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 (HVTs), we address the following general question:
(i) Given $\mathbf{r}, \mathbf{c} \in \mathbb{R}_+^{n\times 1}$, with $\mathbf{1}^{\mathrm{T}}\mathbf{r} = \mathbf{1}^{\mathrm{T}}\mathbf{c} = \gamma$, how does one construct $\mathbf{P} \in \mathbb{R}_+^{n\times n}$ with row and column sums satisfying $\mathbf{P1} = \mathbf{r}, \mathbf{P}^{\mathrm{T}}\mathbf{1} = \mathbf{c}$? 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 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: $r_i \le r_{i+1}$ 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 $m_i \coloneqq \min(r_i, c_i)$ 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

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

of, in general, $1 + \frac{n(n-1)}{2}$ distinct matrices where $\mathbf{P}_{(i,j)} = \mathbf{P}^* + m_1 \cdot (\mathbf{e}_i\mathbf{e}_j^{\mathrm{T}} + \mathbf{e}_j\mathbf{e}_i^{\mathrm{T}} - \mathbf{e}_i\mathbf{e}_i^{\mathrm{T}} - \mathbf{e}_j\mathbf{e}_j^{\mathrm{T}})$ 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 $r_1 \le c_1 \le c_2 \le r_2 \le r_3 \le c_3$, 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

Lemma 1. *(a) $\mathcal{P}_{(\mathbf{r},\mathbf{c})} \subseteq \mathcal{S}_{(\mathbf{r},\mathbf{c})}$ for $n > 2$. (b) $\mathcal{P}_{(\mathbf{r},\mathbf{c})} = \mathcal{S}_{(\mathbf{r},\mathbf{c})}$ for $n = 2$.*

Proof. (a) To show that every matrix in $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ is a solution of (i), the convexity of $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ makes it sufficient to show that matrices in $\mathcal{V}_{(\mathbf{r},\mathbf{c})}$ are solutions to (i). The construction (❖) 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 verify these properties in order:

- *Row sums*: Denote $\mathbf{P}^*_{i,.}$ to be the i^{th} row of $\mathbf{P}^*$. For $i \in [n-1]$, $\mathbf{P}^*_{i,.}\mathbf{1} = m_i + r_i - m_i = r_i$. $\mathbf{P}^*_{n,.}\mathbf{1} = \sum_{i=1}^{n-1}(c_i - m_i) + p^*_{n,n} = r_n + (\sum_{i=1}^{n} c_i) - \gamma = r_n$.

- *Column sums*: Verification is analogous to *Row sums*.

- *Nonnegativity of off-diagonal terms; diagonal terms $\geq m_1$*: Readily follows from (❖) 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.

(b) For $n = 2$, $\mathcal{V}_{(\mathbf{r},\mathbf{c})}$ contains two elements $\mathbf{P}^*$ and $\mathbf{P}_{(1,2)}$. For $m_1 > 0$, every purported solution $\mathbf{P}$ of (i), can be written as $\mathbf{P} = \phi\mathbf{P}^* + (1-\phi)\mathbf{P}_{(1,2)}$ where $0 \leq \phi = \frac{p_{11}}{m_1} \leq 1$. The case $m_1 = 0$ is trivial. □

$\mathcal{P}_{(\mathbf{r},\mathbf{c})}$ 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 $n-1$.

Questions about $\mathcal{S}_{(\mathbf{r},\mathbf{c})} \setminus \mathcal{P}_{(\mathbf{r},\mathbf{c})}$:

- Define the *diameter* of a bounded convex set of matrices as the maximum of $\|\mathbf{M}_i - \mathbf{M}_j\|_\infty$, for any two matrices $\mathbf{M}_i$ and $\mathbf{M}_j$ in the set. Does $\mathcal{S}_{(\mathbf{r},\mathbf{c})}$ have a larger diameter than $\mathcal{P}_{(\mathbf{r},\mathbf{c})}$?

- $\mathbf{P}^*$ 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. Is $\mathbf{P}^*$ uniquely sparsest in $\mathcal{S}_{(\mathbf{r},\mathbf{c})}$?