# Enumerating signed permutations by reversal distance

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# Brief Introduction to Genetics

- **DNA:** Double helix of nucleotides, complementary pairs A–T, G–C.
- **Gene:** Sequence of nucleotides, codes a specific protein.
- **Chromosome:** Ordering device for genes.
- **Genome:** Collection of chromosomes.
- **Mutations:** Two types:
  - **Point Mutations:** Mutations at the level of nucleotides.
  - **Genome Rearrangements:** Structural mutations to chromosomes at level of genes. Types: deletions, duplications, **translocation**, **inversion**, fission, fusion, etc.
- **Edit Distance:** The minimum number of genome rearrangements required to transform one genome into another. Approximates evolutionary distance.
  - mouse $\xrightarrow{251}$ human (149 inversions, 93 translocations, 9 fissions)
  - cabbage $\xrightarrow{3}$ turnip (all inversions)

# Mathematical Model

- Two closely-related species typically have similar gene orders. Comparing two similar sequences of genes yields two permutations or signed permutations (depending on the mutation you want to model), one for each species.
- Each number in the permutation or signed permutation represents either a single gene or a conserved block of genes (sign of the number indicates the orientation of the block).
- Translocation = Block Interchange:

$$5 \quad \boxed{2 \quad 1} \quad 4 \quad \boxed{3 \quad 7 \quad 6} \mapsto 5 \quad \boxed{3 \quad 7 \quad 6} \quad 4 \quad \boxed{2 \quad 1}$$

- Inversion = Reversal:

$$5 \boxed{-2 \ -1 \quad 4 \ -3} -7 \quad 6 \mapsto 5 \boxed{\ 3 \ -4 \quad 1 \quad 2} -7 \quad 6$$

**Definition**

Let $T$ be generating set for $S_n$ (respectively, $S_n^{\pm}$) such that $\rho^{-1} = \rho$ for all $\rho \in T$. For permutations (respectively, signed permutations) $\pi$, we define the distance $d_T(\pi)$ to be the minimum number of generators $\rho_1, \ldots, \rho_k \in T$ such that

$$\pi \circ \rho_1 \circ \cdots \circ \rho_k = \text{identity}.$$

**Notation and Terminology**

- $\mathrm{Rk}_k(S_n, d_T) := \{\pi \in S_n \mid d_T(\pi) = k\}$ = perms in $S_n$ of distance $k$
- $\mathrm{rk}_k(S_n, d_T) := |\mathrm{Rk}_k(S_n, d_T)| = \#$ of perms in $S_n$ of distance $k$
- $d_T^{\max}(S_n) := \max\{d_T(\pi) \mid \pi \in S_n\}$ = diameter of Cayley diagram
- A maximal permutation is a permutation that attains maximal distance.
- $\mathrm{rk}_{\max}(S_n, d_T) := \#$ of maximal perms in $S_n$

# Sorting By Adjacent Transpositions

Let $T$ be the collection of adjacent transpositions in $S_n$ and let $d_{at}(\cdot)$ be the corresponding distance. ($at$ = adjacent transposition)

- $d_{at}(\pi) = \text{inv}(\pi) = \#$ of inversions in $\pi$ = Coxeter length
- $\text{rk}_K(S_n, d_{at}) = \#$ of perms in $S_n$ with $k$ inversions $= I(n, k)$
  $=$ Inversion/Mahonian numbers
- $d_{at}^{\max}(S_n) = \binom{n}{2}$
- $\text{Rk}_{\max}(S_n, d_{at}) = \{[n \cdots 321]\}$
- $\text{rk}_{\max}(S_n, d_{at}) = 1$

# Sorting By Transpositions

Let $T$ be the collection of transpositions in $S_n$ and let $d_t(\cdot)$ be the corresponding distance ($t =$ transposition).

- $d_t(\pi) = n - \text{cyc}(\pi)$
- $\text{rk}_k(S_n, d_t) = \#$ of perms in $S_n$ with $n - k$ cycles $= S(n, n-k)$
  $= $ Stirling numbers of the 1st kind
- $d_t^{\max}(S_n) = n - 1$
- $\text{Rk}_{\max}(S_n, d_t) =$ collection of $n$-cycles in $S_n$
- $\text{rk}_{\max}(S_n, d_t) = (n-1)!$

## Sorting By Block Interchanges

Let $T$ be the collection of block interchanges in $S_n$ and let $d_{bi}(\cdot)$ be the corresponding distance. ($bi$ = block interchange)

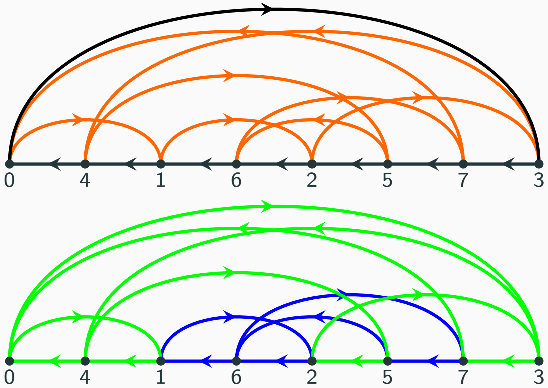
- $d_{bi}(\pi) = \dfrac{n+1-\text{cyc}(\text{DBG}(\pi))}{2}$
- $\text{rk}_k(S_n, d_{bi}) = \#$ of perms in $S_n$ such that DBG has $n+1-2k$ cycles $= H(n, n+1-2k) =$ Hultman numbers
- $d_{bi}^{\max}(S_n) = \left\lfloor \dfrac{n}{2} \right\rfloor$
- $\text{rk}_{\max}(S_n, d_{bi}) = \begin{cases} H(n,1), & \text{if } n \text{ even} \\ H(n,2), & \text{if } n \text{ odd} \end{cases}$

Note that

$$H(n,1) = \begin{cases} \frac{2n!}{n+2}, & \text{if } n \text{ even} \\ 0, & \text{if } n \text{ odd.} \end{cases}$$

# Example of Directed Breakpoint Graph

Directed breakpoint graph for $\pi = [4, 1, 6, 2, 5, 7, 3]$:




$$d_{bi}(\pi) = \frac{n + 1 - \text{cyc}(\text{DBG}(\pi))}{2} = \frac{7 + 1 - 2}{2} = 3$$

# Sorting By Adjacent Block Interchanges

Let $T$ be the collection of adjacent block interchanges in $S_n$ and let $d_{abi}(\cdot)$ be the corresponding distance. ($abi$ = adjacent block interchange)

- $d_{abi}(\pi) = ???$ (numerous formulas for lower and upper bounds)
- Special case: $d_{abi}([n \cdots 321]) = \left\lceil \frac{n+1}{2} \right\rceil$
- $\mathrm{rk}_k(S_n, d_{abi}) = ???$
- $d_{abi}^{\max}(S_n) = ???$
- $\mathrm{rk}_{\max}(S_n, d_{abi}) = ???$

# Sorting by Reversals

Let $S_n^{\pm}$ be the set of signed permutations on $\{1, 2, \ldots, n\}$. A reversal $\rho_{ij}$ acts on a signed permutation $\pi$ by reversing the order of values in positions $i$ through $j$ and changing all of their signs:

$$\pi \circ \rho_{ij} = [\pi_1, \ldots, \pi_{i-1}, -\pi_j, -\pi_{j-1}, \ldots, -\pi_{i+1}, -\pi_i, \pi_{j+1}, \ldots, \pi_n].$$

Note that $\rho_{i,i}$ is the reversal that changes the sign in the $i$th position. Let $T$ be the collection of reversals, so that $S_n^{\pm} = \langle T \rangle$ and let $d_r(\cdot)$ be the corresponding distance. ($r =$ reversal)

$$|T| = \binom{n+1}{2}.$$

# Example

Consider the permutation $\pi = [-5, \quad 1, \quad 2, -7, -6, -4, -3] \in S_7^{\pm}$.

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$$\pi = [-5, \ 1, \ 2, -7, -6, -4, -3]$$

$$\downarrow \rho_{4,7}$$

$$[-5, \ 1, \ 2, \ 3, \ 4, \ 6, \ 7]$$

$$\downarrow \rho_{2,5}$$

$$[-5, -4, -3, -2, -1, \ 6, \ 7]$$

$$\downarrow \rho_{1,5}$$

$$\mathrm{id} = [\ 1, \ 2, \ 3, \ 4, \ 5, \ 6, \ 7]$$

# Expansion Transformation

**Definition**

Define $S^0_{2n}$ to be the set of unsigned permutations on $\{0, 1, 2, \ldots, 2n+1\}$ such that 0 and $2n+1$ are fixed points. We define the expansion transformation from a signed permutation $\pi \in S^{\pm}_n$ to an unsigned permutation $\pi' \in S^0_{2n}$ as follows:

$$\pi'_0 = 0, \pi'_{2n+1} = 2n+1,$$

and for all other values, if $\pi_i > 0$, then

$$\pi'_{2i-1} = 2\pi_i - 1, \pi'_{2i} = 2\pi_i,$$

while if $\pi_i < 0$, then

$$\pi'_{2i-1} = 2|\pi_i|, \pi'_{2i} = 2|\pi_i| - 1.$$

Note that the expansion transformation is injective, which implies that the process is uniquely reversible for an unsigned permutation in the image.

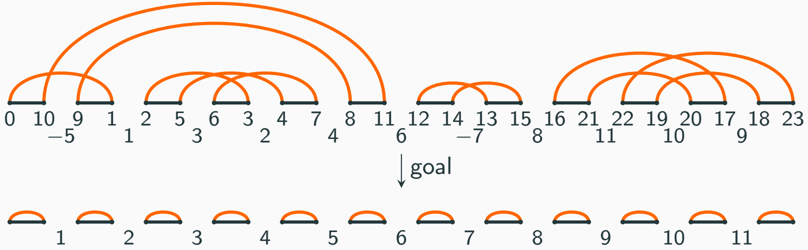
# Breakpoint Diagram

**Definition**

The breakpoint diagram of $\pi$, denoted $\mathrm{BG}(\pi)$, is a graph with colored edges constructed as follows.

- vertex set: $\{\pi'_0, \pi'_1, \ldots, \pi'_{2n+1}\}$;
- black edge set: $\{\{\pi'_{2i}, \pi'_{2i+1}\} \mid 0 \leq i \leq n\}$;
- orange edge set: $\{\{2i, 2i+1\} \mid 0 \leq i \leq n\}$.

**Example**



**Theorem (Hannenhalli & Pevzner)**

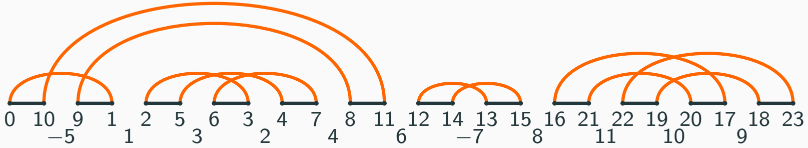
The reversal distance of any signed permutation $\pi \in S_n^{\pm}$ is given by

$$d_r(\pi) = n + 1 - c(\pi) + h(\pi) + f(\pi)$$

- $c(\pi) := \#$ of cycles in BG($\pi$),
- $h(\pi) := \#$ of "hurdles" in BG($\pi$),
- $f(\pi)$ is 1 if $\pi$ is a "fortress" and 0 otherwise.

**Example**

For $\pi = [-5, 1, 3, 2, 4, 6, -7, 8, 11, 10, 9]$, it turns out that $c(\pi) = 5$, $h(\pi) = 2$, and $\pi$ is not a fortress, and so $d_r(\pi) = 11 + 1 - 5 + 2 + 0 = 9$.

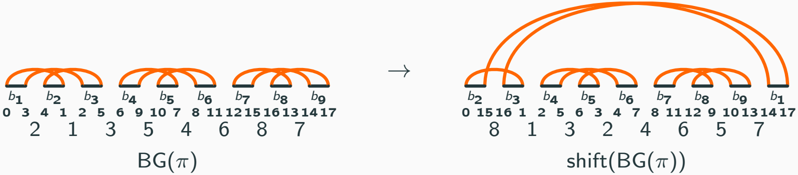


# Cyclic Shift of Breakpoint Diagram

**Definition**

Let $b_1, \ldots, b_{n+1}$ denote the black edges of $\mathrm{BG}(\pi)$ (from left to right). The cyclic shift of $\mathrm{BG}(\pi)$, denoted $\mathrm{shift}(\mathrm{BG}(\pi))$, is the diagram obtained by shifting $b_i$ to $b_{i-1}$ (mod $n+1$) while preserving the connections of the orange and black edges between vertices.

**Example**



**Theorem**

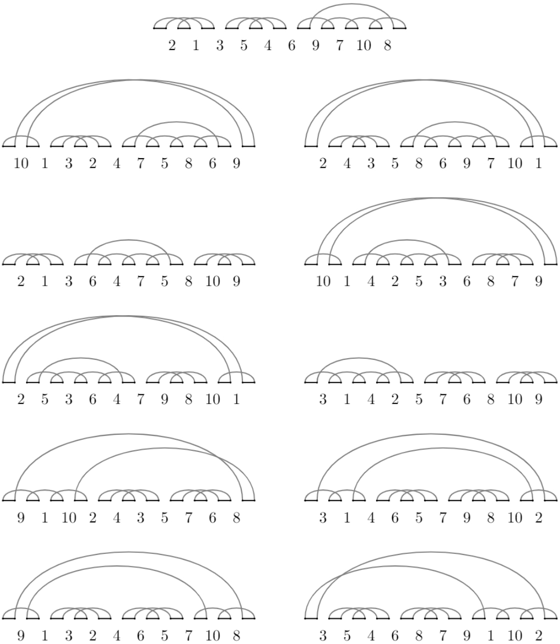
If $\pi \in S_n^{\pm}$, then shift(BG($\pi$)) is the breakpoint diagram for a signed permutation in $S_n^{\pm}$, denoted shift($\pi$). Moreover, $d_r(\pi) = d_r(\text{shift}(\pi))$.

**Definition**

For $\pi, \gamma \in S_n^{\pm}$, define $\pi \sim \gamma$ if we can obtain BG($\gamma$) from BG($\pi$) by a sequence of cyclic shifts. If $\pi \sim \gamma$, we say that $\pi$ and $\gamma$ are shift equivalent. Define the shift equivalence class of $\pi \in S_n^{\pm}$ via

$$[\pi] = \{\gamma \in S_n^{\pm} \mid \gamma \sim \pi\}.$$

# Example



2 1 3 5 4 6 9 7 10 8
10 1 3 2 4 7 5 8 6 9
2 4 3 5 8 6 9 7 10 1
2 1 3 6 4 7 5 8 10 9
10 1 4 2 5 3 6 8 7 9
2 5 3 6 4 7 9 8 10 1
3 1 4 2 5 7 6 8 10 9
9 1 10 2 4 3 5 7 6 8
3 1 4 6 5 7 9 8 10 2
9 1 3 2 4 6 5 7 10 8
3 5 4 6 8 7 9 1 10 2

# Maximal Signed Permutations

**Theorem (Folklore?)**

$$d_r^{\max}(S_n^{\pm}) = \begin{cases} n, & n = 1, 3 \\ n+1, & \text{otherwise.} \end{cases}$$

**Theorem**

Let $\pi \in S_n^{\pm}$ be a maximal signed permutation. Then

1. $\pi$ is not a fortress;
2. $\pi$ only contains positive entries;
3. All cycles of $\mathrm{BG}(\pi)$ are hurdles $\Longrightarrow$ all cycles "sit side by side" or there is one that "covers" and the rest sit "side by side";
4. Every element of $[\pi]$ is also a maximal signed permutation.

# Compositions

**Definition**

A composition of $n$ is an ordered list of positive integers whose sum is $n$, denoted

$$\alpha = (\alpha_1, ..., \alpha_k).$$

We refer to each $\alpha_i$ as a part of the composition. Let $C(n)$ denote the set of all compositions on $n$.

**Example**

$$C(4) = \{(1,1,1,1),(1,2,1),(1,1,2),(2,1,1),(3,1),(1,3),(2,2),(4)\}.$$

**Definition**

We define

$$C^{>1}_{\text{odd}}(n) := \{(\alpha_1, \ldots, \alpha_k) \in C(n) \mid \text{ each } \alpha_i \text{ is odd and greater than } 1\}$$

and let $c^{>1}_{\text{odd}}(n) := |C^{>1}_{\text{odd}}(n)|$.

**Theorem**

We have $c^{>1}_{\text{odd}}(1) = c^{>1}_{\text{odd}}(2) = 0, c^{>1}_{\text{odd}}(3) = 1$ and for $n \geq 4$

$$c^{>1}_{\text{odd}}(n) = c^{>1}_{\text{odd}}(n-2) + c^{>1}_{\text{odd}}(n-3).$$

The first few terms of the sequence are

$$0, 0, 1, 0, 1, 1, 1, 2, 2, 3.$$

It turns out that $c^{>1}_{\text{odd}}(n)$ is the Padovan sequence (OEIS A000931).

# Enumerating Maximal Signed Permutations

**Theorem**

For $n \neq 1, 3$, we have

$$\mathrm{rk}_{\max}(S_n^{\pm}, d_r) = \sum_{(\alpha_1,\ldots,\alpha_k)\in C_{\mathbf{odd}}^{>1}(n+1)} \left(\prod_{i=1}^{k} \frac{2(\alpha_i - 1)!}{\alpha_i + 1}\right) \cdot \begin{cases} \alpha_1, & \text{if } k \neq 1 \\ 1, & \text{if } k = 1. \end{cases}.$$

**Remark**

- Note that $\dfrac{2(\alpha_i - 1)!}{\alpha_i + 1} = H(\alpha_i - 1, 1)$ (where $\alpha_i$ is always odd).
- The complexity is subject to finding the compositions in $C_{\mathbf{odd}}^{>1}(n+1)$.
- The first few terms of $\mathrm{rk}_{\max}(S_n^{\pm}, d_r)$ when $n \neq 1, 3$ are $1, 8, 3, 180, 64, 8067$.

# Distribution of Maximal Signed Permutations

**Conjecture**

We conjecture that

$$\lim_{n\to\infty} \frac{\mathrm{rk}_{\max}(S_n^{\pm}, d_r)}{2(n-1)!} = 1 \quad \text{if } n \text{ is odd,}$$
$$\lim_{n\to\infty} \frac{\mathrm{rk}_{\max}(S_n^{\pm}, d_r)}{2(n-3)!} = 1 \quad \text{if } n \text{ is even.}$$

If true, then if we choose a signed permutation uniformly at random, the probability of selecting a maximal signed permutation is about $n/2^n$ for $n$ odd and $n(n-1)(n-2)/2^n$ for $n$ even. That is, as $n$ grows, it is exponentially unlikely to choose a maximal signed permutation at random.

# Further Enumeration

We can partition the collection of signed permutations in $S_n^{\pm}$ of reversal distance $k$ according to the number of "trivial cycles" in their breakpoint diagrams. This yields

$$\mathrm{rk}_k(S_n^{\pm}, d_r) = \sum_{i=0}^{n+1} a_{i,k} \binom{n+1}{i+1},$$

where $a_{i,k} := \#$ signed perms in $S_i^{\pm}$ of reversal distance $k$ with no trivial cycles. But some leading terms and trailing terms are 0.

**Theorem**

$$\mathrm{rk}_k(S_n^{\pm}, d_r) = a_{k-1,k}\binom{n+1}{k} + a_{k,k}\binom{n+1}{k+1} + \cdots + a_{2k-1,k}\binom{n+1}{2k}.$$

This is a polynomial in $n$ of degree $2k$ with rational coefficients.

Determining closed forms for $\mathrm{rk}_k(S_n^{\pm}, d_r)$ using the above theorem is dependent on having values for $a_{k-1,k}, \ldots, a_{2k-1,k}$. These values are independent of $n$.

Using brute-force computations (Python and Java), we have obtained data for $a_{k-1,k}, \ldots, a_{2k-1,k}$ when $1 \leq k \leq 5$. This yields the following:

- $\mathrm{rk}_1(S_n^{\pm}, d_r) = \dfrac{n(n+1)}{2} = \dbinom{n+1}{2}$
- $\mathrm{rk}_2(S_n^{\pm}, d_r) = \dfrac{n(n-1)(n+1)^2}{6}$ (OEIS A004320... Aztec diamonds)
- $\mathrm{rk}_3(S_n^{\pm}, d_r) = \dfrac{n^2(n-1)(n+1)(n+2)(7n-11)}{144}$
- $\mathrm{rk}_4(S_n^{\pm}, d_r) =$ Ugly (not real-rooted)
- $\mathrm{rk}_5(S_n^{\pm}, d_r) =$ Ugly (not real-rooted)

Moreover, for $n \neq 1, 3$, we have

$$\mathrm{rk}_{\max}(S_n^{\pm}, d_r) = a_{n,n+1}.$$

# Terminal Permutations

Interesting side story...

**Definition**

We call a signed permutation $\pi \in S_n^{\pm}$ terminal if $d_r(\pi \circ \rho_{ij}) \leq d_r(\pi)$ for all $\rho_{ij}$.

Note that every maximal signed permutation in $S_n^{\pm}$ is terminal. However, there exist terminal permutations that are not maximal! Terminal means maximal in the language of posets as opposed to distance.

**Example**

Let $\pi = [2, -3, 1, -4] \in S_4^{\pm}$. It turns out that $d_r(\pi) = 4$ while $d_r(\pi \circ \rho_{ij}) \leq 4$ for all reversals $\rho_{ij}$, which implies that $\pi$ is terminal but not maximal. However, the maximal reversal distance in $S_4^{\pm}$ is 5.

# Something Cool?

Computing the first several terms of $\sum_{k=0}^{n+1} a_{n,k}$ coincides with OEIS A061714, which counts the number of circular permutations on $0, 1, \ldots, 2n-1$ where every two elements $2i, 2i+1$ are adjacent and no two elements $2i-1, 2i$ are adjacent. There is a connection to the Traveling Salesman Problem. . .

# Open Problems

Adjacent block interchanges in $S_n$:

- $d_{abi}(\pi) = ???$ (numerous formulas for lower and upper bounds)
- $\text{rk}_k(S_n, d_{abi}) = ???$
- $d_{abi}^{\max}(S_n) = ???$
- $\text{rk}_{\max}(S_n, d_{abi}) = ???$

Reversals in $S_n^{\pm}$:

- Wrap up proof for limit results for $\text{rk}_{\max}(S_n, d_r)$.
- Push results for $\text{rk}_k(S_n^{\pm}, d_r)$ for $k \geq 6$.
- "Closed form" for $rk_{\max}(S_n^{\pm}, d_r)$? Or at least an enumeration that does not rely on determining compositions in $C_{\textbf{odd}}^{>1}(n+1)$.
- Enumerate/classify terminal non-maximal permutations.
- Generating functions?

# Generalizations

$\xrightarrow{?} \cdots \xrightarrow{?}$

Þakka þér fyrir / takk