So we have

$$\operatorname{rank}_{\otimes}(A \otimes \mathbf{e}_1^{(k+1)} \otimes \cdots \otimes \mathbf{e}_1^{(k+\ell)}) = \operatorname{rank}_{\otimes}(A).$$

The general case for arbitrary nonzero $\mathbf{u}_i \in \mathbb{R}^{d_i}$ follows from applying to $A \otimes \mathbf{e}_1^{(k+1)} \otimes \cdots \otimes \mathbf{e}_1^{(k+\ell)}$ a multiplication $(I_{d_1}, \ldots, I_{d_k}, L_1, \ldots, L_\ell) \in \operatorname{GL}_{d_1, \ldots, d_{k+\ell}}(\mathbb{R})$, where I_d is the $d \times d$ identity matrix and L_i is a nonsingular matrix with $L_i \mathbf{e}_i = \mathbf{u}_i$. It then follows from Lemma 2.3 that

$$\operatorname{rank}_{\otimes}(A \otimes \mathbf{u}_{k+1} \otimes \cdots \otimes \mathbf{u}_{k+\ell}) = \operatorname{rank}_{\otimes}[(I_{d_1}, \dots, I_{d_k}, L_1, \dots, L_\ell) \cdot (A \otimes \mathbf{e}_1^{(k+1)} \otimes \cdots \otimes \mathbf{e}_1^{(k+\ell)})] = \operatorname{rank}_{\otimes}(A \otimes \mathbf{e}_1^{(k+1)} \otimes \cdots \otimes \mathbf{e}_1^{(k+\ell)}). \quad \Box$$

Let $E = \mathbf{u}_{k+1} \otimes \mathbf{u}_{k+2} \otimes \cdots \otimes \mathbf{u}_{k+\ell} \in \mathbb{R}^{d_{k+1} \times \cdots \times d_{k+\ell}}$. So $\operatorname{rank}_{\otimes}(E) = 1$ and Corollary 3.3 says that $\operatorname{rank}_{\otimes}(A \otimes E) = \operatorname{rank}_{\otimes}(A) \operatorname{rank}_{\otimes}(E)$. Note that this last relation does not generalize. If $\operatorname{rank}_{\otimes}(A) > 1$ and $\operatorname{rank}_{\otimes}(B) > 1$, then it is true that

$$\operatorname{rank}_{\otimes}(A \otimes B) \leq \operatorname{rank}_{\otimes}(A) \operatorname{rank}_{\otimes}(B)$$

since one can multiply decompositions of A, B term by term to obtain a decomposition of $A \otimes B$, but it can happen (cf. [12]) that

$$\operatorname{rank}_{\otimes}(A \otimes B) < \operatorname{rank}_{\otimes}(A) \operatorname{rank}_{\otimes}(B).$$

The corresponding statement for direct sum is still an open problem for tensors of order 3 or higher. It has been conjectured by Strassen [70] that

(3.1)
$$\operatorname{rank}_{\otimes}(A \oplus B) \stackrel{?}{=} \operatorname{rank}_{\otimes}(A) + \operatorname{rank}_{\otimes}(B)$$

for all order-k tensors A and B. However JáJá and Takche [43] have shown that for the special case when A and B are of order 3 and at least one of them is a matrix pencil (i.e., a tensor of size $p \times q \times 2$, $p \times 2 \times q$, or $2 \times p \times q$ that may be regarded as a pair of $p \times q$ matrices), then the direct sum conjecture holds.

THEOREM 3.4 (JáJá–Takche [43]). Let $A \in \mathbb{R}^{c_1 \times c_2 \times c_3}$ and $B \in \mathbb{R}^{d_1 \times d_2 \times d_3}$. If $2 \in \{c_1, c_2, c_3, d_1, d_2, d_3\}$, then

$$\operatorname{rank}_{\otimes}(A \oplus B) = \operatorname{rank}_{\otimes}(A) + \operatorname{rank}_{\otimes}(B).$$

It is not hard to define tensors of arbitrarily high rank so long as we have sufficiently many linearly independent vectors in every factor.

LEMMA 3.5. For $\ell = 1, ..., k$, let $\mathbf{x}_1^{(\ell)}, ..., \mathbf{x}_r^{(\ell)} \in \mathbb{R}^{d_i}$ be linearly independent. Then the tensor defined by

$$A := \sum_{j=1}^{r} \mathbf{x}_{j}^{(1)} \otimes \mathbf{x}_{j}^{(2)} \otimes \cdots \otimes \mathbf{x}_{j}^{(k)} \in \mathbb{R}^{d_{1} \times d_{2} \times \cdots \times d_{k}}$$

has $\operatorname{rank}_{\otimes}(A) = r$.

Proof. Note that $\operatorname{rank}_{\boxplus}(A) = (r, r, \dots, r)$. By (2.17), we get

$$\operatorname{rank}_{\otimes}(A) \ge \max\{r_i(A) \mid i = 1, \dots, k\} = r$$

On the other hand, it is clear that $\operatorname{rank}_{\otimes}(A) \leq r$. \Box

Thus, in $\mathbb{R}^{d_1 \times \cdots \times d_k}$, it is easy to write down tensors of any rank r in the range $0 \leq r \leq \min\{d_1, \ldots, d_k\}$. For matrices, this exhausts all possibilities; the rank of $A \in \mathbb{R}^{d_1 \times d_2}$ is at most $\min\{d_1, d_2\}$. In contrast, for $k \geq 3$, there will always be tensors in $\mathbb{R}^{d_1 \times d_k}$ that have rank exceeding $\min\{d_1, \ldots, d_k\}$. We will see this in Theorem 4.10.

4. The topology of tensor rank. Let $A = [\![a_{i_1 \cdots i_k}]\!] \in \mathbb{R}^{d_1 \times \cdots \times d_k}$. The Frobenius norm of A and its associated inner product are defined by

$$||A||_F^2 := \sum_{i_1,\dots,i_k=1}^{d_1,\dots,d_k} |a_{i_1\dots i_k}|^2, \quad \langle A,B\rangle_F := \sum_{i_1,\dots,i_k=1}^{d_1,\dots,d_k} a_{i_1\dots i_k} b_{i_1\dots i_k}.$$

Note that for a decomposable tensor, the Frobenius norm satisfies

(4.1)
$$\|\mathbf{u} \otimes \mathbf{v} \otimes \cdots \otimes \mathbf{z}\|_F = \|\mathbf{u}\|_2 \|\mathbf{v}\|_2 \cdots \|\mathbf{z}\|_2,$$

where $\|\cdot\|_2$ denotes the l^2 -norm of a vector, and more generally

$$(4.2) ||A \otimes B||_F = ||A||_F ||B||_F$$

for arbitrary tensors A, B. Another important property which follows from (2.13) and (4.1) is orthogonal invariance:

(4.3)
$$\|(L_1, \dots, L_k) \cdot A\|_F = \|A\|_F$$

whenever $(L_1, \ldots, L_k) \in O_{d_1, \ldots, d_k}(\mathbb{R})$. There are of course many other natural choices of norms on tensor product spaces [25, 36]. The important thing to note is that $\mathbb{R}^{d_1 \times \cdots \times d_k}$ being finite dimensional, all these norms will induce the same topology.

We define the following (topological) subspaces of $\mathbb{R}^{d_1 \times \cdots \times d_k}$:

$$\mathcal{S}_r(d_1,\ldots,d_k) = \left\{ A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}_{\otimes}(A) \leq r \right\},\\ \overline{\mathcal{S}}_r(d_1,\ldots,d_k) = \text{closure of } \mathcal{S}_r(d_1,\ldots,d_k) \subset \mathbb{R}^{d_1 \times \cdots \times d_k}.$$

Clearly the only reason to define \overline{S}_r is the sad fact that S_r is not necessarily (or even usually) closed—the theme of this paper. See section 4.2.

We occasionally refer to elements of S_r as "rank-*r* tensors." This is slightly inaccurate, since lower-rank tensors are included, but convenient. However, the direct assertions "*A* has rank *r*" and "rank(*A*) = *r*" are always meant in the precise sense. The same remarks apply to "border rank," which is defined in section 5.5. We refer to elements of \overline{S}_r as "border-rank-*r* tensors" and describe them as being "rank-*r*approximable."

Theorem 5.1 asserts that $\overline{S}_2(d_1, d_2, d_3) \subset S_3(d_1, d_2, d_3)$ for all d_1, d_2, d_3 , and that the exceptional tensors $\overline{S}_2(d_1, d_2, d_3) \setminus S_2(d_1, d_2, d_3)$ are all of a particular form.

4.1. Upper semicontinuity. Discrete-valued rank functions on spaces of matrices or tensors cannot usefully be continuous, because they would then be constant and would not have any classifying power. As a sort of compromise, matrix rank is well known to be an upper semicontinuous function; if $\operatorname{rank}(A) = r$, then $\operatorname{rank}(B) \ge r$ for all matrices B in a neighborhood of A. This is not true for the outer-product rank of tensors (as we will see in section 4.2). There are several equivalent ways of formulating this assertion.

PROPOSITION 4.1. Let $r \geq 2$ and $k \geq 3$. Given the norm-topology on $\mathbb{R}^{d_1 \times \cdots \times d_k}$, the following statements are equivalent:

- (a) The set $\mathcal{S}_r(d_1, \ldots, d_k) := \{A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}_{\otimes}(A) \leq r\}$ is not closed.
- (b) There exists a sequence $A_n \in \mathbb{R}^{d_1 \times \cdots \times d_k}$, $\operatorname{rank}_{\otimes}(A_n) \leq r, n \in \mathbb{N}$, converging to $B \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ with $\operatorname{rank}_{\otimes}(B) > r$.
- (c) There exists $B \in \mathbb{R}^{d_1 \times \cdots \times d_k}$, rank_{\otimes}(B) > r, that may be approximated arbitrarily closely by tensors of strictly lower rank, i.e.,

$$\inf\{\|B - A\| \mid \operatorname{rank}_{\otimes}(A) \le r\} = 0.$$

(d) There exists $C \in \mathbb{R}^{d_1 \times \cdots \times d_k}$, rank_{\otimes}(C) > r, that does not have a best rank-r approximation; i.e.,

$$\inf\{\|C - A\| \mid \operatorname{rank}_{\otimes}(A) \le r\}$$

is not attained (by any A with rank_{\otimes}(A) $\leq r$).

Proof. It is obvious that (a) \Rightarrow (b) \Rightarrow (c) \Rightarrow (d). To complete the chain, we just need to show that (d) \Rightarrow (a). Suppose $S := S_r(d_1, \ldots, d_k)$ is closed. Since the closed ball of radius ||C|| centered at C, $\{A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid ||C - A|| \leq ||C||\}$, intersects

 \mathcal{S} nontrivially (e.g., 0 is in both sets), their intersection $\mathcal{T} = \{A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}_{\otimes}(A) \leq r, \|C - A\| \leq \|C\|\}$ is a nonempty compact set. Now observe that

$$\delta := \inf\{ \|C - A\| \mid A \in \mathcal{S} \} = \inf\{ \|C - A\| \mid A \in \mathcal{T} \}$$

since any $A' \in S \setminus T$ must have ||C - A'|| > ||C|| while we know that $\delta \leq ||C||$. By the compactness of T, there exists $A_* \in T$ such that $||C - A_*|| = \delta$. So the required infimum is attained by $A_* \in T \subset S$. \Box

We caution the reader that there exist tensors of rank > r that do not have a best rank-r approximation but cannot be approximated arbitrarily closely by rankr tensors, i.e., $\inf\{\|C - A\| \mid \operatorname{rank}_{\otimes}(A) \leq r\} > 0$. In other words, statement (d) applies to a strictly larger class of tensors than statement (c) (cf. section 8). The tensors in statement (d) are sometimes called "degenerate" in the psychometrics and chemometrics literature (e.g., [49, 51, 63, 68, 69]), but we prefer to avoid this term since it is inconsistent (and often at odds) with common usage in Mathematics. For example, in Table 7.1, the tensors in the orbit classes of D_2, D'_2, D''_2 are all degenerate, but statement (d) does not apply to them; on the other hand, the tensors in the orbit class of G_3 are nondegenerate, but Theorem 8.1 tells us that they are all of the form in statement (d).

We begin by getting three well-behaved cases out of the way. The proofs shed light on what can go wrong in all the other cases.

PROPOSITION 4.2. For all d_1, \ldots, d_k , we have $\overline{S}_1(d_1, \ldots, d_k) = S_1(d_1, \ldots, d_k)$. Proof. Suppose $A_n \to A$, where rank_{\otimes} $(A_n) \leq 1$. We can write

$$A_n = \lambda_n \mathbf{u}_{1,n} \otimes \mathbf{u}_{2,n} \otimes \cdots \otimes \mathbf{u}_{k,n},$$

where $\lambda_n = ||A_n||$ and the vectors $\mathbf{u}_{i,n} \in \mathbb{R}^{d_i}$ have unit norm. Certainly $\lambda_n = ||A_n|| \rightarrow ||A|| =: \lambda$. Moreover, since the unit sphere in \mathbb{R}^{d_i} is compact, each sequence $\mathbf{u}_{i,n}$ has a convergent subsequence, with limit \mathbf{u}_i , say. It follows that there is a subsequence of A_n which converges to $\lambda \mathbf{u}_1 \otimes \cdots \otimes \mathbf{u}_k$. This must equal A, and it has rank at most 1. \Box

PROPOSITION 4.3. For all r and d_1, d_2 , we have $\overline{S}_r(d_1, d_2) = S_r(d_1, d_2)$. In other words, matrix rank is upper-semicontinuous.

Proof. Suppose $A_n \to A$, where rank $(A_n) \leq r$, so we can write

$$A_n = \lambda_{1,n} \mathbf{u}_{1,n} \otimes \mathbf{v}_{1,n} + \dots + \lambda_{r,n} \mathbf{u}_{r,n} \otimes \mathbf{v}_{r,n}.$$

Convergence of the sequence A_n does not imply convergence of the individual terms $\lambda_{i,n}$, $\mathbf{u}_{i,n}$, $\mathbf{v}_{i,n}$, even in a subsequence. However, if we take the singular value decomposition, then the $\mathbf{u}_{i,n}$ and $\mathbf{v}_{i,n}$ are unit vectors and the $\lambda_{i,n}$ satisfy

$$\lambda_{1,n}^2 + \dots + \lambda_{r,n}^2 = \|A_n\|.$$

Since $||A_n|| \to ||A||$ this implies that the $\lambda_{i,n}$ are uniformly bounded. Thus we can find a subsequence with convergence $\lambda_{i,n} \to \lambda_i$, $\mathbf{u}_{i,n} \to \mathbf{u}_i$, $\mathbf{v}_{i,n} \to \mathbf{v}_i$ for all *i*. Then

$$A = \lambda_1 \mathbf{u}_1 \otimes \mathbf{v}_1 + \dots + \lambda_r \mathbf{u}_r \otimes \mathbf{v}_r,$$

which has rank at most r.

PROPOSITION 4.4. The multilinear rank function $\operatorname{rank}_{\boxplus}(A) = (r_1(A), \ldots, r_k(A))$ is upper-semicontinuous.

Proof. Each r_i is the rank of a matrix obtained by rearranging the entries of A, and is therefore upper-semicontinuous in A by Proposition 4.3.

COROLLARY 4.5. Every tensor has a best rank-1 approximation. Every matrix has a best rank-r approximation. Every order-k tensor has a best approximation with rank_{\boxplus} $\leq (r_1, \ldots, r_k)$ for any specified (r_1, \ldots, r_k) .

Proof. These statements follow from Propositions 4.2, 4.3, and 4.4, together with the implication $(d) \Rightarrow (a)$ from Proposition 4.1.

4.2. Tensor rank is not upper-semicontinuous. Here is the simplest example of the failure of outer-product rank to be upper-semicontinuous. This is the first example of a more general construction which we discuss in section 4.7. A formula similar to (4.4) appeared as Exercise 62 in section 4.6.4 of Knuth's *The Art of Computer Programming* [48] (the original source is [8]). Other examples have appeared in [7] (the earliest known to us) and [63], as well as in unpublished work of Kruskal.

PROPOSITION 4.6. Let $\mathbf{x}_1, \mathbf{y}_1 \in \mathbb{R}^{d_1}, \mathbf{x}_2, \mathbf{y}_2 \in \mathbb{R}^{d_2}$, and $\mathbf{x}_3, \mathbf{y}_3 \in \mathbb{R}^{d_3}$ be vectors such that each pair $\mathbf{x}_i, \mathbf{y}_i$ is linearly independent. Then the tensor

$$(4.4) A := \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 \in \mathbb{R}^{d_1 \times d_2 \times d_3}$$

has rank 3 but can be approximated arbitrarily closely by tensors of rank 2. In particular, A does not have a best rank-2 approximation.

Proof. For each $n \in \mathbb{N}$, define

(4.5)
$$A_n := n\left(\mathbf{x}_1 + \frac{1}{n}\mathbf{y}_1\right) \otimes \left(\mathbf{x}_2 + \frac{1}{n}\mathbf{y}_2\right) \otimes \left(\mathbf{x}_3 + \frac{1}{n}\mathbf{y}_3\right) - n\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3.$$

Clearly, $\operatorname{rank}_{\otimes}(A_n) \leq 2$, and since, as $n \to \infty$,

$$\begin{split} \|A_n - A\|_F &\leq \frac{1}{n} \|\mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|_F \\ &+ \frac{1}{n^2} \|\mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|_F \to 0, \end{split}$$

we see that A is approximated arbitrary closely by tensors A_n .

It remains to establish that $\operatorname{rank}_{\otimes}(A) = 3$. From the three-term format of A, we deduce only that $\operatorname{rank}_{\otimes}(A) \leq 3$. A clean proof that $\operatorname{rank}_{\otimes}(A) > 2$ is included in the proof of Theorem 7.1, but this depends on the properties of the polynomial Δ defined in section 5.3. A more direct argument is given in the next lemma.

LEMMA 4.7. Let $\mathbf{x}_1, \mathbf{y}_1 \in \mathbb{R}^{d_1}, \mathbf{x}_2, \mathbf{y}_2 \in \mathbb{R}^{d_2}, \mathbf{x}_3, \mathbf{y}_3 \in \mathbb{R}^{d_3}, and$

$$A = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3.$$

Then rank_{\otimes}(A) = 3 if and only if $\mathbf{x}_i, \mathbf{y}_i$ are linearly independent for i = 1, 2, 3.

Proof. Only two distinct vectors are involved in each factor of the tensor product, so rank_{\mathbb{H}} $(A) \leq (2, 2, 2)$ and we can work in $\mathbb{R}^{2 \times 2 \times 2}$ (Corollary 3.2). More strongly, if any of the pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$ is linearly dependent, then A is GL-equivalent to a tensor in $\mathbb{R}^{1 \times 2 \times 2}$, $\mathbb{R}^{2 \times 1 \times 2}$, or $\mathbb{R}^{2 \times 2 \times 1}$. These spaces are isomorphic to $\mathbb{R}^{2 \times 2}$, so the maximum possible rank of A is 2.

Conversely, suppose each pair $\{\mathbf{x}_i, \mathbf{y}_i\}$ is linearly independent. We may as well assume that

(4.6)
$$A = \begin{bmatrix} 0 & 1 & | & 1 & 0 \\ 1 & 0 & | & 0 & 0 \end{bmatrix}$$

since we can transform A to that form using a multilinear transformation (L_1, L_2, L_3) , where $L_i(\mathbf{x}_i) = \mathbf{e}_1$ and $L_i(\mathbf{y}_i) = \mathbf{e}_2$ for i = 1, 2, 3.

Suppose, for a contradiction, that $\operatorname{rank}_{\otimes}(A) \leq 2$; then we can write

$$(4.7) A = \mathbf{u}_1 \otimes \mathbf{u}_2 \otimes \mathbf{u}_3 + \mathbf{v}_1 \otimes \mathbf{v}_2 \otimes \mathbf{v}_3$$

for some $\mathbf{u}_i, \mathbf{v}_i \in \mathbb{R}^{d_i}$.

Claim 1. The vectors $\mathbf{u}_1, \mathbf{v}_1$ are independent. If they are not, then let $\varphi : \mathbb{R}^2 \to \mathbb{R}$ be a nonzero linear map such that $\varphi(\mathbf{u}_1) = \varphi(\mathbf{v}_1) = 0$. Using the expressions in (4.7) and (4.6), we find that

$$\mathbf{0} = (\varphi, I, I) \cdot A = \begin{bmatrix} \varphi(\mathbf{e}_2) & \varphi(\mathbf{e}_1) \\ \varphi(\mathbf{e}_1) & 0 \end{bmatrix}$$

in $\mathbb{R}^{1 \times 2 \times 2} \cong \mathbb{R}^{2 \times 2}$, which is a contradiction because $\varphi(\mathbf{e}_1)$ and $\varphi(\mathbf{e}_2)$ cannot both be zero.

Claim 2. The vectors $\mathbf{u}_1, \mathbf{e}_1$ are dependent. Indeed, let $\varphi_u : \mathbb{R}^2 \to \mathbb{R}$ be a linear map whose kernel is spanned by \mathbf{u}_1 . Then

$$\varphi_u(\mathbf{v}_1)(\mathbf{v}_2 \otimes \mathbf{v}_3) = (\varphi_u, I, I) \cdot A = \begin{bmatrix} \varphi_u(\mathbf{e}_2) & \varphi_u(\mathbf{e}_1) \\ \varphi_u(\mathbf{e}_1) & 0 \end{bmatrix}$$

in $\mathbb{R}^{1 \times 2 \times 2} \cong \mathbb{R}^{2 \times 2}$. The left-hand side (LHS) has rank at most 1, which implies on the right-hand side (RHS) that $\varphi_u(\mathbf{e}_1) = 0$, and hence $\mathbf{e}_1 \in \operatorname{span}{\mathbf{u}_1}$.

Claim 3. The vectors $\mathbf{v}_1, \mathbf{e}_1$ are dependent. Indeed, let $\varphi_v : \mathbb{R}^2 \to \mathbb{R}$ be a linear map whose kernel is spanned by \mathbf{v}_1 . Then

$$\varphi_{v}(\mathbf{u}_{1})(\mathbf{u}_{2}\otimes\mathbf{u}_{3}) = (\varphi_{v}, I, I) \cdot A = \begin{bmatrix} \varphi_{v}(\mathbf{e}_{2}) & \varphi_{v}(\mathbf{e}_{1}) \\ \varphi_{v}(\mathbf{e}_{1}) & 0 \end{bmatrix}$$

in $\mathbb{R}^{1\times 2\times 2} \cong \mathbb{R}^{2\times 2}$. The LHS has rank at most 1, which implies on the RHS that $\varphi_v(\mathbf{e}_1) = 0$, and hence $\mathbf{e}_1 \in \operatorname{span}\{\mathbf{v}_1\}$.

Taken together, the three claims are inconsistent. This is the desired contradiction. Thus $\operatorname{rank}_{\otimes}(A) > 2$, and therefore $\operatorname{rank}_{\otimes}(A) = 3$. \Box

Remark. Note that if we take $d_1 = d_2 = d_3 = 2$, then (4.4) is an example of a tensor whose outer-product rank exceeds min $\{d_1, d_2, d_3\}$.

4.3. Diverging coefficients. What goes wrong in the example of Proposition 4.6? Why do the rank-2 decompositions of the A_n fail to converge to a rank-2 decomposition of A? We can attempt to mimic the proofs of Propositions 4.2 and 4.3 by seeking convergent subsequences for the rank-2 decompositions of the A_n . We fail because we cannot simultaneously keep all the variables bounded. For example, in the decomposition

$$A_n = n\left(\mathbf{x}_1 + \frac{1}{n}\mathbf{y}_1\right) \otimes \left(\mathbf{x}_2 + \frac{1}{n}\mathbf{y}_2\right) \otimes \left(\mathbf{x}_3 + \frac{1}{n}\mathbf{y}_3\right) - n\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3$$

the vector terms converge but the coefficients $\lambda_1 = \lambda_2 = n$ tend to infinity. In spite of this, the sequence A_n itself remains bounded.

In fact, rank-jumping always occurs like this (see also [49]).

PROPOSITION 4.8. Suppose $A_n \to A$, where $\operatorname{rank}_{\otimes}(A) \ge r+1$ and $\operatorname{rank}_{\otimes}(A_n) \le r$ for all n. If we write

$$A_n = \lambda_{1,n} \mathbf{u}_{1,n} \otimes \mathbf{v}_{1,n} \otimes \mathbf{w}_{1,n} + \dots + \lambda_{r,n} \mathbf{u}_{r,n} \otimes \mathbf{v}_{r,n} \otimes \mathbf{w}_{r,n},$$

where the vectors $\mathbf{u}_{i,n}$, $\mathbf{v}_{i,n}$, $\mathbf{w}_{i,n}$ are unit vectors, then $\max_i\{|\lambda_{i,n}|\} \to \infty$ as $n \to \infty$. Moreover, at least two of the coefficient sequences $\{\lambda_{i,n} \mid n = 1, 2, ...\}$ are unbounded.

Proof. If the sequence $\max_i\{|\lambda_{i,n}|\}$ does not diverge to ∞ , then it has a bounded subsequence. In this subsequence, the coefficients and vectors are all bounded, so we can pass to a further subsequence in which each of the coefficient sequences and vector sequences is convergent:

$$\lambda_{i,n} \to \lambda_i, \quad \mathbf{u}_{i,n} \to \mathbf{u}_i, \quad \mathbf{v}_{i,n} \to \mathbf{v}_i, \quad \mathbf{w}_{i,n} \to \mathbf{w}_i.$$

It follows that $A = \lambda_1 \mathbf{u}_1 \otimes \mathbf{v}_1 \otimes \mathbf{w}_1 + \cdots + \lambda_r \mathbf{u}_r \otimes \mathbf{v}_r \otimes \mathbf{w}_r$, so it has rank at most r, which is a contradiction.

Thus $\max_i\{|\lambda_{i,n}|\}$ diverges to ∞ . It follows that at least one of the coefficient sequences has a divergent subsequence. If there were only one such coefficient sequence, all the others being bounded, then (on the subsequence) A_n would be dominated by this term and consequently $||A_n||$ would be unbounded. Since $A_n \to A$, this cannot happen. Thus there are at least two unbounded coefficient sequences. \Box

For a minimal rank-jumping example, all the coefficients must diverge to ∞ .

PROPOSITION 4.9. Suppose $A_n \to A$, where $\operatorname{rank}_{\otimes}(A) = r + s$ and $\operatorname{rank}_{\otimes}(A_n) \leq r$ for all n. If we write

$$A_n = \lambda_{1,n} \mathbf{u}_{1,n} \otimes \mathbf{v}_{1,n} \otimes \mathbf{w}_{1,n} + \dots + \lambda_{r,n} \mathbf{u}_{r,n} \otimes \mathbf{v}_{r,n} \otimes \mathbf{w}_{r,n},$$

where the vectors $\mathbf{u}_{i,n}$, $\mathbf{v}_{i,n}$, $\mathbf{w}_{i,n}$ are unit vectors, then there are two possibilities: either (i) all of the sequences $|\lambda_{i,n}|$ diverge to ∞ as $n \to \infty$ or (ii) in the same tensor space there exists $B_n \to B$, where $\operatorname{rank}_{\otimes}(B) \ge r' + s$ and $\operatorname{rank}_{\otimes}(B_n) \le r'$ for all n, for some r' < r.

Proof. Suppose one of the coefficient sequences, say, $|\lambda_{i,n}|$, fails to diverge as $n \to \infty$; so it has a bounded subsequence. In a further subsequence, the *i*th term $R_n = \lambda_{i,n} \mathbf{u}_{i,n} \otimes \mathbf{v}_{i,n} \otimes \mathbf{w}_{i,n}$ converges to a tensor R of rank (at most) 1. Writing $B_n = A_n - R_n$, we find that $B_n \to B = A - R$ on this subsequence, with rank $\otimes (B_n) \le r - 1$. Moreover, $r + s \le \operatorname{rank}_{\otimes}(A) \le \operatorname{rank}_{\otimes}(B) + \operatorname{rank}_{\otimes}(R)$, so $\operatorname{rank}_{\otimes}(B) \ge (r - 1) + s$.

Remark. Clearly the arguments in Propositions 4.8 and 4.9 apply to tensors of all orders, not just order 3. We also note that the vectors $(\mathbf{u}_{i,n}, \text{ etc.})$ need not be unit vectors; they just have to be uniformly bounded.

One interpretation of Proposition 4.8 is that if one attempts to minimize

$$\|A - \lambda_1 \mathbf{u}_1 \otimes \mathbf{v}_1 \otimes \mathbf{w}_1 - \dots - \lambda_r \mathbf{u}_r \otimes \mathbf{v}_r \otimes \mathbf{w}_r\|$$

for a tensor A which does not have a best rank-r approximation, then (at least some of) the coefficients λ_i become unbounded. This phenomenon of diverging summands has been observed in practical applications of multilinear models in psychometrics and chemometrics and is commonly referred to in those circles as "CANDECOMP/PARAFAC degeneracy" or "diverging CANDECOMP/PARAFAC components" [49, 51, 63, 68, 69]. More precisely, these are called "k-factor degeneracies" when there are k diverging summands whose sum stays bounded. 2- and 3-factor degeneracies were exhibited in [63] and 4- and 5-factor degeneracies were exhibited in [68]. There are uninteresting (see section 4.4) and interesting (see section 4.7) ways of generating k-factor degeneracies for arbitrarily large k.

4.4. Higher orders, higher ranks, arbitrary norms. We will now show that the rank-jumping phenomenon—that is, the failure of $S_r(d_1, \ldots, d_k)$ to be closed—is independent of the choice of norms and can be extended to arbitrary order. The norm

independence is a trivial consequence of a basic fact in functional analysis: all norms on finite dimensional vector spaces are equivalent; in particular, any norm will induce the same unique topology on a finite dimensional vector space.

THEOREM 4.10. For $k \geq 3$ and $d_1, \ldots, d_k \geq 2$, the problem of determining a best rank-r approximation for an order-k tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ has no solution in general for any $r = 2, \ldots, \min\{d_1, \ldots, d_k\}$. In particular, there exists $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ with

$$\operatorname{rank}_{\otimes}(A) = r + 1$$

that has no best rank-r approximation. The result is independent of the choice of norms.

Proof. We begin by assuming k = 3.

Higher rank. Let $2 \leq r \leq \min\{d_1, d_2, d_3\}$. By Lemma 3.5, we can construct a tensor $B \in \mathbb{R}^{(d_1-2)\times(d_2-2)\times(d_3-2)}$ with rank r-2. By Proposition 4.6, we can construct a convergent sequence of tensors $C_n \to C$ in $\mathbb{R}^{2\times2\times2}$ with rank $\otimes(C_n) \leq 2$ and rank $\otimes(C) = 3$. Let $A_n = B \oplus C_n \in \mathbb{R}^{d_1 \times d_2 \times d_3}$. Then $A_n \to A := B \oplus C$ and rank $\otimes(A_n) \leq \operatorname{rank}_{\otimes}(B) + \operatorname{rank}_{\otimes}(C_n) \leq r$. The result of JáJá–Takche (Theorem 3.4) implies that $\operatorname{rank}_{\otimes}(A) = \operatorname{rank}_{\otimes}(B) + \operatorname{rank}_{\otimes}(C) = r+1$.

Arbitrary order. Let $\mathbf{u}_4 \in \mathbb{R}^{d_4}, \ldots, \mathbf{u}_k \in \mathbb{R}^{d_k}$ be unit vectors and set

$$\tilde{A}_n := A_n \otimes \mathbf{u}_4 \otimes \cdots \otimes \mathbf{u}_k, \qquad \tilde{A} := A \otimes \mathbf{u}_4 \otimes \cdots \otimes \mathbf{u}_k$$

By (4.2),

$$\|\tilde{A}_n - \tilde{A}\|_F = \|A_n - A\| = \|B \oplus C_n - B \oplus C\| = \|C_n - C\| \to 0 \text{ as } n \to \infty.$$

Moreover, Corollary 3.3 ensures that $\operatorname{rank}_{\otimes}(\tilde{A}) = r + 1$ and $\operatorname{rank}_{\otimes}(\tilde{A_n}) \leq r$.

Norm independence. Whether the sequence \tilde{A}_n converges to \tilde{A} is entirely dependent on the norm-induced topology on $\mathbb{R}^{d_1 \times \cdots \times d_k}$. Since it has a unique topology induced by any of its equivalent norms as a finite dimensional vector space, the convergence is independent of the choice of norms. \Box

We note that the proof above exhibits an order-k tensor, namely, \tilde{A} , that has rank strictly larger than min $\{d_1, \ldots, d_k\}$.

4.5. Tensor rank can leap an arbitrarily large gap. How can we construct a sequence of tensors of rank r that converge to a tensor of rank r + 2? An easy trick is to take the direct sum of two sequences of rank-2 tensors of the form shown in (4.5). The resulting sequence converges to a limiting tensor that is the direct sum of two rank-3 tensors, each of the form shown in (4.4). To show that the limiting tensor has rank 6 (and does not have some miraculous lower-rank decomposition), we once again turn to the theorem of JáJá–Takche, which contains just enough of the direct sum conjecture (3.1) for our purposes.

PROPOSITION 4.11. Given any $s \in \mathbb{N}$ and $r \geq 2s$, there exists a sequence of order-3 tensors B_n such that $\operatorname{rank}_{\otimes}(B_n) \leq r$ and $\lim_{n\to\infty} B_n = B$ with $\operatorname{rank}_{\otimes}(B) = r + s$.

Proof. Let d = r - 2s. By Lemma 3.5, there exists a rank-*d* tensor $C \in \mathbb{R}^{d \times d \times d}$. Let $A_n \to A$ be a convergent sequence in $\mathbb{R}^{2 \times 2 \times 2}$ with rank_{\otimes} $(A) \leq 2$ and rank_{\otimes}(A) = 3. Define

$$B_n = C \oplus A_n \oplus \cdots \oplus A_n, \quad B = C \oplus A \oplus \cdots \oplus A,$$

where there are s terms A_n and A. Then $B_n \to B$, and $\operatorname{rank}_{\otimes}(B_n) \leq r - 2s + 2s = r$. By applying the JáJá–Takche theorem sequentially s times, once for each summand A, we deduce that $\operatorname{rank}_{\otimes}(B) = r - 2s + 3s = r + s$. \Box As usual the construction can be extended to order-k tensors by taking an outer product with a suitable number of nonzero vectors in the new factors.

COROLLARY 4.12. Given any $s \ge 1$, $r \ge 2$, and $k \ge 3$, with $r \ge 2s$, there exists $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ such that $\operatorname{rank}_{\otimes}(A) = r + s$ and A has no best rank-r approximation. Proof. This follows from Proposition 4.11 and the previous remark. \Box

4.6. Brègman divergences and other continuous measures of proximity. In data analytic applications, one frequently encounters low-rank approximations with respect to "distances" that are more general than norms. Such a "distance" may not even be a metric, an example being the Brègman divergence [10, 26] (sometimes also known as the Brègman distance). The definition here is based on the definition given in [26]. Recall first that if $S \subset \mathbb{R}^n$, the *relative interior* of S is simply the interior of S considered as a subset of its affine hull and is denoted by ri(S).

DEFINITION 4.13. Let $S \subseteq \mathbb{R}^{d_1 \times \cdots \times d_k}$ be a convex set. Let $\varphi : S \to \mathbb{R}$ be a lower-semicontinuous, convex function that is continuously differentiable and strictly convex in $\operatorname{ri}(S)$. Let φ have the property that for any sequence $\{C_n\} \subset \operatorname{ri}(S)$ that converges to $C \in S \setminus \operatorname{ri}(S)$, we have

$$\lim_{n \to \infty} \|\nabla \varphi(C_n)\| = +\infty.$$

The Brègman divergence $D_{\varphi}: S \times ri(S) \to \mathbb{R}$ is defined by

$$D_{\varphi}(A,B) = \varphi(A) - \varphi(B) - \langle \nabla \varphi(B), A - B \rangle.$$

It is natural to ask if the analogous problem APPROX(A, r) for Brègman divergence will always have a solution. Note that a Brègman divergence, unlike a metric, is not necessarily symmetric in its two arguments, and thus there are *two* possible problems:

 $\operatorname{argmin}_{\operatorname{rank}_{\otimes}(B) < r} D_{\varphi}(A, B) \quad \text{and} \quad \operatorname{argmin}_{\operatorname{rank}_{\otimes}(B) < r} D_{\varphi}(B, A).$

As the following proposition shows, the answer is no in both cases.

PROPOSITION 4.14. Let D_{φ} be a Brègman divergence. Let A and A_n be defined as in (4.4) and (4.5), respectively. Then

$$\lim_{n \to \infty} D_{\varphi}(A, A_n) = 0 = \lim_{n \to \infty} D_{\varphi}(A_n, A).$$

Proof. The Brègman divergence is jointly continuous in both arguments with respect to the norm topology, and $A_n \to A$ in the norm, so $D_{\varphi}(A, A_n) \to D_{\varphi}(A, A) = 0$ and $D_{\varphi}(A_n, A) \to D_{\varphi}(A, A) = 0$. \Box

Proposition 4.14 extends trivially to any other measure of nearness that is continuous with respect to the norm topology in at least one argument.

4.7. Difference quotients. We thank Landsberg [53] for the insight that the expression in (4.4) is best regarded as a derivative. Indeed, if

$$f(t) = (\mathbf{x} + t\mathbf{y})^{\otimes 3} = (\mathbf{x} + t\mathbf{y}) \otimes (\mathbf{x} + t\mathbf{y}) \otimes (\mathbf{x} + t\mathbf{y}),$$

then

$$\left. \frac{df}{dt} \right|_{t=0} = \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{x} + \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{x} + \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{y}$$

by the Leibniz rule. On the other hand,

$$\left. \frac{df}{dt} \right|_{t=0} = \lim_{t \to 0} \left[\frac{(\mathbf{x} + t\mathbf{y}) \otimes (\mathbf{x} + t\mathbf{y}) \otimes (\mathbf{x} + t\mathbf{y}) - \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}}{t} \right],$$

and the difference quotient on the RHS has rank 2. The expression in (4.5) can be obtained from this by taking t = 1/N.

We can extend Landsberg's idea to more general partial differential operators. It will be helpful to use the degree-k Veronese map [37], which is $V_k(\mathbf{x}) = \mathbf{x}^{\otimes k} = \mathbf{x} \otimes \cdots \otimes \mathbf{x}$ (a k-fold product). Then, for example, the six-term symmetric tensor

$$\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z} + \mathbf{x} \otimes \mathbf{z} \otimes \mathbf{y} + \mathbf{y} \otimes \mathbf{z} \otimes \mathbf{x} + \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{z} + \mathbf{z} \otimes \mathbf{x} \otimes \mathbf{y} + \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{x}$$

can be written as a partial derivative

$$\frac{\partial^2}{\partial s \,\partial t} \bigg|_{s=t=0} \, (\mathbf{x} + s\mathbf{y} + t\mathbf{z})^{\otimes 3},$$

which is a limit of a four-term difference quotient:

$$\lim_{s,t\to 0} \left[\frac{V_3(\mathbf{x}+s\mathbf{y}+t\mathbf{z})-V_3(\mathbf{x}+s\mathbf{y})-V_3(\mathbf{x}+t\mathbf{z})+V_3(\mathbf{x})}{st} \right].$$

This example lies naturally in $\mathbb{R}^{3\times3\times3}$, taking $\mathbf{x}, \mathbf{y}, \mathbf{z}$ to be linearly independent. Another example, in $\mathbb{R}^{2\times2\times2\times2}$, is the six-term symmetric order-4 tensor

$$\begin{aligned} \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{y} + \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{y} + \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{x} \\ &+ \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{y} + \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{y} \otimes \mathbf{x} + \mathbf{y} \otimes \mathbf{y} \otimes \mathbf{x} \otimes \mathbf{x}. \end{aligned}$$

This can be written as the second-order derivative

$$\left. \frac{\partial^2}{\partial t^2} \right|_{t=0} \frac{(\mathbf{x} + t\mathbf{y})^{\otimes 4}}{2!}$$

which is a limit of a three-term difference quotient:

$$\lim_{t\to 0} \left[\frac{V_4(\mathbf{x}+2t\mathbf{y})-2V_4(\mathbf{x}+t\mathbf{y})+V_4(\mathbf{x})}{2!\,t^2} \right].$$

We call these examples symmetric Leibniz tensors for the differential operators $\partial^2/\partial s \,\partial t$ and $\partial^2/\partial t^2$, of orders 3 and 4, respectively. More generally, given positive integers k and a_1, \ldots, a_j with $a_1 + \cdots + a_j = a \leq k$, the symmetric tensor

$$L_k(a_1,\ldots,a_j) := \sum_{\text{Sym}} \mathbf{x}^{\otimes (k-a)} \otimes \mathbf{y}_1^{\otimes a_1} \otimes \cdots \otimes \mathbf{y}_j^{\otimes a_j}$$

can be written as a partial derivative,

$$\left. \frac{\partial^a}{\partial t_1^{a_1} \dots \partial t_j^{a_j}} \right|_{t_1 = \dots = t_j = 0} \frac{V_k(\mathbf{x} + t_1 \mathbf{y}_1 + \dots + t_j \mathbf{y}_j)}{(a_1!) \cdots (a_j!)},$$

which is a limit of a difference quotient with $(a_1 + 1) \cdots (a_j + 1)$ terms. On the other hand, the number of terms in the limit $L_k(a_1, \ldots, a_j)$ is given by a multinomial coefficient, and that is usually much bigger.

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This construction gives us a ready supply of candidates for rank-jumping. However, we do not know—even for the two explicit six-term examples above — whether the limiting tensors actually have the ranks suggested by their formulas. We can show that $\operatorname{rank}_{\otimes}(L_k(1)) = k$ for all k and over any field, generalizing Lemma 4.7. Beyond that it is not clear to us what is likely to be true. The optimistic conjecture is

(4.8)
$$\operatorname{rank}_{\otimes}(L_k(a_1,\ldots,a_j)) \stackrel{?}{=} \binom{k}{k-a,a_1,\ldots,a_j} = \frac{k!}{(k-a)!\,a_i!\,\cdots\,a_j!}$$

Comon et al. [18] show that the symmetric rank of $L_k(1)$ over the complex numbers is k, so that is another possible context in which (4.8) may be true.

5. Characterizing the limit points of order-3 rank-2 tensors. If an order-3 tensor can be expressed as a limit of a sequence of rank-2 tensors but itself has rank greater than 2, then we show in this section that it takes a particular form. This kind of result may make it possible to overcome the ill-posedness of APPROX(A, r) by defining weak solutions.

THEOREM 5.1. Let $d_1, d_2, d_3 \geq 2$. Let $A_n \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ be a sequence of tensors with rank_{\otimes} $(A_n) \leq 2$ and

$$\lim_{n \to \infty} A_n = A,$$

where the limit is taken in any norm topology. If the limiting tensor A has rank higher than 2, then rank_{\otimes}(A) must be exactly 3, and there exist pairs of linearly independent vectors $\mathbf{x}_1, \mathbf{y}_1 \in \mathbb{R}^{d_1}, \mathbf{x}_2, \mathbf{y}_2 \in \mathbb{R}^{d_2}, \mathbf{x}_3, \mathbf{y}_3 \in \mathbb{R}^{d_3}$ such that

(5.1)
$$A = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3.$$

The proof of this theorem will occupy the next few subsections.

5.1. Reduction. Our first step is to show that we can limit our attention to the particular tensor space $\mathbb{R}^{2\times 2\times 2}$. Here the orthogonal group action is important. Recall that the actions of $O_{d_1,\ldots,d_k}(\mathbb{R})$ and $\operatorname{GL}_{d_1,\ldots,d_k}(\mathbb{R})$ on $\mathbb{R}^{d_1\times\cdots\times d_k}$ are continuous and carry decomposable tensors to decomposable tensors. It follows that the subspaces S_r and \overline{S}_r are preserved. The next theorem provides a general mechanism for passing to a tensor subspace.

THEOREM 5.2. Let $r_i = \min(r, d_i)$ for all *i*. The restricted maps

$$O_{d_1,\dots,d_k}(\mathbb{R}) \times S_r(r_1,\dots,r_k) \to S_r(d_1,\dots,d_k),$$

$$O_{d_1,\dots,d_k}(\mathbb{R}) \times \overline{S}_r(r_1,\dots,r_k) \to \overline{S}_r(d_1,\dots,d_k)$$

given by $((L_1, \ldots, L_k), A) \mapsto (L_1, \ldots, L_k) \cdot A$ are both surjective.

In other words, every rank-*r* tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ is equivalent by an orthogonal transformation to a rank-*r* tensor in the smaller space $\mathbb{R}^{r_1 \times \cdots \times r_k}$. Similarly every rank-*r*-approximable tensor in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ is equivalent to a rank-*r*-approximable tensor in $\mathbb{R}^{r_1 \times \cdots \times r_k}$.

Proof. If $A \in S_r(d_1, \ldots, d_k)$ is any rank-*r* tensor then we can write $A = \sum_{j=1}^r \mathbf{x}_1^j \otimes \cdots \otimes \mathbf{x}_k^j$ for vectors $\mathbf{x}_i^j \in \mathbb{R}^{d_i}$. For each *i*, the vectors $\mathbf{x}_i^1, \ldots, \mathbf{x}_i^r$ span a subspace $V_i \subset \mathbb{R}^{d_i}$ of rank at most r_i . Choose $L_i \in O_{d_i}(\mathbb{R})$ so that $L_i(\mathbb{R}^{d_i}) \supseteq V_i$. Let $B = (L_1^{-1}, \ldots, L_k^{-1}) \cdot A$. Then $A = (L_1, \ldots, L_k) \cdot B$ and $B \in S_r(d_1, \ldots, d_k)$. This argument shows that the first of the maps is surjective.

Now let $A \in \overline{S}_r(d_1, \ldots, d_k)$ be any rank-*r*-approximable tensor. Let $(A^{(n)})_{n=1}^{\infty}$ be any sequence of rank-*r* tensors converging to *A*. For each *n*, by the preceding result, we can find $B^{(n)} \in \overline{S}_r(d_1, \ldots, d_k)$ and $(L_1^{(n)}, \ldots, L_k^{(n)}) \in O_{d_1, \ldots, d_k}(\mathbb{R})$ with $(L_1^{(n)}, \ldots, L_k^{(n)}) \cdot B^{(n)} = A^{(n)}$. Since $O_{d_1, \ldots, d_k}(\mathbb{R})$ is compact, there is a convergent subsequence $(L_1^{(n_j)}, \ldots, L_k^{(n_j)}) \to (L_1, \ldots, L_k)$. Let $B = (L_1, \ldots, L_k)^{-1} \cdot A$. Then $A = (L_1, \ldots, L_k) \cdot B$; and $B^{(n_j)} = (L_1^{(n_j)}, \ldots, L_k^{(n_j)})^{-1} \cdot A^{(n_j)} \to (L_1, \ldots, L_k)^{-1} \cdot A = B$, so $B \in \overline{S}_r(d_1, \ldots, d_k)$. Thus the second map is also surjective. \Box

COROLLARY 5.3. If Theorem 5.1 is true for the tensor space $\mathbb{R}^{2\times 2\times 2}$ then it is true in general.

Proof. The general case is $V_1 \otimes V_2 \otimes V_3 \cong \mathbb{R}^{d_1 \times d_2 \times d_3}$. Suppose $A \in \overline{S}_2(d_1, d_2, d_3)$ and $\operatorname{rank}_{\otimes}(A) \geq 3$. By Theorem 5.2, there exists $(L_1, L_2, L_3) \in O_{d_1, d_2, d_3}(\mathbb{R})$ and $B \in \overline{S}_2(2, 2, 2)$ with $(L_1, L_2, L_3) \cdot B = A$. Moreover, $\operatorname{rank}_{\otimes}(B) = \operatorname{rank}_{\otimes}(A) \geq 3$ in $\mathbb{R}^{l \times m \times n}$ and hence $\operatorname{rank}_{\otimes}(B) \geq 3$ in $\mathbb{R}^{2 \times 2 \times 2}$ by Proposition 3.1. Since the theorem is assumed true for $\mathbb{R}^{2 \times 2 \times 2}$ and B satisfies the hypotheses, it can be written in the specified form in terms of vectors $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ and $\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3$. It follows that A takes the same form with respect to the vectors $L_1\mathbf{x}_1, L_2\mathbf{x}_2, L_3\mathbf{x}_3$ and $L_1\mathbf{y}_1, L_2\mathbf{y}_2, L_3\mathbf{y}_3$.

5.2. Tensors of rank 1 and 2. We establish two simple facts for later use.

PROPOSITION 5.4. If $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ has rank 1, then we can write $A = (L_1, \ldots, L_k) \cdot B$, where $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R})$ and $B = \mathbf{e}_1 \otimes \cdots \otimes \mathbf{e}_k$.

Proof. Write $A = \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k$ and choose the L_i so that $L_i(\mathbf{e}_i) = \mathbf{x}_i$.

PROPOSITION 5.5. Assume $d_i \geq 2$ for all *i*. If $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ has rank 2, then we can write $A = (L_1, \ldots, L_k) \cdot B$, where $(L_1, \ldots, L_k) \in \operatorname{GL}_{d_1, \ldots, d_k}(\mathbb{R})$ and $B \in \mathbb{R}^{2 \times \cdots \times 2}$ is of the form $B = \mathbf{e}_1 \otimes \cdots \otimes \mathbf{e}_1 + \mathbf{f}_1 \otimes \cdots \otimes \mathbf{f}_k$. Here \mathbf{e}_1 denotes the standard basis vector $(1, 0)^\top$; each \mathbf{f}_i is equal either to \mathbf{e}_1 or to $\mathbf{e}_2 = (0, 1)^\top$; and at least two of the \mathbf{f}_i are equal to \mathbf{e}_2 .

Proof. We can write $A = \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k + \mathbf{y}_1 \otimes \cdots \otimes \mathbf{y}_k$. Since $\operatorname{rank}_{\otimes}(A) = 2$ all of the \mathbf{x}_i and \mathbf{y}_i must be nonzero. We claim that $\mathbf{y}_i, \mathbf{x}_i$ must be linearly independent for at least two different indices *i*. Otherwise, suppose $\mathbf{y}_i = \lambda_i \mathbf{x}_i$ for k - 1 different indices, say, $i = 1, \ldots, k - 1$. It would follow that

$$A = \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_{k-1} \otimes (\mathbf{x}_k + (\lambda_1 \cdots \lambda_{k-1}) \mathbf{y}_k),$$

contradicting rank_{\otimes}(A) = 2.

For each *i* choose $L_i : \mathbb{R}^2 \to \mathbb{R}^{d_i}$ such that $L_i \mathbf{e}_1 = \mathbf{x}_i$ and such that $L_i \mathbf{e}_2 = \mathbf{y}_i$ if \mathbf{y}_i is linearly independent of \mathbf{x}_i ; otherwise $L_i \mathbf{e}_2$ may be arbitrary. It is easy to check that $(L_1, \ldots, L_k)^{-1} \cdot A = \mathbf{e}_1 \otimes \cdots \otimes \mathbf{e}_1 + \lambda \mathbf{f}_1 \otimes \cdots \otimes \mathbf{f}_k$, where the \mathbf{f}_i are as specified in the theorem, and λ is the product of the λ_i over those indices where $\mathbf{y}_i = \lambda_i \mathbf{x}_i$. This is almost in the correct form. To get rid of the λ , replace $L_i \mathbf{e}_2 = \mathbf{y}_i$ with $L_i \mathbf{e}_2 = \lambda \mathbf{y}_i$ at one of the indices *i* for which $\mathbf{x}_i, \mathbf{y}_i$ are linearly independent. This completes the construction. \Box

5.3. The discriminant polynomial Δ **.** The structure of tensors in $\mathbb{R}^{2\times2\times2}$ is largely governed by a quartic polynomial Δ which we define and discuss here. This same polynomial was discovered by Cayley in 1845 [15]. More generally, Δ is the $2 \times 2 \times 2$ special case of an object called the *hyperdeterminant* revived in its modern form by Gelfand, Kapranov, and Zelevinsky [30, 31]. We give an elementary treatment of the properties we need.

As in our discussion in section 2.1, we identify a tensor $\mathbf{A} \in \mathbb{R}^2 \otimes \mathbb{R}^2 \otimes \mathbb{R}^2$ with the array $A \in \mathbb{R}^{2 \times 2 \times 2}$ of its eight coefficients with respect to the standard basis

 $\{\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k : i, j, k = 1, 2\}$. Pictorially, we can represent it as a pair of side-by-side 2×2 slabs:

$$\mathbf{A} = \sum_{i=1}^{2} \sum_{j=1}^{2} \sum_{k=1}^{2} a_{ijk} \mathbf{e}_{i} \otimes \mathbf{e}_{j} \otimes \mathbf{e}_{k} = \begin{bmatrix} a_{111} & a_{112} \\ a_{121} & a_{122} \end{bmatrix} \begin{bmatrix} a_{211} & a_{212} \\ a_{221} & a_{222} \end{bmatrix} = A.$$

The general strategy is to find ways of simplifying the representation of A by applying transformations in $\operatorname{GL}_{2,2,2}(\mathbb{R}) = \operatorname{GL}_2(\mathbb{R}) \times \operatorname{GL}_2(\mathbb{R}) \times \operatorname{GL}_2(\mathbb{R})$. This group is generated by the following operations: decomposable row operations applied to both slabs simultaneously; decomposable column operations applied to both slabs simultaneously; decomposable slab operations (for example, adding a multiple of one slab to the other).

Slab operations on a tensor $A = [A_1 | A_2]$ generate new 2×2 slabs of the form $S = \lambda_1 A_1 + \lambda_2 A_2$. One can check that

(5.2)
$$\det(S) = \lambda_1^2 \det(A_1) + \lambda_1 \lambda_2 \frac{\det(A_1 + A_2) - \det(A_1 - A_2)}{2} + \lambda_2^2 \det(A_2).$$

We define Δ to be the discriminant of this quadratic polynomial:

(5.3)
$$\Delta([A_1 | A_2]) = \left[\frac{\det(A_1 + A_2) - \det(A_1 - A_2)}{2}\right]^2 - 4\det(A_1)\det(A_2).$$

Explicitly, if $A = \llbracket a_{ijk} \rrbracket_{i,j,k=1,2} \in \mathbb{R}^{2 \times 2 \times 2}$, then

$$\Delta(A) = (a_{111}^2 a_{222}^2 + a_{112}^2 a_{221}^2 + a_{121}^2 a_{212}^2 + a_{122}^2 a_{211}^2) - 2(a_{111}a_{112}a_{221}a_{222} + a_{111}a_{121}a_{212}a_{222} + a_{111}a_{122}a_{211}a_{222} + a_{112}a_{121}a_{212}a_{221} + a_{112}a_{122}a_{221}a_{211} + a_{121}a_{122}a_{212}a_{211}) + 4(a_{111}a_{122}a_{212}a_{221} + a_{112}a_{121}a_{212}a_{221}).$$

PROPOSITION 5.6. Let $A \in \mathbb{R}^{2 \times 2 \times 2}$, let A' be obtained from A by permuting the three factors in the tensor product, and let $(L_1, L_2, L_3) \in \operatorname{GL}_{2,2,2}(\mathbb{R})$. Then $\Delta(A') = \Delta(A)$ and $\Delta((L_1, L_2, L_3) \cdot A) = \det(L_1)^2 \det(L_2)^2 \det(L_3)^2 \Delta(A)$.

Proof. To show that Δ is invariant under all permutations of the factors of $\mathbb{R}^{2\times2\times2}$, it is enough to check invariance in the cases of two distinct transpositions. It is clear from (5.3) that Δ is invariant under the transposition of the second and third factors, since this amounts to replacing A_1, A_2 with their transposes A_1^{\top}, A_2^{\top} . To show that Δ is invariant under transposition of the first and third factors, write $A = [\mathbf{u}_{11}, \mathbf{u}_{12} | \mathbf{u}_{21}, \mathbf{u}_{22}]$, where the \mathbf{u}_{ij} are column vectors. One can verify that

$$\Delta(A) = \det[\mathbf{u}_{11}, \mathbf{u}_{22}]^2 + \det[\mathbf{u}_{21}, \mathbf{u}_{12}]^2 - 2 \det[\mathbf{u}_{11}, \mathbf{u}_{12}] \det[\mathbf{u}_{21}, \mathbf{u}_{22}] - 2 \det[\mathbf{u}_{11}, \mathbf{u}_{21}] \det[\mathbf{u}_{12}, \mathbf{u}_{22}],$$

which has the desired symmetry.

In view of the permutation invariance of Δ , it is enough to verify the second claim in the case $(L_1, L_2, L_3) = (I, L_2, I)$. Then $(L_1, L_2, L_3) \cdot A = [L_2A_1 | L_2A_2]$ and an extra factor det $(L_2)^2$ appears in all terms of (5.3), exactly as required. \Box

COROLLARY 5.7. The sign of Δ is invariant under the action of $\text{GL}_{2,2,2}(\mathbb{R})$.

COROLLARY 5.8. The value of Δ is invariant under the action of $O_{2,2,2}(\mathbb{R})$.

Using the properties of Δ , we can easily prove, in a slightly different way, a result due originally to Kruskal (unpublished work) and ten Berge [73].

PROPOSITION 5.9. If $\Delta(A) > 0$ then $\operatorname{rank}_{\otimes}(A) \leq 2$.

PROPOSITION 5.10. If $\operatorname{rank}_{\otimes}(A) \leq 2$ then $\Delta(A) \geq 0$.

Proof of Proposition 5.9. If the discriminant $\Delta(A)$ is positive then the homogeneous quadratic equation (5.2) has two linearly independent root pairs $(\lambda_{11}, \lambda_{12})$ and $(\lambda_{21}, \lambda_{22})$. It follows that we can use slab operations to transform $[A_1 | A_2] \rightarrow [B_1 | B_2]$, where $B_i = \lambda_{i1}A_1 + \lambda_{i2}A_2$. By construction $\det(B_i) = 0$, so we can write $B_i = \mathbf{f}_i \otimes \mathbf{g}_i$ for some $\mathbf{f}_i, \mathbf{g}_i \in \mathbb{R}^2$ (possibly zero). It follows that $[B_1 | B_2] = \mathbf{e}_1 \otimes \mathbf{f}_1 \otimes \mathbf{g}_1 + \mathbf{e}_2 \otimes \mathbf{f}_2 \otimes \mathbf{g}_2$; so rank $\otimes(A) = \operatorname{rank}_{\otimes}([B_1 | B_2]) \leq 2$. \Box

Proof of Proposition 5.10. It is easy to check that $\Delta(A) = 0$ if rank $\otimes(A) \leq 1$, since we can write $A = (L_1, L_2, L_3) \cdot (\mathbf{e}_1 \otimes \mathbf{e}_1 \otimes \mathbf{e}_1)$ or else A = 0.

It remains to be shown that $\Delta(A)$ is not negative when rank_{\otimes}(A) = 2. Proposition 5.5 implies that A can be transformed by an element of $\operatorname{GL}_{2,2,2}(\mathbb{R})$ (and a permutation of factors, if necessary) into one of the following tensors:

$$I_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{or} \quad I_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

Since $\Delta(I_1) = 1$ and $\Delta(I_2) = 0$, it follows that $\Delta(A) \ge 0$. \Box

Kruskal and also ten Berge deserve complete credit for discovering the above result. In fact, the hyperdeterminant for $2 \times 2 \times 2$ tensor Δ is known by the name *Kruskal polynomial* in the psychometrics community [73]. Our goal is not so much to provide alternative proofs for Propositions 5.9 and 5.10 but to include them so that our proof of Theorem 5.1 can be self-contained. We are now ready to give that proof, thereby characterizing all limit points of order-3 rank-2 tensors.

Proof of Theorem 5.1. Note that the theorem is stated for order-3 tensors of any size $d_1 \times d_2 \times d_3$. We begin with the case $A \in \mathbb{R}^{2 \times 2 \times 2}$. Suppose $A \in \overline{S}_2(2,2,2) \setminus S_2(2,2,2)$. Then we claim that $\Delta(A) = 0$. Indeed, since $A \notin S_2$, Proposition 5.9 implies that $\Delta(A) \leq 0$. On the other hand, since $A \in \overline{S}_2$, it follows from Proposition 5.10 and the continuity of Δ that $\Delta(A) \geq 0$.

Since $\Delta(A) = 0$, the homogeneous quadratic equation (5.2) has a nontrivial root pair (λ_1, λ_2) . It follows that A can be transformed by slab operations into the form $[A_i | S]$, where $S = \lambda_1 A_1 + \lambda_2 A_2$ and i = 1 or 2. By construction det(S) = 0, but $S \neq 0$ for otherwise rank_{\otimes} $(A) = \text{rank}(A_i) \leq 2$. Hence rank(S) = 1 and by a further transformation we can reduce A to the form

$$B = \left[\begin{array}{cc|c} p & q & 1 & 0 \\ r & s & 0 & 0 \end{array} \right]$$

In fact we may assume p = 0 (the operation "subtract p times the second slab from the first slab" will achieve this), and moreover $s^2 = \Delta(B) = 0$. Both q and r must be nonzero; otherwise rank_{\otimes}(A) = rank_{\otimes}(B) ≤ 2 . If we rescale the bottom rows by 1/rand the right-hand columns by 1/q we are finally reduced to

$$B' = \begin{bmatrix} 0 & 1 & | & 1 & 0 \\ 1 & 0 & | & 0 & 0 \end{bmatrix} = \mathbf{e}_2 \otimes \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_1 \otimes \mathbf{e}_2 \otimes \mathbf{e}_1 + \mathbf{e}_1 \otimes \mathbf{e}_2 \otimes \mathbf{e}_2.$$

By reversing all the row, column, and slab operations we can obtain a transformation $(L_1, L_2, L_3) \in \operatorname{GL}_{2,2,2}(\mathbb{R})$ such that $A = (L_1, L_2, L_3) \cdot B'$. Then A can be written in the required form, with $\mathbf{x}_i = L_i \mathbf{e}_1$, $\mathbf{y}_i = L_i \mathbf{e}_2$ for i = 1, 2, 3.

This completes the proof of Theorem 5.1 in the case of the tensor space $\mathbb{R}^{2 \times 2 \times 2}$. By Corollary 5.3 this implies the theorem in general. \Box

5.4. Ill-posedness and ill-conditioning of the best rank-r approximation problem. Recall that a problem is called *well-posed* if a solution exists, is unique, and is stable (i.e., depends continuously on the input data). If one or more of these three criteria are not satisfied, the problem³ is called *ill-posed*.

From sections 4 and 8, we see that tensors will often fail to have a best rankr approximation. In all applications that rely on APPROX(A, r) or a variant of it as the underlying mathematical model, we should fully expect the ill-posedness of APPROX(A, r) to pose a serious difficulty. Even if it is known a priori that a tensor Ahas a best rank-r approximation, we should remember that in applications, the data array \hat{A} available at our disposal is almost always one that is corrupted by noise, i.e., $\hat{A} = A + E$, where E denotes the collective contributions of various errors, limitations in measurements, background noise, rounding off, etc. Clearly there is no guarantee that \hat{A} will also have a best rank-r approximation.

In many situations, one needs only a "good" rank-r approximation rather than the best rank-r approximation. It is tempting to argue, then, that the nonexistence of the best solution does not matter—it is enough to seek an "approximate solution." We discourage this point of view for two main reasons. First, there is a serious conceptual difficulty: if there is no solution, then what is the "approximate solution" an approximation of? Second, even if one disregards this and ploughs ahead to compute an "approximate solution," we argue below that this task is ill-conditioned and the computation is unstable.

For notational simplicity and since there is no loss of generality (cf. Theorem 4.10 and Corollary 4.12), we will use the problem of finding a best rank-2 approximation to a rank-3 tensor to make our point. Let $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ be an instance where

(5.4)
$$\operatorname{argmin}_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \| A - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 \|$$

does not have a solution (such examples abound; cf. section 8). If we disregard the fact that a solution does not exist and plug the problem into a computer program,⁴ we will still get some sort of "approximate solution" because of the finite-precision error inherent in the computer. What really happens here [77] is that we are effectively solving a problem perturbed by some small $\varepsilon > 0$; the "approximate solution" $\mathbf{x}_i^*(\varepsilon), \mathbf{y}_i^*(\varepsilon) \in \mathbb{R}^{d_i}$ (i = 1, 2, 3) is really a solution to the perturbed problem

(5.5)
$$\|A - \mathbf{x}_1^*(\varepsilon) \otimes \mathbf{x}_2^*(\varepsilon) \otimes \mathbf{x}_3^*(\varepsilon) - \mathbf{y}_1^*(\varepsilon) \otimes \mathbf{y}_2^*(\varepsilon) \otimes \mathbf{y}_3^*(\varepsilon) \|$$
$$= \varepsilon + \inf_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \|A - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 \|.$$

Since we are attempting to find a solution of (5.4) that does not exist, in exact arithmetic the algorithm will never terminate, but in reality the computer is limited by its finite precision, and so the algorithm terminates at an "approximate solution," which may be viewed as a solution to a perturbed problem (5.5). This process of forcing a solution to an ill-posed problem is almost always guaranteed to be ill-conditioned because of the infamous rule of thumb in numerical analysis [22, 23, 24]:

A well-posed problem near an ill-posed one is ill-conditioned.

 $^{^{3}}$ Normally, existence is taken for granted, and an ill-posed problem often means one whose solution lacks either uniqueness or stability. In this paper, the ill-posedness is of a more serious kind—the existence of a solution is itself in question.

⁴While there is no known globally convergent algorithm for APPROX(A, r), we will ignore this difficulty for a moment and assume that the ubiquitous alternating least squares algorithm would yield the required solution.

The root of the ill-conditioning lies in the fact that we are solving the (well-posed but ill-conditioned) problem (5.5) that is a slight perturbation of the ill-posed problem (5.4). The ill-conditioning manifests itself as the phenomenon described in Proposition 4.8, namely,

 $\|\mathbf{x}_1^*(\varepsilon) \otimes \mathbf{x}_2^*(\varepsilon) \otimes \mathbf{x}_3^*(\varepsilon)\| \to \infty$ and $\|\mathbf{y}_1^*(\varepsilon) \otimes \mathbf{y}_2^*(\varepsilon) \otimes \mathbf{y}_3^*(\varepsilon)\| \to \infty$

as $\varepsilon \to 0$. The ill-conditioning described here was originally observed in numerical experiments by psychometricians and chemometricians, who named the phenomenon "diverging CANDECOMP/PARAFAC components" or "CANDECOMP/PARAFAC degeneracy" [49, 51, 63, 68, 69].

To fix the ill-conditioning, we should first fix the ill-posedness, i.e., find a wellposed problem. This leads us to the subject of the next section.

5.5. Weak solutions. In the study of PDEs [29], there often arise systems of PDEs that have no solutions in the traditional sense. A standard way around this is to define a so-called *weak solution*, which may not be a continuous function or even a function (which is a tad odd since one would expect a *solution* to a PDE to be at least differentiable). Without going into the details, we will just say that weak solution turns out to be an extremely useful concept and is indispensable in modern studies of PDEs. Under the proper context, a weak solution to an ill-posed PDE may be viewed as the limit of strong or classical solutions to a sequence of well-posed PDEs that are slightly perturbed versions of the ill-posed one in question. Motivated by the PDE analogies, we will define weak solutions to APPROX(A, r).

We let $\mathcal{S}_r(d_1, \ldots, d_k) := \{A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}_{\otimes}(A) \leq r\}$ and let $\overline{\mathcal{S}}_r(d_1, \ldots, d_k)$ denote its closure in the (unique) norm-topology. DEFINITION 5.11. An order-k tensor $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ has border rank r if

 $A \in \overline{\mathcal{S}}_r(d_1, \dots, d_k)$ and $A \notin \overline{\mathcal{S}}_{r-1}(d_1, \dots, d_k)$.

This is denoted by $\underline{\operatorname{rank}}_{\otimes}(A)$. Note that

$$\overline{\mathcal{S}}_r(d_1,\ldots,d_k) = \{ A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \underline{\operatorname{rank}}_{\otimes}(S) \le r \}.$$

Remark. Clearly $\underline{\operatorname{rank}}_{\otimes}(A) \leq \operatorname{rank}_{\otimes}(A)$ for any tensor A. Since $\overline{\mathcal{S}}_0 = \mathcal{S}_0$ (trivially) and $\overline{\mathcal{S}}_1 = \mathcal{S}_1$ (by Proposition 4.2), it follows that $\underline{\operatorname{rank}}_{\otimes}(A) = \operatorname{rank}_{\otimes}(A)$ whenever rank_{\otimes}(A) ≤ 2 . Moreover, <u>rank_{\otimes}(A) ≥ 2 if rank_{\otimes}(A) ≥ 2 .</u>

Our definition differs slightly from the usual definition of border rank in the algebraic computational complexity literature [5, 6, 12, 48, 54], which uses the Zariski topology (and is normally defined for tensors over \mathbb{C}).

Let $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ with $d_i \geq 2$ and $k \geq 3$. Then the way to ensure that APPROX(A, r), the optimal rank-r approximation problem

(5.6)
$$\operatorname{argmin}_{\operatorname{rank}_{\otimes}(B) \leq r} \|A - B\|,$$

always has a meaningful solution for any $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ is to instead consider the optimal border-rank-r approximation problem

(5.7)
$$\operatorname{argmin}_{\operatorname{rank}_{\infty}(B) < r} \|A - B\|.$$

It is an obvious move to propose to fix the ill-posedness of APPROX(A, r) by taking the closure. However, without a characterization of the limit points such a proposal will at best be academic—it is not enough to simply say that weak solutions are limits of rank-2 tensors without giving an explicit expression (or a number of expressions) for them that may be plugged into the objective function to be minimized.

Theorem 5.1 solves this problem in the order-3 rank-2 case—it gives a complete description of these limit points with an explicit formula and, in turn, a constructive solution to the border-rank approximation problem. In case this is not obvious, we will spell out the implication of Theorem 5.1.

COROLLARY 5.12. Let $d_1, d_2, d_3 \geq 2$. Let $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank_{\otimes}(A) = 3. A is the limit of a sequence $A_n \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank_{\otimes} $(A_n) \leq 2$ if and only if

$$A = \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3$$

for some $\mathbf{x}_i, \mathbf{y}_i$ linearly independent vectors in \mathbb{R}^{d_i} , i = 1, 2, 3.

This implies that every tensor in $\overline{S}_2(d_1, \ldots, d_k)$ can be written in one of two forms:

(5.8)
$$\mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3$$

or

(5.9)
$$\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3.$$

These expressions may then be used to define the relevant objective function(s) in the minimization of (5.7). As in the case of PDEs, every classical (strong) solution is also a weak solution to APPROX(A, r).

PROPOSITION 5.13. If B is a solution to (5.6) then B is a solution to (5.7). Proof. If $||A - B|| \leq ||A - B'||$ for all $B' \in S_r$, then $||A - B|| \leq ||A - B'||$ for all $B' \in \overline{S}_r$ by continuity. \Box

6. Semialgebraic description of tensor rank. One may wonder whether the result in Propositions 5.9 and 5.10 extends to more general *hyperdeterminants*. We know from [30, 31] that a hyperdeterminant may be uniquely defined (up to a constant scaling) in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ whenever d_1, \ldots, d_k satisfy

(6.1)
$$d_i - 1 \le \sum_{j \ne i} (d_j - 1)$$
 for $i = 1, \dots, k$.

(Note that for matrices, (6.1) translates to $d_1 = d_2$, which may be viewed as one reason why the determinant is defined only for square matrices.) Let $\text{Det}_{d_1,\ldots,d_k}$: $\mathbb{R}^{d_1 \times \cdots \times d_k} \to \mathbb{R}$ be the polynomial function defined by the hyperdeterminant whenever (6.1) is satisfied. Propositions 5.9 and 5.10 tell us that the rank of a tensor is 2 on the set $\{A \mid \text{Det}_{2,2,2}(A) > 0\}$ and 3 on the set $\{A \mid \text{Det}_{2,2,2}(A) < 0\}$. One may start by asking whether the tensor rank in $\mathbb{R}^{d_1 \times \cdots \times d_k}$ is constant-valued on the sets

$$\{A \mid \text{Det}_{d_1,\dots,d_k}(A) < 0\}$$
 and $\{A \mid \text{Det}_{d_1,\dots,d_k}(A) > 0\}.$

The answer, as Sturmfels has kindly communicated to us [71], is *no* with explicit counterexamples in cases $2 \times 2 \times 2 \times 2$ and $3 \times 3 \times 3$. We will not reproduce Sturmfels's examples here (one reason is that $\text{Det}_{2,2,2,2}$ already contains close to 3 million monomial terms [35]) but instead refer our readers to his forthcoming paper.

We will prove that although there is no single polynomial Δ that will separate $\mathbb{R}^{d_1 \times \cdots \times d_k}$ into regions of constant rank as in the case of $\mathbb{R}^{2 \times 2 \times 2}$, there is always a finite number of polynomials $\Delta_1, \ldots, \Delta_m$ that will achieve this.

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Before we state and prove the result, we will introduce a few notions and notations. We will write $\mathbb{R}[X_1, \ldots, X_m]$ for the ring of polynomials in m variables X_1, \ldots, X_m with real coefficients. Subsequently, we will be considering polynomial functions on tensor spaces and will index our variables in a consistent way (for example, when discussing polynomial functions on $\mathbb{R}^{l \times m \times n}$, the polynomial ring in question will be denoted $\mathbb{R}[X_{111}, X_{112}, \ldots, X_{lmn}]$). Given $A = [\![a_{ijk}]\!] \in \mathbb{R}^{l \times m \times n}$ and $p(X_{111}, X_{112}, \ldots, X_{lmn}) \in \mathbb{R}[X_{111}, X_{112}, \ldots, X_{lmn}]$, p(A) will mean the obvious thing, namely, $p(A) = p(a_{111}, a_{112}, \ldots, a_{lmn}) \in \mathbb{R}$.

A polynomial map is a function $F : \mathbb{R}^n \to \mathbb{R}^m$, defined for each $\mathbf{a} = [a_1, \ldots, a_n]^\top \in \mathbb{R}^n$ by $F(\mathbf{a}) = [f_1(\mathbf{a}), \ldots, f_m(\mathbf{a})]^\top$, where $f_i \in \mathbb{R}[X_1, \ldots, X_n]$ for all $i = 1, \ldots, m$. A semialgebraic set in \mathbb{R}^n is a union of finitely many sets of the form⁵

$$\{\mathbf{a} \in \mathbb{R}^n \mid p(\mathbf{a}) = 0, q_1(\mathbf{a}) > 0, \dots, q_\ell(\mathbf{a}) > 0\},\$$

where $\ell \in \mathbb{N}$ and $p, q_1, \ldots, q_\ell \in \mathbb{R}[X_1, \ldots, X_n]$. Note that we do not exclude the possibility of p or any of the q_i being constant (degree-0) polynomials. For example, if p is the zero polynomial, then the first relation 0 = 0 is trivially satisfied and the semialgebraic set will be an open set in \mathbb{R}^n .

It is easy to see that the class of all semialgebraic sets in \mathbb{R}^n is closed under finite unions, finite intersections, and taking the complement. Moreover, if $S \subseteq \mathbb{R}^{n+1}$ is a semialgebraic set and $\pi : \mathbb{R}^{n+1} \to \mathbb{R}^n$ is the projection onto the first *n* coordinates, then $\pi(S)$ is also a semialgebraic set; this seemingly innocuous statement is in fact the Tarski–Seidenberg theorem [65, 72], possibly the most celebrated result about semialgebraic sets. We will restate it in a (somewhat less common) form that better suits our purpose.

THEOREM 6.1 (Tarski–Seidenberg). If $S \subseteq \mathbb{R}^n$ is a semialgebraic set and $F : \mathbb{R}^n \to \mathbb{R}^m$ is a polynomial map, then the image $F(S) \subseteq \mathbb{R}^m$ is also a semialgebraic set.

These and other results about semialgebraic sets may be found in [19, Chapter 2], which, in addition, is a very readable introduction to semialgebraic geometry.

THEOREM 6.2. The set $\mathcal{R}_r(d_1, \ldots, d_k) := \{A \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}_{\otimes}(A) = r\}$ is a semialgebraic set.

Proof. Let $\psi_r : (\mathbb{R}^{d_1} \times \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k})^r \to \mathbb{R}^{d_1 \times d_2 \times \cdots \times d_k}$ be defined by

 $\psi_r(\mathbf{u}_1,\mathbf{v}_1,\ldots,\mathbf{z}_1;\ldots;\mathbf{u}_r,\mathbf{v}_r,\ldots,\mathbf{z}_r)=\mathbf{u}_1\otimes\mathbf{v}_1\otimes\cdots\otimes\mathbf{z}_1+\cdots+\mathbf{u}_r\otimes\mathbf{v}_r\otimes\cdots\otimes\mathbf{z}_r.$

It is clear that the image of ψ_r is exactly $S_r(d_1, \ldots, d_k) = \{A \mid \operatorname{rank}_{\otimes}(A) \leq r\}$. It is also clear that ψ_r is a polynomial map.

It follows from Theorem 6.1 that $S_r(d_1, \ldots, d_k)$ is semialgebraic. This holds for arbitrary r. So $\mathcal{R}_r(d_1, \ldots, d_k) = S_r(d_1, \ldots, d_k) \setminus S_{r-1}(d_1, \ldots, d_k)$ is also semialgebraic. \Box

COROLLARY 6.3. There exist $\Delta_0, \ldots, \Delta_m \in \mathbb{R}[X_{1\dots 1}, \ldots, X_{d_1\dots d_k}]$ from which the rank of a tensor $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ can be determined purely from the signs (i.e., + or - or 0) of $\Delta_0(A), \ldots, \Delta_m(A)$.

In the next section, we will see examples of such polynomials for the tensor space $\mathbb{R}^{2\times2\times2}$. We will stop short of giving an explicit semialgebraic characterization of rank, but it should be clear to the reader how to get one.

⁵Only one *p* is necessary, because multiple equality constraints $p_1(\mathbf{a}) = 0, \ldots, p_k(\mathbf{a}) = 0$ can always be amalgamated into a single equation $p(\mathbf{a}) = 0$ by setting $p = p_1^2 + \cdots + p_k^2$.

7. Orbits of real $2 \times 2 \times 2$ tensors. In this section, we study the equivalence of tensors in $\mathbb{R}^{2 \times 2 \times 2}$ under multilinear matrix multiplication. We will use the results and techniques of this section later on in section 8 where we determine *which* tensors in $\mathbb{R}^{2 \times 2 \times 2}$ have an optimal rank-2 approximation.

Recall that A and $B \in \mathbb{R}^{2 \times 2 \times 2}$ are said to be $(\operatorname{GL}_{2,2,2}(\mathbb{R}))$ -equivalent if and only if there exists a transformation $(L, M, N) \in \operatorname{GL}_{2,2,2}(\mathbb{R})$ such that $A = (L, M, N) \cdot B$. The question is whether there is a finite list of "canonical tensors" so that every $A \in \mathbb{R}^{2 \times 2 \times 2}$ is equivalent to one of them. For matrices $A \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A) = r$ if and only if there exist $M \in \operatorname{GL}_m(\mathbb{R}), N \in \operatorname{GL}_n(\mathbb{R})$ such that

$$(M,N) \cdot A = MAN^{\top} = \begin{bmatrix} I_r & 0\\ 0 & 0 \end{bmatrix}.$$

So every matrix of rank r is equivalent to one that takes the canonical form $\begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}$. Note that this is the same as saying that the matrix A can be transformed into $\begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}$ using elementary row and column operations—adding a scalar multiple of a row/column to another, scaling a row/column by a nonzero scalar, interchanging two rows/columns—since every $(L_1, L_2) \in \operatorname{GL}_{m,n}(\mathbb{R})$ is a sequence of such operations.

We will see that there is indeed a finite number of canonical forms for tensors in $\mathbb{R}^{2\times2\times2}$, although the classification is somewhat more intricate than the case of matrices; two tensors in $\mathbb{R}^{2\times2\times2}$ can have the same rank but be inequivalent (i.e., reduce to different canonical forms).

In fancier language, what we are doing is classifying the *orbits* of the group action $\operatorname{GL}_{2,2,2}(\mathbb{R})$ on $\mathbb{R}^{2\times2\times2}$. We are doing for $\mathbb{R}^{2\times2\times2}$ what Gelfand, Kapranov, and Zelevinsky did for $\mathbb{C}^{2\times2\times2}$ in the last sections of [30, 31]. Not surprisingly, the results that we obtained are similar but not identical; there are *eight* distinct orbits for the action of $\operatorname{GL}_{2,2,2}(\mathbb{R})$ on $\mathbb{R}^{2\times2\times2}$ as opposed to *seven* distinct orbits for the action of $\operatorname{GL}_{2,2,2}(\mathbb{C})$ on $\mathbb{C}^{2\times2\times2}$ —a further reminder of the dependence of such results on the choice of field.

THEOREM 7.1. Every tensor in $\mathbb{R}^{2 \times 2 \times 2}$ is equivalent via a transformation in $\operatorname{GL}_{2,2,2}(\mathbb{R})$ to precisely one of the canonical forms indicated in Table 7.1, with its invariants taking the values shown.

Proof. Write $A = [A_1 \mid A_2], A_i \in \mathbb{R}^{2 \times 2}$ for $\llbracket a_{ijk} \rrbracket \in \mathbb{R}^{2 \times 2 \times 2}$. If rank $(A_1) = 0$, then

$$A = \left[\begin{array}{cc|c} 0 & 0 \\ 0 & 0 \end{array} \middle| \begin{array}{c} \times & \times \\ \times & \times \end{array} \right].$$

Using matrix operations, A must then be equivalent to one of the forms (depending on $\operatorname{rank}(A_2)$)

$$\left[\begin{array}{cc|c} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right], \qquad \left[\begin{array}{cc|c} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right], \qquad \left[\begin{array}{cc|c} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right], \qquad \left[\begin{array}{cc|c} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right],$$

which correspond to D_0 , D_1 , and D_2 , respectively (after reordering the slabs).

If $rank(A_1) = 1$, then we may assume that

$$A = \left[\begin{array}{ccc} 1 & 0 \\ 0 & 0 \end{array} \middle| \begin{array}{c} a & b \\ c & d \end{array} \right]$$

TABLE 7.1									
GL-orbits of $\mathbb{R}^{2 \times 2 \times 2}$.	The letters D, G stand for	• "degenerate" and	"generic," respectively.						

tensor	$\operatorname{sign}(\Delta)$	rank	rank_{\otimes}	$rank_{\otimes}$
$D_0 = \left[\begin{array}{cc c} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	0	(0, 0, 0)	0	0
$D_1 = \left[\begin{array}{ccc c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$	0	(1, 1, 1)	1	1
$D_2 = \left[\begin{array}{ccc c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array} \right]$	0	(1, 2, 2)	2	2
$D_2' = \left[\begin{array}{ccc c} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{array} \right]$	0	(2, 1, 2)	2	2
$D_2'' = \left[\begin{array}{ccc c} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right]$	0	(2, 2, 1)	2	2
$G_2 = \left[\begin{array}{ccc c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right]$	+	(2, 2, 2)	2	2
$D_3 = \left[\begin{array}{ccc c} 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right]$	0	(2, 2, 2)	3	2
$G_3 = \left[\begin{array}{ccc c} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \end{array} \right]$	_	(2, 2, 2)	3	3

If $d \neq 0$ then we may transform this to G_2 as follows:

$$\left[\begin{array}{cc|c} 1 & 0 & a & b \\ 0 & 0 & c & d \end{array}\right] \rightsquigarrow \left[\begin{array}{cc|c} 1 & 0 & \times & 0 \\ 0 & 0 & 0 & d \end{array}\right] \rightsquigarrow \left[\begin{array}{cc|c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right].$$

If d = 0, then

$$\left[\begin{array}{cc|c} 1 & 0 & a & b \\ 0 & 0 & c & 0 \end{array}\right] \rightsquigarrow \left[\begin{array}{cc|c} 1 & 0 & 0 & b \\ 0 & 0 & c & 0 \end{array}\right].$$

In this situation we can normalize b, c separately, reducing these matrices to one of the following four cases (according to whether b, c are zero):

 $\left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right], \quad \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{array}\right], \quad \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{array}\right], \quad \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array}\right], \quad \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right],$

which are D_1, D'_2, D''_2 , and D_3 , respectively.

Finally, if $rank(A_1) = 2$, then we may assume that

$$A = [A_1 \mid A_2] = \begin{bmatrix} 1 & 0 \mid \times & \times \\ 0 & 1 \mid & \times & \times \end{bmatrix}.$$

By applying a transformation of the form (I, L, L^{-1}) , we can keep A_1 fixed while conjugating A_2 into (real) Jordan canonical form. There are four cases.

If A_2 has repeated real eigenvalues and is diagonalizable, then we get D_2 :

$\begin{bmatrix} 1 & 0 \end{bmatrix}$	$\lambda 0$] [1	0	0	0]
0 1	$\begin{vmatrix} 0 & \lambda \end{vmatrix}$	$\left] \rightsquigarrow \left[\begin{array}{c} 1 \\ 0 \end{array} \right]$	1	0	0].

If A_2 has repeated real eigenvalues and is not diagonalizable, then we have

[1	0	λ	1]	1	0	0	1]
0	1	0	λ	$] \sim $	0	1	0	0	,

which is equivalent (after swapping columns and swapping slabs) to D_3 .

If A_2 has distinct real eigenvalues, then A reduces to G_2 :

[1	0	λ	0		[1	0	0	0]	1	0	0	0	
0	1	0	μ	\sim	0	1	0	$\begin{array}{c} 0 \\ \mu - \lambda \end{array}$		0	0	0	1	•

If A_2 has complex eigenvalues, then we can reduce A to G_3 :

$$\left[\begin{array}{ccc|c} 1 & 0 & a & -b \\ 0 & 1 & b & a \end{array}\right] \rightsquigarrow \left[\begin{array}{ccc|c} 1 & 0 & 0 & -b \\ 0 & 1 & b & 0 \end{array}\right] \rightsquigarrow \left[\begin{array}{ccc|c} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \end{array}\right].$$

Thus, every $2 \times 2 \times 2$ tensor can be transformed into one of the canonical forms listed in the statement of the theorem. Moreover, the invariants $\operatorname{sign}(\Delta)$ and $\operatorname{rank}_{\mathbb{H}}$ are easily computed for the canonical forms and suffice to distinguish them. It follows that the listed forms are pairwise inequivalent.

We confirm the given values of rank_{\otimes}. It is clear that rank_{\otimes}(D_0) = 0 and rank_{\otimes}(D_1) = 1. By Proposition 5.4, any tensor of rank 1 must be equivalent to D_1 . Thus D_2 , D'_2 , D''_2 , and G_2 are all of rank 2. By Proposition 5.5, every tensor of rank 2 must be equivalent to one of these. In particular, D_3 and G_3 must have rank at least 3. Evidently rank_{\otimes}(D_3) = 3 from its definition; and the same is true for G_3 by virtue of the less obvious relation

$$G_3 = (\mathbf{e}_1 + \mathbf{e}_2) \otimes \mathbf{e}_2 \otimes \mathbf{e}_2 + (\mathbf{e}_1 - \mathbf{e}_2) \otimes \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes (\mathbf{e}_1 + \mathbf{e}_2) \otimes (\mathbf{e}_1 - \mathbf{e}_2).$$

Finally, we confirm the tabulated values of $\underline{\operatorname{rank}}_{\otimes}$. By virtue of the remark after Definition 5.11, it is enough to verify that $\underline{\operatorname{rank}}_{\otimes}(D_3) \leq 2$ and that $\underline{\operatorname{rank}}_{\otimes}(G_3) = 3$. The first of these assertions follows from Proposition 4.6. The set of tensors of type G_3 is an open set, which implies the second assertion. \Box

Remark. We note that D_3 is equivalent to any of the tensors obtained from it by permutations of the three factors. Indeed, all of these tensors have rank_{\mathbb{H}} = (2, 2, 2) and $\Delta = 0$. Similar remarks apply to G_2 , G_3 .

Remark. The classification of $GL_{2,2,2}(\mathbb{C})$ -orbits in $\mathbb{C}^{2\times2\times2}$ differs only in the treatment of G_3 , since there is no longer any distinction between real and complex eigenvalues.

We caution the reader that the *finite* classification in Theorem 7.1 is, in general, not possible for tensors of arbitrary size and order simply because the dimension or "degrees of freedom" of $\mathbb{R}^{d_1 \times \cdots \times d_k}$ exceeds that of $\operatorname{GL}_{d_1,\ldots,d_k}(\mathbb{R})$ as soon as $d_1 \cdots d_k > d_1^2 + \cdots + d_k^2$ (which is almost always the case). Any attempt at an explicit classification must necessarily include continuous parameters. For the case of $\mathbb{R}^{2 \times 2 \times 2}$ this argument is not in conflict with our finite classification, since $2 \cdot 2 \cdot 2 < 2^2 + 2^2 + 2^2$.

7.1. Generic rank. We called the tensors in the orbit classes of G_2 and G_3 generic in the sense that the property of being in either one of these classes is an open condition. One should note that there is often no one single generic outer-product rank for tensors over \mathbb{R} [50, 74]. (For tensors over \mathbb{C} such a generic rank always exists [18].) The "generic outer-product rank" for tensors over \mathbb{R} should be regarded as set-valued:

generic-rank_{$$\otimes$$}($\mathbb{R}^{d_1 \times \cdots \times d_k}$) = { $r \in \mathbb{N} \mid S_r(d_1, \ldots, d_k)$ has nonempty interior}.

So the generic outer-product rank in $\mathbb{R}^{2 \times 2 \times 2}$ is $\{2,3\}$. Another term, preferred by some and coined originally by ten Berge, is *typical rank* [74].

Given $d_1, \ldots d_k$, the determination of the generic outer-product rank is an open problem in general and a nontrivial problem even in simple cases; see [13, 14] for results over \mathbb{C} and [73, 74] for results over \mathbb{R} . Fortunately, the difficulty does not extend to multilinear rank; a single unique generic multilinear rank always exists and depends only on $d_1, \ldots d_k$ (and not on the base field; cf. Proposition 7.4).

PROPOSITION 7.2. Let $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$. If $\operatorname{rank}_{\boxplus}(A) = (r_1(A), \ldots, r_k(A))$, then

$$r_i(A) = \min\left(d_i, \prod_{j \neq i} d_j\right), \quad i = 1, \dots, k,$$

generically.

Proof. Let $\mu_i : \mathbb{R}^{d_1 \times \cdots \times d_k} \to \mathbb{R}^{d_i \times \prod_{j \neq i} d_j}$ be the forgetful map that "flattens" or "unfolds" a tensor into a matrix in the *i*th mode. It is easy to see that

(7.1)
$$r_i(A) = \operatorname{rank}(\mu_i(A)),$$

where "rank" here denotes matrix rank. The results then follow from the fact that the generic rank of a matrix in $\mathbb{R}^{d_i \times \prod_{j \neq i} d_j}$ is $\min(d_i, \prod_{j \neq i} d_j)$. \Box

For example, for order-3 tensors,

generic-rank_{\mathbb{H}}(
$$\mathbb{R}^{l \times m \times n}$$
) = (min(l, mn), min(m, ln), min(n, lm)).

7.2. Semialgebraic description of orbit classes. For a general tensor $A \in \mathbb{R}^{2 \times 2 \times 2}$, its orbit class is readily determined by computing the invariants $\operatorname{sign}(\Delta(A))$ and $\operatorname{rank}_{\boxplus}(A)$ and comparing with the canonical forms. The ranks $r_i(A)$ which constitute $\operatorname{rank}_{\boxplus}(A)$ can be evaluated algebraically as follows. If $A \neq 0$, then each $r_i(A)$ is either 1 or 2. For example, note that $r_1(A) < 2$ if and only if the vectors $A_{\bullet 11}$, $A_{\bullet 12}$, $A_{\bullet 21}$, $A_{\bullet 22}$ are linearly dependent, which happens if and only if all the 2-by-2 minors of the matrix

$$\begin{bmatrix} a_{111} & a_{112} & a_{121} & a_{122} \\ a_{211} & a_{212} & a_{221} & a_{222} \end{bmatrix}$$

are zero. Explicitly, the following six equations must be satisfied:

 $(7.2) a_{111}a_{212} = a_{211}a_{112}, a_{111}a_{221} = a_{211}a_{121}, a_{111}a_{222} = a_{211}a_{122},$ $a_{112}a_{221} = a_{212}a_{121}, a_{112}a_{222} = a_{212}a_{122}, a_{121}a_{222} = a_{221}a_{122}.$

Similarly, $r_2(A) < 2$ if and only if

$$(7.3) a_{111}a_{122} = a_{121}a_{112}, a_{111}a_{221} = a_{121}a_{211}, a_{111}a_{222} = a_{121}a_{212}, a_{112}a_{122} = a_{122}a_{211}, a_{112}a_{222} = a_{122}a_{212}, a_{211}a_{222} = a_{221}a_{212};$$

and $r_3(A) < 2$ if and only if

$$(7.4) a_{111}a_{122} = a_{112}a_{121}, a_{111}a_{212} = a_{112}a_{211}, a_{111}a_{222} = a_{112}a_{221}, a_{121}a_{212} = a_{122}a_{211}, a_{121}a_{222} = a_{122}a_{221}, a_{211}a_{222} = a_{212}a_{221}.$$

The equations (7.2)-(7.4) lead to twelve distinct polynomials (beginning with $\Delta_1 = a_{111}a_{212}-a_{211}a_{112}$) which, together with $\Delta_0 := \Delta$, make up the collection $\Delta_0, \ldots, \Delta_{12}$ of polynomials used in the semialgebraic description of the orbit structure of $\mathbb{R}^{2\times2\times2}$, as in Corollary 6.3. Indeed, we note that in Table 7.1 the information in the fourth and fifth columns (rank_{\otimes}(A), <u>rank_{\otimes}(A)</u>) is determined by the information in the second and third columns (sign(Δ), rank_{\boxplus}(A)).

7.3. Generic rank on $\Delta = 0$. The notion of generic rank also makes sense on subvarieties of $\mathbb{R}^{2 \times 2 \times 2}$ —for instance, on the $\Delta = 0$ hypersurface.

PROPOSITION 7.3. The tensors on the hypersurface $\mathcal{D}_3 = \{A \in \mathbb{R}^{2 \times 2 \times 2} \mid \Delta(A) = 0\}$ are all of the form

$$\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3,$$

and they have rank 3 generically.

Proof. From the canonical forms in Table 7.1, we see that if $\Delta(A) = 0$, then

$$A = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3$$

for some $\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^2$, not necessarily linearly independent. It remains to be shown that rank_{\otimes}(A) = 3 generically.

From Theorem 7.1 and the subsequent discussion, if $\Delta(A) = 0$, then rank_{\otimes} $(A) \leq 2$ if and only if at least one of the equation sets (7.2), (7.3), (7.4) is satisfied. Hence $\mathcal{D}_2 := \{A \mid \Delta(A) = 0, \operatorname{rank}_{\otimes}(A) \leq 2\}$ is an algebraic subset of \mathcal{D}_3 .

On the other hand, $\mathcal{D}_3 \setminus \mathcal{D}_2$ is dense in \mathcal{D}_3 with respect to the Euclidean, and hence the Zariski, topology. Indeed, each of the tensors D_0 , D_1 , D_2 , D'_2 , D''_2 can be approximated by tensors of type D_3 ; for instance,

$$\begin{bmatrix} 1 & 0 & | & 0 & \epsilon \\ 0 & 1 & | & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & | & 0 & 0 \\ 0 & 1 & | & 0 & 0 \end{bmatrix} = D_2 \quad \text{as } \epsilon \rightarrow 0.$$

Multiplying by an arbitrary $(L, M, N) \in GL_{2,2,2}(\mathbb{R})$, it follows that any tensor in \mathcal{D}_2 can be approximated by tensors of type D_3 .

It follows that the rank-3 tensors $\mathcal{D}_3 \setminus \mathcal{D}_2$ in \mathcal{D}_3 constitute a generic subset of \mathcal{D}_3 in the Zariski sense (and hence in all the other usual senses).

Remark. In fact, it can be shown that \mathcal{D}_3 is an irreducible variety. If we accept that, then the fact that \mathcal{D}_2 is a proper subvariety of \mathcal{D}_3 immediately implies that the rank-3 tensors form a generic subset of \mathcal{D}_3 . The denseness argument becomes unnecessary.

7.4. Base field dependence. It is interesting to observe that the $GL_{2,2,2}(\mathbb{R})$ orbit classes of G_2 and G_3 merge into a single orbit class over \mathbb{C} (under the action of $GL_{2,2,2}(\mathbb{C})$). Explicitly, if we write $\mathbf{z}_k = \mathbf{x}_k + i\mathbf{y}_k$ and $\bar{\mathbf{z}}_k = \mathbf{x}_k - i\mathbf{y}_k$, then

(7.5)
$$\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 - \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{x}_3$$

= $\frac{1}{2} (\bar{\mathbf{z}}_1 \otimes \mathbf{z}_2 \otimes \bar{\mathbf{z}}_3 + \mathbf{z}_1 \otimes \bar{\mathbf{z}}_2 \otimes \mathbf{z}_3).$

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The LHS is in the $\operatorname{GL}_{2,2,2}(\mathbb{R})$ -orbit class of G_3 and has outer-product rank 3 over \mathbb{R} . The RHS is in the $\operatorname{GL}_{2,2,2}(\mathbb{C})$ -orbit class of G_2 and has outer-product rank 2 over \mathbb{C} . To see why this is unexpected, recall that an $m \times n$ matrix with real entries has the same rank whether we regard it as an element of $\mathbb{R}^{m \times n}$ or of $\mathbb{C}^{m \times n}$. Note, however, that G_2 and G_3 have the same multilinear rank; this is not coincidental but is a manifestation of the following result.

PROPOSITION 7.4. The multilinear rank of a tensor is independent of the choice of base field. If \mathbb{K} is an extension field of \mathbb{k} , the value rank_{\mathbb{H}}(A) is the same whether A is regarded as an element of $\mathbb{k}^{d_1 \times \cdots \times d_k}$ or of $\mathbb{K}^{d_1 \times \cdots \times d_k}$.

Proof. This follows immediately from (7.1) and the base field independence of matrix rank. \Box

In 1969, Bergman [4] considered linear subspaces of matrix spaces, and showed that the minimum rank on a subspace can become strictly smaller upon taking a field extension. He gave a class of examples, the simplest instance being the 2-dimensional subspace

$$s \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + t \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

of $\mathbb{R}^{2\times 2}$. Every (nonzero) matrix in this subspace has rank 2, but the complexified subspace contains a matrix of rank 1. Intriguingly, this example is precisely the subspace spanned by the slabs of G_3 . We suspect a deeper connection.

7.5. Injectivity of orbits. The tensor rank has the property of being invariant under the general multilinear group (cf. (2.15)). Indeed, much of its relevance comes from this fact. Moreover, from Proposition 3.1 we know that tensor rank is preserved when a tensor space is included in a larger tensor space. Similar assertions are true for the multilinear rank (cf. (2.19)).

The situation is more complicated for the function Δ defined on $\mathbb{R}^{2\times2\times2}$. The sign of Δ is $\operatorname{GL}_{2,2,2}(\mathbb{R})$ -invariant, and Δ itself is invariant under $\operatorname{O}_{2,2,2}(\mathbb{R})$. For general $d_1, d_2, d_3 \geq 2$, we do not have an obvious candidate function Δ defined on $\mathbb{R}^{d_1 \times d_2 \times d_3}$. However, there is a natural definition of Δ restricted to the subset of tensors A for which $\operatorname{rank}_{\mathbb{H}}(A) \leq (2, 2, 2)$. Such a tensor can be expressed as

$$A = (L, M, N) \cdot (B \oplus 0),$$

where $B \in \mathbb{R}^{2 \times 2 \times 2}$, $0 \in \mathbb{R}^{(d_1-2) \times (d_2-2) \times (d_3-2)}$, and $(L, M, N) \in O_{d_1, d_2, d_3}(\mathbb{R})$. We provisionally define $\Delta(A) = \Delta(B)$, subject to a check that this is independent of the choices involved. Given an alternative expression $A = (L', M', N') \cdot (B' \oplus 0)$, it follows that $B \oplus 0$ and $B' \oplus 0$ are in the same $O_{d_1, d_2, d_3}(\mathbb{R})$ -orbit. Indeed,

$$B \oplus 0 = (L^{-1}L', M^{-1}M', N^{-1}N') \cdot (B' \oplus 0).$$

If we can show, more strongly, that B, B' belong to the same $O_{2,2,2}(\mathbb{R})$ -orbit, then the desired equality $\Delta(B) = \Delta(B')$ follows from the orthogonal invariance of Δ .

The missing step is supplied by the next theorem, which we state in a basis-free form for abstract vector spaces. If V is a vector space, we write $\operatorname{GL}(V)$ for the group of invertible linear maps from $V \to V$. If, in addition, V is an inner-product space, we write $\operatorname{O}(V)$ for the group of norm-preserving linear maps $V \to V$. In particular, $\operatorname{GL}(\mathbb{R}^d) \cong \operatorname{GL}_d(\mathbb{R})$ and $\operatorname{O}(\mathbb{R}^d) \cong \operatorname{O}_d(\mathbb{R})$.

THEOREM 7.5 (injectivity of orbits). Let $\mathbb{k} = \mathbb{R}$ or \mathbb{C} and V_1, \ldots, V_k be \mathbb{k} -vector spaces. Let $U_1 \leq V_1, \ldots, U_k \leq V_k$. (1) Suppose $B, B' \in U_1 \otimes \cdots \otimes U_k$ are in

distinct $\operatorname{GL}(U_1) \times \cdots \times \operatorname{GL}(U_k)$ -orbits of $U_1 \otimes \cdots \otimes U_k$; then B and B' are in distinct $\operatorname{GL}(V_1) \times \cdots \times \operatorname{GL}(V_k)$ -orbits of $V_1 \otimes \cdots \otimes V_k$. (2) Suppose $B, B' \in U_1 \otimes \cdots \otimes U_k$ are in distinct $\operatorname{O}(U_1) \times \cdots \times \operatorname{O}(U_k)$ -orbits of $U_1 \otimes \cdots \otimes U_k$; then B and B' are in distinct $\operatorname{O}(V_1) \times \cdots \times \operatorname{O}(V_k)$ -orbits of $V_1 \otimes \cdots \otimes V_k$.

LEMMA 7.6. Let $W \leq U \leq V$ be vector spaces and $L \in GL(V)$. Suppose $L(W) \leq U$. Then there exists $\tilde{L} \in GL(U)$ such that $L|_W = \tilde{L}|_W$. Moreover, if $L \in O(V)$, then we can take $\tilde{L} \in O(U)$.

Proof. Extend $L|_W$ to U by mapping the orthogonal complement of W in U by a norm-preserving map to the orthogonal complement of L(W) in U. The resulting linear map \tilde{L} has the desired properties and is orthogonal if L is orthogonal. \Box

Proof of Theorem 7.5. We prove the contrapositive form of the theorem. Suppose $B' = (L_1, \ldots, L_k) \cdot B$, where $L_i \in \operatorname{GL}(V_i)$. Let $W_i \leq U_i$ be minimal subspaces such that B is in the image of $W_1 \otimes \cdots \otimes W_k \hookrightarrow U_1 \otimes \cdots \otimes U_k$. It follows that $L_i(W_i) \leq U_i$, for otherwise we could replace W_i by $L_i^{-1}(L_i(W_i) \cap U_i)$. We can now use Lemma 7.6 to find $\tilde{L}_i \in \operatorname{GL}(U_i)$ which agree with L_i on W_i . By construction, $(\tilde{L}_1, \ldots, \tilde{L}_k) \cdot B = (L_1, \ldots, L_k) \cdot B = B'$. In the orthogonal case, where $L_i \in \operatorname{O}(V_i)$, we may choose $\tilde{L}_i \in \operatorname{O}(U_i)$.

COROLLARY 7.7. Let φ be a $\operatorname{GL}_{d_1,\ldots,d_k}(\mathbb{R})$ -invariant (respectively, $\operatorname{O}_{d_1,\ldots,d_k}(\mathbb{R})$ invariant) function on $\mathbb{R}^{d_1 \times \cdots \times d_k}$. Then φ naturally extends to a $\operatorname{GL}_{d_1,\ldots,d_k}(\mathbb{R})$ invariant (respectively, $\operatorname{O}_{d_1,\ldots,d_k}(\mathbb{R})$ -invariant) function on the subset

$$\{A \in \mathbb{R}^{(d_1+e_1) \times \dots \times (d_k+e_k)} \mid r_i(A) \le d_i \text{ for } i = 1, \dots, k\}$$

of $\mathbb{R}^{(d_1+e_1)\times\cdots\times(d_k+e_k)}$.

Proof. As with Δ above, write $A = (L_1, \ldots, L_k) \cdot B$ for $B \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ and define $\varphi(A) = \varphi(B)$. By Theorem 7.5 this is independent of the choices involved. \Box

The problem of classification is closely related to finding invariant functions. We end this section with a strengthening of Theorem 7.1.

COROLLARY 7.8. The eight orbits in Theorem 7.1 remain distinct under the embedding $\mathbb{R}^{2\times2\times2} \hookrightarrow \mathbb{R}^{d_1\times d_2\times d_3}$ for any $d_1, d_2, d_3 \geq 2$. Thus, Theorem 7.1 immediately gives a classification of tensors $A \in \mathbb{R}^{d_1\times d_2\times d_3}$ with $\operatorname{rank}_{\boxplus}(A) \leq (2, 2, 2)$, into eight classes under $\operatorname{GL}_{d_1, d_2, d_3}(\mathbb{R})$ -equivalence.

The corollary allows us to extend the notion of tensor type to $\mathbb{R}^{d_1 \times d_2 \times d_3}$. For instance, we will say that $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ has type G_3 if and only if A is GL-equivalent to $G_3 \in \mathbb{R}^{2 \times 2 \times 2} \subset \mathbb{R}^{d_1 \times d_2 \times d_3}$.

Note that order-k tensors can be embedded in order-(k+1) tensors by taking the tensor product with a 1-dimensional factor. Distinct orbits remain distinct, so the results of this subsection extend to inclusions into tensor spaces of higher order.

8. Volume of tensors with no optimal low-rank approximation. At this point, it is clear that there exist tensors that can fail to have optimal low-rank approximations. However, it is our experience that practitioners have sometimes expressed optimism that such failures might be rare abnormalities that are not encountered in practice. In truth, such optimism is misplaced: the set of tensors with no optimal low-rank approximation has positive volume. In other words, a randomly chosen tensor will have a nonzero chance of failing to have a optimal low-rank approximation.

We begin this section with a particularly striking instance of this.

THEOREM 8.1. No tensor of rank 3 in $\mathbb{R}^{2\times 2\times 2}$ has an optimal rank-2 approximation (with respect to the Frobenius norm). In particular, APPROX(A, 2) has no solution for tensors of type G_3 , which comprise a set that is open and therefore of positive volume. LEMMA 8.2. Let $A \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ with $\operatorname{rank}_{\otimes}(A) \geq r$. Suppose $B \in \mathcal{S}_r(d_1, \ldots, d_k)$ is an optimal rank-r approximation for A. Then $\operatorname{rank}_{\otimes}(B) = r$.

Proof. Suppose $\operatorname{rank}_{\otimes}(B) \leq r-1$. Then $B \neq A$, and so B-A has at least one nonzero entry in its array representation. Let $E \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ be the rank-1 tensor which agrees with B-A at that entry and is zero everywhere else. Then $\operatorname{rank}_{\otimes}(B+E) \leq r$ but $||A-(B+E)||_F < ||A-B||_F$, so B is not optimal. \Box *Proof of Theorem* 8.1. Let $A \in \mathbb{R}^{2 \times 2 \times 2}$ have rank 3, and suppose that B is an

Proof of Theorem 8.1. Let $A \in \mathbb{R}^{2 \times 2 \times 2}$ have rank 3, and suppose that B is an optimal rank-2 approximation to A. Propositions 5.9 and 5.10, together with the continuity of Δ , imply that $\Delta(B) = 0$. Lemma 8.2 implies that rank_{\otimes}(B) = 2. By Theorem 7.1, it follows that B is of type D_2 , D'_2 , or D''_2 .

We may assume without loss of generality that B is of type D_2 . The next step is to put B into a helpful form by making an orthogonal change of coordinates. This gives an equivalent approximation problem, thanks to the O-invariance of the Frobenius norm. From Table 7.1, we know that $\operatorname{rank}_{\boxplus}(B) = (1, 2, 2)$. Such a B is orthogonally equivalent to a tensor of the following form:

(8.1)
$$\begin{bmatrix} \lambda & 0 & | & 0 & 0 \\ 0 & \mu & | & 0 & 0 \end{bmatrix}.$$

Indeed, a rotation in the first tensor factor brings B entirely into the first slab, and further rotations in the second and third factors put the resulting matrix into diagonal form, with singular values $\lambda, \mu \neq 0$.

Henceforth we assume that B is equal to the tensor in (8.1). We will consider perturbations of the form $B + \epsilon H$, which will be chosen so that $\Delta(B + \epsilon H) = 0$ for all $\epsilon \in \mathbb{R}$. Then $B + \epsilon H \in \overline{S}_2(2, 2, 2)$, and we must have

$$||A - B||_F \le ||A - (B + \epsilon H)||_F$$

for all ϵ . In fact

$$||A - (B + \epsilon H)||_F^2 - ||A - B||_F^2 = -2\epsilon \langle A - B, H \rangle_F + \epsilon^2 ||H||_F^2,$$

so if this is to be nonnegative for all small values of ϵ , it is necessary that

(8.2)
$$\langle A - B, H \rangle_F = 0.$$

Tensors H which satisfy the condition $\Delta(B + \epsilon H) \equiv 0$ include the following:

$$\begin{bmatrix} \times & \times & & 0 & 0 \\ \times & \times & & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & & 0 & 1 \\ 0 & 0 & & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & & 0 & 0 \\ 0 & 0 & & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & & \lambda & 0 \\ 0 & 0 & & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & & \lambda & 0 \\ 0 & 0 & & 0 & \mu \end{bmatrix}$$

since the resulting tensors have types D_2 , D_3 , D_3 , and D_2 , respectively.

Each of these gives a constraint on A - B, by virtue of (8.2). Putting the constraints together, we find that

$$A - B = \begin{bmatrix} 0 & 0 & | & a\mu & 0 \\ 0 & 0 & | & 0 & -a\lambda \end{bmatrix} \quad \text{or} \quad A = \begin{bmatrix} \lambda & 0 & | & a\mu & 0 \\ 0 & \mu & | & 0 & -a\lambda \end{bmatrix}$$

for some $a \in \mathbb{R}$. Thus $A = (\lambda \mathbf{e}_1 + a\mu \mathbf{e}_2) \otimes \mathbf{e}_1 \otimes \mathbf{e}_1 + (\mu \mathbf{e}_1 - a\lambda \mathbf{e}_2) \otimes \mathbf{e}_2 \otimes \mathbf{e}_2$ has rank 2, which is a contradiction. \Box

COROLLARY 8.3. Let $d_1, d_2, d_3 \geq 2$. If $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ is of type G_3 , then A does not have an optimal rank-2 approximation.

Proof. We use the projection Π_A defined in subsection 2.6. For any $B \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, Pythagoras's theorem (2.20) gives

$$||B - A||_F^2 = ||\Pi_A(B - A)||_F^2 + ||(1 - \Pi_A)(B - A)||_F^2$$

= $||\Pi_A(B) - A||_F^2 + ||B - \Pi_A(B)||_F^2.$

If B is an optimal rank-2 approximation, then it follows that $B = \prod_A(B)$; for otherwise $\prod_A(B)$ would be a better approximation. Thus $B \in U_1 \otimes U_2 \otimes U_3$, where U_1, U_2, U_3 are the supporting subspaces of A. These are 2-dimensional, since $\operatorname{rank}_{\boxplus}(A) = (2, 2, 2)$, so $U_1 \otimes U_2 \otimes U_3 \cong \mathbb{R}^{2 \times 2 \times 2}$. The optimality of B now contradicts Theorem 8.1.

Our final result is that the set of tensors A for which APPROX(A, 2) has no solution is a set of positive volume for all tensor spaces of order 3 except those isomorphic to a matrix space—in other words, Theorem 1.3. Note that the G_3 -tensors comprise a set of zero volume in all cases except $\mathbb{R}^{2 \times 2 \times 2}$. Here is the precise statement.

THEOREM 8.4. Let $d_1, d_2, d_3 \geq 2$. The set of tensors $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ for which APPROX(A, 2) does not have a solution (in the Frobenius norm) contains an open neighborhood of the set of tensors of type G_3 . In particular, this set is nonempty and has positive volume.

For $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, let $\mathcal{B}(A)$ denote the set of optimal border-rank-2 approximations for A. Since $\overline{\mathcal{S}}_2(d_1, d_2, d_3)$ is nonempty and closed, it follows that $\mathcal{B}(A)$ is nonempty and compact.

We can restate the theorem as follows. Let A_0 be an arbitrary G_3 -tensor. We must show that if A is close to A_0 , and $B \in \mathcal{B}(A)$, then rank_{\otimes}(B) > 2, i.e., B is a D_3 -tensor. Our proof strategy is contained in the steps of the following lemma.

LEMMA 8.5. Let $A_0 \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ be a fixed tensor of type G_3 . Then there exist positive numbers $\rho = \rho(A_0)$, $\delta = \delta(A_0)$ such that the following statements are true for all $A \in \mathbb{R}^{d_1 \times d_2 \times d_3}$.

- (1) If A is a G_3 -tensor and $B \in \mathcal{B}(A)$, then B is a D_3 -tensor and $\Pi_B = \Pi_A$.
- (2) If $||A A_0||_F < \rho$ and $\operatorname{rank}_{\boxplus}(A) \le (2, 2, 2)$, then A is a G_3 -tensor.
- (3) If $||A A_0||_F < \delta$ and $B \in \mathcal{B}(A)$, define $A' = \Pi_B(A)$. Then $||A' A_0||_F < \rho$ and $B \in \mathcal{B}(A')$.

Proof of Theorem 8.4, assuming Lemma 8.5. Fix $A_0 \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and suppose $||A - A_0||_F < \delta$. It is not generally true that $\operatorname{rank}_{\boxplus}(A) \leq (2, 2, 2)$, so we cannot apply (2) directly to A. Let $B \in \mathcal{B}(A)$. Then $A' = \prod_B(A)$ is close to A_0 , by (3). Since $\operatorname{rank}_{\boxplus}(B) \leq (2, 2, 2)$ and \prod_B is the projection onto the subspace spanned by B, it follows that $\operatorname{rank}_{\boxplus}(A') \leq (2, 2, 2)$. Now (2) implies that A' is a G_3 -tensor. Since $B \in \mathcal{B}(A')$, by (3), it follows from (1) that B is a D_3 -tensor. \Box

Proof of Lemma 8.5 (1). This is essentially Corollary 8.3: B cannot have rank 2 or less, but it has border-rank 2, so B must be a D_3 -tensor. Since $B = \prod_A(B)$ it follows that the supporting subspaces of B are contained in the supporting subspaces of A. However, rank_{\boxplus}(B) = (2,2,2) = rank_{\boxplus}(A), so the two tensors must have the same supporting subspaces, and so $\prod_B = \prod_A$. \Box

Proof of Lemma 8.5 (2). Let $\overline{\mathcal{S}}_2^+(d_1, d_2, d_3)$ denote the set of non G_3 tensors in $\mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank_{\mathbb{H}} $\leq (2, 2, 2)$. Since $A_0 \notin \overline{\mathcal{S}}_2^+(d_1, d_2, d_3)$, it is enough to show that $\overline{\mathcal{S}}_2^+(d_1, d_2, d_3)$ is closed, for then it would be disjoint from the ρ -ball about A_0 for some $\rho > 0$. Note that

$$\overline{\mathcal{S}}_{2}^{+}(d_{1}, d_{2}, d_{3}) = O_{d_{1}, d_{2}, d_{3}}(\mathbb{R}) \cdot \overline{\mathcal{S}}_{2}^{+}(2, 2, 2).$$

Now $\overline{\mathcal{S}}_2^+(2,2,2) = \{A \in \mathbb{R}^{2 \times 2 \times 2} \mid \Delta(A) \ge 0\}$ is a closed subset of $\mathbb{R}^{2 \times 2 \times 2}$, and the

action of the compact group $O_{d_1,d_2,d_3}(\mathbb{R})$ is proper. It follows that $\overline{\mathcal{S}}_2^+(d_1,d_2,d_3)$ is closed, as required. \Box

Proof of Lemma 8.5 (3). We begin with the easier part of the statement, which is that $B \in \mathcal{B}(A')$. To prove this, we will show that $||A' - B||_F \leq ||A' - B'||_F$ whenever $B' \in \mathcal{B}(A')$, establishing the optimality of B as an approximation to A'. Accordingly, let $B' \in \mathcal{B}(A')$. Since $\Pi_B(A') = A'$, it follows from (2.20) with Π_B that

$$||A' - B'||_F^2 = ||A' - \Pi_B(B')||_F^2 + ||B' - \Pi_B(B')||_F^2$$

so, since B' is optimal, we must have $\Pi_B(B') = B'$. We can now apply (2.20) with Π_B to both sides of the inequality $||A - B||_F^2 \leq ||A - B'||_F^2$ to get

$$||A' - B||_F^2 + ||A - A'||_F^2 \le ||A' - B'||_F^2 + ||A - A'||_F^2,$$

and hence $||A' - B||_F \le ||A' - B'||_F$, as claimed.

We now turn to the proof that $\Pi_B(A)$ is close to A_0 if A is close to A_0 . This is required to be uniform in A and B. In other words, there exists $\delta = \delta(A_0) > 0$ such that for all A and all $B \in \mathcal{B}(A)$ if $||A - A_0||_F < \delta$, then $||\Pi_B(A) - A_0|| < \rho$. Here $\rho = \rho(A_0)$ is fixed from part (2) of this lemma.

We need control over the location of *B*. Let $\mathcal{B}_{\epsilon}(A_0)$ denote the ϵ -neighborhood of $\mathcal{B}(A_0)$ in $\overline{\mathcal{S}}_2(d_1, d_2, d_3)$.

PROPOSITION 8.6. Given $\epsilon > 0$, there exists $\delta > 0$ such that if $||A - A_0||_F < \delta$ then $\mathcal{B}(A) \subset \mathcal{B}_{\epsilon}(A_0)$.

Proof. The set $\overline{S}_2(d_1, d_2, d_3) \setminus \mathcal{B}_{\epsilon}(A_0)$ is closed, and so it attains its minimum distance from A_0 . This must exceed the absolute minimum $||A_0 - B_0||_F$ for $B_0 \in \mathcal{B}(A_0)$ by a positive quantity 2δ , say. If $||A - A_0||_F < \delta$ and $B' \in \overline{S}_2(d_1, d_2, d_3) \setminus \mathcal{B}_{\epsilon}(A_0)$ then

$$||A - B'||_F \ge ||B' - A_0||_F - ||A - A_0||_F$$

> $||A_0 - B_0||_F + 2\delta - \delta$
= $||A_0 - B_0||_F + \delta$
> $||A_0 - B_0||_F + ||A - A_0||_F$
 $\ge ||A - B_0||_F$

using the triangle inequality in the first and last lines. Thus $B' \notin \mathcal{B}(A)$.

We claim that if ϵ is small enough, then $\operatorname{rank}_{\boxplus}(B) = (2, 2, 2)$ for all $B \in \mathcal{B}_{\epsilon}(A_0)$. Indeed, this is already true on $\mathcal{B}(A_0)$, by part (1). Since $\operatorname{rank}_{\boxplus}$ is upper-semicontinuous and does not exceed (2, 2, 2) on $\overline{\mathcal{S}}_2(d_1, d_2, d_3)$, it must be constant on a neighborhood of $\mathcal{B}(A_0)$ in $\overline{\mathcal{S}}_2(d_1, d_2, d_3)$. Since $\mathcal{B}(A_0)$ is compact, the neighborhood can be taken to be an ϵ -neighborhood.

Part (1) implies that $\Pi_{B_0} = \Pi_{A_0}$ for all $B_0 \in \mathcal{B}(A_0)$. If ϵ is small enough that $\operatorname{rank}_{\boxplus}(B) = (2, 2, 2)$ on $\mathcal{B}_{\epsilon}(A_0)$, then Π_B depends continuously on $B \in \mathcal{B}_{\epsilon}(A_0)$, by Proposition 2.5. Since $\mathcal{B}(A_0)$ is compact, we can choose ϵ small enough so that the operator norm of $\Pi_B - \Pi_{A_0}$ is as small as we like, uniformly over $\mathcal{B}_{\epsilon}(A_0)$.

We are now ready to confine $\Pi_B(A)$ to the ρ -neighborhood of A_0 . Suppose, initially, that $||A - A_0||_F \leq \rho/2$ and $B \in \mathcal{B}_{\epsilon}(A_0)$. Then

$$\begin{aligned} \|\Pi_B(A) - A_0\|_F &\leq \|(\Pi_B - \Pi_{A_0}) \cdot A\|_F + \|\Pi_{A_0} \cdot A - A_0\|_F \\ &\leq \|\Pi_B - \Pi_{A_0}\| \|A\|_F + \|\Pi_{A_0} \cdot (A - A_0)\|_F \\ &\leq \|\Pi_B - \Pi_{A_0}\| (\|A_0\|_F + \rho/2) + \|A - A_0\|_F \\ &\leq \|\Pi_B - \Pi_{A_0}\| (\|A_0\|_F + \rho/2) + \rho/2. \end{aligned}$$

Now choose $\epsilon > 0$ so that the operator norm $\|\Pi_B - \Pi_{A_0}\|$ is kept small enough to guarantee that the RHS is less than ρ . For this ϵ , choose δ as given by Proposition 8.6. Ensure also that $\delta < \rho/2$.

Then, if $||A - A_0||_F < \delta$ and $B \in \mathcal{B}(A)$, we have $B \in \mathcal{B}_{\epsilon}(A_0)$. By the preceding calculation, $||A' - A_0||_F < \rho$. This completes the proof. \Box

9. Closing remarks. We refer interested readers to [17, 18, 57, 58] for a discussion of similar issues for symmetric tensors and nonnegative tensors. In particular, the reader will find in [18] an example of a symmetric tensor of symmetric rank r (r may be chosen to be arbitrarily large) that does not have a best symmetric-rank-2 approximation. In [57, 58], we show that such failures do not occur in the context of nonnegative tensors; a nonnegative tensor of nonnegative-rank r will always have a best nonnegative-rank-s approximation for any $s \leq r$.

In this paper we have focused our attention on the real case; the complex case has been studied in great detail in algebraic computational complexity theory and algebraic geometry. For the interested reader, we note that the rank-jumping phenomenon still occurs: Proposition 4.6 and its proof carry straight through to the complex case. On the other hand, there is no distinction between G_{3} - and G_{2} -tensors over the complex numbers; if $\Delta(A) \neq 0$, then A has rank 2. The results of section 8 have no direct analogue.

The major open question in tensor approximation is how to overcome the illposedness of APPROX(A, r). In general this will conceivably require an equivalent of Theorem 5.1 that characterizes the limit points of rank-r order-k tensors. It is our hope that some of the tools developed in our study, such as Theorems 5.2 and 7.5 (both of which apply to general r and k), may be used in future studies. The type of characterization in Corollary 5.12, for r = 2 and k = 3, is an example of what one might hope to achieve.

Acknowledgments. We thank the anonymous reviewers for some exceptionally helpful comments. We also gratefully acknowledge Joseph Landsberg and Bernd Sturmfels for enlightening pointers that helped improved sections 4.7 and 6. Lek-Heng Lim thanks Gene Golub for his encouragement and helpful discussions. Both authors thank Gunnar Carlsson and the Department of Mathematics, Stanford University, where some of this work was done.

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