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PARTIAL TRANSPOSES OF PERMUTATION MATRICES

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Abstract

The partial transpose of a block matrix M is the matrix obtained by transposing the blocks of M independently. We approach the notion of the partial transpose from a combinatorial point of view. In this perspective, we solve some basic enumeration problems concerning the partial transpose of permutation matrices. More specifically, we count the number of permutations matrices which are invariant under the partial transpose and the number of permutation matrices whose partial transposes are still permutations. We solve these problems also when restricted to transposition matrices only.

1. Introduction

The *partial transpose* (or, equivalently, *partial transposition*) is a linear algebraic concept, which can be interpreted as a simple generalization of the usual matrix transpose. In the present paper, we consider the partial transpose from a combinatorial point of view. More specifically, we solve some enumeration problems concerning the partial transpose of permutation matrices.

Even if this notion is a natural one, to the knowledge of the authors, it has never been directly studied by the linear algebra community. On the other hand, the partial transpose is an important tool in the mathematical theory of quantum entanglement. For this reason, the partial transpose appears often in works contextual with quantum information theory. We will spend a few paragraphs on this, just for taking a snapshot of the scenario in which this notion arises.

Bruß and Macchiavello [3] give an excellent explanation of the meaning of the partial transpose in quantum information theory. Its primary use is materialized in the so-called *PPT-criterion*, where "PPT" stands for *Positive Partial Transpose*. The criterion, firstly discovered by Peres [13] and the Horodeckis [10] (see also [12]), is as follows: if the density matrix (or, equivalently, the state) of a quantum mechanical system with composite dimension pq is entangled, with respect to the subsystems of dimension p and q, then its partial transpose is positive. The converse of the implication is not necessarily true. However, under certain restrictions, for example, when the dimension of the density matrix is six, the PPT-criterion is necessary and sufficient.

There is a number of problems suggested by the PPT-criterion. In particular, in order to shed light onto the structure of the set of density matrices, it would be important to characterize those for which the criterion is valid. An open question of practical importance is to prove or disprove that certain states, which are said to be non-distillable, have positive partial transpose. However, there is strong evidence that there exist non-distillable states with negative partial transpose, which would be then called NPT-bound entangled states. Regarding this topic, see the important references [6, 7], or [4], for an account on recent discussions.

Looking at the notion of the partial transpose from the combinatorial point of view is an appealing topic, because it has the potential to uncover patterns in the set of density matrices and indicate connections with other mathematical objects, and this may turn out to be helpful in understanding physical properties. As a matter of fact there have been a number of recent papers considering entanglement in discrete settings (see, *e.g.*, [1, 8, 11]).

Here we state and solve some basic enumeration problems involving the partial transposes of permutation matrices. Permutations appear in fact to be a simple, yet a rich territory to explore. Enumeration is a good first step towards the quantitative understanding of the structure of a set.

In particular, we count the number of permutation matrices which are invariant under the partial transpose and the number of permutation matrices whose partial transposes are still permutations. We solve these problems also when restricted to transposition matrices only (*i.e.*, induced by transpositions).

Apart from considerations related to symmetry, given that symmetry often predisposes to relations between different combinatorial objects, a further reason to look at involutions comes from [1]. A permutation matrix associated to a involution can be seen as the adjacency matrix of the disjoint union of matchings and self-loops. Since the combinatorial Laplacian of any graph is a density matrix after appropriate normalization [1], counting the number of involutions whose partial transposes are permutations is equivalent to counting the number of these states with positive partial transposes. However, the PPT-criterion is not sufficient also for this extremely restricted class. There actually are disconnected graphs whose Laplacians are entangled even if their partial transposes are positive [9].

The organization of the paper is as follows. In the next section, we give the required definitions and formally state our problems. Section 3 deals with permutations whose partial transposes are permutations; Section 4, with permutations which are invariant under the partial transpose; Section 5, with involutions whose partial transposes are permutations.

2. Definitions, Statements of the Problems, and Examples

The following is a formal definition of the partial transpose of a matrix:

Definition 1 *Let M be an $n \times n$ matrix with real entries. Let us assume that $n = pq$, where p and q are chosen arbitrarily. Under this assumption, we can look at the matrix M as partitioned into p^2 blocks each of size $q \times q$. The* partial transpose *of M, denoted by M^{Γ_p}, is the matrix obtained from M, by transposing independently each of its p^2 blocks. Formally, if*

$$M = \begin{pmatrix} \mathcal{B}_{1,1} & \cdots & \mathcal{B}_{1,p} \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1} & \cdots & \mathcal{B}_{p,p} \end{pmatrix}$$

then

$$M^{\Gamma_p} = \begin{pmatrix} \mathcal{B}_{1,1}^T & \cdots & \mathcal{B}_{1,p}^T \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1}^T & \cdots & \mathcal{B}_{p,p}^T \end{pmatrix},$$

where $\mathcal{B}_{i,j}^T$ denotes the transpose of the block $\mathcal{B}_{i,j}$, for $1 \leq i, j \leq p$.

Notice that, by taking the adjoint $\mathcal{B}_{i,j}^\dagger$, instead of the transpose $\mathcal{B}_{i,j}^T$, the notion of the partial transpose can be easily extended to matrices with complex entries. This is something which we will not need here. The term "partial transpose" also indicates the actual operation required to obtain the matrix partial transposed as defined here.

We will consider the partial transposes of permutation matrices. Let us recall that a *permutation matrix* of *size* n is an $n \times n$ matrix, with entries in the set $\{0, 1\}$, such that each row and each column contains exactly one nonzero entry. A *permutation* of *length* n is a bijection $\pi : [n] \longrightarrow [n]$, where $[n] = \{1, 2, ..., n\}$. In standard linear notation, a permutation $\pi \in S_n$ can be written as a word of the form $\pi(1)\pi(2) \cdots \pi(n)$. Given an $n \times n$ permutation matrix P, there is a unique permutation π of length n associated to P, such that $\pi(i) = j$ if and only if $P_{i,j} = 1$. We then say P is the permutation matrix of π, denoted by $P = P_\pi$.

Let us denote by S_n the set of all $n \times n$ permutation matrices. With an innocuous abuse of notation, we write S_n also for the set of all permutations of length n.

The transpose of a permutation matrix is still a permutation matrix. But this does not hold for the partial transpose. See the following example.

Example 2 *Let*

$$P_{3142} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

be the permutation matrix corresponds to the permutation $\pi = 3142$. *Then*

$$P_{3142}^{\Gamma_2} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix},$$

which is not a permutation matrix.

The following table lists all permutation matrices P_π in S_4 and their partial transposes $P_\pi^{\Gamma_2}$.

$1234, 1234$	$1243, 1243$	$1324, NP$	$1342, NP$	$1423, NP$	$1432, 1432$
$2134, 2134$	$2143, 2143$	$2314, NP$	$2341, 4123$	$2413, NP$	$2431, NP$
$3124, NP$	$3142, NP$	$3214, 3214$	$3241, NP$	$3412, 3412$	$3421, 3421$
$4123, 2341$	$4132, NP$	$4213, NP$	$4231, NP$	$4312, 4312$	$4321, 4321$

Table 1: Permutation matrices and their partial transposes. The notation "NP" means that $P_\pi^{\Gamma_2}$ is not a permutation matrix.

It may be interesting to point out that a permutation matrix P and its partial transpose P^Γ have the same sum of the row (or column) indices of the 1 entries, whatever P^Γ is a permutation matrix or not. More precisely, if $n = pq$ and P is a permutation matrix of size $n \times n$, then

$$\sum_{P_{i,j}=1} i = \sum_{(P^{\Gamma_p})_{i,j}=1} i = n(n+1)/2.$$

Let us recall that a permutation π is said to be a *transposition* if there is $i \neq j$ such that $\pi(i) = j$, $\pi(j) = i$ and $\pi(k) = k$ for $k \neq i, j$. As usual, we write $\pi = (i, j)$ and call P_π a *transposition matrix*.

We will solve the following three problems.

Problem 3 *Count the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$.*

Example 4 *Suppose that $p = q = 2$. From Table 1, there are all together 12 matrices $P \in S_4$ such that $P^{\Gamma_2} \in S_4$. Among them, 8 are the block-matrices of the forms*

$$\begin{pmatrix} * & \mathbf{0} \\ \mathbf{0} & * \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathbf{0} & * \\ * & \mathbf{0} \end{pmatrix}. \tag{1}$$

The remaining 4 matrices are

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

Problem 5 *Count the number of permutation matrices $P \in S_{pq}$ which are invariant under the partial transpose, i.e., $P^{\Gamma_p} = P$.*

Example 6 *Suppose that $p = q = 2$. By Table 1, there are all together 10 matrices $P \in S_4$ such that $P^{\Gamma_2} = P$. Among them, 8 are the block matrices of the form (1). The remaining 2 matrices are the first and the last matrix in (2).*

Problem 7 *Count the number of transposition matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$.*

We will show in Section 5 that a transposition matrix $P \in S_{pq}$ satisfy $P^{\Gamma_p} \in S_{pq}$ if and only if $P^{\Gamma_p} = P$. Therefore, Problem 7 also counts the number of transposition matrices which are invariant under the partial transpose.

Example 8 *Suppose that $p = q = 2$. There are all together 4 transposition matrices $P \in S_4$ such that $P^{\Gamma_2} \in S_4$:*

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

3. Permutations Whose Partial Transposes are Permutations

To solve Problems 3 and 5, we introduce the following notations. Let $P \in S_n$ be a permutation matrix of order $n = pq$, where p, q are positive integers. We divide P into p^2 blocks, each of size $q \times q$, and denote by $\mathcal{B}_{i,j}$ the (i,j)-th block. Further, let $A_{i,j}, B_{i,j} \subseteq [q] = \{1, 2, \ldots, q\}$ be the sets of relative row indices and column indices of the 1's in the block $\mathcal{B}_{i,j}$, called the *row sets* and the *column sets* of P, respectively. For example, given $p = q = 2$ and

$$P = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

we have $A_{1,1} = \{2\}, A_{1,2} = \{1\}, A_{2,1} = \{1\}, A_{2,2} = \{2\}$, and $B_{1,1} = \{1\}, B_{1,2} = \{2\}$, $B_{2,1} = \{2\}, B_{2,2} = \{1\}$.

Clearly, we have

$$|A_{i,j}| = |B_{i,j}|, \tag{3}$$

where $|S|$ denotes the cardinality of a set S. Since P is a permutation matrix, we have

$$A_{i,j} \cap A_{i,k} = \emptyset, \quad \text{for every } i,j,k \text{ with } j \neq k, \tag{4}$$

$$B_{i,j} \cap B_{k,j} = \emptyset, \quad \text{for every } i,j,k \text{ with } i \neq k, \tag{5}$$

and

$$\bigcup_{j=1}^{p} A_{i,j} = [q], \text{ for } i = 1, 2, ..., p, \qquad \bigcup_{i=1}^{p} B_{i,j} = [q], \text{ for } j = 1, 2, ..., p. \tag{6}$$

Conversely, let $A_{i,j}, B_{i,j}$ be $2p^2$ subsets of $[q]$ satisfying (3)–(6). Since we have $r_{i,j}!$ ways to place 1's in $\mathcal{B}_{i,j}$, there are $\prod_{i,j} r_{i,j}!$ permutation matrices whose row indices and column indices are exactly $A_{i,j}$ and $B_{i,j}$, respectively. Therefore, we may solve Problems 3 and 5 by counting the number of $A_{i,j}, B_{i,j}$'s satisfying certain conditions.

We begin with Problem 3. Suppose that P and its partial transpose P^{Γ_p} are both permutation matrices. Let $A_{i,j}$ and $B_{i,j}$ be the row sets and the column sets of P, respectively. Then we see that $B_{i,j}$ and $A_{i,j}$ are the row sets and the column sets of P^{Γ_p}. Therefore, we have

$$B_{i,j} \cap B_{i,k} = \emptyset, \quad \text{for every } i,j,k \text{ with } j \neq k, \tag{7}$$

$$A_{i,j} \cap A_{k,j} = \emptyset, \quad \text{for every } i,j,k \text{ with } i \neq k, \tag{8}$$

and

$$\bigcup_{j=1}^{p} B_{i,j} = [q], \text{ for } i = 1, 2, ..., p, \qquad \bigcup_{i=1}^{p} A_{i,j} = [q], \text{ for } j = 1, 2, ..., p. \tag{9}$$

Conversely, let $A_{i,j}, B_{i,j}$ be $2p^2$ subsets of $[q]$ which satisfy (3)–(9). As stated before, there are all together $\prod_{i,j} r_{i,j}!$ permutation matrices whose row indices and column indices are $A_{i,j}$ and $B_{i,j}$ respectively. Since $A_{i,j}, B_{i,j}$ satisfy (7)–(9), the partial transposes of these permutation matrices are still permutation matrices. Therefore, the number of permutation matrices whose partial transposes are still permutation matrices equals the number of $A_{i,j}, B_{i,j}$ satisfying (3)–(9) multiplied by $\prod_{i,j} r_{i,j}!$.

Let

$$A_\pi = \bigcap_{i=1}^{p} A_{i,\pi_i} \quad \text{and} \quad B_\pi = \bigcap_{i=1}^{p} B_{i,\pi_i}, \quad \forall\, \pi \in S_p.$$

By Eqs. (4)–(6), we know that

$$A_{i,j} = \bigcup_{\pi_i=j} A_\pi, \quad B_{i,j} = \bigcup_{\pi_i=j} B_\pi. \tag{10}$$

From (4)–(8), we can then write

$$A_\pi \cap A_\sigma = B_\pi \cap B_\sigma = \emptyset, \quad \text{for every } \pi, \sigma \in S_p \text{ with } \pi \neq \sigma. \tag{11}$$

Furthermore, by (6) and (9),

$$\bigcup_{\pi \in S_p} A_\pi = \bigcup_{\pi \in S_p} B_\pi = [q]. \tag{12}$$

Conversely, given two set partitions $\{A_\pi\}$ and $\{B_\pi\}$ of $[q]$, satisfying Eqs. (11) and (12), we may define $A_{i,j}$ and $B_{i,j}$ by Eq. (10). One can easily check that Eqs. (4)–(9) hold. The only restriction on the A_π's and the B_π's is that the cardinalities of $A_{i,j}$ and $B_{i,j}$ should be the equal. Let a_π and b_π denote the cardinalities of A_π and B_π, respectively. On the basis of the above lines, we can state the following result:

Theorem 9 *Let $Z(p,q)$ be the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$. Then*

$$Z(p,q) = \sum_{\substack{\sum a_\pi = \sum b_\pi = q \\ \sum_{\pi_i=j} a_\pi = \sum_{\pi_i=j} b_\pi}} \frac{q!^2}{\prod_\pi a_\pi! b_\pi!} \prod_{i,j=1}^{p} \left(\sum_{\pi_i=j} a_\pi \right)!, \tag{13}$$

where the sum runs over all non-negative integers a_π, b_π.

For $p = 2$, we have

$$\begin{aligned} Z(p,q) &= \sum_{\substack{a_{12}+a_{21}=b_{12}+b_{21}=q \\ a_{12}=b_{12}, a_{21}=b_{21}}} \frac{q!^2}{a_{12}!a_{21}!b_{12}!b_{21}!} a_{12}!a_{21}!a_{21}!a_{12}! \\ &= \sum_{a_{12}=0}^{q} q!^2 = q!(q+1)!. \end{aligned}$$

Thus, we have a neat expression for the special case $P \in S_{2q}$:

Corollary 10 *The number of permutation matrices $P \in S_{2q}$ such that $P^{\Gamma_2} \in S_{2q}$ is*

$$Z(2,q) = q!(q+1)!.$$

The pattern avoidance language is now a standard tool for characterizing classes of permutations (see [16]). It would be natural to find a characterization of the set of permutations given in Theorem 9 in terms of pattern avoidance.

4. Permutations Invariant Under the Partial Transpose

We now turn to Problem 5. Let P be invariant under the partial transpose. Then each block $\mathcal{B}_{i,j}$ of P is invariant under the usual transpose. Hence, $A_{i,j} = B_{i,j}$. Additionally, given $A_{i,j}$ with $|A_{i,j}| = r_{i,j}$, there are $I(r_{i,j})$ ways to put 1's in the block $\mathcal{B}_{i,j}$, where $I(m)$ denotes the number of involutions in S_m. It is well-known that (see, *e.g.*, [15, Example 5.2.10])

$$I(m) = \sum_{\substack{j=0 \\ j \text{ even}}}^{m} \binom{m}{j} \frac{j!}{2^{j/2}(j/2)!} \tag{14}$$

and $I(m+1) = I(m) + m \cdot I(m-1)$. With the same analysis carried on for Theorem 9, we can directly obtain the number of desired matrices:

Theorem 11 *Let $Z_e(p,q)$ be the number of permutation matrices $P \in S_{pq}$ such that $P = P^{\Gamma_p}$. Then*

$$Z_e(p,q) = \sum_{\sum a_\pi = q} \frac{q!}{\prod_\pi a_\pi!} \prod_{i,j=1}^{p} I\left(\sum_{\pi_i = j} a_\pi\right), \tag{15}$$

where the sum runs over all non-negative integers a_π and $I(m)$ denotes the number of involutions in S_m.

Taking $p = 2$, we obtain

Corollary 12 *The number of permutation matrices $P \in S_{2q}$ such that $P = P^{\Gamma_2}$ is*

$$Z_e(2,q) = \sum_{r=0}^{q} \binom{q}{r}^2 I(r)^2 I(q-r)^2.$$

5. Transpositions Whose Partial Transposes are Permutations

In this section, we present a solution of Problem 7. Let $n = pq$ as before. Suppose that P is a transposition matrix whose corresponding permutation is $\pi = (aq+i, bq+j)$, where $0 \le a, b \le p-1$, $1 \le i, j \le q$ and $(a,i) \ne (b,j)$. Notice that there are $n-2$ 1's lie in the diagonal of P and the partial transpose keeps them fixed. So, the only possible permutation matrices after partial transpose would be the identity matrix Id or P itself. In the first case, we have $P = \mathrm{Id}$, since we get back the original matrix by applying twice the partial transpose operation. While by definition Id is not a transposition. Therefore, we must fall in the second case, that is, P remains invariant under partial transpose. Since $\pi = (aq+i, bq+j)$, the

$(aq+i, bq+j)$-th and the $(bq+j, aq+i)$-th entry of P are 1's. After partial transpose, the $(aq+j, bq+i)$-th and the $(bq+i, aq+j)$-th entry are 1's. Thus we have

$$\begin{aligned}(aq+i, bq+j) &= (aq+j, bq+i),\\ (bq+j, aq+i) &= (bq+i, aq+j),\end{aligned}$$

or

$$\begin{aligned}(aq+i, bq+j) &= (bq+i, aq+j),\\ (bq+j, aq+i) &= (aq+j, bq+i).\end{aligned}$$

Solving the equations, we derive that $i = j$ or $a = b$. Hence, the desired transpositions are $(aq+i, aq+j)$, with $i \neq j$, or, $(aq+i, bq+i)$, with $a \neq b$. This leads to the following fact:

Theorem 13 *Let $Z_t(p, q)$ be the number of transposition matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$, or, equivalently, $P^{\Gamma_p} = P$. Then $Z_t(p, q) = p\binom{q}{2} + q\binom{p}{2}$.*

Corollary 14 *The following statements hold true:*

- $Z_t(q+1, q) = q(q+1)(2q-1)/2$;
- $Z_t(q, q) = (q^3 - q^2)$.

The numbers $Z_t(q+1, q)$ are called *octagonal pyramidal numbers*, and count the ways of covering a $2q \times 2q$ lattice with $2q^2$ dominoes with exactly 2 horizontal dominoes ([14], Seq. A002414).

To conclude this section, even if these are simple facts, it may be clarifying to remark the following:

Proposition 15 *The following statements hold for all p and q:*

- $Z(p, q) = Z(q, p)$;
- *In general,* $Z_e(p, q) \neq Z_e(p, q)$;
- $Z_t(p, q) = Z_t(q, p)$.

Proof. While the second point is obvious, the other two can be verified by the following bijection. Suppose that the $(ap+i, b(a,i)p + j(a,i))$-th entry of P is 1. Then let the $((i-1)q+(a+1), (j(a,i)-1)q+(b(a,i)+1))$-th entry of P' be 1. If the partial transpose of P is a permutation, then $ap+j(a,i)$ and $b(a,i)p+i$ run from 1 to n, for $0 \leq a \leq q-1, 1 \leq i \leq p$.

Thus, $(i-1)q+(b(a,i)+1)$ and $(j(a,i)-1)q+(a+1)$ run from 1 to n also. This implies that the partial transpose of P' is a permutation. $\square$

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