

Sorting Genomes by Prefix Double-Cut-and-Joins

Guillaume Fertin Géraldine Jean **Anthony Labarre**



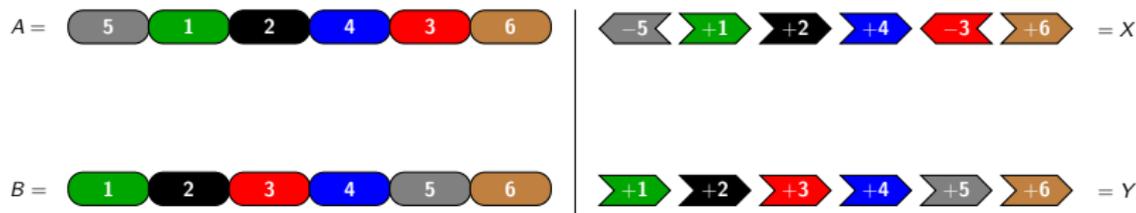
March 23rd, 2023



Genome rearrangements for permutations

- (Signed) permutations model duplication-free genomes with the same contents;
- The actual numbering is irrelevant, so we assume either genome is the **identity** $Id = \langle 1 \ 2 \ \dots \ n \rangle$;

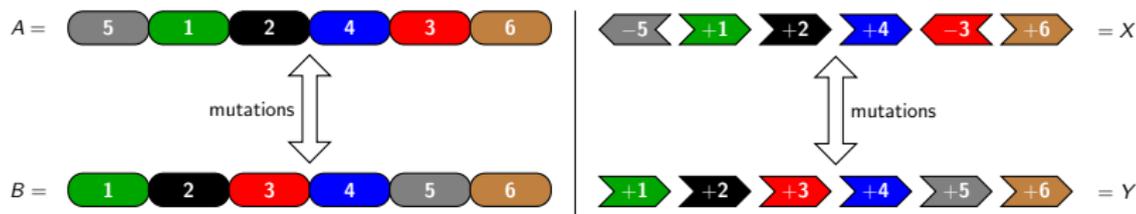
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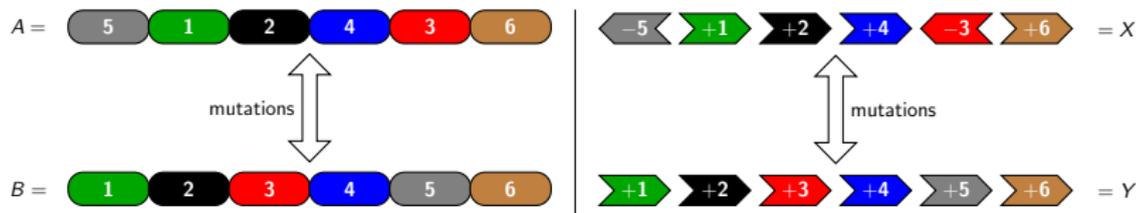
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GENOME SORTING (PERMUTATIONS)

Input: a (signed) permutation π , a set S of (per)mutations;

Goal: find a shortest sorting sequence of elements of S for π .
(the length of that sequence is the **distance** of π)

Example (disregarding / considering gene orientation)



Modelling genomes

A more unified treatment is provided by:

- 1 **unsigned genomes**: paths on $\{0, 1, 2, \dots, n + 1\}$;
- 2 **signed genomes**: perfect matchings on $\{0, 1, 2, \dots, 2n + 1\}$;

Example (from permutations to genomes)

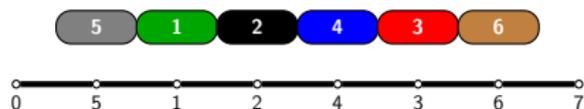


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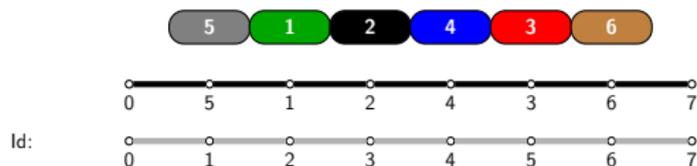


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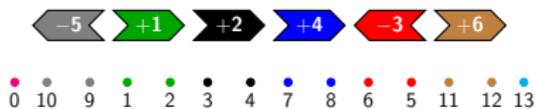
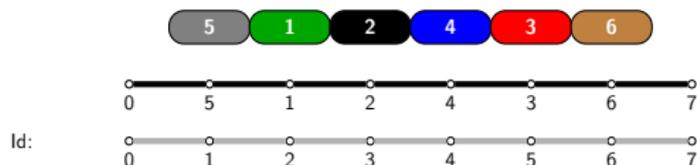


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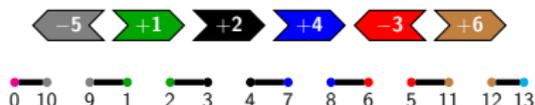
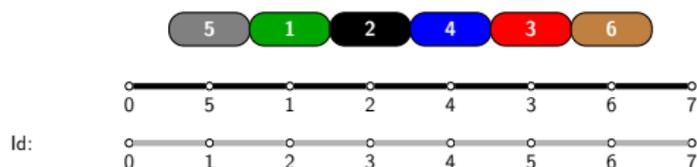
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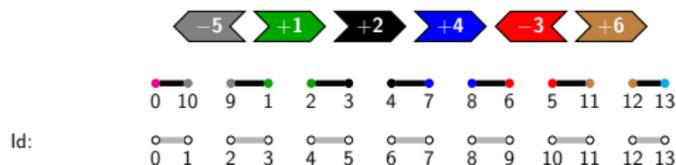
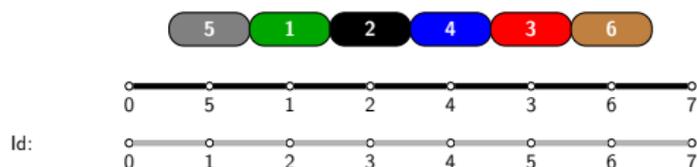
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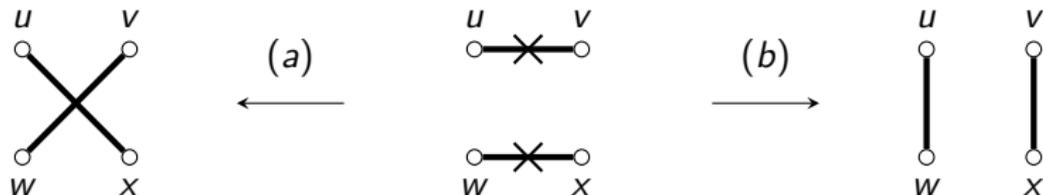


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The double cut-and-join (DCJ) operation

A **double cut-and-join** (DCJ) removes two edges $\{u, v\}$ and $\{w, x\}$ from a graph, then connects the four endpoints in one of two ways.

Example



The graph might be directed, belong to a particular class, ... which may restrict our options for reconnecting the endpoints (see examples later on).

DCJs in a biological setting

- DCJs generalise several well-studied mutations, e.g.:

- transpositions;

$$3 \boxed{1} 5 \boxed{4} 2 6 \rightarrow 3 \boxed{4} 5 \boxed{1} 2 6$$

- reversals;

$$3 \underline{1} \underline{5} \underline{4} \underline{2} 6 \rightarrow 3 \underline{2} \underline{4} \underline{5} \underline{1} 6$$

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$$3 \underline{-1} \underline{5} \underline{-4} \underline{2} 6 \rightarrow 3 \underline{-2} \underline{4} \underline{-5} \underline{1} 6$$

- block-transpositions;

$$3 \boxed{15} \boxed{42} 6 \rightarrow 3 \boxed{42} \boxed{15} 6$$

- block-interchanges;

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- Sorting genomes by DCJs is:

- in P in the signed case [7];
- NP-hard in the unsigned case [5];

The prefix constraint

- We study **prefix DCJs**: one of the cut edges must be incident with 0;
- The constraint has no biological relevance: it originates from interconnection network design;
- Theoretical interest: many “unrestricted” problems remain open under the prefix constraint;

Results

We obtain:

- new lower bounds for sorting by prefix reversals or DCJs (signed or unsigned);
- a polynomial time algorithm for sorting by signed prefix DCJs;
- a $3/2$ -approximation for sorting by unsigned prefix DCJs;

To the best of our knowledge, this is the first $(2 - \varepsilon)$ -approximation for a prefix sorting problem not known to be in P.

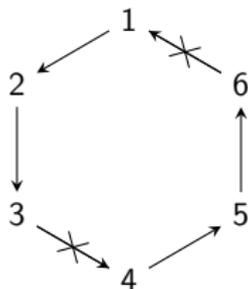
Mimicking other rearrangements using DCJs

Algebraic transpositions as DCJs

Let π be a permutation and $\Gamma(\pi)$ be its graph; i.e., the cycles of π are exactly those of $\Gamma(\pi)$.

Example

Let us compute $(1, 2, 3)(4, 5, 6) = (1, 4) \circ (1, 2, 3, 4, 5, 6)$.

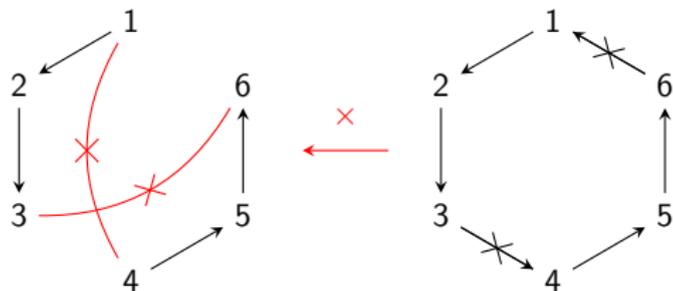


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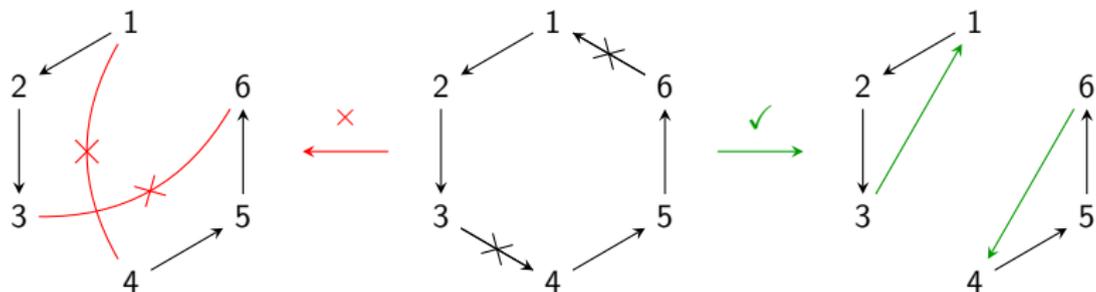
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Viewing permutations of $\{1, 2, \dots, n\}$ as paths on $\{0, 1, 2, \dots, n, n+1\}$ allows us to express reversals as DCJs.

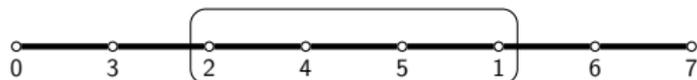
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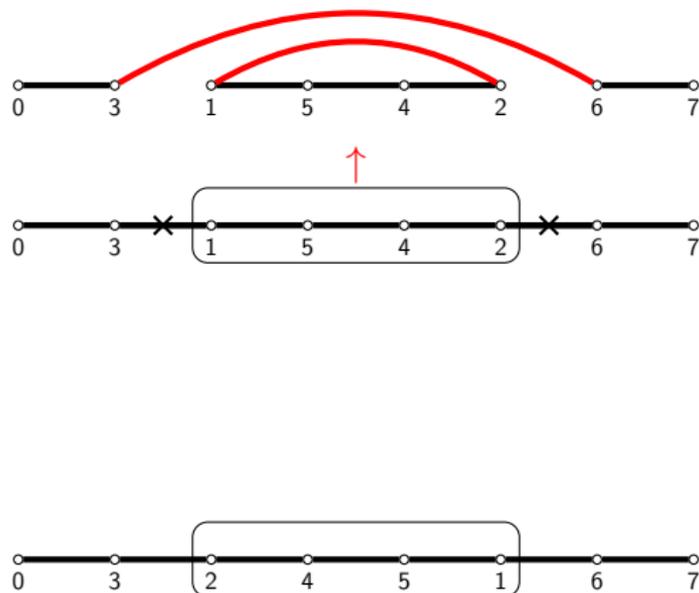
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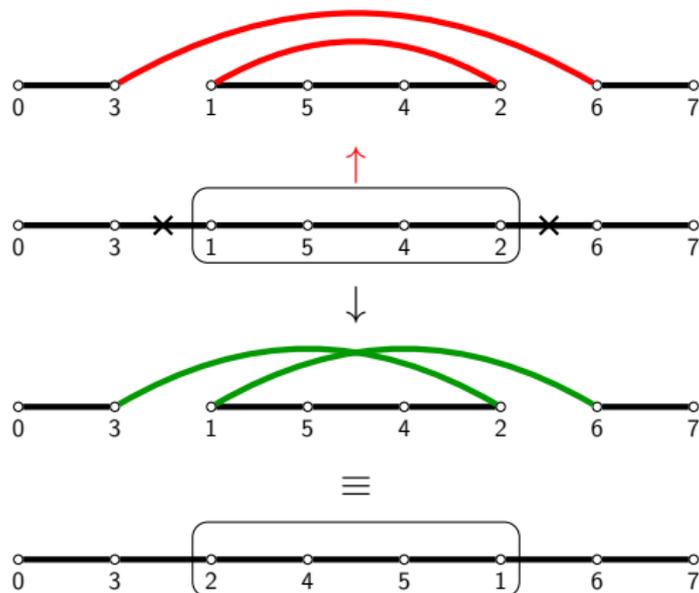


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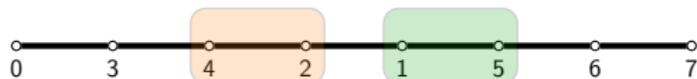


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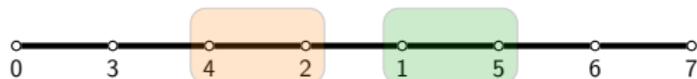
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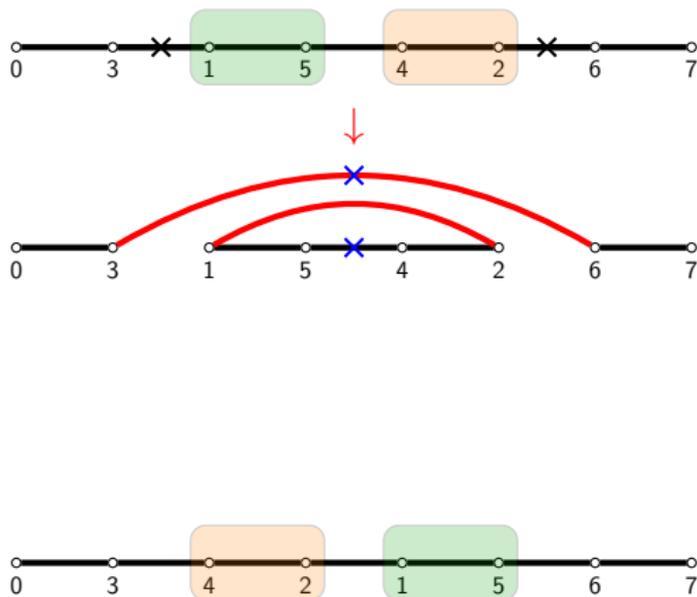
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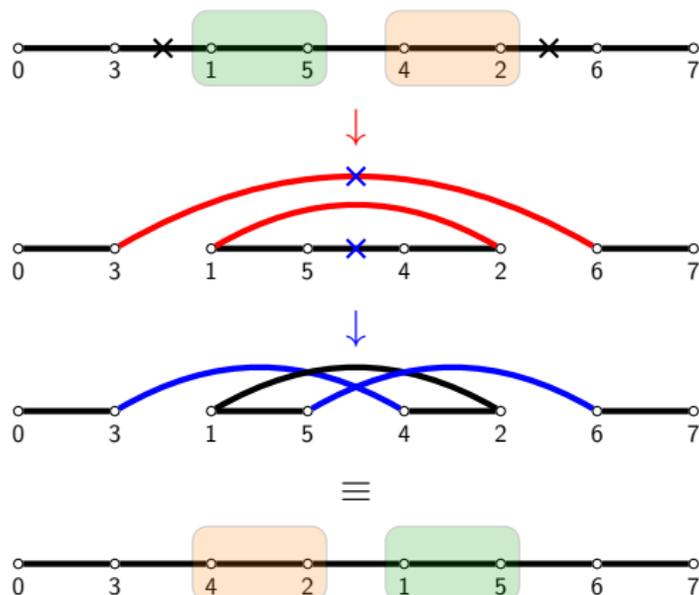
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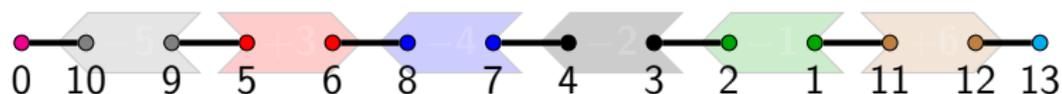
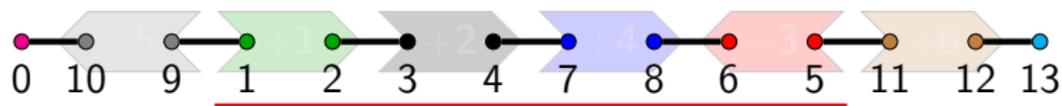
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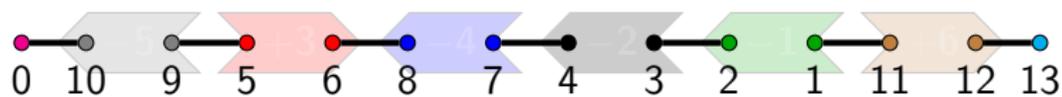
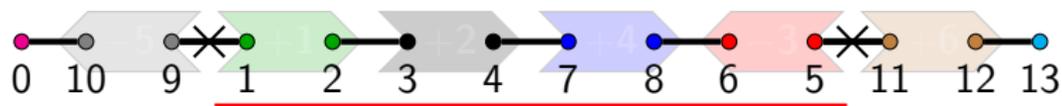
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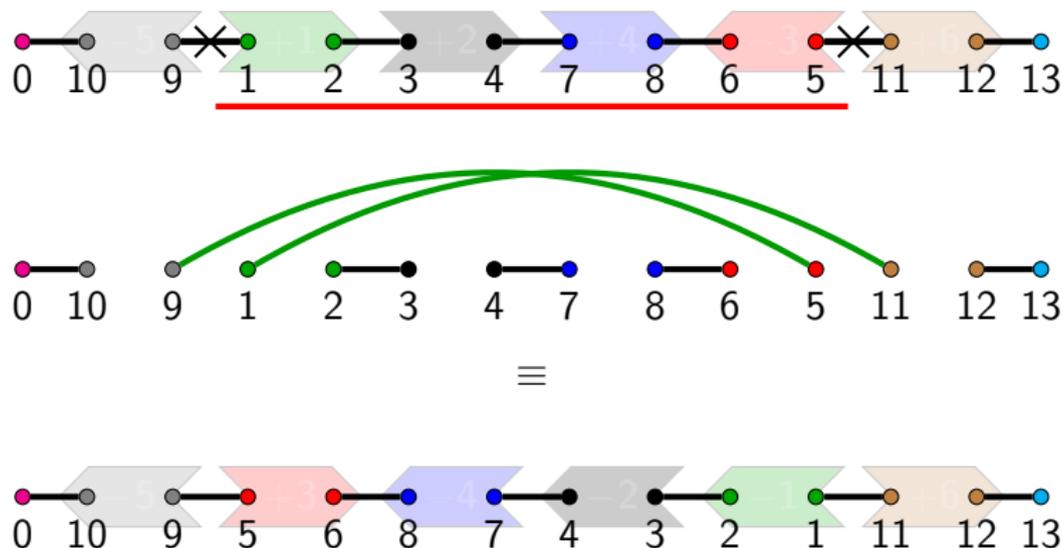
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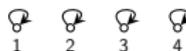
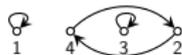
Results

Preliminary results

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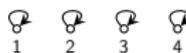
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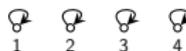
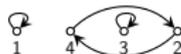
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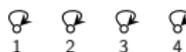
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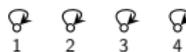
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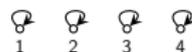
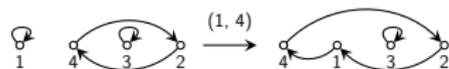
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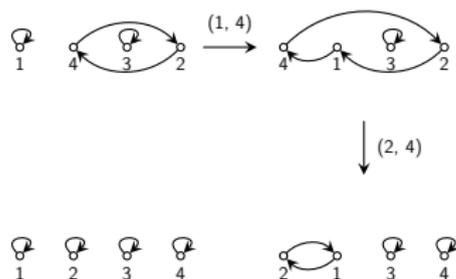
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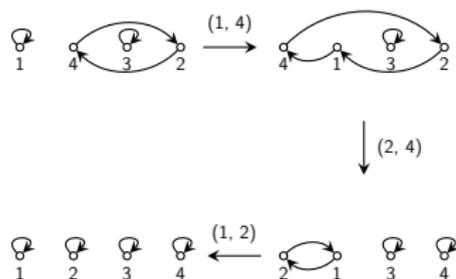
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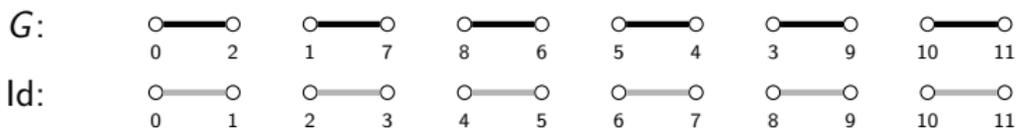
Approach

- As we have seen, (prefix) transpositions are (prefix) DCJs;
- Strategy:
 - find “the right graph” representation for pairs of genomes, depending on the mutations we want to use;
 - rely on the prefix Cayley distance to obtain bounds based on that graph;

Signed prefix DCJs

- A **signed genome** is a perfect matching G over $\{0, 1, \dots, 2n + 1\}$;
- We want to obtain $Id = \{\{0, 1\}, \{2, 3\}, \dots, \{2n, 2n + 1\}\}$;

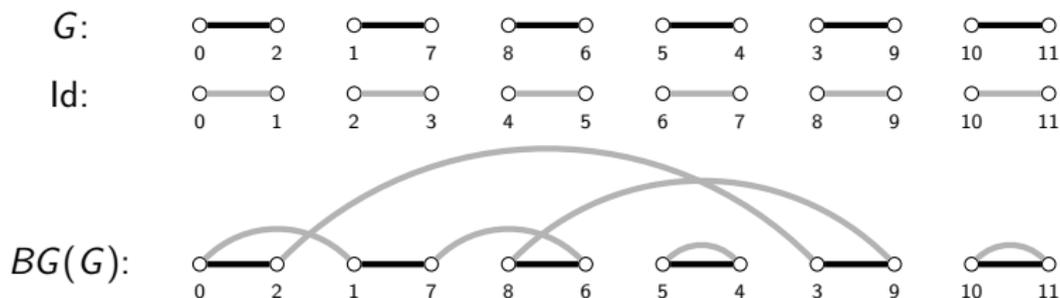
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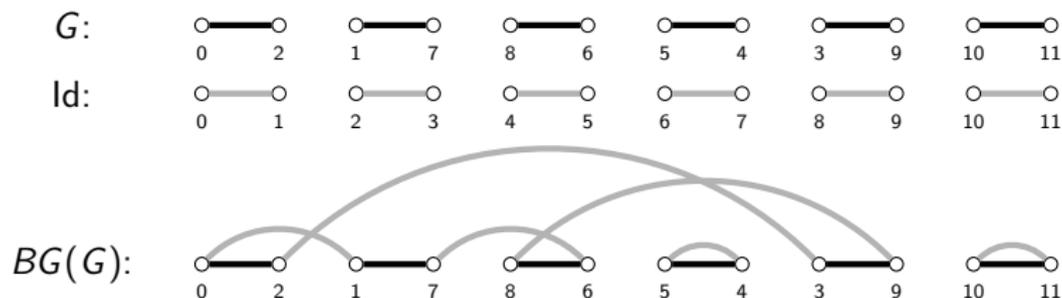
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Every vertex has degree 2 \Rightarrow collection of cycles.

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For any signed genome G , we have

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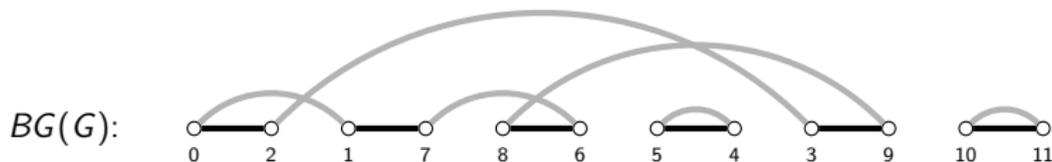
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Example

With G as in the previous slide:



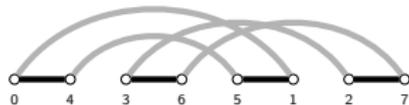
we have $psdcj(G) \geq 6 + 3 - 2 \times 2 - 2 = 3$.

Sorting by signed prefix DCJs is in P

Algorithm outline

Until $G = \text{Id}$, check edge $\{0, v\} \in G$:

Example



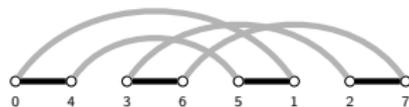
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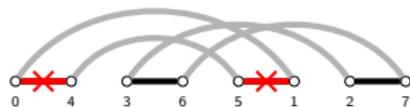
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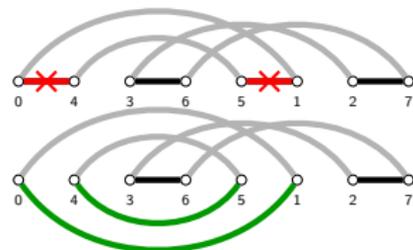
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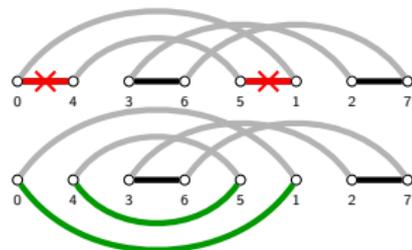
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Until $G = \text{Id}$, check edge $\{0, v\} \in G$:

- 1 if $v \neq 1$: connect v to its “grey neighbour” in Id ;
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Example



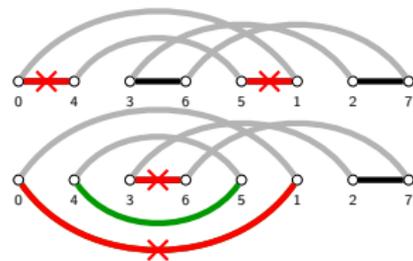
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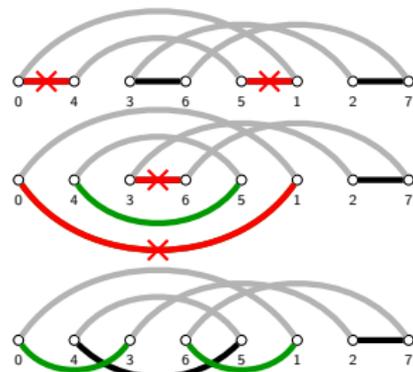
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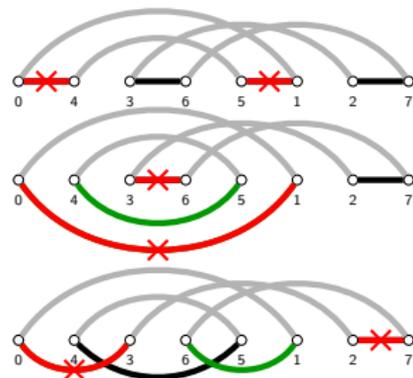
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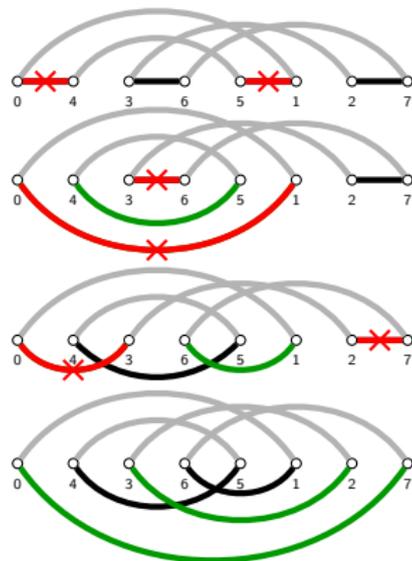
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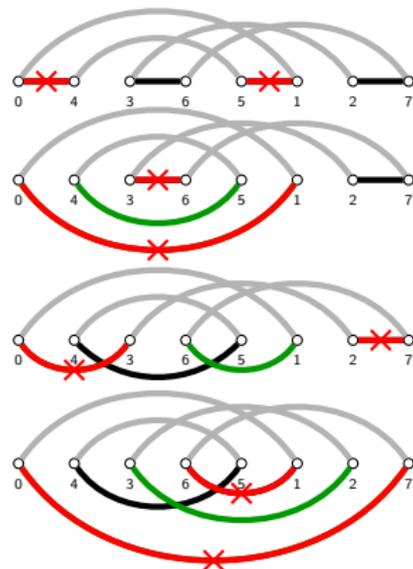
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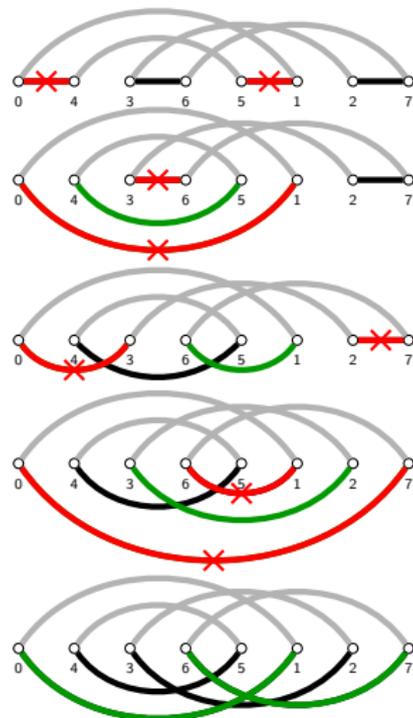
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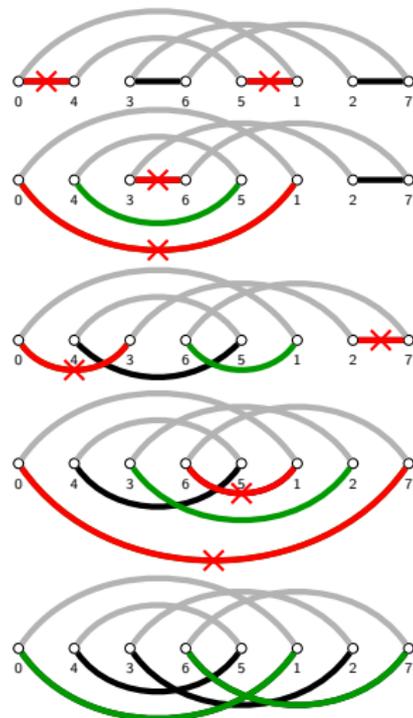
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Every operation decreases the value of our lower bound by 1 \Rightarrow algorithm is optimal.

Example



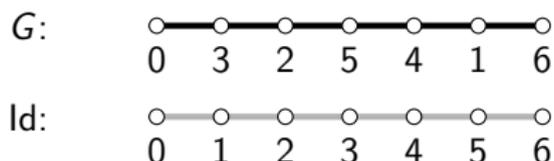
Signed prefix reversals

- Signed prefix reversals are signed prefix DCJs that must preserve an additional structural constraint (details omitted);
 - ✓ therefore, $psrd(G) \geq psdcj(G)$;
 - ✗ but previous algorithm cannot be used;

Unsigned prefix DCJs

- An **unsigned genome** is a path G over $\{0, 1, \dots, n + 1\}$;
- We want to obtain the path $Id = (0, 1, \dots, n + 1)$;

Example



- An unsigned version of the breakpoint graph yields a similar lower bound to the signed case (no time for details);

A lower bound for sorting by unsigned prefix DCJs

Theorem

For any genome G , we have:

$$pdcj(G) \geq n + 1 + c^*(UBG(G)) - 2c_1^*(UBG(G)) - \begin{cases} 0 & \text{if } \{0, 1\} \in G \text{ and } \{1, 2\} \in G, \\ 1 & \text{if } \{0, 1\} \in G \text{ and } \{1, 2\} \notin G, \\ 2 & \text{otherwise.} \end{cases}$$

where $c^*(\cdot)$ (resp. $c_1^*(\cdot)$) is the number of (trivial) cycles in an **optimal decomposition** of $UBG(G)$.

An optimal decomposition can be computed as follows:

- 1 remove all edges that belong to trivial cycles;
- 2 each connected component that remains is Eulerian and therefore constitutes a nontrivial cycle.

Approximating the unsigned prefix DCJ distance

An edge $e \in G$ is a **breakpoint** if $0 \notin e$ and $e \notin Id$, and an **adjacency** otherwise;

Example

The following genome has 3 breakpoints and 3 adjacencies:



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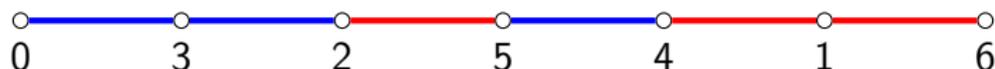
For any genome G , we have $pdcj(G) \geq b(G)$.

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The following genome has 3 breakpoints and 3 adjacencies:



Lemma

For any genome G , we have $pdcj(G) \geq b(G)$.

Proof.

A prefix DCJ cuts $\{0, v\}$ and another edge, then reconnects their endpoints. But $\{0, v\}$ is never a breakpoint, so $b(G)$ can only decrease by 1. □

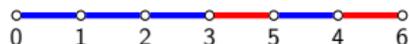
A 3/2-approximation algorithm for unsigned prefix DCJs

Algorithm outline

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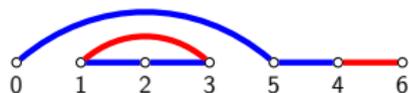
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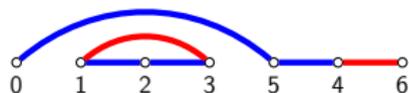
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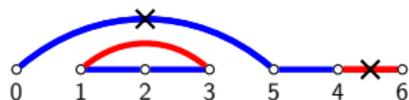
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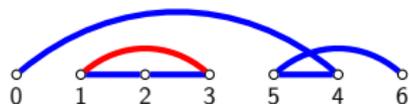
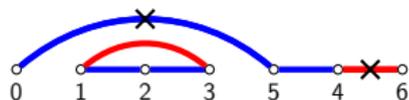
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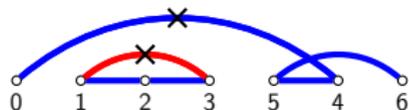
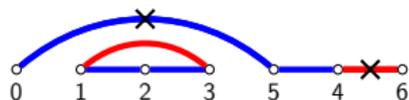
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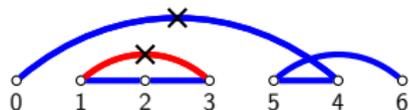
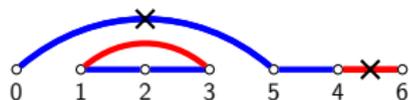
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Approximation guarantee

- Case 1: $b(G)$ decreases by 1;

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Unsigned prefix reversals

- Unsigned prefix reversals are unsigned prefix DCJs that must yield a path at each step;
 - ✓ therefore, $prd(G) \geq pdcj(G)$;
 - ✗ but previous algorithm cannot be used;

Open problems

- Complexity issues:

	reversals		DCJs	
	unsigned	signed	unsigned	signed
unrestricted	NP-hard [4]	in P [6]	NP-hard [5]	in P [7]
prefix	NP-hard [3]	???	???	in P(here)

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Thanks!

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