

Polytope of Matrices with Invariant Row- and Column- Sums

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Motivated by Aaronson's ¹ description of the role of transition matrices (those with nonnegative entries summing to 1) in hidden variable theories, we address the following general question:

(i) Given $\mathbf{r}, \mathbf{c} \in \mathbb{R}_+^{n \times 1}$, with $\mathbf{1}^T \mathbf{r} = \mathbf{1}^T \mathbf{c} = \gamma$, how does one construct $\mathbf{P} \in \mathbb{R}_+^{n \times n}$ with row and column sums satisfying $\mathbf{P} \mathbf{1} = \mathbf{r}, \mathbf{P}^T \mathbf{1} = \mathbf{c}$? Here, $\mathbf{1}$ is the vector of all ones. The case $\gamma = 1$ corresponds to requiring that \mathbf{P} be a transition matrix.

Construction

$\mathcal{S}_{(\mathbf{r}, \mathbf{c})}$, the set of all solutions to (i), is convex. We present a simple and explicit construction of $\mathcal{V}_{(\mathbf{r}, \mathbf{c})}$, the set of vertices of a polytope $\mathcal{P}_{(\mathbf{r}, \mathbf{c})} \subseteq \mathcal{S}_{(\mathbf{r}, \mathbf{c})}$.

Without loss of generality, we assume that the elements of \mathbf{r} and \mathbf{c} are arranged in increasing order: $r_i \leq r_{i+1}$ for $i \in [n-1]$, likewise for \mathbf{c} ($[k]$ denotes the set of positive integers not exceeding k). If one solves for this case, then the rows and columns of \mathbf{P} can always be permuted back to their original order without changing the values of the respective sums.

We define $m_i := \min(r_i, c_i)$ and \mathbf{e}_i as the column vector with 1 in the i^{th} position and zeros in the other $(n-1)$ positions.

The polytope $\mathcal{P}_{(\mathbf{r}, \mathbf{c})}$ is then defined as the convex hull of the set

$$\mathcal{V}_{(\mathbf{r}, \mathbf{c})} = \mathbf{P}^* \bigcup_{\substack{i, j \in [n], \\ i < j}} \mathbf{P}_{(i, j)} \quad (\diamond)$$

of, in general, $1 + \frac{n(n-1)}{2}$ distinct matrices where $\mathbf{P}_{(i, j)} = \mathbf{P}^* + m_i \cdot (\mathbf{e}_i \mathbf{e}_j^T + \mathbf{e}_j \mathbf{e}_i^T - \mathbf{e}_i \mathbf{e}_i^T - \mathbf{e}_j \mathbf{e}_j^T)$ and \mathbf{P}^* has entries $p_{i, j}^*$ equal to zero except for the following elements:

$p_{i, i}^* = m_i$, $p_{n, i}^* = c_i - m_i$, $p_{i, n}^* = r_i - m_i$ for $i \in [n-1]$ and

$p_{n, n}^* = r_n + c_n - \gamma + \sum_{i=1}^{n-1} m_i$.

For example, in the case $n = 3$ with ordering $r_1 \leq c_1 \leq c_2 \leq r_2 \leq r_3 \leq c_3$, every element in the polytope defined by these four matrices will be a solution to (i):

$$\mathbf{P}^* = \begin{bmatrix} r_1 & 0 & 0 \\ 0 & c_2 & r_2 - c_2 \\ c_1 - r_1 & 0 & r_3 + c_3 - \gamma + (r_1 + c_2) \end{bmatrix}, \mathbf{P}_{(1,2)} = \begin{bmatrix} 0 & r_1 & 0 \\ r_1 & c_2 - r_1 & r_2 - c_2 \\ c_1 - r_1 & 0 & r_3 + c_3 - \gamma + (r_1 + c_2) \end{bmatrix},$$

$$\mathbf{P}_{(1,3)} = \begin{bmatrix} 0 & 0 & r_1 \\ 0 & c_2 & r_2 - c_2 \\ c_1 & 0 & r_3 + c_3 - \gamma + c_2 \end{bmatrix}, \mathbf{P}_{(2,3)} = \begin{bmatrix} r_1 & 0 & 0 \\ 0 & c_2 - r_1 & r_2 - c_2 + r_1 \\ c_1 - r_1 & r_1 & r_3 + c_3 - \gamma + c_2 \end{bmatrix}.$$

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¹<https://www.scottaaronson.com/papers/qchvpra.pdf>

The construction (\diamond) makes it clear that any $\mathbf{P}_{(i,j)}$ has the same row and columns sums as \mathbf{P}^* . So it suffices to show that \mathbf{P}^* satisfies (i) and that $p_{i,i}^* \geq m_1$ for $i \in [n]$, the additional condition ensuring that the diagonal elements of $\mathbf{P}_{(i,j)}$ are nonnegative. We prove these properties in order:

- *Row sums:* Denote $\mathbf{P}_{i,\cdot}^*$ to be the i^{th} row of \mathbf{P}^* . For $i \in [n-1]$, $\mathbf{P}_{i,\cdot}^* \mathbf{1} = m_i + r_i - m_i = r_i$.
 $\mathbf{P}_{n,\cdot}^* \mathbf{1} = \sum_{i=1}^{n-1} (c_i - m_i) + p_{n,n}^* = r_n + (\sum_{i=1}^n c_i) - \gamma = r_n$.
- *Column sums:* The calculation is analogous to the one for row sums.
- *Nonnegativity of off-diagonal terms; diagonal terms $\geq m_1$:* Readily follows from (\diamond) for all elements except $p_{n,n}^*$.
 Requiring $p_{n,n}^* \geq m_1$ is equivalent to requiring $r_n + c_n + \sum_{i=2}^{n-1} m_i \geq \gamma$. By the inequality of arithmetic and geometric means, the left hand side is minimized when each of the n terms is equal, say, to M . The orderings $r_i \leq r_{i+1}$ and $c_i \leq c_{i+1}$ then imply that $r_i = c_i = M$ for $2 \leq i \leq n$, $M \geq m_1$ and thus $(n-1)M + m_1 = \gamma$. $p_{n,n}^* \geq m_1$ follows.

This shows that all matrices in $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ are solutions to (i). But $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ does not necessarily contain all solutions to (i), i.e., $\mathcal{P}_{(\mathbf{r},\mathbf{c})} \subseteq \mathcal{S}_{(\mathbf{r},\mathbf{c})}$; indeed, the construction shows that any matrix in $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ has a symmetric principal minor of order $n-1$.

\mathbf{P}^* has at most $2n-1$ nonzero entries and any solution in $\mathcal{S}_{(\mathbf{r},\mathbf{c})}$ must in general have at least as many; but it is not clear if \mathbf{P}^* is uniquely sparsest in $\mathcal{S}_{(\mathbf{r},\mathbf{c})}$. It is also unclear if $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ is the largest polytope in $\mathcal{S}_{(\mathbf{r},\mathbf{c})}$.