Matrix Completion for the Independence Model

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joint work with Zvi Rosen
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Main problem

Problem

Given some entries of a matrix, is it possible to add the missing entries so that the matrix has rank 1*, its entries sum to one, and it is nonnegative?*

Example

For example, the partial matrix

$$\begin{pmatrix} 0.16 & & & \\ & 0.09 & & \\ & & 0.04 & \\ & & & 0.01 \end{pmatrix}$$

has a unique completion:

$$\begin{pmatrix} 0.16 & 0.12 & 0.08 & 0.04 \\ 0.12 & 0.09 & 0.06 & 0.03 \\ 0.08 & 0.06 & 0.04 & 0.02 \\ 0.04 & 0.03 & 0.02 & 0.01 \end{pmatrix}.$$

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On the other hand, perturbing any entry of the original matrix by $\epsilon > 0$ makes the matrix have no eligible completions, and perturbing any entry by $\epsilon < 0$ introduces an infinite number of completions.

Motivation

Let X and Y be two independent discrete random variables with m and n states respectively, i.e.

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for all i, j.

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$$Pr(X = i, Y = j) = Pr(X = i) \cdot Pr(Y = j)$$

for all i, j. Their joint probabilities are recorded in the matrix

$$P = \begin{pmatrix} Pr(X = 1) \\ Pr(X = 2) \\ \vdots \\ Pr(X = m) \end{pmatrix} \begin{pmatrix} Pr(Y = 1) & Pr(Y = 2) & \cdots & Pr(Y = n) \end{pmatrix},$$

which is rank 1, nonnegative, and its entries sum to one.

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- A situation in which this might arise in applications is a pair of compounds in a laboratory that only react when in certain states.
- A complete answer to our question will allow us to reject a hypothesis of independence of the events X and Y, based only on this collection of probabilities.

2×2 diagonal matrices

Example

Let M be the partial probability matrix given by:

$$M = \begin{pmatrix} a & \\ & b \end{pmatrix}.$$

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Set the off-diagonal entries to x and ab/x and set the sum of all entries $a + ab/x + x + b$ equal to 1. The equivalent quadratic equation is $x^2 + (a + b - 1)x + ab = 0$.

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Set the off-diagonal entries to x and ab/x and set the sum of all entries $a + ab/x + x + b$ equal to 1. The equivalent quadratic equation is $x^2 + (a + b - 1)x + ab = 0$. In order for a real solution for x to exist, the discriminant must be ≥ 0, i.e.

$$(a + b - 1)^2 - 4ab \geq 0.$$

This inequality, along with the requirement that $a + b \leq 1$ and both $a, b > 0$, is sufficient to guarantee that x gives a completion of M.

2×2 diagonal matrices

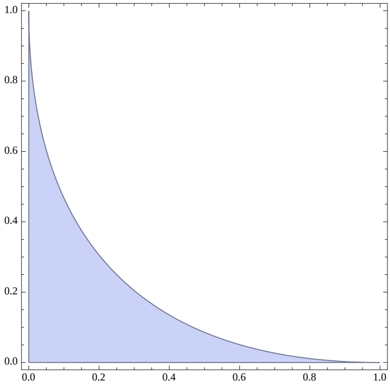

Figure: The colored region corresponds to completable probability matrices of 2×2 matrices with diagonal entries a, b observed.

Diagonal partial matrices

Theorem (K.,Rosen)

Let M be an $n \times n$ partial probability matrix, where $n \geq 2$, with nonnegative observed entries along the diagonal:

$$M = \begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}.$$

Then M is completable if and only if $\sum_{i=1}^{n} \sqrt{a_i} \leq 1$, or equivalently, $||(a_1, \dots, a_n)||_{1/2} \leq 1$. In the special case $\sum_{i=1}^{n} \sqrt{a_i} = 1$, the partial matrix M has a unique completion.

Diagonal partial matrices

Corollary

Let $\sum_{i=1}^{n} \sqrt{a_i} < 1$. For $n = 2$, the probability matrix M has exactly two completions. If $n > 2$, then the set of completions of M is $(n-2)$-dimensional.

Diagonal partial matrices

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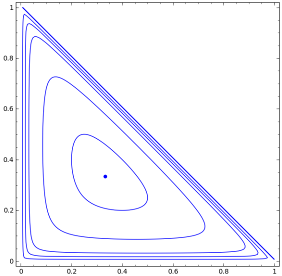

Figure: Each curve represents values of $\mathbf{u}$ that parametrize a completion of the 3×3 diagonal partial matrix with $1/9, 1/10, 1/16, 1/36, 1/64$, and $1/150$ on the diagonal.

2×2 diagonal matrices

The analysis of the previous theorem works to derive the constraint for the 2×2 diagonal probability matrix as in the example. Assuming $a, b \geq 0$:

$$\sqrt{a} + \sqrt{b} \leq 1 \Leftrightarrow a + b + 2\sqrt{ab} \leq 1 \Leftrightarrow 2\sqrt{ab} \leq 1 - a - b$$
$$\Leftrightarrow 4ab \leq (1 - a - b)^2 \text{ and } 0 \leq 1 - a - b.$$

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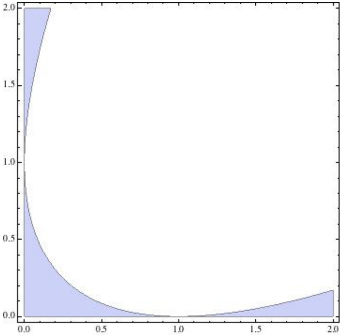

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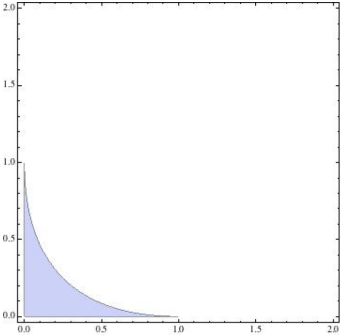

Example: General partial matrices

$$\begin{pmatrix} * & * & * \\ .06 & .09 & * \\ .08 & * & * \\ * & * & .15 \end{pmatrix}$$

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$$\to \begin{pmatrix} .06 & .09 & * \\ .08 & .12 & * \\ * & * & .15 \end{pmatrix} \to \begin{pmatrix} .35 & * \\ * & .15 \end{pmatrix}$$

$$\sqrt{.35} + \sqrt{.15} = .98 < 1$$

General partial matrices

Theorem

Let M be a feasible partial matrix such that after carefully removing zeros, it has s blocks. Let b_i be the sum of the entries in the i-th block after completing by 2×2 minors. If $s = 1$, then M is completable if and only if $b_1 = 1$. For $s > 1$, the partial matrix M is completable to a probability matrix if and only if:

$$\sum_{i=1}^{s} \sqrt{b_i} \leq 1.$$

Example: General partial matrices

Example

The probability matrix

$$\begin{pmatrix} x_{11} & x_{12} & \\ x_{21} & & \\ & & x_{33} \end{pmatrix}$$

with all observed entries nonnegative has a completion if and only if

$$\sqrt{x_{11} + x_{12} + x_{21} + x_{12}x_{21}/x_{11}} + \sqrt{x_{33}} \leq 1.$$

Tensors

Theorem

Suppose we are given a partial probability tensor $T \in (\mathbb{R}^n)^{\otimes d}$ with nonnegative observed entries a_i along the diagonal, i. e. we have $t_{ii\dots i} = a_i$ for $1 \leq i \leq n$, and all other entries unobserved. Then T is completable if and only if

$$\sum_{i=1}^{n} a_i^{1/d} \leq 1.$$

Semialgebraic sets

Proposition

Partial tensors of fixed type which can be completed to rank-1 probability tensors form a semialgebraic set.

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There exists a unique irreducible polynomial f of degree d^{n-1} with constant term 1 that vanishes on the boundary of diagonal partial tensors which can be completed to rank-1 probability tensors. The semialgebraic description takes the form $f \geq 0$, coordinates ≥ 0 plus additional inequalities that separate our set from other chambers in the region defined by $f \geq 0$.

3×3 diagonal matrices

The region defined by

$$\sqrt{a} + \sqrt{b} + \sqrt{c} \leq 1$$

is the same as

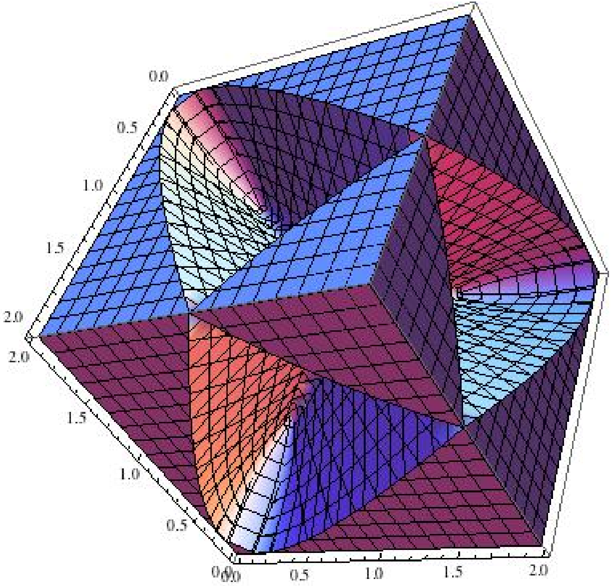
$$((1 - S_1)^2 - 4S_2)^2 - 64S_3 \geq 0$$

together with

$$\begin{aligned} a, b, c &\geq 0, \\ 1 - S_1 &\geq 0, \\ (1 - S_1)^2 - 4S_2 &\geq 0, \end{aligned}$$

where $S_1 = a + b + c$, $S_2 = ab + bc + ca$ and $S_3 = abc$.

3 × 3 diagonal matrices



3 × 3 diagonal matrices

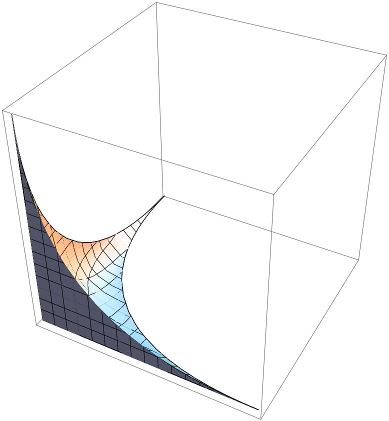


Figure: The colored region corresponds to completable probability matrices of 3×3 matrices with diagonal entries observed.

Completion algorithm for two blocks

Consider the partial matrix

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Step 1: Add in the missing entries using 2×2 minors:

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Step 1: Add in the missing entries using 2×2 minors:

$$\begin{pmatrix} .06 & .08 & \\ .09 & \color{red}{.12} & \\ & & .15 \end{pmatrix}$$

Step 2: Add in X and the rest of entries:

$$\begin{pmatrix} .06 & .08 & \color{blue}{X} \\ .09 & \color{red}{.12} & \color{blue}{1.5X} \\ \color{blue}{.009/X} & \color{blue}{.012/X} & .15 \end{pmatrix}$$

Completion algorithm for two blocks

Step 3: Set $\sum p_{ij} = 1$ and solve for X:

$$(.06 + .08 + .09 + .12 + .15) + X + 1.5X + .009/X + .012/X = 1$$

$$\Rightarrow .5 + 2.5X + .021/X = 1 \Rightarrow 2.5X^2 - .5X + .021 = 0$$

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The two solutions for X yield the following two completions:

$$\begin{pmatrix} .06 & .08 & .06 \\ .09 & .12 & .09 \\ .15 & .2 & .15 \end{pmatrix} \qquad \begin{pmatrix} .06 & .08 & .14 \\ .09 & .12 & .21 \\ .06 & .09 & .15 \end{pmatrix}$$

Completion algorithm for more blocks

Proposition

Let $A = \operatorname{diag}(a_1, \ldots, a_n)$*, such that* $n > 2$ *and* $S = \sum \sqrt{a_i} < 1$*. Then, a completion of the matrix is given by:*

$$\mathbf{u} = \left(\frac{\sqrt{a_1}}{S} + t, \frac{\sqrt{a_2}}{S} - t, \frac{\sqrt{a_3}}{S}, \ldots, \frac{\sqrt{a_n}}{S} \right),$$

where t *is one of the solutions to the following quadratic equation:*

$$\left(\frac{\sqrt{a_1} + \sqrt{a_2}}{S} \right) t^2 + \left(a_2 - a_1 - \left(\frac{\sqrt{a_1} + \sqrt{a_2}}{S} \right)^2 \right) t + \left(\frac{a_1\sqrt{a_2} + a_2\sqrt{a_1}}{S} - \frac{\sqrt{a_1 a_2}(\sqrt{a_1} + \sqrt{a_2})}{S^3} \right) = 0,$$

both of which lie in the interval $[-\sqrt{a_1}/S, \sqrt{a_2}/S]$*.*

Completion algorithm for more blocks

Example

We want to find a completion of $A = \text{diag}(1/4, 1/25, 1/36)$ that minimizes the Pearson χ^2 distance from the uniform distribution:

$$d = \frac{1}{n^2} \sum_{i,j} \left(p_{ij} - \frac{1}{n^2} \right)^2 = \frac{1}{n^2} \sum_{i,j} \left(u_i v_j - \frac{1}{n^2} \right)^2 .$$

This can be done using Lagrange multipliers. The minimum is achieved at

$$M = \begin{pmatrix} 0.250 & 0.049 & 0.215 \\ 0.204 & 0.040 & 0.176 \\ 0.032 & 0.006 & 0.028 \end{pmatrix} \text{ and } M^T.$$

The Pearson χ^2 distance from the uniform distribution is 0.683.

$2 \times 2 \times 2$ tensors

1. (Size 1) Any singleton, e.g. p_{000}. The only condition is $p_{000} \leq 1$.
2. (Size 2) Three orbits of pairs:
    1. p_{000}, p_{001}: $p_{000} + p_{001} \leq 1$.
    2. p_{000}, p_{011}: $\sqrt{p_{000}} + \sqrt{p_{011}} \leq 1$.
    3. p_{000}, p_{111}: $\sqrt[3]{p_{000}} + \sqrt[3]{p_{111}} \leq 1$.
3. (Size 3) Three orbits of triples:
    1. $p_{000}, p_{001}, p_{010}$: $p_{000} + p_{001} + p_{010} + (p_{001}p_{010}/p_{000}) \leq 1$.
    2. $p_{000}, p_{001}, p_{110}$: $\sqrt{p_{000} + p_{001}} + \sqrt{p_{110} + p_{001}p_{110}/p_{000}} \leq 1$.
    3. $p_{000}, p_{101}, p_{011}$: The tensor is completable if and only if the equation

$$x^3 + (p_{000} + p_{101} + p_{011} - 1)x^2 + (p_{000}p_{101} + p_{000}p_{011} + p_{101}p_{011})x + p_{000}p_{101}p_{011} = 0$$

has a root in the interval $[0, 1]$.

Thank you!