Note

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A short note on extreme points of certain polytopes

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Abstract: We give a short proof of Mirsky's result regarding the extreme points of the convex polytope of doubly substochastic matrices via Birkhoff's Theorem and the doubly stochastic completion of doubly substochastic matrices. In addition, we give an alternative proof of the extreme points of the convex polytopes of symmetric doubly substochastic matrices via its corresponding loopy graphs.

Keywords: Doubly (sub)stochastic matrices; Symmetric doubly (sub)stochastic matrices, Extreme points.

MSC: 15A51, 15A83

1 Introduction

An $n \times n$ nonnegative matrix is called a *doubly (sub) stochastic matrix* if the sum of each row and each column is (less than or) equal to 1. The convex sets of all $n \times n$ doubly stochastic matrices and doubly substochastic matrices are denoted by Ω_n and ω_n , respectively. Both Ω_n and ω_n have been studied intensively in [4]. A matrix A is an *extreme point* of a convex set S if every convex decomposition of the form

$$A = \lambda A_1 + (1 - \lambda) A_2, (0 \leq \lambda \leq 1)$$

where A_1 and A_2 in S implies that $A_1 = A_2 = A$.

We let $\Omega_n^t = \{A \in \Omega_n \mid A = A^t\}$ denote the set of all $n \times n$ symmetric doubly stochastic matrices and let $\omega_n^t = \{B \in \omega_n \mid B = B^t\}$ denote the set of all $n \times n$ symmetric doubly substochastic matrices.

A well known result of Birkhoff [1] characterized all extreme points of Ω_n , stated as the following theorem.

Theorem 1.1. ([1]) P_n is an extreme point of Ω_n if and only if P is an $n \times n$ permutation matrix.

A square $(0, 1)$ -matrix is called a subpermutation matrix or a partial permutation matrix if it has at most one 1 in each row and each column. The extreme points of ω_n were characterized by Mirsky [6] in the following theorem.

Theorem 1.2. ([6]) Q_n is an extreme point of ω_n if and only if Q is an $n \times n$ subpermutation matrix.

In Section 2, we provide an alternative proof of Theorem 2.2. In Section 3, we give equivalent characterizations of the extreme points of Ω_n^t and ω_n^t in the language of graph theory and a concise proof of the extreme points of ω_n^t .

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2 Classical Case

Given an $n \times n$ doubly substochastic matrix $B_n = (b_{ij})_{i,j=1}^n$, there always exists an $m \times m$ doubly stochastic completion matrix A_m such that B_n is an $n \times n$ submatrix of A_m , where $n \leq m$. Indeed, denote r_i the i th row sum of B_n and c_j the j th column sum of B_n , then

$$\begin{pmatrix} B_n & D_n \\ E_n & B_n^t \end{pmatrix}$$

is a $2n \times 2n$ doubly stochastic matrix where D_n is the diagonal matrix with diagonal entries $1-r_1, 1-r_2, \dots, 1-r_n$ and E_n is the diagonal matrix with diagonal entries $1-c_1, 1-c_2, \dots, 1-c_n$. In [3], the authors give the lower bound of m and provide methods to construct A_m when m minimal. The results in [3] imply the following proposition.

Proposition 2.1. *Let B_n be an $n \times n$ doubly substochastic matrix, then there always exists an $m \times m$ doubly stochastic matrix A_m such that B_n is the $n \times n$ principal submatrix on the upper left corner of A_m .*

We are now in the position to provide an alternate proof of Theorem 1.2.

Theorem 2.2. ([6]) *Let n be a positive integer. Q is an extreme point of ω_n if and only if Q is an $n \times n$ subpermutation matrix.*

Proof. On the one hand, it is clear that all $n \times n$ subpermutation matrices are extreme points of ω_n .

On the other hand, let $B_n \in \omega_n$. According to Proposition 2.1, there exists

$$A_{n+k} = \begin{pmatrix} B_n & C_k \\ R_k & M_k \end{pmatrix} \in \Omega_{n+k},$$

where C_k is an $n \times k$ matrix, R_k is a $k \times n$ matrix and M_k is a $k \times k$ matrix. Applying Theorem 1.1, there exists $(n+k) \times (n+k)$ permutation matrices $P_1, P_2, \dots, P_t$ such that

$$A_{n+k} = \sum_{i=1}^t c_i P_i \quad (1)$$

where $c_i > 0$ and $\sum c_i = 1$. Truncate the last k rows and k columns of each matrix in (1), we have

$$B_n = \sum_{i=1}^t c_i Q_i$$

where Q_i are subpermutation matrices. Since B_n is arbitrary, any $n \times n$ doubly substochastic matrix can be written as a convex combination of subpermutation matrices, meaning that there are no more extreme points besides subpermutation matrices. □

3 Symmetric Case

The extreme points of the set Ω_n^t , all symmetric $n \times n$ doubly stochastic matrices, were characterized by Katz ([5], also see [2]) which can be generalized as the following theorem.

Theorem 3.1. ([5], Lemma 1 in [2]) *Let P be an $n \times n$ permutation matrix. Then $\frac{1}{2}(P + P^t)$ is an extreme point of Ω_n^t if and only if P does not contain any even cycle longer than 2.*

For an $n \times n$ symmetric matrix A , we associate a loopy graph in the following way to represent the structure of the non-zeros of A . Let $V = \{v_1, v_2, \dots, v_n\}$ be the set of vertices. The *loopy graph* associated with A is the graph $G(A)$ with vertex set V such that there is an edge connecting v_i and v_j if and only if $a_{i,j} \neq 0$.

Let P be an $n \times n$ permutation matrix. Then there is a one to one correspondence between cycles longer than 2 contained in P and cycles in the loopy graph associated with $\frac{1}{2}(P + P^t)$. Indeed, if $\sigma = (i_1, i_2, \dots, i_k)$ is a cycle contained in P longer than 2, then there is a cycle

$$v_{i_1} \rightarrow v_{i_2} \rightarrow \dots \rightarrow v_{i_k} \rightarrow v_{i_1}$$

contained in the associated loopy graph of $\frac{1}{2}(P + P^t)$ and vice versa. Hence, Theorem 3.1 in [5] can be stated as the following.

Corollary 3.2. *Let P be an $n \times n$ permutation matrix. Then $\frac{1}{2}(P + P^t)$ is an extreme point of Ω_n^t if and only if the loopy graph associated with $\frac{1}{2}(P + P^t)$ does not contain even cycles longer than 2.*

Proposition 3.3. *Any $n \times n$ symmetric doubly substochastic matrix A can be written as a convex combination of the matrices of the form $\frac{1}{2}(Q + Q^t)$ where Q is an $n \times n$ subpermutation matrix.*

The proof of Proposition 3.3 is essentially the same as the proof of Theorem 9 in [2]. Before we give the following lemma, we would like to mention that we do not consider loops to be cycles, and since loopy graphs are undirected, the shortest possible cycle is on three vertices.

Lemma 3.4. *Let Q be an $n \times n$ subpermutation matrix. Then $\frac{1}{2}(Q + Q^t)$ is not an extreme point of ω_n^t if the loopy graph associated with $\frac{1}{2}(Q + Q^t)$ contains at least one even cycle.*

Proof. Denote the loopy graph associated with $\frac{1}{2}(Q + Q^t)$ by G . Suppose G contains an even cycle $\mathcal{C}_{2k}$

$$v_{i_1} \rightarrow v_{i_2} \rightarrow \dots \rightarrow v_{i_{2k}} \rightarrow v_{i_1}$$

where $k \geq 2$. Denote the submatrix of $\frac{1}{2}(Q + Q^t)$ corresponding to $\mathcal{C}_{2k}$ by A_{2k} . We construct the matrix A_1 by putting 1 in the places

$$(i_1, i_2), (i_2, i_1), (i_3, i_4), (i_4, i_3), \dots, (i_{2k-1}, i_{2k}), (i_{2k}, i_{2k-1})$$

and the matrix A_2 by putting 1 in the places

$$(i_2, i_3), (i_3, i_2), (i_4, i_5), (i_5, i_4), \dots, (i_{2k}, i_1), (i_1, i_{2k}).$$

Note that both A_1 and A_2 are symmetric permutation matrices and

$$A_{2k} = \frac{1}{2}A_1 + \frac{1}{2}A_2,$$

and hence $\frac{1}{2}(Q + Q^t)$ is not an extreme point. $\square$

Lemma 3.5. *Let Q be an $n \times n$ subpermutation matrix. Then $\frac{1}{2}(Q + Q^t)$ is not an extreme point of ω_n^t if the loopy graph associated with $\frac{1}{2}(Q + Q^t)$ contains a path longer than 1.*

Proof. Denote the loopy graph associated with $\frac{1}{2}(Q + Q^t)$ by G . Suppose G contains a path $\mathcal{P}_k$

$$v_{i_1} \rightarrow v_{i_2} \rightarrow \dots \rightarrow v_{i_k}$$

where $k \geq 3$. Denote the $k \times k$ submatrix of $\frac{1}{2}(Q + Q^t)$ corresponding to $\mathcal{P}_k$ by P_k .

We may construct symmetric subpermutation matrices A_1 and A_2 similarly in Lemma 3.4 such that

$$P_k = \frac{1}{2}A_1 + \frac{1}{2}A_2,$$

and hence $\frac{1}{2}(Q + Q^t)$ is not an extreme point. $\square$

Theorem 3.6. *Let Q be an $n \times n$ subpermutation matrix. Then $\frac{1}{2}(Q + Q^t)$ is an extreme point of ω_n^t if and only if each connected component of the loopy graph associated with $\frac{1}{2}(Q + Q^t)$ is one of the following:*

- (a) a loop
- (b) an isolated vertex
- (c) an independent edge (a path with length 1)
- (d) an odd cycle.

Proof. Let $A = \frac{1}{2}(Q + Q^t)$. Since Q is a subpermutation matrix, it contains at most one nonzero element in each row and each column, and hence $\frac{1}{2}(Q + Q^t)$ contains at most two nonzero elements in each row and each column which implies that the degree of each vertex in the associated loopy graph $G(A)$ is at most 2. Therefore, each connected component of $G(A)$ must be one of the following:

- (a) a loop
- (b) a path longer than 1
- (c) an isolated vertex
- (d) an independent edge (a path with length 1)
- (e) an odd cycle
- (f) an even cycle.

Lemma 3.4 and Lemma 3.5 rule out the possibilities that $G(A)$ contains a connected component which is a path longer than 1 or an even cycle.

On the other hand, if each of connected component of A is one of the four types listed in the theorem, then there exists a permutation matrix P such that PAP^T is a direct sum of some square matrices with smaller orders denoted by $A_1, A_2, \dots, A_k$, and $G(A_i)$, the associated loopy graph of A_i , is one of these four types. It is suffice to show that each A_i is extreme for $i = 1, 2, \dots, k$.

If $G(A_i)$ is a loop, then A_i is the 1×1 matrix I_1 which is extreme. If $G(A_i)$ is an isolated vertex, then A_i is the 1×1 zero matrix. If $G(A_i)$ is an independent edge, then A_i is the 2×2 matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ which is a permutation matrix and hence extreme. If $G(A_i)$ is an odd cycle, then according to Theorem 3.1, each A_i is an extreme point. Hence, A is an extreme point. $\square$

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