AUSTRALASIAN JOURNAL OF COMBINATORICS
Volume **91(3)** (2025), Pages 366–386

Near-derangements and their polytopes

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Abstract

A derangement is a permutation with no fixed point. We refer to permutations of $\{1, 2, \ldots, n\}$ with at most one fixed point as near-derangements, and study the corresponding set of permutation matrices $\mathcal{P}_n^{(\leq 1)}$. We determine a basis of the linear span of $\mathcal{P}_n^{(\leq 1)}$ consisting of matrices in $\mathcal{P}_n^{(\leq 1)}$. Also, we study the polytope determined by $\mathcal{P}_n^{(\leq 1)}$. In addition, we investigate the polytope of all $n \times n$ doubly stochastic matrices with trace at most 1 and determine its extreme points, not all of which are permutation matrices.

1 Introduction

Let $\mathcal{S}_n$ be the set of permutations of $\{1, 2, \ldots, n\}$ with corresponding set $\mathcal{P}_n$ of $n \times n$ permutation matrices. We call a permutation with at most one fixed point a *near-derangement* and call the corresponding permutation matrix a *near-derangement matrix.* Near-derangement matrices have at most one 1 on its main diagonal. We denote the set of near-derangements of $\{1, 2, \ldots, n\}$ by $\mathcal{S}_n^{(\leq 1)}$ and the corresponding set of $n \times n$ near-derangement matrices by $\mathcal{P}_n^{(\leq 1)}$. The set $\mathcal{P}_n^{(\leq 1)}$ strictly contains the set $\mathcal{D}_n$ of permutation matrices corresponding to the derangements of size n (permutations without fixed points).

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ISSN: 2202-3518

Let $D_n = |\mathcal{D}_n|$ be the n th *derangement number*. It follows that

$$|\mathcal{P}_n^{(\leq 1)}| = D_n + nD_{n-1}$$

where $D_n = \lfloor (n! + 1)/e \rfloor$ with e as Euler's number. Derangements have been studied extensively in combinatorics, and we refer to [3] for a survey of the subject, including an historic account starting with a question by Montmort in 1708 on a certain card game.

Let M_n denote the (linear) space of real $n \times n$ matrices. A matrix $A = [a_{ij}] \in M_n$ is *doubly stochastic* provided that

$$a_{ij} \geq 0 \ \ (i, j \leq n), \ \ \sum_{j=1}^{n} a_{ij} = 1 \ \ (i \leq n) \text{ and } \sum_{i=1}^{n} a_{ij} = 1 \ \ (j \leq n).$$

We let Ω_n denote the *Birkhoff polytope* consisting of all $n \times n$ doubly stochastic matrices. A classical result in combinatorial matrix theory [11] is the Birkhoff-von Neumann theorem that the convex hull $\mathrm{conv}\,(\mathcal{P}_n)$ of the $n \times n$ permutation matrices equals the set of $n \times n$ doubly stochastic matrices. This result is also central in combinatorial optimization and matching theory, see [19, 20, 21]. A general discussion of many properties of Ω_n is found in [7]. In [6] it is shown that every d-dimensional polytope whose vertices are (0,1)-vectors is affinely equivalent to a face of Ω_n, indeed a face of the subpolytope of Ω_n determined by the $(n-1)!$ permutation matrices that are cycles of length n, the *asymmetric traveling salesman polytope*. The Chan-Robbins-Yuen polytope CRY_n defined as the convex hull of the $n \times n$ permutation matrices $P = [p_{ij}]$ such that $p_{ij} = 0$ for all i, j with $i - j \geq 2$ is a face of the Birkhoff polytope (see e.g. [16]).

In particular, there are several related studies on doubly stochastic matrices constrained in some way, such as [9, 14]. The goal of this paper is to investigate the class $\mathcal{P}_n^{(\leq 1)}$ and the related polytope

$$\Omega_n^{(\leq 1)} = \{A \in \Omega_n : \mathrm{trace}(A) \leq 1\}.$$

We observe that the set $\mathcal{P}_n^{(\leq 1)}$ of near-derangement matrices consists of the integral matrices in $\Omega_n^{(\leq 1)}$.

The following inclusions hold

$$\mathcal{D}_n \subseteq \mathcal{P}_n^{(\leq 1)}, \text{ and } \mathrm{conv}\,(\mathcal{D}_n) \subseteq \mathrm{conv}\,(\mathcal{P}_n^{(\leq 1)}) \subseteq \Omega_n^{(\leq 1)} \subseteq \Omega_n. \qquad (1)$$

We call $\mathrm{conv}\,(\mathcal{D}_n)$ the *derangement polytope*, $\mathrm{conv}\,(\mathcal{P}^{(\leq 1)})$ the *near-derangement polytope*, and $\Omega_n^{(\leq 1)}$ the *extended near-derangement polytope*. The polytope $\mathrm{conv}\,(\mathcal{D}_n)$ is a face of the Birkhoff polytope Ω_n; it consists of all doubly stochastic matrices A that satisfy $A \leq J_n - I_n$ where J_n is the $n \times n$ matrix of all 1's.

This paper is devoted to a study of these polytopes and the corresponding sets of permutation matrices.

We assume hereafter that $n \geq 2$. Then all of the inclusions in (1) are strict. The polytopes $\Omega_n^{(\leq 1)}$ and $\mathrm{conv}\,(\mathcal{P}_n^{(\leq 1)})$ are both closed under taking the transpose of a matrix. Later we show that the dimension of $\Omega_n^{(\leq 1)}$ is $(n-1)^2$, the same as the dimension of Ω_n.

We remark that a related subpolytope of Ω_n, defined as the convex hull of all permutation matrices except the identity matrix, was investigated in detail in [7].

Example 1.1. Let $n=2$. Then Ω_2 consists of all matrices

$$A(\alpha) = \begin{bmatrix} \alpha & 1-\alpha \\ 1-\alpha & \alpha \end{bmatrix}$$

where $0 \leq \alpha \leq 1$. The identity matrix $I_2 \in \Omega_2$, but it is not in $\Omega_2^{(\leq 1)}$ as its trace is 2. The following two matrices both lie in $\Omega_2^{(\leq 1)}$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}.$$

It follows from a general result we establish later that $\Omega_2^{(\leq 1)}$ is the convex hull of these two matrices, and, in fact, both matrices are extreme points of $\Omega_2^{(\leq 1)}$. $\diamond$

Let

$$I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ and } L_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

An *interchange* in a permutation matrix $P = [p_{ij}]$ is to replace a 2×2 submatrix equal to I_2 with L_2, or vice versa. Let $G(\mathcal{D}_n)$ denote the graph with vertex set $\mathcal{D}_n$ and edges corresponding to interchanges. Then it can be shown that $G(\mathcal{D}_n)$ is connected for all n except $n=3$; see Theorem 1 in [15]. A similar problem was discussed in connection with Gray codes in [4]. Concerning near-derangement matrices one can also show that the graph $G(\mathcal{P}_n^{(\leq 1)})$ is connected (this graph has vertex set $\mathcal{P}_n^{(\leq 1)}$ and edges corresponding to interchanges). We refer to [15] for closely related results.

The rest of the paper is organized as follows. In Section 2 we consider certain decompositions of J_n and use these to construct bases for the linear span of $\mathcal{P}_n^{(\leq 1)}$ and also for the linear span of $\mathcal{D}_n$. In Section 3, we study the polytope $\Omega_n^{(\leq 1)}$ and determine all the extreme points of this polytope. Then, in Section 4, we give some results on the convex hull of $\mathcal{P}_n^{(\leq 1)}$ while Section 5 deals with a relation between faces of $\Omega_n^{(\leq 1)}$ and faces of Ω_n. The faces of Ω_n are determined by $n \times n$ (0,1)-matrices A of *total support*, matrices in which every 1 is part of a permutation matrix $P \leq A$ (entrywise inequality). The matrix A is *fully indecomposable* provided that each $(n-1) \times (n-1)$ submatrix obtained by crossing out the row and column of an entry (0 or 1) contains an $(n-1) \times (n-1)$ permutation matrix. It follows that fully indecomposable matrices have total support.

Notation: We use the symbol $\square$ to denote as usual the end of a proof and the symbol $\diamond$ as above to denote the end of an example, remark, and question. Vectors in $\mathbb{R}^n$ are column vectors and we identify these with real n-tuples. The i th component of a vector $x \in \mathbb{R}^n$ is usually denoted by x_i $(i \leq n)$. A zero matrix, or vector, is denoted by O, and an all ones vector is denoted by e. M_n denotes the space of square real matrices of order n. The diagonal of a matrix $A = [a_{ij}] \in M_n$ is $\mathrm{diag}(A)$, so $\mathrm{diag}(A) = (a_{11}, a_{22}, \ldots, a_{nn})$. The transpose of a matrix A is denoted by A^t. Finally, L_n is the $n \times n$ backward identity matrix where $L_n \in \mathcal{P}_n^{(\leq 1)}$.

2 Decompositions and bases of subspaces

Let $\langle \mathcal{T}_n \rangle$ be the linear span of any subset $\mathcal{T}_n$ of $n \times n$ permutation matrices. The dimension of $\langle \mathcal{P}_n \rangle$ is known to be equal to $(n-1)^2 + 1$. In fact, the subspace $\langle \mathcal{P}_n \rangle$ of M_n is determined by the $2(n-1)$ linear equations saying that row sums are equal and column sums are equal. Several bases have been constructed for $\langle \mathcal{P}_n \rangle$. The convex hull Ω_n of $\mathcal{P}_n$ has dimension $(n-1)^2$.

We will make use of the *cyclic-Toeplitz decomposition* $J_n = T_1 + T_2 + \cdots + T_n$ and the *cyclic-Hankel decomposition* $J_n = H_1 + H_2 + \cdots + H_n$ of the $n \times n$ matrix J_n of all 1's into n permutation matrices as defined in [8]. The matrices T_i are obtained from the identity matrix I_n ($=T_1$) by successively rotating its rows. The matrices H_i are obtained from the matrix L_n ($=H_1$) by successively rotating its columns. These are illustrated below for $n = 5$ using letters a, b, c, d, e, respectively, to distinguish the permutation matrices $T_1 = I_5, T_2, T_3, T_4, T_5$, and the permutation matrices H_5, H_4, H_3, H_2, H_1:

$$\left[\begin{array}{c|c|c|c|c} a & b & c & d & e \\ \hline e & a & b & c & d \\ \hline d & e & a & b & c \\ \hline c & d & e & a & b \\ \hline b & c & d & e & a \end{array}\right], \quad \left[\begin{array}{c|c|c|c|c} e & d & c & b & a \\ \hline d & c & b & a & e \\ \hline c & b & a & e & d \\ \hline b & a & e & d & c \\ \hline a & e & d & c & b \end{array}\right].$$

For n odd the permutation matrices in the cyclic-Hankel decomposition have exactly one 1 on the main diagonal and thus correspond to permutations with exactly one fixed point. This is not the case for n even as illustrated for $n = 4$ below:

$$\left[\begin{array}{c|c|c|c} d & c & b & a \\ \hline c & b & a & d \\ \hline b & a & d & c \\ \hline a & d & c & b \end{array}\right].$$

The cyclic-Toeplitz decomposition contains the identity matrix and thus the other permutation matrices correspond to permutations without any fixed point, that is, to derangements.

Theorem 2.1. *Let $n \geq 3$. Every permutation matrix P in $\mathcal{P}_n$ is a ± 1 linear combination of permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. In particular, there is a basis of $\langle \mathcal{P}_n \rangle$ consisting of $(n-1)^2 + 1$ permutation matrices in $\mathcal{P}_n^{(\leq 1)}$.*

Proof. First assume that $P \in \mathcal{P}_n$ has an odd number $k \geq 3$ of fixed points.

Using the cyclic-Hankel decomposition and the cyclic-Toeplitz decomposition of J_k with the identity matrix $T_1 = I_k$ removed, we obtain for k odd that

$$I_k = (H_1 + H_2 + \cdots + H_k) - (T_2 + T_3 + \cdots + T_k),$$

a decomposition of I_k into matrices in $\mathcal{P}_k^{(\leq 1)}$. For example with $k = 3$,

$$\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} = \begin{bmatrix} & & 1 \\ & 1 & \\ 1 & & \end{bmatrix} + \begin{bmatrix} & 1 & \\ 1 & & \\ & & 1 \end{bmatrix} + \begin{bmatrix} 1 & & \\ & & 1 \\ & 1 & \end{bmatrix} - \begin{bmatrix} & 1 & \\ & & 1 \\ 1 & & \end{bmatrix} - \begin{bmatrix} & & 1 \\ 1 & & \\ & 1 & \end{bmatrix}. \tag{2}$$

Without loss of generality, we assume that the k fixed points of $P \in \mathcal{P}_n$ are $\{1, 2, \ldots, k\}$. Thus $P = I_k \oplus R$ where $R \in \mathcal{D}_{n-k}$. Then the desired decomposition is

$$P = I_k \oplus R = \sum_{i=1}^{k} (H_i \oplus R) - \sum_{i=2}^{k} (T_i \oplus R). \tag{3}$$

We now consider $k \geq 4$ even. Let K_k^* be the complete digraph of n vertices obtained from K_k by replacing each edge with two directed edges in opposite directions. For instance, consider $k = 4$ and the decomposition of J_4 given by

$$J_4 = \begin{bmatrix} 1 & & & \\ & & 1 & \\ & & & 1 \\ & 1 & & \end{bmatrix} + \begin{bmatrix} & 1 & & \\ & & & 1 \\ & & 1 & \\ 1 & & & \end{bmatrix} + \begin{bmatrix} & & 1 & \\ 1 & & & \\ & 1 & & \\ & & & 1 \end{bmatrix} + \begin{bmatrix} & & & 1 \\ & 1 & & \\ 1 & & & \\ & & 1 & \end{bmatrix}.$$

This corresponds to a decomposition of K_4^* into directed cycles of length 3, where an additional 1 on the main diagonal has been included in each matrix. By subtracting the permutation matrices in the cyclic-Toeplitz decomposition of J_4 with the identity matrix I_4 removed, that is,

$$-\begin{bmatrix} & 1 & & \\ & & 1 & \\ & & & 1 \\ 1 & & & \end{bmatrix} - \begin{bmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{bmatrix} - \begin{bmatrix} & & & 1 \\ 1 & & & \\ & 1 & & \\ & & 1 & \end{bmatrix}$$

we get I_4 expressed as a ± 1 linear combination of permutation matrices in $\mathcal{P}_4^{(\leq 1)}$.

In [2] it is shown that there is a decomposition of the complete digraph K_n^* into directed cycles of length m if and only if $m | n(n-1)$ and $(n, m) \notin \{(4, 4), (6, 3), (6, 6)\}$. Thus if $m = n - 1$, such a decomposition exists into n cycles of length $n - 1$. In fact, in [5] it is proved directly that K_n^* can always be decomposed into directed cycles of length $n - 1$. Generalizing the preceding construction for $k = 4$ in the obvious way, we see that for k even, I_k is a ± 1 linear combination of permutation matrices in $\mathcal{P}_k^{(\leq 1)}$. Then, as in the odd case (see (3)), we see that every permutation matrix in $\mathcal{P}_n$ is a ± 1 linear combination of permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. Thus there is a basis of $\langle \mathcal{P}_n \rangle$ consisting of permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. $\square$

Corollary 2.2.

$$\dim\langle \mathcal{P}_n^{(\leq 1)} \rangle = \dim\langle \mathcal{P}_n \rangle = (n-1)^2 + 1.$$

Proof. This follows from the proof of Theorem 2.1. See also Theorem 2.5 for a different proof. ∎

Example 2.3. We illustrate the construction in [5] in the case of even $k = 8$. Consider K_9^* with vertices $\mathbb{Z}_8 \cup \{\infty\} = \{\infty, 0, 1, \ldots, 7\}$ and the cycle in K_9^* given by

$$\infty \to 0 \to 7 \to 1 \to 6 \to 2 \to 5 \to 3 \to 4 \to \infty.$$

Using arithmetic in $\mathbb{Z}_8$ with $\infty + x = \infty$ for all $x \in \mathbb{Z}_8$, we get by adding 1, the eight cycles in K_9^*:

$$\begin{aligned}
&\infty \to 0 \to 7 \to 1 \to 6 \to 2 \to 5 \to 3 \to \infty,\\
&\infty \to 1 \to 0 \to 2 \to 7 \to 3 \to 6 \to 4 \to \infty,\\
&\infty \to 2 \to 1 \to 3 \to 0 \to 4 \to 7 \to 5 \to \infty,\\
&\infty \to 3 \to 2 \to 4 \to 1 \to 5 \to 0 \to 6 \to \infty,\\
&\infty \to 4 \to 3 \to 5 \to 2 \to 6 \to 1 \to 7 \to \infty,\\
&\infty \to 5 \to 4 \to 6 \to 3 \to 7 \to 2 \to 0 \to \infty,\\
&\infty \to 6 \to 5 \to 7 \to 4 \to 0 \to 3 \to 1 \to \infty,\\
&\infty \to 7 \to 6 \to 0 \to 5 \to 1 \to 4 \to 2 \to \infty.
\end{aligned}$$

With the additional cycle

$$0 \to 1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 0,$$

we get a decomposition of K_9^* into 9 cycles of length 8. This corresponds to the decomposition of J_9:

$$\left[\begin{array}{c||c|c|c|c|c|c|c|c|c}
 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & \infty \\ \hline\hline
0 & (e) & i & b & g & c & h & d & a & f \\ \hline
1 & b & (f) & i & c & h & d & a & e & g \\ \hline
2 & f & c & (g) & i & d & a & e & b & h \\ \hline
3 & c & g & d & (h) & i & e & b & f & a \\ \hline
4 & g & d & h & e & (a) & i & f & c & b \\ \hline
5 & d & h & e & a & f & (b) & i & g & c \\ \hline
6 & h & e & a & f & b & g & (c) & i & d \\ \hline
7 & i & a & f & b & g & c & h & (d) & e \\ \hline
\infty & a & b & c & d & e & f & g & h & (i)
\end{array}\right].$$

◇

In the previous theorem we assumed $n \geq 3$. In fact, for $n = 2$, since $\mathcal{P}_2^{(\leq 1)}$ contains only the matrix

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

I_2 is not a ± 1 linear combination of permutation matrices in $\mathcal{P}_2^{(\leq 1)}$. Thus $\langle \mathcal{P}_2^{(\leq 1)} \rangle \neq \langle \mathcal{P}_2 \rangle$.

We now consider the subspace $\langle \mathcal{D}_n \rangle$ spanned by the derangements of $\{1, 2, \ldots, n\}$ represented, as we do, by permutation matrices. First we consider an example.

Example 2.4. If $n = 3$, there are only two derangements

$$\left[\begin{array}{c|c|c} & & 1 \\ \hline 1 & & \\ \hline & 1 & \end{array}\right] \text{ and } \left[\begin{array}{c|c|c} & 1 & \\ \hline & & 1 \\ \hline 1 & & \end{array}\right],$$

and these are linearly independent. Thus $\dim\langle \mathcal{D}_3 \rangle = 2$.

Now let $n = 4$. We have $D_4 = 9$, and $\mathcal{D}_4$ consists of the matrices

$$P_1 = \left[\begin{array}{c|c|c|c} & 1 & & \\ \hline 1 & & & \\ \hline & & & 1 \\ \hline & & 1 & \end{array}\right], P_2 = \left[\begin{array}{c|c|c|c} & & 1 & \\ \hline & & & 1 \\ \hline 1 & & & \\ \hline & 1 & & \end{array}\right], P_3 = \left[\begin{array}{c|c|c|c} & & & 1 \\ \hline & & 1 & \\ \hline & 1 & & \\ \hline 1 & & & \end{array}\right],$$

$$Q_1 = \left[\begin{array}{c|c|c|c} & & & 1 \\ \hline & & 1 & \\ \hline 1 & & & \\ \hline & 1 & & \end{array}\right], Q_2 = \left[\begin{array}{c|c|c|c} & & & 1 \\ \hline 1 & & & \\ \hline & 1 & & \\ \hline & & 1 & \end{array}\right], Q_3 = \left[\begin{array}{c|c|c|c} & & 1 & \\ \hline & & & 1 \\ \hline & 1 & & \\ \hline 1 & & & \end{array}\right],$$

$$Q_4 = \left[\begin{array}{c|c|c|c} & 1 & & \\ \hline & & 1 & \\ \hline & & & 1 \\ \hline 1 & & & \end{array}\right], Q_5 = \left[\begin{array}{c|c|c|c} & 1 & & \\ \hline & & & 1 \\ \hline 1 & & & \\ \hline & & 1 & \end{array}\right], Q_6 = \left[\begin{array}{c|c|c|c} & & 1 & \\ \hline 1 & & & \\ \hline & & & 1 \\ \hline & 1 & & \end{array}\right].$$

The first three, the P_i's, correspond to two cycles of length 2; the last six, the Q_i's correspond to 4-cycles.

We have

$$Q_1 + Q_3 = P_2 + P_3 = \left[\begin{array}{c|c|c|c} & & 1 & 1 \\ \hline & & 1 & 1 \\ \hline 1 & 1 & & \\ \hline 1 & 1 & & \end{array}\right],$$

$$Q_2 + Q_4 = P_1 + P_3 = \left[\begin{array}{c|c|c|c} & 1 & & 1 \\ \hline 1 & & 1 & \\ \hline & 1 & & 1 \\ \hline 1 & & 1 & \end{array}\right],$$

and

$$Q_5 + Q_6 = P_1 + P_2 = \left[\begin{array}{c|c|c|c} & 1 & 1 & \\ \hline 1 & & & 1 \\ \hline 1 & & & 1 \\ \hline & 1 & 1 & \end{array}\right].$$

Thus, for example, Q_3, Q_4, Q_6 are redundant and a basis is contained in $\{P_1, P_2, P_3, Q_1, Q_2, Q_5\}$. P_1, P_2, P_3 are clearly linearly independent as each has a 1 where the other two have 0's; similarly, Q_1, Q_2, Q_5 are linearly independent. Moreover, $P_1, P_2, P_3, Q_1, Q_2, Q_5$ are linearly independent, since each of P_1, P_2, P_3 has a 1 where all of Q_1, Q_2, Q_5 have a 0. Hence we have: $\dim\langle\mathcal{D}_4\rangle = 6$ and $P_1, P_2, P_3, Q_1, Q_2, Q_5$ is a basis of $\langle\mathcal{D}_4\rangle$.

Since $\dim\langle\mathcal{P}_4^{(\leq 1)}\rangle = 10$, including four permutation matrices each with exactly one 1 on the main diagonal in different positions, gives a basis of $\langle\mathcal{P}_4^{(\leq 1)}\rangle$. $\diamond$

We now give a different proof of the dimension formulas which is also constructive.

Theorem 2.5. *There is a basis of $\langle\mathcal{P}_n^{(\leq 1)}\rangle$, so of $\langle\mathcal{P}_n\rangle$, containing exactly n permutation matrices with a 1 in different positions on the main diagonal and so*

$$\dim\langle\mathcal{P}_n^{(\leq 1)}\rangle = \dim\langle\mathcal{P}_n\rangle = \dim\langle\mathcal{D}_n\rangle + n.$$

Proof. Consider the $n \times n$ $(0,1)$-matrix $J_n^* = J_n - I_n$. Then J_n^* determines a face $\mathcal{F}(J_n^*)$ of Ω_n consisting of all the $n \times n$ doubly stochastic matrices with only 0's on the main diagonal. From the formula for faces of Ω_n corresponding to fully indecomposable matrices, given e.g. in Theorem 9.2.1 in [7], the dimension of this face is

$$(n^2 - n) - 2n + 1 = n^2 - 3n + 1 = (n-1)^2 - n.$$

Thus this face determines an affine set (translation of a linear space) $\mathrm{aff}(\mathcal{F}(J_n^*))$ of dimension $n^2 - 3n + 1$, so containing $t := n^2 - 3n + 2$ affinely independent permutation matrices $P_1, P_2, \ldots, P_t$ (all in the face $\mathcal{F}(J_n^*)$, so derangements). Now, the zero matrix O does not lie in $\mathrm{aff}(\mathcal{F}(J_n^*))$ and hence $O, P_1, P_2, \ldots, P_t$ are affinely independent. This implies that $P_1 - O, P_2 - O, \ldots, P_t - O$, i.e., $P_1, P_2, \ldots, P_t$, are linearly independent. By choosing for $1 \leq i \leq n$ an $n \times n$ permutation matrix W_i with a 1 in the i th position of the main diagonal and 0's elsewhere we get an additional n linearly independent permutation matrices. Since

$$(n^2 - 3n + 2) + n = n^2 - 2n + 1 = (n-1)^2 = \dim\Omega_n,$$

it follows that

$$\dim\langle\mathcal{D}_n\rangle = n^2 - 3n + 2 = (n-1)^2 - n + 1$$

and thus there is a basis of $\langle\mathcal{P}_n^1\rangle = \langle\mathcal{P}_n\rangle$ containing exactly n permutation matrices (freely chosen) with a 1 on the main diagonal (in different positions). $\square$

Example 2.6. We construct a basis of $\langle\mathcal{D}_n\rangle$ as follows. Consider the $n \times n$ fully indecomposable matrix F_n illustrated in (4) for $n = 6$ (all $(n^2 - 3n)$ unspecified entries are assumed to equal 0). In general. $F_n = U_n + V_n$ where U_n is the permutation matrix in F_n containing a 1 in position $(1, n)$ and V_n is the permutation matrix in F_n containing the 1 in positions $(1, n-1)$. These are the only two permutation matrices contained in F_n.

$$F_6 = \left[\begin{array}{c|c|c|c|c|c} 0 & & & & 1 & 1 \\ \hline 1 & 0 & & & & 1 \\ \hline 1 & 1 & 0 & & & \\ \hline & 1 & 1 & 0 & & \\ \hline & & 1 & 1 & 0 & \\ \hline & & & 1 & 1 & 0 \end{array}\right]. \tag{4}$$

Since F_n is easily seen to be fully indecomposable, each of the $n^2 - 3n$ positions of F_n with an unspecified 0 belongs to a permutation matrix with a 1 in that position where all of its other 1's are 1's in F_n. This gives a set $\mathcal{R}_n$ of $n^2 - 3n$ linearly independent derangements. The permutation matrices U_n and V_n are clearly linearly independent of the permutation matrices in $\mathcal{R}_n$. This gives a total of $n^2 - 3n + 2$ linearly independent derangements. Since $\dim\langle\mathcal{D}_n\rangle = n^2 - 3n + 2$, we have a basis of $\langle\mathcal{D}_n\rangle$. $\diamond$

Remark 2.7. Let A be an $n \times n$ $(0, 1)$-matrix (or a nonnegative integral matrix). Then A is the sum of permutation matrices in $\mathcal{D}_n$ if and only if A has constant row and column sums and all 0's on its main diagonal. On the other hand, characterizing those A that are sums of permutation matrices in $\mathcal{P}_n^{(\leq 1)}$ seems to be a difficult problem since there may be many nonzeros on the main diagonal of A. Let $\mathcal{T}_n^{(\leq 1)}$ be the class of $(0, 1)$-matrices that are a sum of matrices in $\mathcal{P}_n^{(\leq 1)}$. Then $A \in \mathcal{T}_n^{(\leq 1)}$ satisfies:

(i) A has constant row and column sums k.

(ii) If A has t 1's on the diagonal, then $k \geq t$. (This is because A must be a sum of at least t permutation matrices.)

Thus, for instance, if A is the identity matrix I_n, with $n > 1$, then condition (ii) is violated. $\diamond$

Example 2.8. Consider the $(0, 1)$-matrix

$$A = \left[\begin{array}{c|c|c|c} 1 & & 1 & \\ \hline & 1 & & 1 \\ \hline 1 & & & 1 \\ \hline & 1 & 1 & \end{array}\right].$$

Then A satisfies the conditions (i) and (ii) with $k = t = 2$. However, $A \notin \mathcal{T}_4^1$. In fact, A has the following unique decomposition as a sum of two permutation matrices

$$A = \left[\begin{array}{c|c|c|c} 1 & & 1 & \\ \hline & 1 & & 1 \\ \hline 1 & & & 1 \\ \hline & 1 & 1 & \end{array}\right] = \left[\begin{array}{c|c|c|c} 1 & & & \\ \hline & 1 & & \\ \hline & & & 1 \\ \hline & & 1 & \end{array}\right] + \left[\begin{array}{c|c|c|c} & & 1 & \\ \hline & & & 1 \\ \hline 1 & & & \\ \hline & 1 & & \end{array}\right]$$

and the first matrix is not in $\mathcal{P}_4^1$. $\diamond$

This example shows that further conditions than (i) and (ii) are required to characterize the class $\mathcal{T}_n^1$. In fact, at least the following additional condition is needed:

(iii) For each 1 on the main diagonal of A the submatrix obtained by deleting the row and column of that 1 must contain a derangement matrix.

This condition (iii) is violated by the matrix A above.

Example 2.9. Consider the $n \times n$ matrix J_n of all 1's. If n is odd, then the cyclic-Hankel decomposition shows that J_n is a sum of n permutation matrices of $\mathcal{P}_n^{(\leq 1)}$. Now assume that n is even so that the cyclic-Hankel decomposition fails. As already discussed, in [2] it is shown that there is a decomposition of the complete digraph K_n^* into directed cycles of length $(n-1)$. Using a 1 on the main diagonal, it follows that J_n has a decomposition into permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. ◇

3 The extended near-derangement polytope $\Omega_n^{(\leq 1)}$

We study the polytope $\Omega_n^{(\leq 1)}$ and begin by computing its dimension. We refer to [20] for polyhedral theory. In general, for a polyhedron C, its dimension is the dimension of its affine hull $\text{aff}(C)$, Moreover, $\text{aff}(C)$ may be determined as the solutions of all the implicit equalities in the linear system that defines C where an *implicit equality* is an inequality that holds with equality for *all* points in C.

Lemma 3.1.

$$\dim \Omega_n^{(\leq 1)} = (n-1)^2.$$

Proof. Consider the polyhedron $\Omega_n^{(\leq 1)}$. Clearly all the line sum equations are implicit equalities, and $a_{ij} \geq 0$ is not an implicit equality $(i, j \leq n)$. Consider the final defining inequality, $\sum_{i=1}^n a_{ii} \leq 1$ for $A = [a_{ij}] \in M_n$. This is not an implicit equality since every derangement satisfies the inequality strictly. It follows that the affine hull of $\Omega_n^{(\leq 1)}$ equals the affine hull of Ω_n, and therefore $\dim \Omega_n^{(\leq 1)} = (n-1)^2$. The result may also be derived from Theorem 2.1. □

The next result deals with the facets of the polytope $\Omega_n^{(\leq 1)}$.

Theorem 3.2. $\Omega_n^{(\leq 1)}$ *has* $n^2 + 1$ *facets. These facets are induced by each of the inequalities* $a_{ij} \geq 0$ *(where* $A = [a_{ij}] \in \Omega_n^{(\leq 1)}$*) for* $i, j \leq n$ *and the trace inequality* $\sum_i a_{ii} \leq 1$.

Proof. Of the linear inequalities defining a polyhedron Q, those that are not implicit equalities are called *plus-inequalities*. There is a one-to-one correspondence between the facets and the plus-inequalities, and the facet is obtained by setting that plus-inequality to equality [20] . The desired result follows from this as (i) for each i, j there is a near-derangement matrix with a 1 in position (i, j), and (ii) there is a derangement matrix (so satisfying the trace inequality strictly). □

In particular, the facet of $\Omega_n^{(\leq 1)}$

$$\{A \in \Omega_n^{(\leq 1)} : \sum_i a_{ii} = 1\},$$

induced by the trace inequality has dimension $(n-1)^2 - 1$. This facet clearly contains the permutation matrices with exactly one 1 on the main diagonal, and these are extreme points. But there are many other extreme points. The next goal is to determine the extreme points of $\Omega_n^{(\leq 1)}$. To this end we define a new class of sparse doubly stochastic matrices. Let

$$\mathcal{P}_n^{(\geq 2)} = \{P \in \mathcal{P}_n : \mathrm{tr}(P) \geq 2\}.$$

Thus, $\mathcal{P}_n^{(\leq 1)}$, $\mathcal{P}_n^{(\geq 2)}$ is a partition of the set $\mathcal{P}_n$ of permutation matrices of order n. Let $P \in \mathcal{P}_n^{(\geq 2)}$ and $Q \in \mathcal{D}_n$, and consider the convex combination

$$R = R(P, Q) = (1/k)P + (1 - 1/k)Q \tag{5}$$

where $k = \mathrm{tr}(P) \geq 2$ is the number of 1's on the diagonal of P. Then $R \in \Omega_n$ and $\mathrm{tr}(R) = (1/k)\mathrm{tr}(P) + (1 - 1/k)\mathrm{tr}(Q) = 1$, so that $R \in \Omega_n^{(\leq 1)}$.

Let $\mathcal{C}_n^*$ be the class of $n \times n$ doubly stochastic matrices of the form (5). Note that each matrix $R \in \mathcal{C}_n^*$ has one or two nonzeros in every line; if there are two nonzeros, these are $1/k$ and $1-1/k$ and they are in positions corresponding to a 1 in P and a 1 in Q, respectively. Consider the bipartite graph G_R with vertices (i, j) $(i, j \leq n)$ and an edge between (two distinct) vertices in the same row or column whenever both entries in R are positive. Then G_R contains vertex-disjoint even cycles $C_1, C_2, \ldots, C_s$ for some $s \geq 1$. The vertices of these cycles alternate between the positions of 1's in P and Q.

Let $\mathcal{C}_n^{**}$ be the subset of $\mathcal{C}_n^*$ consisting of matrices $R \in \mathcal{C}_n^*$ such that G_R has exactly one cycle; such a cycle must contain all the k positions on the main diagonal of P containing a 1 of P. This is because Q is a derangement and thus does not contain any 1's on its main diagonal.

We now determine the set of extreme points of the extended near-derangement polytope $\Omega_n^{(\leq 1)}$.

Theorem 3.3. *The extreme points of $\Omega_n^{(\leq 1)}$ are the permutation matrices in $\mathcal{P}_n^{(\leq 1)}$ and the doubly stochastic matrices in $\mathcal{C}_n^{**}$. Therefore*

$$\Omega_n^{(\leq 1)} = \mathrm{conv}\,(\mathcal{P}_n^{(\leq 1)} \cup \mathcal{C}_n^{**}).$$

Proof. Our main tool will be the so-called double description method, developed by Motzkin et al. [17]; the method is described for polyhedral cones in [19]. The starting point is the Birkhoff polytope Ω_n where we know all extreme points (the $n \times n$ permutation matrices) and a complete linear inequality description. We have

$$\Omega_n^{(\leq 1)} = \Omega_n \cap \{A = [a_{ij}] \in M_n : \sum_{i=1}^{n} a_{ii} \leq 1\}.$$

Clearly every permutation matrix in $\mathcal{P}_n^{(\leq 1)}$ is an extreme point of $\Omega_n^{(\leq 1)}$; this follows by convexity as Ω_n^1 is contained in the unit cube.

First we show that any matrix $A \in \Omega_n^{(\leq 1)}$ can be written as a convex combination of matrices in $\mathcal{P}_n^1 \cup \mathcal{C}_n^*$. As $A \in \Omega_n$ we may write

$$A = \sum_{k=1}^{m} \lambda_k P_k \tag{6}$$

for permutation matrices P_k and positive scalars λ_k $(k \leq m)$ where $\sum_k \lambda_k = 1$. If none of these P_k's are in $\mathcal{P}_n^{(\geq 2)}$, we are done, so assume that $P_{k^*} \in \mathcal{P}_n^{(\geq 2)}$ for some k^*. Then there exists an s where $P_s \in \mathcal{D}_n$; otherwise $\mathrm{tr}(A) > 1$ which is impossible. We can therefore rewrite A as a convex combination of the P_j's with $j \neq k^*$ and the matrix $R = R(P_{k^*}, P_s)$ with a positive weight λ_R associated with R. We here choose λ_R largest possible, and this means that one of the updated weights λ_{k^*} or λ_s will be zero. Thus, the number of positive weights λ_k is reduced by at least 1. We continue this process a finite number of times and gradually change the convex combination by introducing further matrices $R(P_i, P_j) \in \mathcal{C}_n^*$. Eventually we end up with A written as a convex combination of matrices in $\mathcal{P}_n^1 \cup \mathcal{C}_n^*$. The fact that a finite number of such transformations suffices is due to the strict reduction of the number of positive weights λ_k associated with permutation matrices. This proves that $\Omega_n^1 = \mathrm{conv}\,(\mathcal{P}_n^{(\leq 1)} \cup \mathcal{C}_n^*)$. Thus all extreme points of Ω_n^1 are in $\mathcal{P}_n^{(\leq 1)} \cup \mathcal{C}_n^*$. It remains to show that this set of "fractional" extreme points in $\mathcal{C}_n^*$ is precisely $\mathcal{C}_n^{**}$.

Let $R = R(P, Q) \in \mathcal{C}_n^*$ be an extreme point of $\Omega_n^{(\leq 1)}$ where $P \in \mathcal{P}_n^{(\geq 2)}$ and $Q \in \mathcal{D}_n$. Assume G_R contains a cycle C with no position on the main diagonal. Let R_1 be obtained from R by adding a small number $\epsilon > 0$ to each entry in the P-positions (as defined above) and subtracting ϵ from each entry in the Q-positions. Similarly, we construct R_2, but we interchange the role of adding/subtracting. For suitably small ϵ the matrices R_1 and R_2 are doubly stochastic. Moreover, as C has no entry on the main diagonal, $\mathrm{tr}(R_i) = \mathrm{tr}(R) = 1$, so $R_i \in \Omega_n^1$ $(i = 1, 2)$. Finally, $R = (1/2)R_1 + (1/2)R_2$, and this contradicts that R is an extreme point. This proves that each cycle in G_R contains a position on the main diagonal.

Assume G_R has (at least) two cycles C_1 and C_2. Then C_i contains some number $\gamma_i \geq 1$ of positions on the main diagonal $(i = 1, 2)$. Let $\epsilon_1, \epsilon_2 > 0$ be "small" numbers to be determined. Let R_1 be obtained from R by (i) adding ϵ_1 to each entry in the P-positions of C_1 and subtracting ϵ_1 from each entry in the Q-positions of C_1, and (ii) subtracting ϵ_2 from each entry in the P-positions of C_2 and adding ϵ_2 to each entry in the Q-positions of C_1. Then, for suitably small ϵ_i $(i = 1, 2)$ the matrix R_1 is doubly stochastic and

$$\mathrm{tr}(R_1) = \mathrm{tr}(R) + \gamma_1\epsilon_1 - \gamma_2\epsilon_2 = \mathrm{tr}(R) = 1$$

by choosing $\epsilon_2 = (\gamma_1/\gamma_2)\epsilon_1$. Thus, with suitably small ϵ_1, $R_1 \in \Omega_n^{(\leq 1)}$. Now let R_2 be obtained from R_1 by changing the signs of ϵ_1 and ϵ_2. Then $R_2 \in \Omega_n^{(\leq 1)}$, and clearly $R = (1/2)R_1 + (1/2)R_2$, and this contradicts that R is an extreme point. This proves that G_R has exactly one cycle, and this cycle contains a position on the main diagonal. Conversely, if G_R has exactly one such cycle, then it is easy to use the variational technique above to show that R cannot be written as a convex combination of two distinct matrices in $\Omega_n^{(\leq 1)}$, and therefore R is an extreme point. $\square$

We illustrate the construction of extreme points as given in the proof of Theorem 3.3.

Example 3.4. Let $n = 5$,

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } Q = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Then $\mathrm{tr}(P) = 3$, $\mathrm{tr}(Q) = 0$ and

$$R = R(P,Q) = \begin{bmatrix} 1/3 & 0 & 2/3 & 0 & 0 \\ 0 & 0 & 1/3 & 2/3 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/3 & 2/3 \\ 2/3 & 0 & 0 & 0 & 1/3 \end{bmatrix} \in \mathcal{C}_5^*.$$

G_R contains exactly one cycle (with three vertices on the main diagonal), so $R \in \mathcal{C}_5^{**}$ and R is an extreme point of $\Omega_5^{(\leq 1)}$. $\diamond$

Example 3.5. Consider the following two permutation matrices in $\mathcal{P}_5$

$$I_5 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } Q = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

So $I_5 \in \mathcal{P}_5^{(\geq 2)}$ and $Q \in \mathcal{D}_5$. Then

$$R = R(I_5,Q) = \begin{bmatrix} \frac{1}{5} & \frac{4}{5} & 0 & 0 & 0 \\ 0 & \frac{1}{5} & \frac{4}{5} & 0 & 0 \\ \frac{4}{5} & 0 & \frac{1}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{5} & \frac{4}{5} \\ 0 & 0 & 0 & \frac{4}{5} & \frac{1}{5} \end{bmatrix} \in \mathcal{C}_5^*.$$

However, R is not an extreme point of $\Omega_5^{(\leq 1)}$ because G_R contains two cycles. $\diamond$

Example 3.6. Consider the following two permutation matrices in $\mathcal{P}_5$

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \text{ and } Q = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

So $P \in \mathcal{P}_5^{(\geq 2)}$ and $Q \in \mathcal{D}_5$. Then

$$R = R(P,Q) = \begin{bmatrix} \frac{1}{3} & 0 & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \frac{1}{3} & \frac{2}{3} & 0 \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \in \mathcal{C}_5^*.$$

R is an extreme point of $\Omega_5^{(\leq 1)}$ because G_R contains only one cycle. $\diamond$

The matrix R in the previous example has a special form where all the entries equal to $1/k$ are on the main diagonal (where k is the trace of P). This means that the cycle in G_R alternates between a vertex on the main diagonal (corresponding to P) and a vertex not on the main diagonal (corresponding to Q). More generally, a subclass of $\mathcal{C}^{**}$ are matrices such that there exists a permutation matrix U such that $R = UAU^t$ where

$$A = \left[\begin{array}{c|c} \frac{1}{k}I_k + \frac{k-1}{k}S_k & O_{k,n-k} \\ \hline O_{n-k,n} & X_{n-k} \end{array}\right],$$

where

$$S_k = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & \ddots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix} \quad (2 \leq k \leq n),$$

and X_{n-k} is a direct sum of matrices of this form. Here $k \leq n-2$.

4 The convex hull of $\mathcal{P}_n^{(\leq 1)}$

Let M_n be the linear space of $n \times n$ matrices. In this section we initiate a study of the polytope $\mathcal{Q}_n^{(\leq 1)}$ defined as the convex hull of the permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. Since a permutation matrix cannot be expressed as a convex combination of permutation matrices different from itself, the set of extreme points of $\mathcal{Q}_n^{(\leq 1)}$ equals $\mathcal{P}_n^{(\leq 1)}$.

Lemma 4.1.

$$\dim \mathcal{Q}_n^{(\leq 1)} = (n-1)^2, \ \textit{the same as the dimension of } \Omega_n.$$

Proof. By Theorem 2.1 there is a basis of $\langle \mathcal{P}_n \rangle$ consisting of permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. Since the dimension of the linear span $\langle \mathcal{P}_n \rangle$ is $(n-1)^2+1$, such a basis contains $(n-1)^2+1$ permutation matrices in $\mathcal{P}_n^{(\leq 1)}$. Since $\mathcal{Q}_n^{(\leq 1)} \subseteq \langle \mathcal{P}_n \rangle$, the dimension of $\mathcal{Q}_n^{(\leq 1)}$ is also $(n-1)^2$. $\square$

We first consider the case when n is small. Each of $\mathcal{Q}_1^{(\leq 1)}$ and $\mathcal{Q}_2^{(\leq 1)}$ consists of a single matrix, namely J_1, and the 2×2 backward identity matrix L_2, respectively.

Theorem 4.2. *The polytope $\mathcal{Q}_3^{(\leq 1)}$ is a 4-dimensional simplex in M_3. A complete linear description of $A = [a_{ij}] \in \mathcal{Q}_3^{(\leq 1)}$ is*

$$\begin{aligned} a_{ii} &\geq 0 \quad (i \leq 3), \\ \textstyle\sum_{j=1}^{3} a_{ij} &= 1 \quad (i \leq 3), \\ \textstyle\sum_{i=1}^{3} a_{ij} &= 1 \quad (j \leq 3), \\ a_{11} + a_{21} + a_{22} \leq 1 &\text{ and } a_{11} + a_{12} + a_{22} \leq 1. \end{aligned} \tag{7}$$

Each inequality in (7) *defines a facet of $\mathcal{Q}_3^{(\leq 1)}$.*

Proof. Let $A = [a_{ij}] \in \mathcal{Q}_3^{(\leq 1)}$. By Lemma 4.1, $\dim(\mathcal{Q}^{(\leq 1)}) = 4$. Moreover, all entries in the last row and column of A are determined uniquely by the leading 2×2 submatrix

$$A' = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}.$$

$\mathcal{P}_3^{(\leq 1)}$ consists of the following five permutation matrices

$$\left[\begin{array}{c|c|c} 1 & & \\ \hline & & 1 \\ \hline & 1 & \end{array}\right], \left[\begin{array}{c|c|c} & 1 & \\ \hline 1 & & \\ \hline & & 1 \end{array}\right], \left[\begin{array}{c|c|c} & 1 & \\ \hline & & 1 \\ \hline 1 & & \end{array}\right], \left[\begin{array}{c|c|c} & & 1 \\ \hline & 1 & \\ \hline 1 & & \end{array}\right], \left[\begin{array}{c|c|c} & & 1 \\ \hline 1 & & \\ \hline & 1 & \end{array}\right] \tag{8}$$

so that it is only the identity matrix I_3 that is left out (see also (2)). By Lemma 4.1, $\mathcal{Q}_3^{(\leq 1)}$ has dimension 4, and therefore the five matrices in (8) are affinely independent. Since, each of these matrices is an extreme point of $\mathcal{Q}_3^{(\leq 1)}$, it follows by definition of a simplex that $\mathcal{Q}_3^{(\leq 1)}$ is a 4-dimensional simplex in M_3.

Consider the set of the five leading 2×2 submatrices of the matrices in (8), and let K be the simplex equal to their convex hull. The simplex $\mathcal{Q}_3^{(\leq 1)}$ is affinely isomorphic to K. This follows from the fact that all the line sum constraints equal 1. Each facet of a simplex is obtained as the convex hull of all except one of its vertices. Based on this one can compute all facets of K and they correspond to the following five linear inequalities in (the entry) variables a_{ij} $(i, j \leq 2)$:

$$\begin{gathered} a_{11} \geq 0, \quad a_{22} \geq 0, \quad a_{11} + a_{12} + a_{21} + a_{22} \geq 1, \\ a_{11} + a_{12} + a_{22} \leq 1, \quad a_{11} + a_{21} + a_{22} \leq 1. \end{gathered}$$

Thus, by adding the linear equations $\sum_j a_{ij} = 1$ $(i \leq 3)$ and $\sum_i a_{ij} = 1$ $(j \leq 3)$ we obtain a complete and nonredundant linear description of $\mathcal{Q}_3^{(\leq 1)}$. As the inequality $a_{11} + a_{12} + a_{21} + a_{22} \geq 1$ can be seen to be equivalent to $a_{33} \geq 0$ (using the line sum equations), the desired result follows. ∎

Note that for $n = 3$ the set $\mathcal{P}_3^{(\leq 1)}$ consists of all permutations except the identity. Therefore the polytope $\mathcal{Q}_3^{(\leq 1)}$ coincides with the polytope Ω_3^* equal to the convex hull of all non-identity permutation matrices of order 3, and the previous theorem characterizes this polytope for $n = 3$.

The final two facet defining inequalities in (7) can be generalized as follows, for general n. Define first the graph G_n with vertices (i, j) $(1 \leq i, j \leq n)$ corresponding to the positions of an $n \times n$ matrix. Next, define edges between every pair of vertices whose positions are in the same row or column, or both are on the main diagonal. Then the support of a matrix $P \in \mathcal{P}_n^{(\leq 1)}$, that is, the set of positions of its nonzeros, corresponds to a stable set in G_n. Recall that a stable set (or independent set) is a vertex subset where no two of these vertices are adjacent. Conversely, a stable set in G_n corresponds to a subpermutation matrix with at most one 1 on the main diagonal. The line sum inequalities (sum in a line is at most 1) and trace inequality correspond to $2n + 1$ clique inequalities for the stable set polytope of G_n. See [21] for many results concerning stable set polytopes. Another general class consists of the *odd cycle inequalities*: every $A = [a_{ij}] \in \mathcal{Q}_n^{\leq 1}$ satisfies

$$\sum_{(i,j)\in C} a_{ij} \leq (|C| - 1)/2 \tag{9}$$

where C is an odd cycle in the graph G_n. A special case is when $|C| = 3$, so C is a triangle, and we get the *triangle inequality*

$$\sum_{(i,j)\in C} a_{ij} \leq 1.$$

This can also be seen as a clique inequality. In fact, these are the only remaining maximum clique inequalities in G_n, apart from those for lines and the main diagonal. The triangles in G_n are of the form $C = \{(i, i), (i, j), (j, j)\}$ or $C = \{(i, i), (j, i), (j, j)\}$ for $1 \leq i < j \leq n$. The final two facet defining inequalities in (7) are triangle inequalities.

5 A property of faces

A natural question concerning the polytopes considered here is to determine which faces of Ω_n are also faces of the subpolytope $\Omega_n^{(\leq 1)}$. Every face $\mathcal{F}$ of Ω_n is determined by an $n \times n$ $(0, 1)$-matrix A with *total support* (meaning that every 1 of A is part of a permutation matrix $P \leq A$):

$$\mathcal{F} = \mathcal{F}(A) = \{X \in \Omega_n : X \leq A\}.$$

Thus $\mathcal{F}$ is also a face of $\Omega_n^{(\leq 1)}$ if and only if every permutation matrix P with $P \leq A$ is contained in $\mathcal{P}_n^{(\leq 1)}$. The question is to characterize those $(0, 1)$-matrices A having this property.

An example of a matrix with this property is

$$A = \left[\begin{array}{c|c|c|c} 1 & & 1 & 1 \\ \hline & 1 & & 1 \\ \hline 1 & 1 & & \\ \hline & 1 & 1 & \end{array}\right],$$

since it contains only the following permutation matrices in $\mathcal{P}_4^{(\leq 1)}$:

$$\left[\begin{array}{c|c|c|c} 1 & & & \\ \hline & & & 1 \\ \hline & 1 & & \\ \hline & & 1 & \end{array}\right], \left[\begin{array}{c|c|c|c} & & 1 & \\ \hline & & & 1 \\ \hline 1 & & & \\ \hline & 1 & & \end{array}\right], \left[\begin{array}{c|c|c|c} & & & 1 \\ \hline & 1 & & \\ \hline 1 & & & \\ \hline & & 1 & \end{array}\right].$$

A general characterization of this property is given next.

Theorem 5.1. *Let $A = [a_{ij}]$ be an $n \times n$ $(0,1)$-matrix with total support. Then the face $\mathcal{F}(A)$ of Ω_n is also a face of $\Omega_n^{(\leq 1)}$ if and only if there are integers u_i and v_j $(i, j \leq n)$ such that*

$$\begin{aligned} u_i + v_i &\geq 1 && \text{for all } i \text{ with } a_{ii} = 1, \\ u_i + v_j &\geq 0 && \text{for all } i \neq j \text{ with } a_{ij} = 1, \\ \textstyle\sum_i u_i + \sum_j v_j &\leq 1. \end{aligned} \tag{10}$$

Proof. Consider the optimization problem

$$\gamma := \max\{\sum_{i=1}^{n} p_{ii} : P = [p_{ij}] \in \mathcal{P}_n,\ P \leq A\} \tag{11}$$

which asks for a permutation matrix $P \leq A$ with a maximum number of 1's on the main diagonal. Then, clearly, the face $\mathcal{F}(A)$ of Ω_n is also a face of $\Omega_n^{(\leq 1)}$ if and only if $\gamma \leq 1$. Problem (11) can be viewed as a maximum weight perfect matching problem in a bipartite graph with two sets of vertices of cardinality n (corresponding to rows and columns) and edges corresponding to those (i, j) where $a_{ij} = 1$. Let E denote the edge set of this graph. The weight w_{ij} is 1 for edges (i, i), i.e., when $a_{ii} = 1$, and 0 otherwise. By a well-known result from matching theory [20, 21] (due to linear programming duality and total unimodularity) γ equals the optimal value of the dual problem which is

$$\gamma := \min\left\{\sum_i u_i + \sum_j v_j : u_i + v_j \geq w_{ij},\ \text{ for all } ij \in E\right\} \tag{12}$$

and both problems have optimal solutions that are integral. This gives the desired result. □

In the example above, we have $\gamma = 1$ and an optimal dual solution is $u_3 = -1$, $v_1 = v_2 = 1$ while all other variables are 0.

The efficient matching algorithm mentioned in the proof of Theorem 5.1 decides if the face $\mathcal{F}(A)$ of Ω_n is also a face of $\Omega_n^{(\leq 1)}$. Still, an interesting question is to find classes of $(0,1)$-matrices A where this property holds (so no algorithm is needed). We give one such result next.

Let r, s, k, and n be natural numbers with $r, s, k < n$ and $k \geq 2$. Define the $(0,1)$-matrix $A = A^{(k,r,s,n)}$ by the following properties: (i) its lower right corner is an $r \times s$ zero submatrix, (ii) the main diagonal of A consists of k 1's followed by zeros, and (iii) all other entries of the matrix are equal to 1.

Theorem 5.2. *Let $A = A^{(k,r,s,n)} = [a_{ij}]$ be as above with*

$$2 \le k \le \lfloor n/2 \rfloor,\ r = n-k \text{ and } s = k-1.$$

Then (i) A has total support and (ii) the face $\mathcal{F}(A)$ of Ω_n is also a face of $\Omega_n^{(\le 1)}$.

Moreover, A has the maximum number of 1's among $n \times n$ $(0,1)$-matrices with trace k satisfying properties (i) and (ii).

Proof. First we observe that A has total support as it has no zero $p \times q$ submatrix with $p + q = n$.

Next, assume P is a permutation matrix with $P \le A$ and trace $s \ge 2$. So $2 \le s \le k$, and P contains the identity matrix I_s as a principal submatrix. The complementary submatrix P' of I_s (in P) has size $(n-s) \times (n-s)$ and contains an $r \times s$ zero submatrix, due to the fact that $P \le A$ and by construction of A. But

$$r + s = (n-k) + (k-1) = n-1.$$

Note that $n - 1 \ge n - s + 1$ as $s \ge 2$. Therefore, by the Frobenius-König Theorem, this zero submatrix implies that P' cannot contain a permutation matrix. This is a contradiction, and it follows that every permutation matrix P with $P \le A$ must have trace at most 1, i.e., it lies in $\mathcal{P}^{(\le 1)}$. This proves property (ii) in the theorem.

To prove the final statement consider an $n \times n$ $(0,1)$-matrix A' with trace $k \ge 2$ and satisfying properties (i) and (ii). Choose two 1's on the main diagonal of A'; they define a 2×2 submatrix. By property (ii) the complementary submatrix A^* cannot contain a permutation matrix, so by the Frobenius-König Theorem, A^* contains a $p \times q$ zero submatrix with $p+q = n-1$. This implies that the number of zeros in A^* is at least the number of zeros in the matrix A in the theorem. (This is because pq is a strictly decreasing function of p under the constraints $p+q = n-1$, $1 \le p, q \le n-k$ and $p \ge q$.) Therefore A has the maximum number of 1's under the mentioned constraints. □

Example 5.3. Let $n = 9$ and $k = 4$. Then $r = 5$, $s = 3$ and the constructed matrix in Theorem 5.2 is

$$A = \left[\begin{array}{c|c|c|c||c|c|c|c|c}
1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1\\
\hline\hline
1&1&1&1&0&1&0&0&0\\
1&1&1&1&1&0&0&0&0\\
1&1&1&1&1&1&0&0&0\\
1&1&1&1&1&1&0&0&0\\
1&1&1&1&1&1&0&0&0
\end{array}\right].$$

◇

6 Concluding remarks

In this final section we suggest some possible further questions to study in this area.

(i) A natural, and interesting topic, is to investigate the stable set polytope of G_n, defined above as the convex hull of all incidence vectors of stable sets in G_n. This polytope contains the polytope $\mathcal{Q}_n^{(\leq 1)}$ as a face. A lot is known about stable set polytopes (see e.g. [18, 21]), but this graph is special, so we believe there may be interesting questions concerning this polytope.

(ii) In Theorem 3.3 we determined all the extreme points of $\Omega_n^{(\leq 1)}$. An extension is to determine all the faces of $\Omega_n^{(\leq 1)}$, and some of their properties. Each such face F of $\Omega_n^{(\leq 1)}$ which is not a face of Ω_n is obtained as an intersection of a face of Ω_n by the hyperplane $\{A = [a_{ij}] : \sum_i a_{ii} = 1\}$. In particular, the edges of the polytope may be determined based on Theorem 3.3.

(iii) Let $n \geq 2$ be a positive integer. What is the maximum trace k_n of a $n \times n$ (0,1)-matrix A with total support such that every permutation matrix $P \leq A$ is in $\mathcal{P}_n^{(\leq 1)}$?

(iv) What is the maximum number $m_n(k)$ of 1's in an $n \times n$ $(0,1)$-matrix A with total support having k 1's and $(n-k)$ 0's on the main diagonal such that all $P \leq A$ are in $\mathcal{P}_n^{(1)}$?

For $k = 1$, the $n \times n$ matrix A with one 1 and $(n-1)$ 0's on the main diagonal, and 1's everywhere else clearly has the property that all $P \leq A$ are in $\mathcal{P}_n^{(1)}$; hence $m_n(1) = n^2 - (n-1)$. Now consider $k = 2$.

If $n = 3$, then

$$\left[\begin{array}{c|c|c} 1 & 1 & 1 \\ \hline 1 & 1 & 1 \\ \hline 1 & 1 & 0 \end{array}\right]$$

is fully indecomposable so that (in question (iii)) $k_3 = 2$, and $m_3(2) = 8$.

If $n = 4$, then

$$A = \left[\begin{array}{c|c|c|c} 1 & 1 & 1 & 1 \\ \hline 1 & 1 & 1 & 1 \\ \hline 1 & 1 & 0 & 1 \\ \hline 1 & 1 & 0 & 0 \end{array}\right]$$

is fully indecomposable and has the property that all $P \leq A$ are in $\mathcal{P}_4^{(1)}$ implying that $m_4(2) = 13$. In general, for $k = 2$, we have $m_n(2) = n^2 - 2n + 5$. This follows easily from the classical Frobenius-König theorem.

An example with $k = 3$ and $n = 5$ is

$$\left[\begin{array}{c|c|c|c|c} 1 & 0 & 0 & 1 & 1 \\ \hline 0 & 1 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 1 & 1 \\ \hline 1 & 0 & 1 & 0 & 0 \\ \hline 0 & 1 & 1 & 0 & 0 \end{array}\right].$$

To what extent is it sufficient to check only pairs of 1's on the main diagonal?

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(Received 20 May 2024; revised 6 Jan 2025)