Average-case complexity analysis of perfect sorting by reversals

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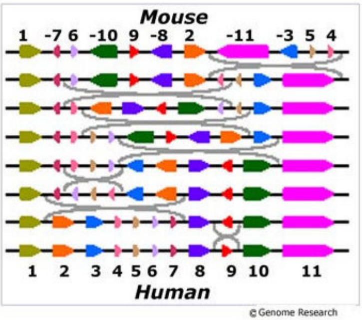
Outline of the talk

Biological motivations



Reconstruction of evolution scenarios
$\hookrightarrow$ Operation on genome = reversal

- Model for genome = signed permutation
- Reversal = reverse a window of the permutation while changing the signs

$$1\ \overline{7}\ 6\ \overline{10}\ 9\ \overline{8}\ 2\ \overline{11}\ \overline{3}\ 5\ 4$$

$\Downarrow$ Reversal $\Downarrow$

$$1\ \overline{7}\ 6\ \overline{10}\ 9\ \overline{8}\ 2\ \overline{4}\ \overline{5}\ 3\ 11$$

Sorting by reversals: the problem and solution

The problem:

- INPUT: Two signed permutations σ_1 and σ_2
- OUTPUT: A parsimonious scenario from σ_1 to σ_2 or $\overline{\sigma_2}$

Parsimonious = shortest, *i.e.* minimal number of reversals.
Without loss of generality, $\sigma_2 = Id = 1\ 2 \dots n$

The solution:

- Hannenhalli-Pevzner theory
- Polynomial algorithms: from $\mathcal{O}(n^4)$ to $\mathcal{O}(n\sqrt{n \log n})$

Remark: the problem is *NP*-hard when permutations are unsigned.

Definition and motivation

Perfect sorting by reversals: do not break common intervals

Common interval between σ_1 and σ_2: windows of σ_1 and σ_2 containing the same elements (with no sign)
Example: $\sigma_1 = 5\ \bar{1}\ \bar{3}\ 7\ 6\ \bar{2}\ 4$ and $\sigma_2 = 6\ \bar{4}\ 7\ 1\ \bar{3}\ 2\ \bar{5}$

When $\sigma_2 = Id$, interval of σ_1 = window forming a range (in $\mathbb{N}$)
Example: $\sigma_1 = 4\ \bar{7}\ \bar{5}\ 6\ 3\ \bar{1}\ 2$

Biological argument: groups of identical (or homologous) genes appearing together in two species are likely to be

- together in the common ancestor
- never separated during evolution

Algorithm and complexity

The problem:

- INPUT: Two signed permutations σ_1 and σ_2
- OUTPUT: A parsimonious perfect scenario (=shortest among perfect scenarios) from σ_1 to σ_2 or $\overline{\sigma_2}$

Without loss of generality, $\sigma_2 = Id = 1\ 2 \ldots n$

Watch out!: Parsimonious perfect $\not\Rightarrow$ parsimonious

Complexity: *NP*-hard problem

Algorithm [Bérard, Bergeron, Chauve, Paul]: take advantage of decomposition trees to produce a *FPT* algorithm $\left(2^p \cdot n^{O(1)}\right)$

Strong intervals of (signed) permutations

- Strong interval = does not overlap any other interval
- Interval I is strong iff $\forall J$, $I \subseteq J$ or $J \subseteq I$ or $I \cap J = \emptyset$

Example of intervals and strong intervals:

$$5 \quad \bar{6} \quad \bar{7} \quad 9 \quad 4 \quad \bar{3} \quad 1 \quad 2 \quad \bar{8} \quad \overline{10} \quad \overline{17} \quad 13 \quad \overline{15} \quad 12 \quad 11 \quad \overline{14} \quad 18 \quad \overline{19} \quad \overline{16}$$

Trivial intervals are always among strong intervals

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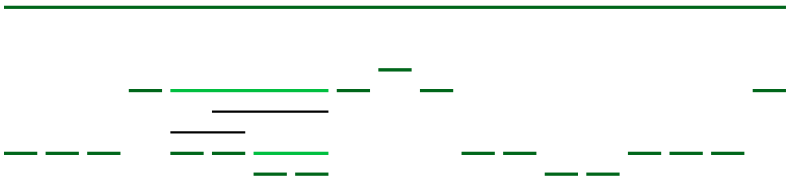

$5 \ \bar{6} \ \bar{7} \ 9 \ 4 \ \bar{3} \ 1 \ 2 \ \bar{8} \ \overline{10} \ \overline{17} \ 13 \ \overline{15} \ 12 \ 11 \ \overline{14} \ 18 \ \overline{19} \ \overline{16}$

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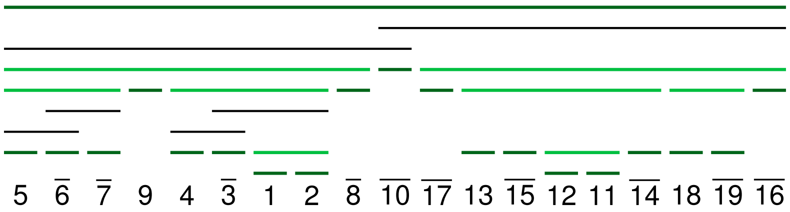
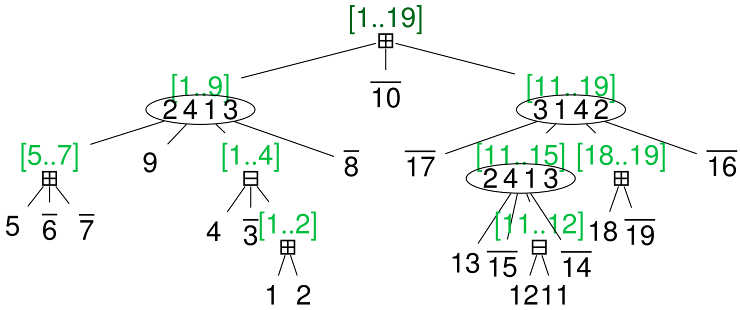


Trivial intervals are always among strong intervals

Decomposition trees of (signed) permutations

Also known as strong interval trees

- Inclusion order on strong intervals: a tree-like ordering

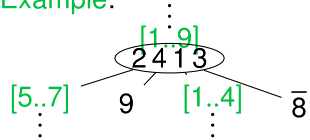


Computation: in linear time

Decomposition trees of (signed) permutations

Quotient permutation $=$
order of the children (that are intervals)

Example:

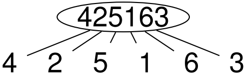


Two types of nodes:

- Linear nodes (□):
  - increasing, *i.e.* quotient permutation = 1 2 . . . k
  - $\Rightarrow$ label ⊞
  - decreasing, *i.e.* quotient permutation = k $(k-1)$ . . . 2 1
  - $\Rightarrow$ label ⊟
- Prime nodes (◯): the quotient permutation is simple

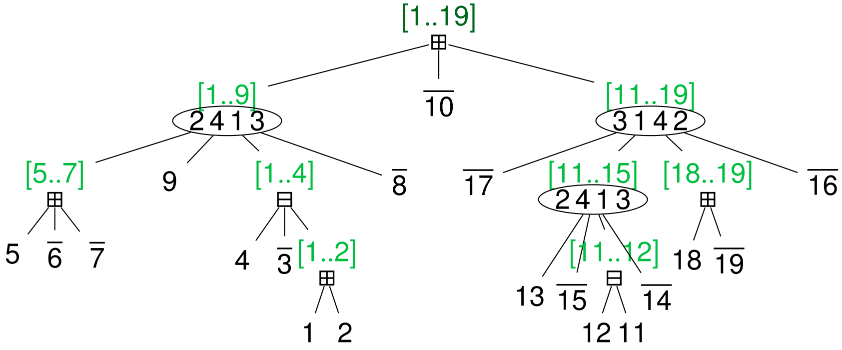
Simple permutations:
the only intervals are 1, 2,. . ., n and σ

Example: 425163, i.e.



Simplified decomposition tree

Remark: redundant information ⇒ forget the leaves and intervals



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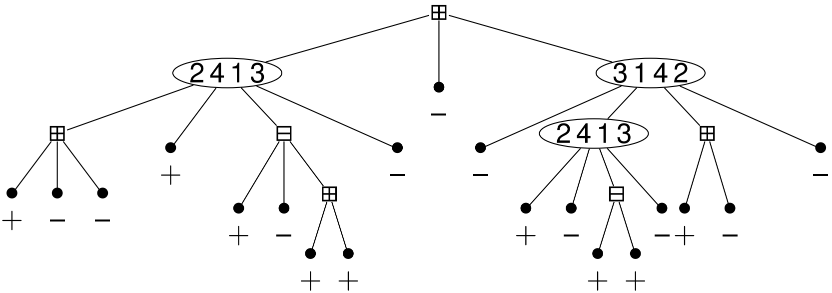


Tree uniquely defined by $\begin{cases}\text{labels of internal nodes} \\ +\text{signs of the leaves}\end{cases}$

Idea of the algorithm to solve perfect sorting

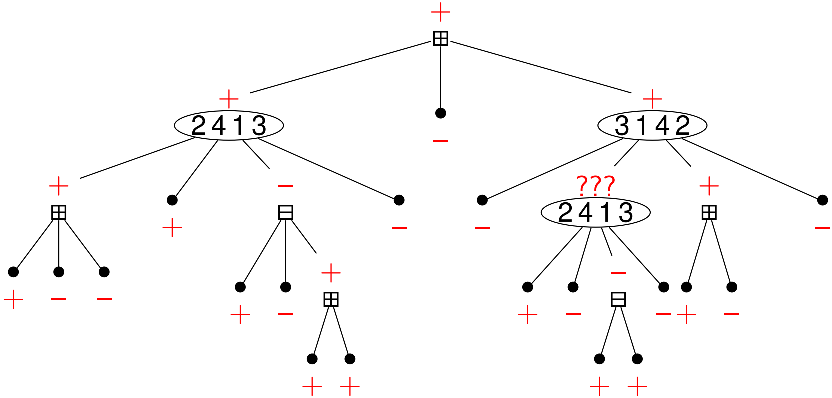
Put labels $+$ or $-$ on the nodes of the decomposition tree of σ

- Leaf: sign of the element in σ
- Linear node: $+$ for ⊞ (increasing) and $-$ for ⊟ (decreasing)
- Prime node whose parent is linear: sign of its parent
- Other prime node: ???
  - $\hookrightarrow$ Test labels $+$ and $-$ and choose the shortest scenario

Algorithm:

- Perform Hannenhalli-Pevzner (or improved version) on prime nodes
- Signed node belongs to scenario **iff** its sign is different from its linear parent

Example of labeled decomposition tree



Complexity results

Complexity:

- $\mathcal{O}(2^p n \sqrt{n \log n})$, with $p = \sharp$ prime nodes
- polynomial on separable permutations ($p = 0$)

Our work:

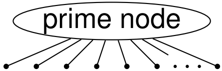
- polynomial with probability 1 asymptotically
- polynomial on average
- in a parsimonious perfect scenario for separable permutations
  - average number of reversals $\sim 1.27n$
  - average length of a reversal $\sim 1.054\sqrt{n}$

Probability distribution: always uniform

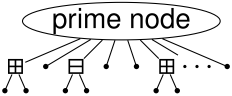
"Average shape" of decomposition trees

Enumeration of simple permutations: asymptotically $\frac{n!}{e^2}$

$\Rightarrow$ Asymptotically, a proportion $\frac{1}{e^2}$ of decom- -position trees are reduced to one prime node.



Thm: Asymptotically, the proportion of decomposition trees made of a prime root with children that are leaves or *twins* is 1.



twin = linear node with only two children, that are leaves

Consequence: Asymptotically, with probability 1, the algorithm runs in polynomial time.

Rem.: The number of *twins* follows a Poisson distribution of parameter 2.

Average complexity

Average complexity on permutations of size n:

$$\frac{\sum_{p=0}^{n} \sharp\{\sigma \text{ with } p \text{ prime nodes}\}\; C\, 2^p n \sqrt{n \log n}}{n!}$$

Thm: When $p \geq 2$, the number of (unsigned) permutations of size n with p prime nodes is at most $\frac{48(n-1)!}{2^p}$.

Proof: induction on p

Consequence: Average complexity on permutations of size n is $\leq 51 C n \sqrt{n \log n}$. In particular, **polynomial on average.**

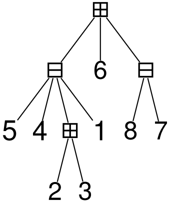
Separable (= commuting) permutations

Def.: Commuting permutation = permutation sorted by a scenario where any pair of reversals commutes (= does not overlap)

Rem.: Here, scenario = set of intervals, in any order

Equivalently: Commuting permutation = permutation with no prime node in its decomposition tree
Also called separable permutations.

Example:
54231687 i.e.



Scenarios for separable permutations

In general, in the computed scenario, reversals are

- linear nodes with label different from its linear parent
- inside prime nodes

Prop.: No ⊞ – ⊞ nor ⊟ – ⊟ edge in decomposition trees

Consequence: For separable permutations,
reversals = linear nodes with label different from its linear parent

$$= \begin{cases} \text{all internal nodes except the root} \\ +\text{leaves with label different from its parent} \end{cases}$$

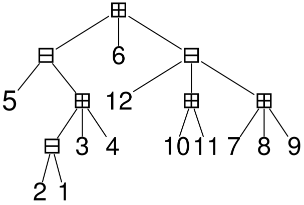
$$\boxed{\text{Reversals} \approx \text{internals nodes} - \text{the root} + \text{half of the leaves}}$$

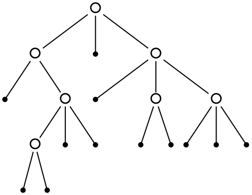
$\Rightarrow$ The shape of the tree is sufficient to study reversals

Bijection between separable perm. and Schröder trees

Decomposition trees of (unsigned) separable permutation

Schröder trees
$+$ label ⊞ or ⊟ on the root





size of σ	$\longleftrightarrow$	number of leaves
reversal of length ≥ 2	$\longleftrightarrow$	internal node except the root
reversal of length 1	$\longleftrightarrow$	some leaves (half of them)
length of a reversal	$\longleftrightarrow$	size ($= \sharp$ leaves) of the subtree

Parameters on Schröder trees

Two parameters on Schröder trees:

- Number of internal nodes
- Pathlength = sum of the sizes of the subtrees

Study their average gives access to:

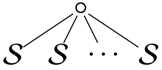
- Average number of reversals
- Average length of a reversal

in a scenario for a separable permutation

Analytic combinatorics:
average from bivariate generating functions $S(x, y) = \sum s_{n,k} x^n y^k$
where $s_{n,k}$ = number of Schröder trees with n leaves and k internal nodes (resp. pathlength k)

Average value of a parameter (number of internal nodes)

Definition: $S(x,y) = \sum s_{n,k} x^n y^k$,
where $s_{n,k}$ = number of Schröder trees with n leaves and k internal nodes

Combinatorial specification: $\mathcal{S} = \bullet \ + $ 

Functional equation: $S(x,y) = x + y\frac{S(x,y)^2}{1-S(x,y)}$

Solution: $S(x,y) = \frac{(x+1)-\sqrt{(x+1)^2-4x(y+1)}}{2(y+1)}$

Average number of internal nodes $= \frac{\sum_k k s_{n,k}}{\sum_k s_{n,k}} = \frac{[x^n]\frac{\partial S(x,y)}{\partial y}|_{y=1}}{[x^n]S(x,1)}$

Asymptotic estimate of $[x^n]S(x,1)$ when $n \to +\infty$: from asymptotic estimate of $S(x,1)$ when $x \to$ dominant singularity

Results

Application of the methodology of [Flajolet, Sedgewick]

In Schröder trees with n leaves:

- Average number of internal nodes: $\sim \frac{n}{\sqrt{2}}$
- Average pathlength: $\sim 1.27 n^{\frac{3}{2}}$

In scenarios for separable permutations of size n:

- Average number of reversals: $\sim \frac{1+\sqrt{2}}{2} n$
- Average length of a reversal: $\sim 1.054 \sqrt{n}$

Results so far and future work

Perfect sorting by reversals for signed permutations:

- *NP*-hard problem
- algorithm running in polynomial time
  - ↪ on average
  - ↪ asymptotically with probability 1
  - ↪ for the uniform distribution on permutations of size n

Special case of separable permutations (no prime nodes):

- expected length of a parsimonious perfect scenario $\sim 1.27n$
- expected length of a reversal in such a scenario $\sim 1.054\sqrt{n}$

using analytic combinatorics techniques

Work in progress: influence on the probability distribution to obtain a model closer to the biological observations

Non-uniform distributions

Results under the uniform distribution: mostly theoretical results
Biological data: not uniformly distributed (few prime nodes,. . .)

Combinatorial specification as decomposition trees: allows to introduce some constraints on the prime nodes (maximal arity, number, . . .) for:

- the study of parameters (on average)
- (Boltzmann) random generation

under non uniform distributions

Comparison between these results (theoretical or simulation) and biological data

$\hookrightarrow$ to describe models that are closer to the biological reality

$\hookrightarrow$ to identify non-random evolution (w.r.t. a *good* distribution)