# 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 $1 \leq i < j \leq n$, (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 inversion-complete 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 $[n] := \{1, 2, \dots, n\}$ (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 $\pi = (\pi(1), \dots, \pi(n))$ *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 $Q' = \{\mathrm{rev}_n\}$, where (using compact notation for permutations) $\mathrm{rev}_n = n(n-1)\dots 21$ is the reverse permutation, is minimally inversion-complete, and has minimum cardinality for this property; whereas the set $P' = \{\mathrm{id}_n, \mathrm{rev}_n\}$, where $\mathrm{id}_n = 12\dots n$ 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 pair-complete 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].[1] 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 $n \geq 2$, 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 $|\mathcal{Q}_n^*| = \left[\left(\frac{n}{2}-1\right)!\right]^{n^2/2}$.*

*(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 $|\mathcal{Q}_n^*| = 2\left[\left(\lfloor \frac{n}{2} \rfloor - 1\right)!\ \lfloor \frac{n}{2} \rfloor!\right]^{\lfloor n^2/4 \rfloor}$.*

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[1] 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 $n \geq 2$, 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., $P = \{\pi, \pi \circ \sigma, \pi \circ \sigma^2, \ldots, \pi \circ \sigma^{n-1}\}$, 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 $E' = \{\{1,2\},\{1,3\}\}$: 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 $\gamma_I(n) = 3 = \lfloor \frac{n^2}{4} \rfloor$ holds for $n = 3$. Similarly, the edge sets $E'' = \{\{1,2\},\{2,3\}\}$ and $E''' = \{\{1,3\},\{2,3\}\}$ define the other two maximum-cardinality minimal inversion-complete subsets $Q'' = \{213, 123\}$ and $Q''' = \{231, 321\}$ of $S_3$. Thus $\mathcal{Q}_3^* = \{Q', Q'', Q'''\}$ and $|\mathcal{Q}_3^*| = 3$.

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:

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

If $c > 1$ the first two conditions imply that $\big(\pi(1), \ldots, \pi(c-1)\big)$ is any permutation of $[c]\setminus\{i\}$; and if $c+1 < n$ the last two conditions imply that $\big(\pi(c+2), \ldots, \pi(n)\big)$ 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 $h \leq c < k$ that is covered by $\pi$. Thus for every fixed $c$ the sets $F_{i,c,j}$ $(1 \leq i \leq c < j \leq n)$ are pairwise disjoint ($F_{i,c,j} \cap F_{i',c,j'} = \emptyset$ whenever $(i, j) \neq (i', j')$). 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 $1 \leq c < n$, every transversal $T$ of the family $\mathcal{F}_c = \{F_{i,c,j} : 1 \leq i \leq c < j \leq n\}$ 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 $i < j \leq c$, then the inversion $(j, i)$ is covered by every $t_{i,j'} \in T$ with $j' > c$.
- Else, $c + 1 \leq i < j$, then the inversion $(j, i)$ is covered by every $t_{i',j} \in T$ with $i' \leq c$.

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. □

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

**Corollary 4.** *For every $n \geq 4$, $\gamma_I(n) = \lfloor n^2/4 \rfloor$ and, for every $c \in \big\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\big\}$, 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 $c \in \big\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\big\}$.*

*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 $c \in \left\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right\}$. 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, $Q = \{q_{j,i} : 1 \leq i \leq c < j \leq n\}$. 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) $c \in \left\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right\}$; 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 $\mathcal{Q}_2^* = 1$, $\mathcal{Q}_3^* = 3$, $\mathcal{Q}_4^* = 1$, $\mathcal{Q}_5^* = 128$ and, as noted in the Introduction, the asymptotic growth rate $|\mathcal{Q}_n^*| = 2^{\theta(n^3 \log n)}$.*

## 2. minimal Pair-Complete Sets of Permutations

In this Section we prove Theorem 2. To simplify the presentation, let $\mu(n) := \max\left\{n, \lfloor n^2/4 \rfloor\right\}$. 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 $c \in \left\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right\}$. 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 $i < j \leq c$ 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 $n \geq 4$, the maximum cardinality $\gamma_P(n)$ of a minimal pair-complete subset of $S_n$ satisfies $\gamma_P(n) \geq \gamma_I(n) = \lfloor n^2/4 \rfloor$.*

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 $|P| - 1 = \lfloor n^2/4 \rfloor - 1 \geq 2$ when $n \geq 5$, $(j, i)$ 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 $n \geq 5$ 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 $|P| - (k-1) \geq \lfloor \frac{n^2}{4} \rfloor - (n-1) \geq 2$ when $n \geq 5$, 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 $|W| \in \left\{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right\}$. 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 $Q_P \in \mathcal{Q}_n^*$.

Consider the mapping $\Phi : \mathcal{P}_n^* \mapsto \binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$ defined by $\Phi(P) = \big(\Phi(P)_1, \Phi(P)_2\big)$ 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 $P \in \mathcal{P}_n^*$.

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 $\binom{[n]}{\lfloor n/2 \rfloor} \times \mathcal{Q}_n^*$. □

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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