Exploiting the algebraic properties of the permutation space in Evolutionary Computation

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Outline

- Permutations in EC
- Permutations in Group Theory
- Algebraic properties of combinatorial spaces
- An algebraic framework for EC
- Algebraic EAs and operators
- Practical applications
- Conclusions and open questions

Why permutations in EC?

- **Represent solutions** of important COPs

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- **Routing among items**: item $\pi(i)$ is connected to item $\pi(i+1)$
  Ex: item 4 is connected to item 7, item 7 is connected to item 2, ...
  Useful in the *Traveling Salesman Problem* (TSP)

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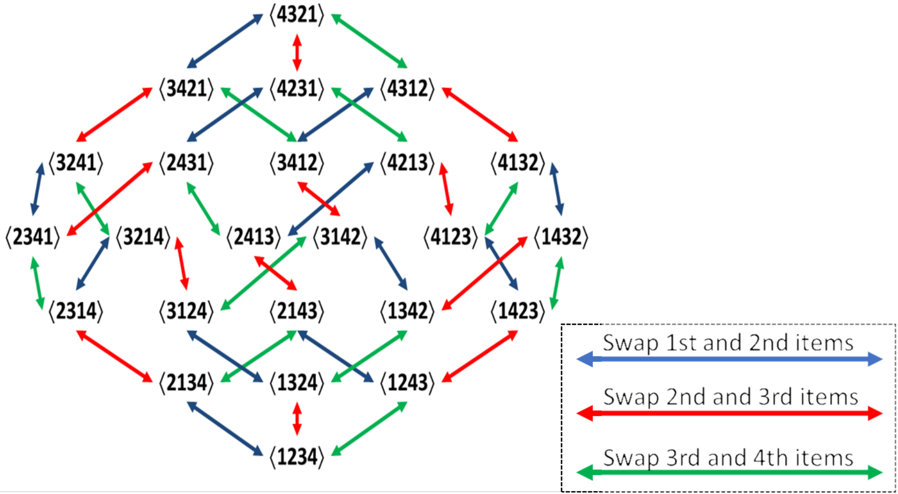
- **REV**: reversals of a chunk of items
  Ex: $\langle 53241 \rangle$ and $\langle 54231 \rangle$ are neighbors
  It modifies only two connections

Permutation space under the ASW neighborhood



Group Theory: permutations form a group

- **Composition** of permutations
  $\tau = \pi \circ \rho$ is defined as $\tau(i) = \pi(\rho(i))$ for $i = 1, \ldots, n$

  Ex: $\left\langle \begin{matrix} 1234 \\ 4213 \end{matrix} \right\rangle \circ \left\langle \begin{matrix} 1234 \\ 2143 \end{matrix} \right\rangle = \left\langle \begin{matrix} 1234 \\ 2431 \end{matrix} \right\rangle$

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- **Inverse** permutation: there exists a unique π^{-1} s.t. $\pi \circ \pi^{-1} = e$
  Ex: $\pi = \left\langle \begin{matrix} 1234 \\ 4213 \end{matrix} \right\rangle \to \left\langle \begin{matrix} 4213 \\ 1234 \end{matrix} \right\rangle \to \left\langle \begin{matrix} 1234 \\ 3241 \end{matrix} \right\rangle \to \left\langle \begin{matrix} 1234 \\ 3241 \end{matrix} \right\rangle = \pi^{-1}$

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- The **Symmetric group** of n items is denoted by $\mathcal{S}_n$

How neighborhoods and algebra relate to each other?

- Under **ASW**, all the neighbors of $\langle 2413 \rangle$ are:
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  - $\langle 2413 \rangle \circ \langle 2134 \rangle = \langle 4213 \rangle$
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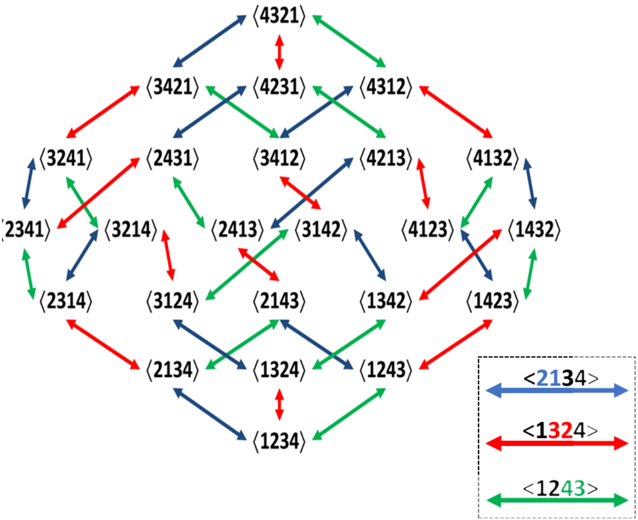
- Let $\sigma_1 = \langle 2134 \rangle$, $\sigma_2 = \langle 1324 \rangle$, $\sigma_3 = \langle 1243 \rangle$ and $\mathtt{ASW} = \{\sigma_1, \sigma_2, \sigma_3\}$ then:
  - $\mathtt{ASW} \subset \mathcal{S}_n$
  - $\mathtt{ASW}$ generates all the permutations in $\mathcal{S}_n$
  - any permutation can be factorized as a product of generators in ASW
  - $\mathcal{S}_n$ is a **finitely generated group**

Cayley graph for the ASW generating set



All the generating sets

- $\texttt{ASW} = \{\sigma_i : 1 \leq i < n\}$, where σ_i is the identity permutation with the items i and $i+1$ exchanged.
  Ex: $\langle 13245 \rangle$ swaps 2nd and 3rd items
  Distance induced: **Kendall's-τ distance**

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  Ex: $\langle 14235 \rangle$ shifts 4th item to 2nd position
  Distance induced: **Ulam distance**

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- $\texttt{REV} = \{\rho_{ij} : 1 \leq i < j \leq n\}$, where ρ_{ij} is the identity permutation where the chunk between positions i and j is reversed.
  Ex: $\langle 14325 \rangle$ reverses the chunk from 2nd to 4th positions
  Distance induced: **reversals' distance**

Relations among the generating sets

- $\mathtt{ASW}$ is a proper subset of $\mathtt{EXC}, \mathtt{INS}, \mathtt{REV}$
- $\mathtt{INS} \cap \mathtt{EXC} = \mathtt{ASW}$
- $\mathtt{INS} \cap \mathtt{REV} = \mathtt{ASW}$
- $\mathtt{EXC} \cap \mathtt{REV} = \mathtt{ASW} \cup \{\epsilon_{ij} \in \mathtt{EXC} : |i - j| = 2\}$
- $\mathtt{INS} = \mathtt{INS}_{\mathtt{bw}} \cup \mathtt{INS}_{\mathtt{fw}}$
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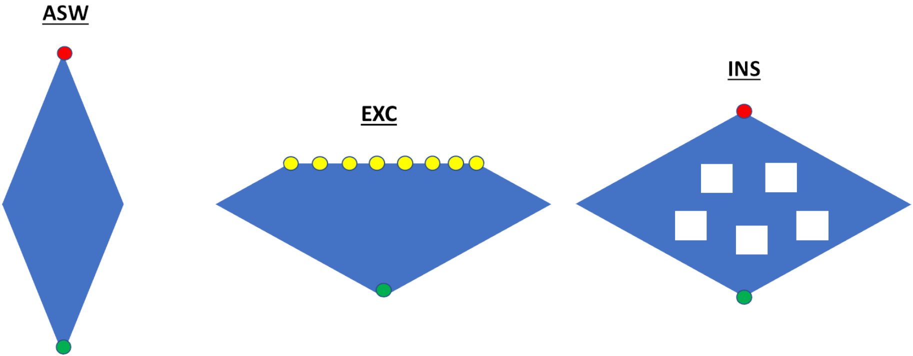
- Useful for:
  - Designing Variable Neighborhood Search algorithms
  - Designing perturbation step in Iterative Local Search algorithms
  - A priori smoothness estimation in Fitness Landscape Analysis

Properties of the generating sets

- **Cardinality** = number of neighbors
- **Diameter** of the Cayley graph (search space)
- **Number of longest permutations** (whose shortest-path distance from the identity equals the diameter)
- **Abstract convexity**: any permutation resides in a shortest path between the identity and a longest permutation?
- **Lattice** structure: *meet* and *join* are well defined?

GSet	Card.	Diameter	#Longest Perm.	Abst.Convex	Lattice
ASW	$n-1$	$\binom{n}{2}$	1	Yes	Yes
EXC	$\binom{n}{2}$	$n-1$	$(n-1)!$	Yes	No
INS	$(n-1)^2$	$n-1$	1	No	No
REV	$\binom{n}{2}$	$\leq n-1$	?	?	?

Visual intuitions about space structures



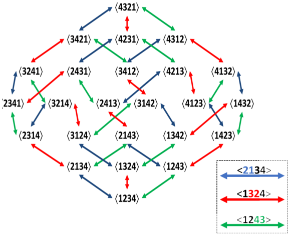
is the identity permutation

is the reversed identity

is a cyclic permutation

is a «hole» (due to «non-convexity»)

From simple search moves to composite search moves



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  = a *special* permutation
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  = **a generic permutation**
  (since a generating set generates the group)

- **Difference permutation** = composition of the **generators in a shortest path**

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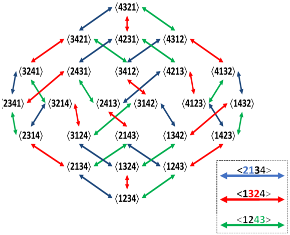

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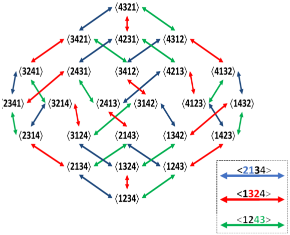

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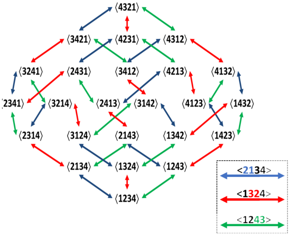

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- **Minimal factorization** of the difference permutation contains generators in a shortest path
- **Distance** = length of a shortest path = length of a minimal factorization of the difference permutation
- **Single representation for solutions and differences**
- **Strong analogy with points and vectors in the Euclidean space**

Equations of Motion in Continuous EAs

Can be consistently redefined for discrete spaces?

Differential Evolution (DE)

$$\boldsymbol{u} \leftarrow \boldsymbol{x_0} + F \cdot (\boldsymbol{x_1} - \boldsymbol{x_2})$$

where: $\boldsymbol{u}, \boldsymbol{x_0}, \boldsymbol{x_1}, \boldsymbol{x_2} \in \mathbb{R}^n$, while $F \in \mathbb{R}^+$

Particle Swarm Optimization (PSO)

$$v \leftarrow w \cdot \boldsymbol{v} + c_1 r_1 \cdot (\boldsymbol{p} - \boldsymbol{x}) + c_2 r_2 \cdot (\boldsymbol{g} - \boldsymbol{x})$$

$$\boldsymbol{x} \leftarrow \boldsymbol{x} + \boldsymbol{v}$$

where: $\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{p}, \boldsymbol{g} \in \mathbb{R}^n$, while $w, c_1, c_2, r_1, r_2 \in \mathbb{R}^+$

Continuous DE vs Algebraic DE

Differential mutation in action

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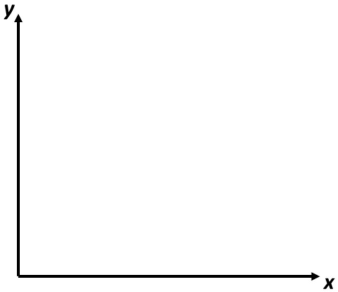
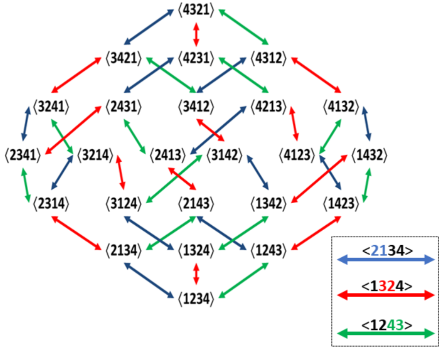


Algebraic DE

$$\upsilon \leftarrow \pi_0 \oplus F \odot (\pi_1 \ominus \pi_2)$$



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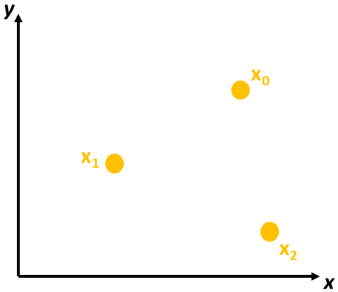

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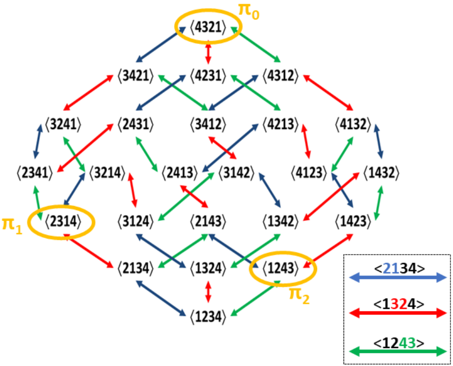

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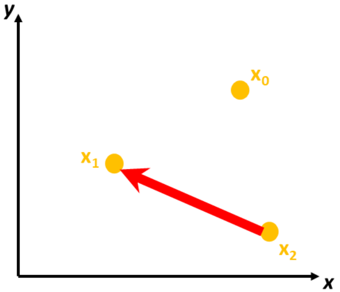

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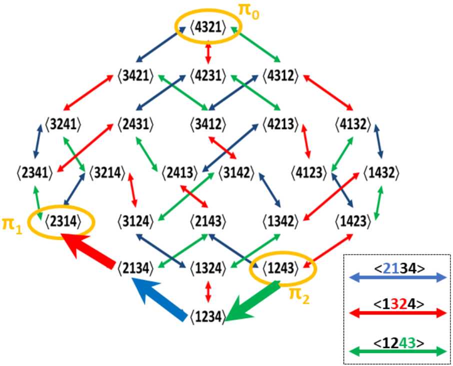

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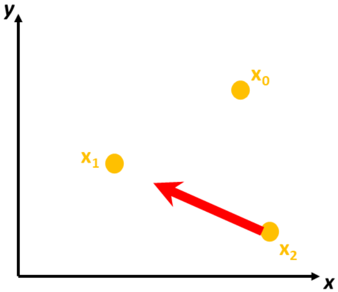

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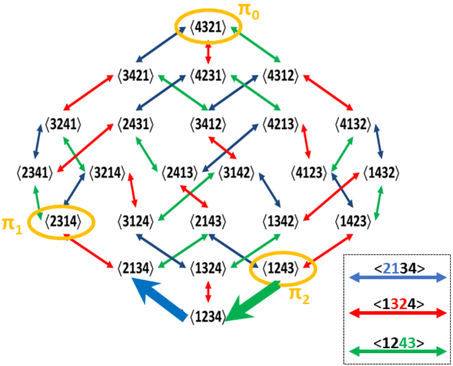

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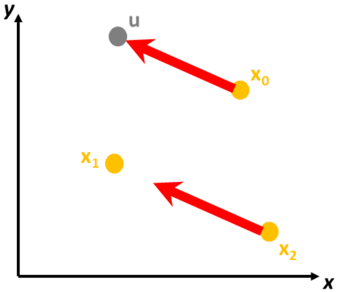

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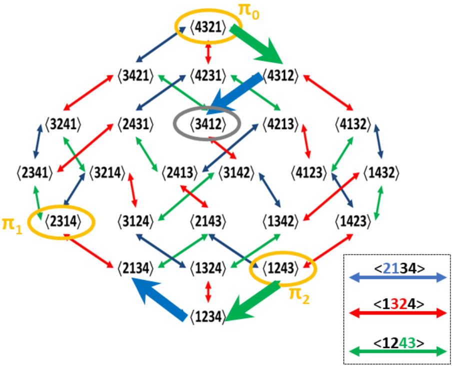

Algebraic Differential Evolution for Permutations

Classical continuous DE

The key operation of DE is the differential mutation which generates a mutant $u \in \mathbb{R}^n$ according to

$$u \leftarrow x_0 + F \cdot (x_1 - x_2)$$

where $x_0, x_1, x_2 \in \mathbb{R}^n$ are three distinct population individuals and $F > 0$ is the *scale factor parameter* of DE.

Algebraic DE for Permutations (ADEP)

The key operation of ADEP is the differential mutation which generates a mutant $\upsilon \in \mathcal{S}_n$ according to

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Algebraic Framework for Permutations

Discrete operators for equations of motion in EAs

Let:

- $\mathtt{ASW}_n = \{\sigma_1, \ldots, \sigma_{n-1}\}$ be the "adjacent swap" generators of $\mathcal{S}_n$
- $\pi, \rho \in \mathcal{S}_n$
- $\langle \sigma_{i_1}, \ldots, \sigma_{i_k}, \ldots, \sigma_{i_l} \rangle$ be a minimal factorization of π whose length is l
- $a \in [0, 1]$

Discrete operators are defined as follows:

- $\pi \oplus \rho := \pi \circ \rho$
- $\pi \ominus \rho := \rho^{-1} \circ \pi$
- $a \odot \pi := \sigma_{i_1} \circ \cdots \circ \sigma_{i_k}$, with $k = \lceil a \cdot l \rceil$

Discrete sum and difference

- Algebraically, they **do not rely on the chosen generating set**
- They are **deterministic**
- They are **consistent to each other**:

$$\pi = \rho \oplus (\pi \ominus \rho) = \rho \circ (\rho^{-1} \circ \pi) = \pi$$

Discrete scalar multiplication

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- Choose one at random $\implies$ **stochastic operator**
- A **stochastic factorization algorithm** is required for every generating set

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  Then:
  - sort the input permutation by only using the chosen moves/generators;
  - keep track of the sequence of selected generators;
  - reverse such sequence and invert every generator;

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- **(REV)** `RandRS`: randomized variant of the Kececioglu-Sankoff algorithm
  Reduces the **number of breakpoints** by only applying reversals.
  Complexity: $\Theta(n^2)$, Optimal: no

How much random we are?

- All the stochastic factorization algorithms perform a **random walk in the sub-graph** formed by the union of all the shortest paths from the identity to the permutation to factorize.
- **Cannot increase entropy** (over the set of minimal factorizations) without increasing computational complexity.

Multiplication by any positive scalar?

- Let $\pi, \rho \in \mathcal{S}_n$ and $a \geq 0$
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- **In line with the geometric interpretation of the Euclidean space** (use L2 norm and linear dependency among vectors)
- Computation when $a \geq 1$: take a shortest path of the inputted permutation and extend it in such way that the extended path is a shortest path in its own, thus the endpoint permutation is the result.

Issues when $a > 1$

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- **Motivation1**: Search space is finite
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- **Issue2**: $a \odot \pi$ may not exists for any $\pi \in \mathcal{S}_n$ when `INS` is used (because of the non-convexity)
- **Motivation2**: *longest increasing subsequence* cannot always be reduced by *shifting away* an item
- **Solution2**: **reverse, consider the longest decreasing subsequence, reverse again** $\implies$ it is like using a surrogate weight which is in (non-strict) monotonic relation with the `INS` weight

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  - **Enumerable subset of real vectors**
    whose entries are "multiples" of a chosen constant $\hbar > 0$
    Operator: $+$
    Generators: vectors with all 0s except one $\pm\hbar$ entry
    Pushing $\hbar \to 0$ tends to replicate the continuous behaviour in discretized equations of motion

Properties of $\oplus, \ominus, \odot$

- Properties which are satisfied:
  (X is the discrete set of solutions, e.g. permutations)

  (i) $\oplus$ is associative;
  (ii) $\oplus$ is commutative iff $\circ$ is commutative;
  (iii) e is the neutral element for $\oplus$;
  (iv) $x \oplus x^{-1} = x^{-1} \oplus x = e$ for each $x \in X$;
  (v) $1 \odot x = x$ for each $x \in X$;
  (vi) $a \odot (b \odot x) = (ab) \odot x$ for each $x \in X$ and $a, b \geq 0$;
  (vii) $0 \odot x = e$ for each $x \in X$;
  (viii) $x \oplus (y \ominus x) = y$ for each $x, y \in X$.

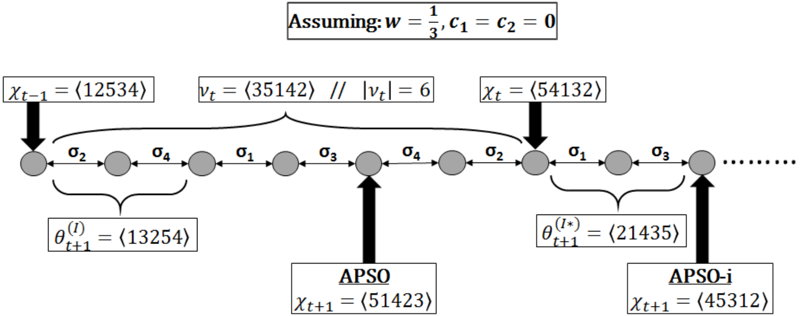
- **Distributive properties are missing**

$$w \odot \nu \neq [(1 + w) \odot \nu] \ominus \nu$$

  where $w \geq 0$ and $\nu \in \mathcal{S}_n$.
  Caution on PSO inertial term

Inertia-preserving Algebraic PSO

- Replace the inertial term $\theta^{(I)} = w \odot \nu$ with $\theta^{(I*)} = [(1+w) \odot \nu] \ominus \nu$



Algebraic Crossover

- **Continuous arithmetic crossover** are convex combinations:
  - $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ are the **parents**
  - $a, b \geq 0$ s.t. $a + b = 1$ are crossover **parameters**
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$$z = \begin{cases} y \oplus a \odot (x \ominus y) & \text{with prob. } 0.5 \\ x \oplus b \odot (y \ominus x) & \text{with prob. } 0.5 \end{cases}$$

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- If greedy strategies are employed $\Longrightarrow$ **Path Relinking**

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- AX has the **Radcliffe properties**:
  - a precedence in z is a precedence in x or y (**AX transmits precedences**)
  - common precedences of x and y are precedences in z (**AX is respectful**)
  - $[x, y]$ contains permutations formed by all the consistent combinations of the precedences in x and y (**AX is assorting** if the scalar parameter is chosen randomly)

Further possibilities

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- **Cycle structure**: interesting for TSP and VRP (future work)

... but is it working?

- ADE and APSO significantly outperform the naive DE and PSO equipped with the popular random-key decoder on a variety of benchmarks (Santucci, Baioletti, & Milani, 2019; Santucci et al., 2020)
- ADE obtained:
  - state-of-the-art results on the PFSP, LOPCC and MDTWNPP (Baioletti et al., 2020b; Santucci et al., 2016; Santucci, Baioletti, Di Bari, et al., 2019)
  - competitive results on the LOP, TSP and SRLFP (Baioletti et al., 2015; Baioletti, Milani, Santucci, & Bartoccini, 2019; Di Bari et al., 2020)
  - peak results among EAs for Bayesian networks learning (Baioletti et al., 2018b)
- Algebraic crossovers are competitive with classical permutation crossover operators (Baioletti et al., 2018a)
- Representation as set of precedences allowed to obtain state-of-the-art results on the LOP (Santucci & Ceberio, 2020)
- Identify preferred pairs of items to exchange in order to exit basins of attraction of QAP instances (Baioletti, Milani, Santucci, & Tomassini, 2019)

Conclusions and Open Questions

- The rich algebraic structure of permutations can be fruitfully exploited for:
  - Study structure and properties of the search space
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- **Open questions**:
  - Can algebraic properties be used to derive expected runtime analyses?
  - Can algebraic properties be used to build a tunable instance generator for the permutation space?
  - Is a review article about EC for permutation problems useful to the community? :-)

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Thanks for the attention!!!

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