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Tensors of nonnegative rank two [☆]

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ABSTRACT

A nonnegative tensor has nonnegative rank at most 2 if and only if it is supermodular and has flattening rank at most 2. We prove this result, then explore the semialgebraic geometry of the general Markov model on phylogenetic trees with binary states, and comment on possible extensions to tensors of higher rank.

1. Introduction

This article offers a journey into *semialgebraic statistics*. By this we mean the systematic study of statistical models as semialgebraic sets. We shall give a semialgebraic description of binary latent class models in terms of binomials expressing supermodularity, and we determine the algebraic boundary of this and related models. Our discussion is phrased in the language of nonnegative tensor factorization [5,9].

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We consider real tensors $P = [p_{i_1 i_2 \cdots i_n}]$ of format $d_1 \times d_2 \times \cdots \times d_n$. Throughout this paper we shall assume that $n \geqslant 3$ and $d_1, d_2, \ldots, d_n \geqslant 2$. Such a tensor has *nonnegative rank at most* 2 if it can be written as

$$P = a_1 \otimes a_2 \otimes \cdots \otimes a_n + b_1 \otimes b_2 \otimes \cdots \otimes b_n, \tag{1}$$

where the vectors $a_i, b_i \in \mathbb{R}^{d_i}$ are nonnegative for $i = 1, 2, \ldots, n$. The set of such tensors is a closed semialgebraic subset of dimension $2(d_1 + d_2 + \cdots + d_n) - 2(n-1)$ in the tensor space $\mathbb{R}^{d_1 \times d_2 \times \cdots \times d_n}$; see [14, §5.5]. We present the following characterization of this semialgebraic set.

Theorem 1.1. *A nonnegative tensor P has nonnegative rank at most* 2 *if and only if P is supermodular and has flattening rank at most* 2.

Here, *flattening* means picking any subset A of $[n] = \{1, 2, \ldots, n\}$ with $1 \leqslant |A| \leqslant n-1$ and writing the tensor P as an ordinary matrix with $\prod_{i \in A} d_i$ rows and $\prod_{j \notin A} d_j$ columns. The *flattening rank* of P (also called the *multilinear rank* in the literature) is the maximal rank of any of these matrices. Landsberg and Manivel [15] proved that flattening rank $\leqslant 2$ is equivalent to border rank $\leqslant 2$, which for nonnegative tensors is equivalent to rank $\leqslant 2$ by [16, Proposition 6.2].

To define supermodularity, we first fix a tuple $\pi = (\pi_1, \pi_2, \ldots, \pi_n)$ where π_i is a permutation of $\{1, 2, \ldots, d_i\}$. Then P is *π-supermodular* if

$$p_{i_1 i_2 \cdots i_n} \cdot p_{j_1 j_2 \cdots j_n} \leqslant p_{k_1 k_2 \cdots k_n} \cdot p_{l_1 l_2 \cdots l_n} \tag{2}$$

whenever $\{i_r, j_r\} = \{k_r, l_r\}$ and $\pi_r(k_r) \leqslant \pi_r(l_r)$ holds for $r = 1, 2, \ldots, n$. We call a tensor P *supermodular* if it is π-supermodular for some π.

Theorem 1.1 says that every tensor of the form (1) is π-supermodular. Here, the tuple of permutations π can be read off from the signs of the 2×2-minors of matrices A_i with two rows given by a_i and b_i. In particular, for $e = (\mathrm{id}, \ldots, \mathrm{id})$ the tensor P is e-supermodular if and only if these minors are all nonnegative (see Lemma 3.3), or all nonpositive. While conditions such as (2) have appeared before in the statistics literature, e.g. [12], the results in this paper are both fundamental and new.

Note that we are using multiplicative notation instead of the additive notation more commonly used for supermodularity. To be specific, if $d_1 = d_2 = \cdots = d_n = 2$, $\pi = (\mathrm{id}, \mathrm{id}, \ldots, \mathrm{id})$, and P is strictly positive, then P being π-supermodular means that $\log(P)$ lies in the convex polyhedral cone [18, §4] of supermodular functions $2^{\{1,2,\ldots,n\}} \to \mathbb{R}$.

The set of π-supermodular nonnegative tensors P of flattening rank $\leqslant 2$ is denoted $\mathcal{M}_\pi$ and called a *toric cell*. The number of toric cells is $d_1! d_2! \cdots d_n!/2$. Theorem 1.1 states that these cells stratify our model:

$$\mathcal{M} = \bigcup_{\pi} \mathcal{M}_\pi. \tag{3}$$

The term *model* refers to the fact that intersection of (3) with the probability simplex, where all coordinates of P sum to one, is a widely used statistical model. It is the mixture model for pairs of independent distributions on n discrete random variables.

The *Zariski closure* $\overline{\mathcal{S}}$ of a semialgebraic subset $\mathcal{S}$ of $\mathbb{R}^N$ is the complex zero set in $\mathbb{C}^N$ of all polynomials that vanish on $\mathcal{S}$. The *boundary* $\partial\mathcal{S}$ is the topological boundary of $\mathcal{S}$ inside $\overline{\mathcal{S}}$. We define the *algebraic boundary* of $\mathcal{S}$ to be the Zariski closure $\overline{\partial\mathcal{S}}$ of its topological boundary.

Our second theorem concerns the algebraic boundaries of the model $\mathcal{M}$ and of toric cells $\mathcal{M}_\pi$. We regard these boundaries as hypersurfaces inside the complex variety of tensors of border rank $\leqslant 2$. A *slice* of our tensor P is a subtensor of some format $d_1 \times \cdots \times d_{s-1} \times 1 \times d_{s+1} \times \cdots \times d_n$. Subtensors of format $d_1 \times \cdots \times d_{s-1} \times 2 \times d_{s+1} \times \cdots \times d_n$ are *double slices*.

Theorem 1.2. *The algebraic boundary of $\mathcal{M}$ has $\sum_{i=1}^n d_i$ irreducible components, given by slices having rank $\leqslant 1$. The algebraic boundary of any toric cell $\mathcal{M}_\pi$ has the same irreducible components plus $\sum_{i=1}^n \binom{d_i}{2}$ additional components given by linearly dependent double slices.*