# LARGEST MINIMAL INVERSION-COMPLETE AND PAIR-COMPLETE SETS OF PERMUTATIONS

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Abstract. We solve two related extremal problems in the theory of permutations. A set Q of permutations of the integers 1 to n is inversion-complete (resp., pair-complete) if for every inversion (j, i), where  $1 \le i < j \le n$ , (resp., for every pair (i, j), where  $i \neq j$ ) there exists a permutation in Q where j is before i. It is minimally inversion-complete if in addition no proper subset of Q is inversion-complete; and similarly for pair-completeness. The problems we consider are to determine the maximum cardinality of a minimal inversioncomplete set of permutations, and that of a minimal pair-complete set of permutations. The latter problem arises in the determination of the Carathéodory numbers for certain abstract convexity structures on the (n-1)-dimensional real and integer vector spaces. Using Mantel's Theorem on the maximum number of edges in a triangle-free graph, we determine these two maximum cardinalities and we present a complete description of the optimal sets of permutations for each problem. Perhaps surprisingly (since there are twice as many pairs to cover as inversions), these two maximum cardinalities coincide whenever  $n \geq 4$ .

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We consider the following extremal problems in the theory of permutations. Given integer  $n \geq 2$ , let  $S_n$  denote the symmetric group of all permutations of  $[n] := \{1, 2, \ldots, n\}$  (so  $|S_n| = n!$ ), and  $A_n = \{(i, j) : i, j \in [n], i \neq j\}$  the set of all (ordered) pairs from [n] (so  $|A_n| = n(n-1)$ ). A permutation  $\pi = (\pi(1), \ldots, \pi(n))$  covers the pair  $(\pi(k), \pi(l)) \in A_n$  iff k < l. An inversion (see, e.g., [1, 4, 5]) is a pair  $(j, i) \in A_n$  with j > i. Let  $I_n \subset A_n$  denote the set of all inversions. A set  $Q \subseteq S_n$  of permutations is inversion-complete (resp., pair-complete) if every inversion in  $I_n$  (resp., pair in  $A_n$ ) is covered by at least one permutation in Q. An inversion-complete set Q is minimally inversion-complete if no proper subset of Q is inversion-complete; and similarly for pair-completeness. For example, the set  $Q' = \{\text{rev}_n\}$ , where (using compact notation for permutations)  $\text{rev}_n = n(n-1) \ldots 21$  is the reverse permutation, is minimally inversion-complete, and has minimum cardinality for this property; whereas the set  $P' = \{\text{id}_n, \text{rev}_n\}$ , where  $\text{id}_n = 12 \ldots n$  is the identity permutation, is minimally pair-complete, and has minimum cardinality.

We determine the maximum cardinality  $\gamma_I(n)$  of a minimal inversion-complete subset  $Q \subseteq S_n$ , as well as the maximum cardinality  $\gamma_P(n)$ , of a minimal paircomplete subset  $P \subseteq S_n$ . The latter problem arose in the determination of the Carathéodory numbers for the integral  $L^{\natural}$  convexity structures on the (n-1)dimensional real and integer vector spaces  $\mathbb{R}^{n-1}$  and  $\mathbb{Z}^{n-1}$ , see [7]. It was posed by the second author as "An Integer Programming Formulation Challenge" at the Integer Programming Workshop, Valparaiso, Chile, March 11-14, 2012.

Stimulated by personal communication of an early version of our results, Malvenuto et al. [2] determine the exact value of, or bounds on, the maximum cardinality of minimal inversion-complete sets in more general classes of finite reflection groups.

Perhaps unexpectedly (since there are twice as many pairs to cover as inversions), the maximum cardinalities  $\gamma_I(n)$  and  $\gamma_P(n)$  considered herein are equal for all  $n \geq 4$  (and they only differ by one unit, viz.,  $\gamma_P(n) = \gamma_I(n) + 1$ , for n = 2 and 3). Furthermore, for all  $n \geq 4$  the family  $\mathcal{Q}_n^*$  of all maximum-cardinality minimal inversion-complete subsets of  $S_n$  is strictly contained in the family  $\mathcal{P}_n^*$  of all maximum-cardinality minimal pair-complete subsets. All our proofs are constructive and produce corresponding optimal sets of permutations.

#### In Section 1 we prove:

**Theorem 1.** (i) For every  $n \ge 2$ , the maximum cardinality of a minimal inversion-complete subset of  $S_n$  is  $\gamma_I(n) = \lfloor n^2/4 \rfloor$ .

- (ii) For every even  $n \geq 4$ , the family  $\mathcal{Q}_n^*$  of all maximum-cardinality minimal inversion-complete subsets of  $S_n$  is the family of all transversals of a family of  $n^2/4$  pairwise disjoint subsets of  $S_n$ , each of cardinality  $\left[\left(\frac{n}{2}-1\right)!\right]^2$ , and thus  $|\mathcal{Q}_n^*| = \left[\left(\frac{n}{2}-1\right)!\right]^{n^2/2}$ .
- thus  $|\mathcal{Q}_n^*| = \left[\left(\frac{n}{2}-1\right)!\right]^{n^2/2}$ .

  (iii) For every odd  $n \geq 5$ ,  $\mathcal{Q}_n^*$  is the disjoint union of the families of all transversals of two families, each one of  $\lfloor n^2/4 \rfloor$  pairwise disjoint subsets of  $S_n$  of cardinality  $\left(\lfloor \frac{n}{2} \rfloor 1\right)! \lfloor \frac{n}{2} \rfloor !$ , and thus  $|\mathcal{Q}_n^*| = 2 \left[\left(\lfloor \frac{n}{2} \rfloor 1\right)! \lfloor \frac{n}{2} \rfloor !\right]^{\lfloor n^2/4 \rfloor}$ .

<sup>&</sup>lt;sup>1</sup>We refer the curious reader to van de Vel's monograph [9] for a general introduction to convexity structures and convexity invariants (such as the Carathéodory number), and to Murota's monograph [6] on various models of discrete convexity, including  $L^{\natural}$  and related convexities.

To prove Theorem 1, we first establish the upper bound  $\gamma_I(n) \leq \lfloor n^2/4 \rfloor$  by applying Mantel's Theorem (which states, [3, 8], that the maximum number of edges in an *n*-vertex triangle-free graph is  $\lfloor n^2/4 \rfloor$ ) to certain "critical selection graphs" associated with the minimal inversion-complete subsets of  $S_n$ . We then show that this upper bound is attained by the families of transversals described in parts (ii)–(iii). We complete the proof by showing that, for  $n \geq 4$ , every  $Q \in \mathcal{Q}_n^*$  must be such a transversal. Note that these results imply the asymptotic growth rate  $|\mathcal{Q}_n^*| = 2^{\theta(n^3 \log n)}$  as n grows.

In Section 2 we prove:

**Theorem 2.** (i) For every integer  $n \ge 2$ , the maximum cardinality of a minimal pair-complete subset of  $S_n$  is  $\gamma_P(n) = \max\{n, \lfloor n^2/4 \rfloor\}$ .

- (ii) For all  $n \geq 5$  the set  $\mathcal{P}_n^*$  of maximum-cardinality minimal pair-complete subset of  $S_n$  is equal to the set  $\tau \circ \mathcal{Q}_n^*$  resulting from applying every possible permutation  $\tau \in S_n$  of the index set [n] to each  $Q \in \mathcal{Q}_n^*$ .
- (iii) For all  $n \geq 5$  there is a one-to-one correspondence between  $\mathcal{P}_n^*$  and the Cartesian product  $\binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$ , where  $\binom{[n]}{\lfloor n/2 \rfloor}$  is the family of all subsets  $S \subset [n]$  with cardinality  $|S| = \lfloor n/2 \rfloor$ .

The intuition for the formula  $\gamma_P(n) = \max\{n, \lfloor n^2/4 \rfloor\}$  in part (i) is that it suffices to consider two classes of minimal pair-complete subsets:

- (1) the subsets P (each of cardinality n) formed by the n circular shifts of any given permutation  $\pi \in S_n$ , i.e.,  $P = \{\pi, \pi \circ \sigma, \pi \circ \sigma^2, \dots, \pi \circ \sigma^{n-1}\}$ , where the (forward) circular shift  $\sigma \in S_n$  is defined by  $\sigma(i) = (i \mod n) + 1$  for all  $i \in [n]$ ; and
- (2) the subsets  $P = \tau \circ Q$  (each of cardinality  $\lfloor n^2/4 \rfloor$ ) defined in part (ii) of Theorem 2.

The characterization in part (ii) of Theorem 2 only implies that  $|\mathcal{P}_n^*| \leq n! |\mathcal{Q}_n^*|$ , because different pairs  $(\tau, Q)$  may give rise to the same set  $\tau \circ Q$  (as will be seen, for example, in Remark 2 at the end of this paper, with the "class-(2) subsets" for the case n=4 therein). Part (iii), on the other hand, refines the preceding result using a "canonical" permutation  $\tau_W$  induced by a balanced partition  $\{W, \overline{W}\}$  of the index set [n] (i.e., with |W| or  $|\overline{W}| = \lfloor n/2 \rfloor$ , a consequence of Mantel's Theorem). This implies that  $|\mathcal{P}_n^*| = \binom{n}{\lfloor n/2 \rfloor} |\mathcal{Q}_n^*|$  for  $n \geq 5$ . Thus, although  $|\mathcal{P}_n^*| > |\mathcal{Q}_n^*|$  for all  $n \geq 5$ , their asymptotic growth rate (as n grows) are similar, differing only in lower order terms in the exponent  $\theta(n^3 \log n)$ .

### 1. MINIMAL INVERSION-COMPLETE SETS OF PERMUTATIONS

In this Section we prove Theorem 1 and present a characterization of the family  $\mathcal{Q}_n^*$  of all maximum-cardinality minimal inversion-complete subsets of  $S_n$ . For n=2, there is a single inversion (2,1), which is covered by the reverse permutation 21, so part (i) of Theorem 1 trivially holds and  $\mathcal{Q}_2^* = \{21\}$ . Hence assume  $n \geq 3$  in the rest of this Section.

Consider any minimal inversion-complete subset Q of  $S_n$ . Since Q is minimally inversion-complete, for every permutation  $\pi \in Q$  there exists an inversion  $(j,i) \in I_n$ , called a *critical inversion*, which is covered by  $\pi$  and by no permutation in  $Q \setminus \{\pi\}$  (for otherwise  $Q \setminus \{\pi\}$  would also be inversion-complete, and thus Q would not be minimally inversion-complete). For every permutation  $\pi \in Q$ , select *one* 

critical inversion that it covers (arbitrarily chosen if  $\pi$  covers more than one critical inversion). Let  $q_{j,i}$  denote the unique permutation in Q that covers the selected critical inversion (j,i). Consider a corresponding critical selection graph  $G_Q = ([n], E_Q)$ , where  $E_Q$  is the set of these |Q| selected critical inversions (one for each permutation in Q), considered as undirected edges. Thus  $|E_Q| = |Q|$ .

Recall that a graph G is triangle-free if there are no three distinct vertices i, j and k such that all three edges  $\{i, j\}$ ,  $\{i, k\}$  and  $\{j, k\}$  are in G.

**Lemma 1.** If subset  $Q \subseteq S_n$  is minimally inversion-complete, then every corresponding critical selection graph  $G_Q$  is triangle-free.

*Proof.* Assume  $Q \subseteq S_n$  is minimally inversion-complete, and let  $G_Q = ([n], E_Q)$  be a corresponding critical selection graph. We need to show that, if  $E_Q$  contains two adjacent edges  $\{i, j\}$  and  $\{j, k\}$ , then it cannot contain edge  $\{i, k\}$ . Thus assume that  $\{i, j\}$  and  $\{j, k\} \in E_Q$  and, without loss of generality, that i < k. We want to show that (k, i) cannot be a selected critical inversion. We consider the possible relative positions of index j relative to i and k:

- If j < i < k, i.e., both (i, j) and (k, j) are selected critical inversions, then  $q_{k,j}$  cannot cover (i, j) and therefore we must have k before j before i in  $q_{k,j}$  (that is, these three indices must be in positions  $\pi^{-1}(i) < \pi^{-1}(j) < \pi^{-1}(k)$  in  $\pi = q_{k,j}$ ). This implies that (k, i) cannot be a selected critical inversion.
- If i < k < j, i.e., both (j,i) and (j,k) are selected critical inversions, then this is dual (in the order-theoretic sense) to the previous case:  $q_{j,i}$  cannot cover (j,k) and therefore we must have k before j before i in  $q_{j,i}$ , implying that (k,i) cannot be a selected critical inversion.
- Else i < j < k, i.e., both (j,i) and (k,j) are selected critical inversions. In every permutation  $\pi \in Q \setminus \{q_{j,i}, q_{k,j}\}$  we must have i before j before k But then (k,i) cannot be a selected critical inversion, since it can only be covered in Q by  $q_{j,i}$  or  $q_{k,j}$ , for each of which another critical inversion has been selected.

Therefore, (k, i) cannot be a selected critical inversion. This implies that no three indices i, j and k can define a triangle in  $G_Q$ .

Since  $|Q| = |E_Q|$ , Mantel's Theorem implies

**Corollary 2.** For every  $n \geq 2$ , the maximum cardinality  $\gamma_I(n)$  of a minimal inversion-complete subset of  $S_n$  satisfies  $\gamma_I(n) \leq \lfloor n^2/4 \rfloor$ .

We prove constructively that the upper bound in Corollary 2 is attained, i.e., that part (i) of Theorem 1 holds. For n=3, we have 3 triangle-free graphs on vertex set  $\{1,2,3\}$ , each consisting of exactly two of the three possible edges. Consider the edge set  $E'=\left\{\left\{1,2\right\},\left\{1,3\right\}\right\}$ : if it is the edge set of a critical selection graph  $G_{Q'}$ , then we must have  $q'_{2,1}=213\in Q'$  (for otherwise,  $q'_{2,1}$  would also cover the inversion (3,1), contradicting that (3,1) is also selected), and similarly  $q'_{3,1}=312\in Q'$ . Thus Q' must be the set  $\{213,312\}$ , which is indeed inversion-complete, and thus a largest minimal inversion-complete subset of  $S_3$ . This implies that  $\gamma_I(n)=3=\left\lfloor\frac{n^2}{4}\right\rfloor$  holds for n=3. Similarly, the edge sets  $E''=\left\{\left\{1,2\right\},\left\{2,3\right\}\right\}$  and  $E'''=\left\{\left\{1,3\right\},\left\{2,3\right\}\right\}$  define the other two maximum-cardinality minimal inversion-complete subsets  $Q''=\left\{213,123\right\}$  and  $Q'''=\left\{231,321\right\}$  of  $S_3$ . Thus  $Q_3^*=\left\{Q',Q'',Q'''\right\}$  and  $|Q_3^*|=3$ .

Thus assume  $n \geq 4$  in the rest of this Section. We now introduce certain subsets of  $S_n$ , which we will use to show that the upper bound in Corollary 2 is attained, and to construct the whole set  $\mathcal{Q}^*$ . For every triple (i, c, j) of integers such that  $1 \leq i \leq c < j \leq n$ , let  $F_{i,c,j}$  denote the set of all permutations  $\pi \in S_n$  such that:

- $\pi(h) \le c$  for all h < c;
- $\pi(c) = j$ ;
- $\pi(c+1) = i$ ; and
- $\pi(k) \ge c + 1$  for all k > c + 1.

If c > 1 the first two conditions imply that  $(\pi(1), \ldots, \pi(c-1))$  is any permutation of  $[c]\setminus\{i\}$ ; and if c+1 < n the last two conditions imply that  $(\pi(c+2), \ldots, \pi(n))$  is any permutation of  $\{c+1, \ldots, n\}\setminus\{j\}$ . Thus the cardinality of  $F_{i,c,j}$  is (c-1)!(n-c-1)!. Note also that, for every  $\pi \in F_{i,c,j}$ , (k,h)=(j,i) is the unique inversion (k,h) with  $h \le c < k$  that is covered by  $\pi$ . Thus for every fixed c the sets  $F_{i,c,j}$  ( $1 \le i \le c < j \le n$ ) are pairwise disjoint  $(F_{i,c,j} \cap F_{i',c,j'} = \emptyset)$  whenever  $(i,j) \ne (i',j')$ . Recall that, given a collection  $\mathcal{F}$  of sets, a transversal is a set containing exactly one element from each member of  $\mathcal{F}$ .

**Lemma 3.** For every integers  $1 \le c < n$ , every transversal T of the family  $\mathcal{F}_c = \{F_{i,c,j} : 1 \le i \le c < j \le n\}$  is minimally inversion-complete.

*Proof.* Given such a transversal T, let  $t_{i,j}$  denote the permutation in  $T \cap F_{i,c,j}$ . For every inversion  $(j,i) \in F_n$ , we consider the relative positions of i and j with respect to c:

- If  $i \leq c < j$ , then  $t_{i,j}$  is the unique permutation in T that covers the inversion (j,i).
- If  $i < j \le c$ , then the inversion (j,i) is covered by every  $t_{i,j'} \in T$  with j' > c.
- Else,  $c+1 \le i < j$ , then the inversion (j,i) is covered by every  $t_{i',j} \in T$  with  $i' \le c$ .

Therefore, T is inversion-complete and for every  $i \leq c < j$  the inversion (j,i), covered by  $t_{i,j}$ , is critical. This implies that T is minimally inversion-complete.  $\square$ 

For a fixed c such that  $1 \le c < n$ , there are c(n-c) subsets  $F_{i,c,j}$  (with  $i \le c < j$ ) (and these subsets are nonempty and pairwise disjoint). Hence the cardinality of every transversal T satisfies  $|T| = |\mathcal{F}_c| = c(n-c) \le \lfloor \frac{n^2}{4} \rfloor$ , with equality iff  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ . Combining with Lemma 2, we obtain:

Corollary 4. For every  $n \geq 4$ ,  $\gamma_I(n) = \lfloor n^2/4 \rfloor$  and, for every  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ , every transversal T of the family  $\mathcal{F}_c = \{F_{i,c,j} : 1 \leq i \leq c < j \leq n\}$  is a maximum-cardinality minimal inversion-complete subset of  $S_n$ .

Part (i) of Theorem 1 follows. To prove parts (ii) and (iii), we invoke the "strong form" of Mantel's Theorem [3, 8]: an *n*-vertex triangle-free graph has the maximum number  $\lfloor n^2/4 \rfloor$  of edges iff it is a balanced bipartite graph, i.e., with  $\lfloor \frac{n}{2} \rfloor$  vertices on one side and  $\lceil \frac{n}{2} \rceil$  on the other.

**Lemma 5.** For  $n \geq 4$ , a subset of  $S_n$  is a maximum-cardinality minimal inversion-complete subset iff it is a transversal of the family  $\mathcal{F}_c$  for some  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ .

*Proof.* Sufficiency was established by Lemma 3. To prove necessity, let  $n \geq 4$  and consider any  $Q \in \mathcal{Q}_n^*$  and a corresponding critical selection graph  $G_Q$ . By Lemma 1,

Corollary 4, and the strong form of Mantel's Theorem,  $G_Q$  is a balanced complete bipartite graph. We first claim that the side W of  $G_Q$  that contains index 1 must be W = [c] with  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ . For this, consider (since  $n \geq 4$ ) any three indices i > 1 in W and j < k on the other side. Thus (j, 1) and (k, 1) are critical inversions. Furthermore, the edges  $\{i, j\}$  and  $\{i, k\}$  in  $G_Q$  are also defined by critical inversions, which depend on the position of index i relative to j and k:

- If 1 < j < i < k, then (i,j) and (k,i) are critical inversions. Then every permutation  $\pi \in Q \setminus \{q_{j,1}, q_{i,j}, q_{k,i}\}$  has 1 before j before i before k, and thus does not cover the inversion (k,1). Thus (k,1) cannot be a critical inversion, a contradiction.
- If 1 < j < k < i, then (i,j) and (i,k) are critical inversions. On one hand, every permutation  $\pi \in Q' = Q \setminus \{q_{j,1}, q_{i,j}\}$  has 1 before j before i, and thus does not cover the inversion (i,1). Similarly, every permutation  $\pi \in Q'' = Q \setminus \{q_{k,1}, q_{i,k}\}$  has 1 before k before i, and thus does not cover the inversion (i,1) either. Therefore  $Q = Q' \cup Q''$  does not cover the inversion (i,1), a contradiction.

This implies that we must have 1 < i < j < k, i.e., that i < j for every  $i \in W$  and every  $j \in [n] \setminus W$ . This proves our claim that W = [c] for some c which, by the strong form of Mantel's Theorem, must be  $\lfloor \frac{n}{2} \rfloor$  or  $\lceil \frac{n}{2} \rceil$ .

As a consequence,  $Q = \{q_{j,i} : 1 \le i \le c < j \le n\}$ . Every  $q_{j,i} \in Q$  must have j before i, and also h before j for every  $h \in [c] \setminus \{i\}$  (for otherwise  $q_{j,i}$  would also cover the inversion (j,h), contradicting the fact that  $q_{j,h}$  is the unique permutation in Q that covers (j,h)) and i before k for every  $k \in \{c+1,\ldots,n\} \setminus \{j\}$  (for otherwise  $q_{j,i}$  would also cover the inversion (k,i)). Therefore  $q_{j,i} \in F_{i,c,j}$ , and thus Q is a transversal of  $\mathcal{F}_c$ . The proof is complete.

Parts (ii) and (iii) of Theorem 1 now follow, noting that: (1)  $\mathcal{F}_c$  consists of c(n-c) pairwise disjoint subsets  $F_{i,c,j}$ ; (2)  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ ; and (3) for n odd, all subsets  $F_{i,\lfloor n/2 \rfloor,j}$  and  $F_{i',\lceil n/2 \rceil,j'}$  are pairwise disjoint (indeed, with n odd, every  $\pi \in F_{i,\lfloor n/2 \rfloor,j}$  has  $\pi(c+1) \in [c]$  while every  $\pi \in F_{i',\lceil n/2 \rceil,j'}$  has  $\pi(c+1) \in [n] \setminus [c]$ ).

**Remark 1.** Thus we have  $Q_2^* = 1$ ,  $Q_3^* = 3$ ,  $Q_4^* = 1$ ,  $Q_5^* = 128$  and, as noted in the Introduction, the asymptotic growth rate  $|Q_n^*| = 2^{\theta(n^3 \log n)}$ .

## 2. MINIMAL PAIR-COMPLETE SETS OF PERMUTATIONS

In this Section we prove Theorem 2. To simplify the presentation, let  $\mu(n) := \max\{n, \lfloor n^2/4 \rfloor\}$ . For n=2, the unique cover of the two pairs (1,2) and (2,1) is  $S_2$  itself, hence  $\gamma_P(2) = 2 = \mu(2)$  and  $\mathcal{P}_2^* = \{S_2\}$ .

Note that, as for inversions, given any minimal pair-complete subset P of  $S_n$ , for every permutation  $\pi \in P$  there exists a *critical pair*  $(i,j) \in F_n$  which is covered by  $\pi$  and by no other permutation in P. Observe however that, in contrast with inversion-completeness, the notion of pair-completeness does not assume any particular order of the indices. Thus, if  $P \subseteq S_n$  is (minimally) pair-complete then for any permutation  $\tau \in S_n$  of the index set [n], the set  $\tau \circ P = \{\tau \circ \pi : \pi \in P\}$  is also (minimally) pair-complete. (Indeed,  $\pi$  covers (i,j) iff  $\tau \circ \pi$  covers  $(\tau(i),\tau(j))$ .)

For n=3 consider the set  $P_3:=\{123,231,312\}$ . It is easily verified that  $P_3$  is pair-complete and the pairs (1,3), (2,1) and (3,2) are critical pairs covered by the permutations 123, 231 and 312, respectively. Hence  $P_3 \in \mathcal{P}_3^*$  and thus

 $\gamma_P(3) \geq |P_3| = 3 = \mu(3)$ . To verify the converse inequality, viz.,  $\gamma_P(3) \leq \mu(3)$ , consider any  $P \in \mathcal{P}_3^*$ : by the preceding observation, we may assume, w.l.o.g., that P contains the identity permutation  $\pi_1 = \mathrm{id}_3$ . This permutation  $\pi_1$  covers all three pairs (i,j) with i < j. Then the permutation  $\pi_2 \in P$  that covers the pair (3,1) must also (depending of the position of index 2) cover at least one of the pairs (2,1) or (3,2). Hence there is at most one pair which is not covered by  $\{\pi_1,\pi_2\}$ , and thus  $\gamma_P(3) = |P| \leq 3 = \mu(3)$ , implying  $\gamma_P(3) = \mu(3)$ . Therefore part (i) of Theorem 2 holds for  $n \in \{2,3\}$ .

**Lemma 6.** If  $n \geq 4$ , for every permutation  $\tau \in S_n$  of the index set [n] and every maximum-cardinality minimal inversion-complete set  $Q \subset S_n$ , the set  $\tau \circ Q$  is minimally pair-complete.

*Proof.* By a preceding observation, it suffices to prove that, for  $n \geq 4$ , every maximum-cardinality minimal inversion-complete set  $Q \in S_n$  is minimally pair-complete. By Lemma 5, every such Q must be a transversal of  $\mathcal{F}_c$  for some  $c \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ . Consider any pair  $(i,j) \in A_n$  and, w.l.o.g., i < j:

- If  $i \leq c < j$  then  $q_{j,i} \in F_{i,c,j} \cap Q$  is the unique permutation in Q that covers the inversion (j,i), and every other permutation in Q covers (i,j).
- If  $i < j \le c$  then, for every  $k \in \{c+1, \ldots, n\}$ ,  $q_{k,i}$  covers (j,i) and  $q_{k,j}$  covers (i,j).
- Else, c < i < j and, dually, for every  $h \in [c]$ ,  $q_{i,h}$  covers (i,j) and  $q_{j,h}$  covers (j,i).

Therefore Q is pair-complete, and every pair (j,i) with  $i \leq c < j$  is critical and covered by  $q_{j,i} \in Q$ . Since  $|Q| = \lfloor \frac{n^2}{4} \rfloor = |\{(j,i) : 1 \leq i \leq c < j \leq n\}|, Q$  is minimally pair-complete.

**Corollary 7.** For every  $n \ge 4$ , the maximum cardinality  $\gamma_P(n)$  of a minimal pair-complete subset of  $S_n$  satisfies  $\gamma_P(n) \ge \gamma_I(n) = \lfloor n^2/4 \rfloor$ .

As we did for inversions, to every minimal pair-complete subset P of  $S_n$  and selection of a critical pair covered by each permutation in P, we associate a corresponding critical selection graph  $G_P = ([n], E_P)$  where  $E_P$  is the set of |P| selected critical pairs (one for each permutation in P), considered as undirected edges. Thus  $|E_P| = |P|$ . Let  $p_{i,j}$  denote the unique permutation in P that covers the selected critical pair (i,j).

**Lemma 8.** If  $n \geq 4$  and  $P \subseteq S_n$  is minimally pair-complete, then every corresponding critical selection graph  $G_P$  is triangle-free.

*Proof.* Assume  $n \geq 4$  and  $P \subseteq S_n$  is minimally pair-complete, and let  $G_P = ([n], E_P)$  be a corresponding critical selection graph. By Corollary 7,  $|P| \geq \lfloor n^2/4 \rfloor \geq 4$ . We have to show that for any three indices i, j, k such that  $\{i, j\}$  and  $\{j, k\} \in E_P$ , we must have  $\{i, k\} \notin E_P$ .

• First, consider the case where both pairs (i,j) and (j,k) are critical. In every permutation  $\pi \in P \setminus \{p_{i,j}, p_{j,k}\}$  we must thus have k before j before i. Since k is before i in all these  $|P|-2 \geq 2$  permutations, (k,i) cannot be a critical pair. Furthermore (i,k) cannot be a selected critical pair, since it can only be covered by  $p_{i,j}$  and  $p_{j,k}$ , for each of which another critical pair has been selected. Therefore, as claimed, we cannot have  $\{i,k\}$  in  $E_P$ .

- A dual argument shows that if both (j,i) and (k,j) are selected critical pairs then  $\{i,k\} \notin E_P$ .
- Now consider the case where (j,i) and (j,k) are selected critical pairs. Since  $p_{j,i}$  does not cover (j,k), we have k before j before i in  $p_{j,i}$ , implying that (k,i) cannot be a selected critical pair. Similarly,  $p_{j,k}$  does not cover (j,i) and therefore we must have i before j before k in  $p_{j,k}$ , implying that (i,k) cannot be a selected critical pair. Therefore, as claimed, we cannot have  $\{i,k\}$  in  $E_P$ .
- A dual argument applies to the remaining case, showing that if both (i, j) and (k, j) are selected critical pairs then  $\{i, k\} \notin E_P$ .

Thus we must have  $\{i, k\} \notin E_P$ . This completes the proof that  $G_P$  is triangle-free.

These results and Mantel's Theorem imply part (i) of Theorem 2. They also imply that, for  $n \geq 4$ , all the sets  $\tau \circ Q$  in Lemma 6 are in  $\mathcal{P}_n^*$ . To complete the proof of part (ii) it now suffices to prove the converse for  $n \geq 5$ .

**Lemma 9.** If  $n \geq 5$ , a subset P of  $S_n$  is a maximum-cardinality minimal pair-complete subset iff  $P = \tau \circ Q$  for some permutation  $\tau$  of the index set [n] and some maximum-cardinality minimal inversion-complete subset Q of  $S_n$ .

*Proof.* Sufficiency was just established. To prove necessity, let  $n \geq 5$  and consider any  $P \in \mathcal{P}_n^*$  and a corresponding critical selection graph  $G_P$ . By Lemma 8, Theorem 2 (i), and the strong form of Mantel's Theorem,  $G_P$  is a balanced complete bipartite graph.

Now, also consider the associated critical selection digraph (directed graph)  $D_P = ([n], A_P)$ , wherein each edge  $\{i, j\}$  is directed as arc  $(i, j) \in A_P$  if the pair (i, j) is critical. If  $(i, j) \in A_P$ , then the reverse pair (j, i) must be covered by every permutation in  $P \setminus \{p_{i,j}\}$ ; since  $|P| - 1 = \lfloor n^2/4 \rfloor - 1 \ge 2$  when  $n \ge 5$ , (j, i) cannot be critical, i.e.,  $(j, i) \notin A_P$ . Thus, every edge  $\{i, j\}$  in the underlying graph  $G_P$  of  $D_P$  corresponds to exactly one arc, (i, j) or (j, i), in  $D_P$ . We now prove that when  $n \ge 5$  the digraph  $D_P$  is acyclic, i.e., it does not contain any (directed) circuit. Indeed, if  $D_P$  contains a directed path  $(i(1), \ldots, i(k))$ , then every permutation  $\pi \in Q \setminus \{p_{i(1),i(2)}, p_{i(2),i(3)}, \ldots, p_{i(k-1),i(k)}\}$  has i(1) after i(2) after i(3), etc, after i(k-1) after i(k), and thus i(k) before i(1). Since  $|P| - (k-1) \ge \lfloor \frac{n^2}{4} \rfloor - (n-1) \ge 2$  when  $n \ge 5$ , pair (i(k), i(1)) cannot be critical, and thus  $(i(k), i(1)) \notin A_P$ .

Since digraph  $D_P$  is acyclic, there is at least one vertex i with in-degree zero. Since the underlying graph  $G_P$  is a balanced complete bipartite graph, the side W of  $G_Q$  that contains index i has cardinality  $|W| \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ . Consider any indices  $j \in W$  and  $k \neq l$  on the other side. Since vertex i has no entering arc, arcs (i,k) and (i,l) are in  $A_P$ , and we consider the possible orientations of the edges  $\{j,k\}$  and  $\{j,l\}$ :

- If both edges are oriented into j, i.e., (k,j) and (l,j) in  $A_P$ , then, on one hand, every permutation  $\pi \in P' = P \setminus \{p_{k,j}, p_{i,k}\}$  has j before k before i, and thus does not cover the pair (i,j). Similarly, every permutation  $\pi \in P'' = P \setminus \{p_{l,j}, p_{i,l}\}$  has j before l before i, and thus does not cover the pair (i,j) either. Therefore  $P = P' \cup P''$  does not cover the pair (i,j), a contradiction.
- If one of these two edges is oriented into j and the other one from j, w.l.o.g., (k, j) and (j, l) in  $A_P$ , then every permutation  $\pi \in P \setminus \{p_{j,l}, p_{k,j}, p_{i,k}\}$  has

l before k before i, and thus does not cover the pair (i, l). Thus (i, l) cannot be a critical inversion, a contradiction.

Thus we must have both (j,k) and (j,l) in  $A_P$ . This implies that all pairs (j,k) with  $j \in W$  and  $k \in \overline{W} := [n] \setminus W$  define arcs in  $A_P$ , i.e., are critical. Let  $c := |\overline{W}| \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$  and consider any permutation  $\tau$  that sends [c] to  $\overline{W}$  (and thus  $\overline{[c]}$  to W): every critical pair in  $Q = \tau^{-1} \circ P$  is an inversion, hence Q is minimally inversion-complete. Since  $|Q| = |P| = \gamma_P(n) = \gamma_I(n)$ , it has maximum cardinality. This completes the proof.

It remains to prove:

**Lemma 10.** (Part (iii) of Theorem 2.) For all  $n \geq 5$  there is a one-to-one correspondence between  $\mathcal{P}_n^*$  and the Cartesian product  $\binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$ .

Proof. Assume  $n \geq 5$  and consider any  $P \in \mathcal{P}_n^*$ . In the proof of Lemma 9 we showed that there exists a unique balanced ordered partition  $(W, \overline{W})$  of [n] such that all critical pairs (j,k) of P have  $j \in W$  and  $k \in \overline{W}$ . Let again  $c := |\overline{W}| \in \{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\}$ , but now select the (unique) "canonical" permutation  $\tau_W$  associated with this ordered partition, that monotonically maps [c] to  $\overline{W}$  (i.e., such that  $1 \leq i < j \leq c$  implies  $\tau_W(i) \in \overline{W}$  and  $\tau_W(i) < \tau_W(j) \in \overline{W}$ ) and monotonically maps  $[\overline{c}] = \{c+1, \ldots, n\}$  to W (i.e., such that  $c+1 \leq k < l \leq n$  implies  $\tau_W(k) \in W$  and  $\tau_W(k) < \tau_W(l) \in W$ ). Then, as also noted in the proof of Lemma 9, every critical pair in  $Q_P := \tau_W^{-1} \circ P$  is an inversion, and thus  $Q_P \in \mathcal{Q}_n^*$ .

pair in  $Q_P := \tau_W^{-1} \circ P$  is an inversion, and thus  $Q_P \in \mathcal{Q}_n^*$ . Consider the mapping  $\Phi : \mathcal{P}_n^* \mapsto \binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$  defined by  $\Phi(P) = \left(\Phi(P)_1, \Phi(P)_2\right)$  with  $\Phi(P)_1 = \overline{W}$  if  $Q_P$  is a transversal of  $\mathcal{F}_{\lfloor n/2 \rfloor}$  (i.e., if  $|\overline{W}| = \lfloor n/2 \rfloor$ , where  $\{W, \overline{W}\}$  is the balanced ordered partition associated with P, as defined in the preceding paragraph), and  $\Phi(P)_1 = W$  otherwise (i.e., if n is odd and  $Q_P$  is a transversal of  $\mathcal{F}_{\lceil n/2 \rceil}$ , and thus  $|W| = \lfloor n/2 \rfloor$ ); and with  $\Phi(P)_2 = Q_P = \tau_W^{-1} \circ P$ . To complete the proof, it suffices to show that every pair  $(X, Q) \in \binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$  is the image  $\Phi(P)$  of exactly one  $P \in \mathcal{P}_n^*$ .

of exactly one  $P \in \mathcal{P}_n^*$ . Thus consider any  $(X,Q) \in \binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$ . Recall that the balanced ordered partition associated with any transversal Q of  $\mathcal{F}_c$  is  $(\overline{[c]}, [c])$ .

If Q is a transversal of  $\mathcal{F}_{\lfloor n/2 \rfloor}$  then we use  $\overline{X}$  to play the role of W, that is, we let  $P:=\tau_{\overline{X}}\circ Q$ , so  $P\in\mathcal{P}_n^*$  and  $\Phi(P)_2=\tau_{\overline{X}}^{-1}\circ P=Q$ . The balanced ordered partition associated with P is  $(\tau_{\overline{X}}\circ \overline{[c]},\,\tau_{\overline{X}}\circ [c])=(\overline{X},X)$ , and therefore  $\Phi(P)_1=X$ . This implies that  $\Phi(P)=(X,Q)$ , as desired. Furthermore, consider any  $P'\in\mathcal{P}_n^*$  such that  $\Phi(P')=(X,Q)$ . Since  $Q_{P'}=\Phi(P')_2=Q$  is a transversal of  $\mathcal{F}_{\lfloor n/2 \rfloor}$  and  $\Phi(P')_1=X$ , the balanced ordered partition associated with P' is  $(W',\overline{W'})=(\overline{X},X)$ . But then  $P'=\tau_{W'}\circ Q_{P'}=\tau_{\overline{X}}\circ Q=P$ . Therefore, for every  $(X,Q)\in\binom{[n]}{\lfloor n/2\rfloor}\times\mathcal{Q}_n^*$  such that Q is a transversal of  $\mathcal{F}_{\lfloor n/2\rfloor}$ , there exists exactly one  $P\in\mathcal{P}_n^*$  such that  $\Phi(P)=(X,Q)$ .

The proof for the remaining case, i.e., when n is odd and Q is a transversal of  $\mathcal{F}_{\lceil n/2 \rceil}$ , is similar, by simply exchanging the roles of X and  $\overline{X}$ . This shows that  $\Phi$  is a one-to-one correspondence from  $\mathcal{P}_n^*$  to  $\binom{[n]}{[n/2]} \times \mathcal{Q}_n^*$ .

The proof of Theorem 2 is complete

**Remark 2.** As seen at the beginning of Section 2,  $\mathcal{P}_2^* = 1 = \mathcal{Q}_2^*$ . For n = 3 it can be verified that  $\mathcal{P}_3^*$  consists of the two orbits  $\{123, 312, 231\}$  and  $\{132, 213, 321\}$  of the circular shift, thus  $|\mathcal{P}_3^*| = 2$  (while  $|\mathcal{Q}_3^*| = 3$ ).

For n = 4 we have two classes of maximum-cardinality minimal pair-complete subsets (mentioned in the introduction):

- (1) the 3! = 6 orbits  $P = \{\pi, \pi \circ \sigma, \pi \circ \sigma^2, \dots, \pi \circ \sigma^{n-1}\}$  of the circular shift  $\sigma$ , one for each permutation  $\pi = \rho 4$  (permutation  $\rho$  followed by 4) defined by each  $\rho \in S_3$ ; and
- (2) the  $\binom{4}{2} = 6$  distinct sets  $P = \tau \circ Q$  where Q is the (unique) maximum-cardinality minimal pair-complete subset of  $S_4$ , namely, the sets  $P_{i,j} = \{ijkl, ilkj, kjil, klij\}$  where  $1 \le i < j \le 4$  and  $\{k,l\} = [4] \setminus \{i,j\}$ .

Thus  $|\mathcal{P}_4^*| = 12$  (while  $|\mathcal{Q}_4^*| = 1$ ).

For  $n \geq 5$ , part (iii) of Theorem 2 implies that  $|\mathcal{P}_n^*| = \binom{n}{\lfloor n/2 \rfloor} |\mathcal{Q}_n^*|$ . Thus, for example,  $|\mathcal{P}_5^*| = 10 |\mathcal{Q}_5^*| = 128$ , and so on, with the same asymptotic growth rate  $|\mathcal{P}_n^*| = 2^{\theta(n^3 \log n)}$  as  $|\mathcal{Q}_n^*|$ .

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