The geometry of rank-one tensor completion

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joint work with Kaie Kubjas, Mario Kummer and Zvi Rosen

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Given some of the entries of a tensor, does there exist a rank-one tensor that has the specified entries?

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Assume given are the diagonal entries of a matrix:

$$X = \begin{pmatrix} x_{11} & ? \\ ? & x_{22} \end{pmatrix}$$

Do there exist values for the ? so that the matrix has rank-one?

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Assume given are the diagonal entries of a matrix:

$$X = \begin{pmatrix} x_{11} & ? \\ ? & x_{22} \end{pmatrix}$$

Do there exist values for the ? so that the matrix has rank-one?

Yes!

Pick one value arbitrary, then $x_{11}x_{22} = x_{12}x_{21}$ fixes the fourth.

*see also Kubjas/Rosen Matrix completion for the independence model.

Answer

This can be answered with computational algebra:

- Rank-one tensors are a binomial algebraic set (Segre variety)
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Problem Solved! Except...

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dimension dimension theory. Using the generic freeness lemma we shall prove
of elimination theory of the main theorem of elimination theorem.
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14.1 Elimination Theory
The following classical result is enormously useful.
Theorem 14.1 (Main Theorem of Elimination Theory). If X is any variety
over an algebraically closed field k, and Y is a Zariski closed subset of
X \times P^n, then the image of Y under projection to X is closed.
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We want $k = \mathbb{R}$ and have inequalities too (probabilities are non-negative!).

Example: joint probability distributions

Given the diagonal entries of a two-variate binary distribution

$$X = \begin{pmatrix} x_{11} & ? \\ ? & x_{22} \end{pmatrix} \quad \text{where } x_{ij} = \mathsf{Prob}(X_1 = i, X_2 = j),$$

Do there exist values for the ? so that X is the distribution of two *independent* binary random variables?

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Do there exist marginal distributions $p, q \in \Delta_1$ such that $x_{ij} = p_i q_j$? ($\Delta_m = m$ -diml. simplex)

The geometric view

Problem

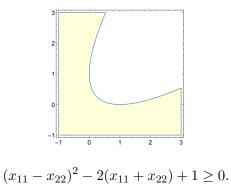
Determine the image of the restricted parametrization map

$$\Delta_1 \times \Delta_1 \to [0, 1]^2$$

(p_1, p_2, q_1, q_2) $\mapsto (x_{11}, x_{22}) = (p_1 q_1, p_2 q_2).$

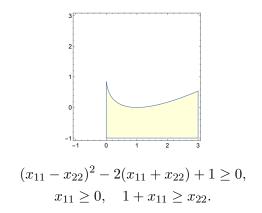
Restrictions on the domain $(p, q \in \Delta_1)$ make this problem interesting.

$$(p_1, p_2, q_1, q_2) \mapsto (x_{11}, x_{22}) = (p_1q_1, p_2q_2).$$
 subject to $p_2 = 1 - p_1, \qquad q_2 = 1 - q_1$



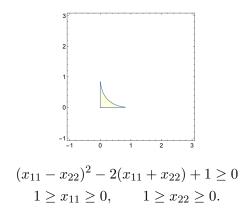
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Tensors

A tensor is an array of numbers from a field ${\mathbb F}$ indexed by

$$D = [d_1] \times \dots \times [d_n]$$

where $d_i \ge 2$ are fixed integers and $[d] = \{1, \ldots, d\}$.

A partial tensor is an array of numbers from \mathbb{F} indexed by a subset $E \subseteq D$. A completion of a partial tensor $S \in \mathbb{F}^E$ is a tensor $T \in \mathbb{F}^D$ such that the restriction $T_{|E}$ agrees with S.

Parametrization of rank one tensors

Let $\mathbb F$ be one of the two fields $\mathbb R$ or $\mathbb C.$ The set of rank-one tensors is the image of the parametrization

 $\mathbb{F}^{d_1} \times \cdots \times \mathbb{F}^{d_n} \to \mathbb{F}^D, \qquad (\theta_1, \dots, \theta_n) \mapsto \theta_1 \otimes \cdots \otimes \theta_n.$

Convenient fact: A real point in the image has a real preimage.

The set of rank-one tensors is a toric variety (product of simplices), cut out by quadratic equations; the (2×2) -minors of its flattenings.

A remark on field dependence

A tensor with real entries and complex rank one has real rank one. This is *false for partial tensors*.

Consider the real $2\times 2\times 2$ partial tensor with third coordinate slices

$$\begin{pmatrix} ? & 1 \\ 1 & ? \end{pmatrix}, \qquad \begin{pmatrix} 1 & ? \\ ? & -1 \end{pmatrix} \in \mathbb{R}^{2 \times 2 \times 2}.$$

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For a rank-one completion T, can assume $T = \begin{pmatrix} 1 \\ a \end{pmatrix} \otimes \begin{pmatrix} 1 \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix}$. Yields

$$bc = 1,$$
 $ac = 1,$ $d = 1,$ $abd = -1.$

Only two solutions:

$$a = \pm i,$$
 $b = \pm i,$ $c = \mp i,$ $d = 1.$

Proposition

The following are equivalent.

- Every real partial tensor T_E with nonzero entries which is completable over the complex numbers is also completeable over the real numbers.
- The index of the lattice spanned by the columns of A_E in its saturation is odd.

Moreover, given complex-completability, real-completability depends only on the signs of observed entries.

Idea of the proof

Diagonalize binomial equations

$$T_e = \theta_{1,e_1} \cdots \theta_{n,e_n} = \theta^{a_e}, \qquad e \in E.$$

via Smith normal form of $A_e = (a_e)_{e \in E}$

Next step

Impose semi-algebraic constraints on the domain of

 $\mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_n} \to \mathbb{R}^D, \qquad (\theta_1, \dots, \theta_n) \mapsto \theta_1 \otimes \cdots \otimes \theta_n.$

For example, $\theta_i \in \Delta_{d_i-1}$ is a probability distribution:

- Non-negativity of entries of θ_i.
- Linear constraints on the entries of θ_i .

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By the way, the Tarski-Seidenberg theorem yields

Semi-algebraic constraints on the parameters yield only semi-algebraic constraints on the image. In principle, they can be computed by eliminating quantifiers from the formula

 $\exists \theta_{1,1}, \ldots, \exists \theta_{n,d_n} \in \mathbb{R}$ such that $x_{1\dots 1} = \ldots$

We study first the algebraic boundary of the image of

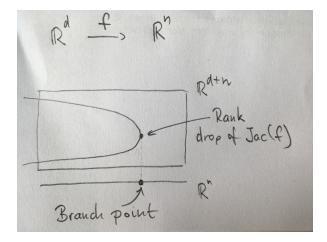
$$\Delta_{d_1-1} \times \cdots \times \Delta_{d_n-1} \to \mathbb{R}^E$$

where $E \subseteq D$, and Δ_m is the probability simplex of dimension m.

The algebraic boundary of a semi-algebraic set $S \subseteq \mathbb{R}^n$ is the Zariskiclosure of the (Euclidean topology) boundary $\partial S = \operatorname{cl}(S) \setminus \operatorname{int}(S)$.

How to compute it

Compute the *branch locus*, the locus in the image where the rank of the Jacobian of the parametrization drops.



Assume now

- the number of observations equals the number of parameters (i.e. Jacobian is square)
- every maximal-dimensional slice is observed

Approach

- Sinn's Lemma: If a semi-algebraic set S ⊆ ℝ^k is nonempty and contained in the closure of its interior and the same holds for ℝ^k \ S, then its algebraic boundary is of pure codimension one.
- Implicit function theorem: If an interior parameter point maps to a boundary tensor, the Jacobian determinant vanishes there.
- Argue that remaining components are all contained in coordinate hyperplanes.

Assume the observed entries of a $2 \times 2 \times 2$ tensor are $x_{211}, x_{121}, x_{112}$. Denote $l_i = 1 - \theta_i$ for i = 1, 2, 3. The graph of the map is defined by

$$I = \langle x_{211} - l_1 \theta_2 \theta_3, x_{121} - \theta_1 l_2 \theta_3, x_{112} - \theta_1 \theta_2 l_3 \rangle.$$

The Jacobian matrix of the parametrization map equals

$$J = \begin{pmatrix} -\theta_2\theta_3 & l_1\theta_3 & l_1\theta_2\\ l_2\theta_3 & -\theta_1\theta_3 & \theta_1l_2\\ \theta_2l_3 & \theta_1l_3 & -\theta_1\theta_2 \end{pmatrix}$$

and has determinant

 $\theta_1^2\theta_2\theta_3 + \theta_1\theta_2^2\theta_3 + \theta_1\theta_2\theta_3^2 - 2\theta_1\theta_2\theta_3 = \theta_1\theta_2\theta_3(-\theta_1 - \theta_2 - \theta_3 + 2).$

 \rightarrow Jacobian determinant is a monomial times a linear polynomial.

Explanation of the linear polynomial

$$\theta_1^2\theta_2\theta_3 + \theta_1\theta_2^2\theta_3 + \theta_1\theta_2\theta_3^2 - 2\theta_1\theta_2\theta_3 = \theta_1\theta_2\theta_3(-\theta_1 - \theta_2 - \theta_3 + 2).$$

Consider the matrix

$$B_E = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix},$$

encoding in its columns which parameters θ_i contribute to a given observed entry, plus an extra column of ones.

The kernel of B_E is spanned by $v = (-1, -1, -1, 2)^T$, which yields the coefficients.

$$I + \langle l_p \rangle = \langle x_{211} - l_1 \theta_2 \theta_3, x_{121} - \theta_1 l_2 \theta_3, x_{112} - \theta_1 \theta_2 l_3, -\theta_1 - \theta_2 - \theta_3 + 2 \rangle.$$

Eliminating θ_1, θ_2 , and θ_3 yields a prime ideal generated by

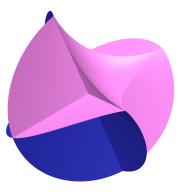
 $\begin{aligned} x_{211}^4 x_{121}^2 &- 2x_{211}^3 x_{121}^{3} + x_{211}^2 x_{121}^4 - 2x_{211}^4 x_{121} x_{112} + 2x_{211}^3 x_{121}^2 x_{112}^2 + 2x_{211}^2 x_{121}^3 x_{121}^2 \\ &- 2x_{211} x_{121}^4 x_{112}^4 + x_{211}^4 x_{112}^2 + 2x_{211}^3 x_{112}^2 - 6x_{211}^2 x_{121}^2 x_{112}^2 + 2x_{211} x_{121}^3 x_{112}^2 + x_{121}^4 x_{121}^2 \\ &- 2x_{211}^3 x_{112}^3 + 2x_{211}^2 x_{112}^3 + 2x_{211} x_{121}^2 x_{112}^3 - 2x_{121}^3 x_{112}^3 + x_{211}^2 x_{112}^4 - 2x_{211} x_{121}^2 x_{112}^4 \\ &+ x_{121}^2 x_{112}^4 - 2x_{211}^3 x_{121}^2 - 2x_{211}^2 x_{121}^3 + 8x_{211}^3 x_{121} x_{112} - 4x_{211}^2 x_{121}^2 + 8x_{211} x_{121}^3 x_{112}^4 \\ &+ x_{121}^2 x_{112}^4 - 4x_{211}^2 x_{121}^2 - 2x_{211}^2 x_{112}^2 - 2x_{121}^3 x_{112}^2 + 2x_{211}^2 x_{112}^3 + 8x_{211} x_{121} x_{112}^3 \\ &- 2x_{211}^2 x_{112}^3 - 4x_{211}^2 x_{121}^2 - 4x_{211} x_{121}^2 x_{112}^2 - 2x_{121}^3 x_{112}^2 + 2x_{211}^2 x_{112}^3 + 8x_{211} x_{121} x_{112}^3 \\ &- 2x_{211}^2 x_{112}^3 + x_{211}^2 x_{121}^2 - 10x_{211}^2 x_{112}^2 - 10x_{211} x_{121}^2 + 2x_{211}^2 x_{112}^2 + 2x_{211}^2 x_{112}$

Observation: Eliminating from

$$I + \langle \theta_1 \theta_2 \theta_3 (-\theta_1 - \theta_2 - \theta_3 + 2) \rangle$$

yields the same (much later).

... and this is how it looks



- The surface is singular in dimension 1 (all along the boundary)
- The interior extends into negative coordinates

Let

- $I = \langle x_e \prod \theta, \dots \rangle$ be the graph ideal of the parametrization.
- *l* be the linear polynomial factor of the Jacobian determinant.
- |E| be equal to the number of parameters.
- $E \subseteq D$ meet every maximal-dimensional slice.

Algebraic boundary theorem

Eliminating the parameter variables from $I + \langle l \rangle$ yields a non-zero principal ideal generated by a non-constant irreducible polynomial f. The polynomial q that defines the algebraic boundary of the completable region is the product of f with some coordinates.

Open Problems

- Determine the degree of f.
- How much do we know from the algebraic boundary?
- Non-square Jacobians (|E| small)



Have some answers for diagonal observations...

Observing diagonal entries

- Consider $d \times d \times \cdots \times d$ tensor of order n.
- Let E consists only of the d diagonal entries (much fewer than number of parameters).
- Let $S_{n,d}$ be the set of diagonal entries that admit a completion to a rank-one "probability tensor" (independent multivariate discrete distribution).

Theorem (Kubjas/Rosen)

 ${\cal S}_{n,d}$ is a semi-algebraic set and its algebraic boundary is known. Furthermore

$$S_{n,d} = \{ x \in \mathbb{R}^d_{\geq 0} : \sum_{i=1}^d x_i^{\frac{1}{n}} \le 1 \}.$$

Theorem

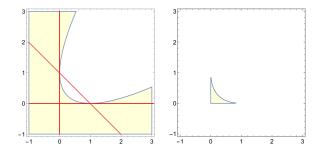
There are explicitly described polynomials $P_{n,d,i}(x)$, $i = 0, \ldots, n^{d-1}$ such that $x \in \mathbb{R}^d_{\geq 0}$ is an element of $S_{n,d}$ if and only if $P_{n,d,i}(x) \geq 0$ for all $0 \leq i < n^{d-1}$. If n is odd, then $S_{n,d} = \{x \in \mathbb{R}^d_{\geq 0} : P_{n,d,0}(x) \geq 0\}$. Let $e_{i,d}$ denote the *i*th elementary symmetric polynomial in x_1, \ldots, x_d .

 $S_{3,2}$ (2 \times 2 \times 2 tensors) is defined by $x_1, x_2 \geq 0$ $(1-e_{1,2})^3 - 27e_{2,2} \geq 0.$

 $S_{2,3}$ (3 × 3 matrices) is defined by

$$\begin{aligned} x_1, x_2, x_3 &\geq 0\\ 1 - e_{1,3} &\geq 0\\ 3(1 - e_{1,3})^2 - 4e_{2,3} &\geq 0\\ (1 - e_{1,3})((1 - e_{1,3})^2 - 4e_{2,3}) - 16e_{3,3} &\geq 0\\ ((1 - e_{1,3})^2 - 4e_{2,3})^2 - 64e_{3,3} &\geq 0. \end{aligned}$$

For d=n=2 the two analyzed classes overlap. We get $x_1,x_2\geq 0$ $1-2(x_1+x_2)+(x_1-x_2)^2\geq 0$ $1-x_1-x_2\geq 0,$



The algebraic boundary misses $1 - x_1 - x_2 \ge 0$ and is thus not the final answer, even in the easiest case.

Conclusion

- The set of partial multi-variate independent probability distributions is semi-algebraic.
- In some cases we can find the algebraic boundary.
- We do want complete semi-algebraic descriptions.
- Semi-algebraic statistics is fun!

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Thank you.