Evolutionary Diversity Optimization for Combinatorial Optimization

Tutorial at GECCO'22, Boston, USA

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Motivation

- Diversity plays a crucial role in evolutionary computation (EC)
- Diversity
  - prevents premature convergence
  - enables successful crossover
  - allows to compute sets of Pareto-optimal solutions for multi-objective problems

Diversity

- Majority of approaches consider diversity in obj. space.
- Ulrich/Thiele [UT11] considered diversity in search space (see, e. g., Tamara Ulrich's PhD thesis [Ulr12])
- Diversity with respect to other properties (features) could be useful in various domains.

Goal

- Compute a set of good solutions that differ in terms of interesting properties/features.

  Think of good designs that vary with respect to important properties.
- The goal is to maximize diversity for a set of high-quality solutions.

  This is different from the standard use of diversity in EC where diversity is used to avoid premature convergence.

Application Areas

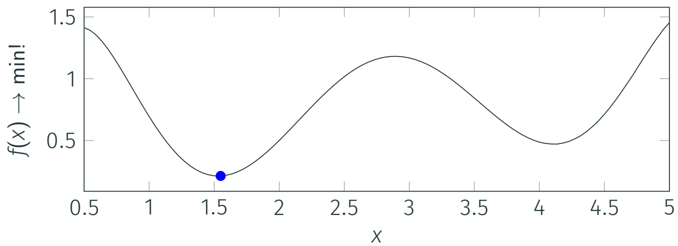
- Present set of diverse high-quality solutions (instead of single one) to enable discussion for further refinement.
- See how good solutions distribute with respect to important features of solutions.
- Understand algorithm performance with respect to important features through diverse instances.
- Construct diverse sets of problem instances or algorithm selection (AS).

Outline

Early Results by Ulrich & Thiele

Evolutionary Diversity Optimization (EDO)

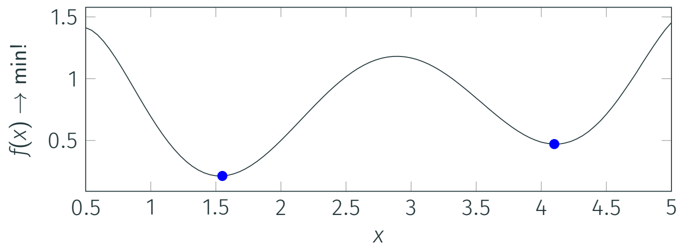
Illustration for single-obj. continuous function $f : \mathcal{X} \to \mathbb{R}$



Global Optimization: Find $x \in \mathcal{X}$ with $f(x) = \min_{x' \in \mathcal{X}} f(x)$.
$\leadsto$ EA: take best solution of n runs.

Evolutionary Diversity Optimization (EDO)

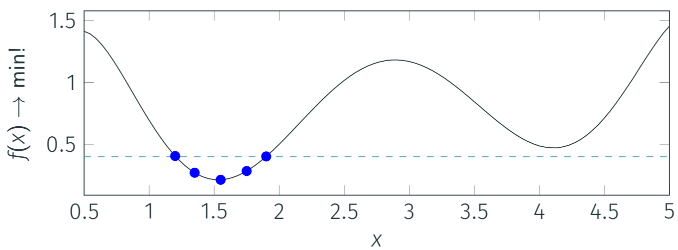
Illustration for single-obj. continuous function $f : \mathcal{X} \to \mathbb{R}$



Multi-Modal Optimization (hand-wavy): find subset $S \subseteq \mathcal{X}$ such that each $x \in S$ is locally (or globally) optimal.
$\leadsto$ EA: take several solutions of one or multiple runs.

Evolutionary Diversity Optimization (EDO)

Illustration for single-obj. continuous function $f : \mathcal{X} \to \mathbb{R}$



(Evol.) Diversity Optimization: Find set P of μ solutions such that

$$P = \arg\max_{P' \subseteq \mathcal{X}_v, |P'|=\mu} D(P') \text{ with } \mathcal{X}_v = \{x \in \mathcal{X} \mid f(x) \leq v\}$$

where $D : \mathcal{P}(\mathcal{X}) \to \mathbb{R}$ measures *diversity* in decision space.

Relation to Similar Approaches

Novelty Search (NS)

- Novelty Search [LS11; DLC19] algorithm only searches for behavioral diversity with no notion of quality.
- Behaviors that are maximally distant from previously discovered behaviors are rewarded.

Quality Diversity[1]

- QD algorithm [PSS16] is used to discover diverse optimal solutions.
- Capable of producing a large array of solutions constituting different low-dimensional behaviors / design features.
- Just recently used to find high-quality solutions for the Traveling Thief Problem [NNN21][2] and for TSP instance generation [BN22][3].

[1] https://www.youtube.com/watch?v=nyOPJxY--kA
[2] https://arxiv.org/abs/2112.08627
[3] https://arxiv.org/abs/2202.02077

Mixed Multi-Objective Optimization

Mixed Multi-Objective Optimization [4]

Goal: Find μ-size population P such that

$$P = \arg\max_{P' \subseteq \mathcal{X}_v, |P'|=\mu} D(P') \text{ with } \mathcal{X}_v = \{x \in \mathcal{X} \mid f(x) \leq v\}.$$

- *Fitness f* maps each individual to an objective value.
- *Diversity measure* $D : \mathcal{P}(\mathcal{X}) \to \mathbb{R}$ maps the whole solution set to an objective / diversity value.

[4] Tamara Ulrich and Lothar Thiele. "Maximizing population diversity in single-objective optimization". In: *13th Annual Genetic and Evolutionary Computation Conference, GECCO 2011, Proceedings, Dublin, Ireland, July 12-16, 2011*. Ed. by Natalio Krasnogor and Pier Luca Lanzi. ACM, 2011, pp. 641–648. DOI: 10.1145/2001576.2001665.

NOAH Algorithm

In a Nutshell

Three steps in each iteration:

1. **Optimize objective** f
   $\rightsquigarrow$ focus on generating good / better solutions.
2. **Adapt quality barrier** b
   $\rightsquigarrow$ balance objective and diversity optimization by maintaining a monotonically decreasing bound b.
3. **Optimize diversity** $D(P)$
   $\rightsquigarrow$ … under the constraint that all solutions stick to quality barrier.

Algorithm 1: Mixed Multi-Objective optimization algorithm NOAH [UT11]

Initialize population P with μ random solutions;
$b \leftarrow \infty$;
while ($b > v$) *and termination condition not satisfied* **do**
  $P \leftarrow \text{ObjOpt}(P, g, b)$; // Optimize f
  $(P, b) \leftarrow \text{BoundChange}(P, b, r)$; // Adapt quality threshold
  $P \leftarrow \text{DivOpt}(P, n, b, c)$; // Optimize diversity D
Return P;

A Suitable Diversity Measure

The authors use the following measure:

Solow-Polasky Diversity [SP94]

Given a μ-size population $P = \{P_1, \ldots, P_\mu\}$ and pairwise *distances* $d(P_i, P_j)$ for $1 \le i, j \le \mu$, let

$$M = [m_{ij}]_{1 \le i,j \le \mu} \text{ with } m_{ij} = \exp\left(-\theta \cdot d(P_i, P_j)\right).$$

Then the *Solow-Polasky measure* is given by

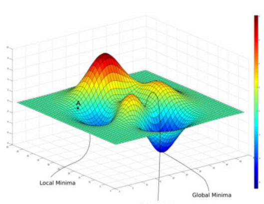
$$D(P) = \sum_{1 \le i,j \le \mu} M_{ij}^{-1} \in [1, \mu].$$

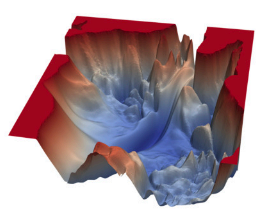
- $D(P)$ *"... can be interpreted as the number of different species found in the population ..."* [UT11].
- Choice of θ not critical under reasonable assumptions.
- Reasonable computational complexity.

Quality Diversity

Quality Diversity (QD)

1. Produce many solutions with a diverse set of features/behaviors.
2. Computing the high quality of solutions.



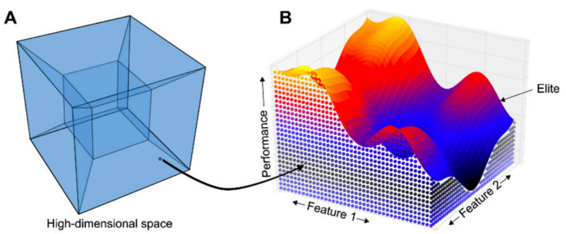


Novelty Search and Local Competition

- Novelty Search (NS) [LS11] algorithm only searches for behavioral diversity.
- Behaviors that are maximally distant from previously discovered behaviors are rewarded.
- NS uses the k-nearest-neighbor (k-NN) algorithm and local fitness completions score.

MAP-Elites

- The *Multi-Dimensional Archive of Phenotypic Elites algorithm* (MAP-Elites; [Mouret]) produces a large diversity of high-performing and qualitatively different solutions.
- The descriptor space is discretize and represented as a grid to form the collection of solutions.



EDO for TSP Instance Generation

Motivation and Goals

- Heuristic algorithms perform very well in many situations.
- Understanding the conditions under which heuristics perform well is curcial for ...
  1. Understanding strengths and weaknesses of said algorithm ⇝ may lead to, e.g., better operator design.
  2. *Automated per instance Algorithm Selection* (AS).

Automated Algorithm Selection

Originally proposed by Rice [Ric76]:

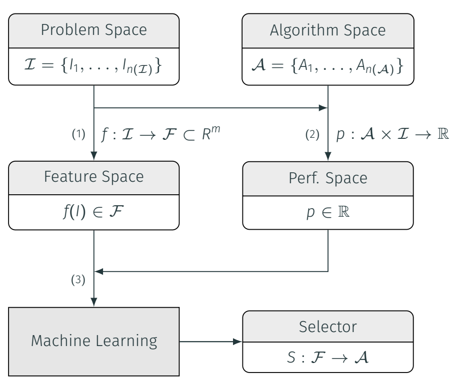


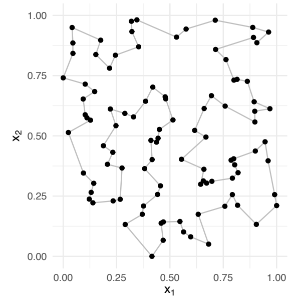
Figure 1: Schema of model building phase of the algorithm selection model with characterizing features. Loosely inspired by Figure 3 in [Ric76].

The Travailing Salesperson Problem

Traveling Salesperson Problem (TSP)

Given a set of n nodes V and pairwise distances $d(v_i, v_j)$ we aim for minimum length round-trip tour, i.e., a permutation $\pi = (\pi_1, \ldots, \pi_n)$ that minimizes

$$TSP(\pi) = d(\pi_n, \pi_1) + \sum_{i=1}^{n-1} d(\pi_i, \pi_{i+1}).$$



TSP Instance Features

It is reasonable to assume that (TSP) solver performance is strongly impacted by structural properties of TSP instances[5] such as:

- The number of nodes.
- Existence of groups / clusters.
- Summary statistics of pairwise distances.
- Number of weak / strong connected components of the k-Nearest Neighbor Graph (k-NNG).
- ...

[5] Imagine a TSP instance where all nodes are aligned on a cycle. Easy for almost all solvers!

Easy and Hard TSP Instances

Q: How do easy (hard) TSP instances for a heuristic, say 2-Opt, look like in feature space?

- If we know that certain feature values / ranges make an instance hard, we could try to construct instances with such feature values
  $\rightsquigarrow$ this is very difficult in general [SHL10]
- Construct by mathematical reasoning
  $\rightsquigarrow$ tedious task; often very artificial instances.
- Let EAs do the work[SHL10; Mer+12; Nal+13]: start with a random instance, perform minor perturbation and optimize the approximation ratio

$$\alpha_A(I) = \frac{A(I)}{OPT(I)}.$$

Diversity in TSP Feature Space

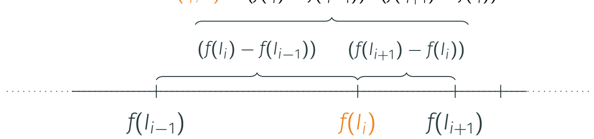
Problem

Feature space range covered by evolved instances rather small in classical approaches, e.g. in [Mer+12].

Measuring Diversity [GNN16]

Let $I_1, \ldots, I_\mu$ be the elements of the population and $f(I_1), \ldots, f(I_k) \in [0, R]$ their feature values. Further assume that $f(I_1) \leq f(I_2) \leq \ldots \leq f(I_\mu)$. Let I_i be such that $f(I_i) \neq f(I_1)$ and $f(I_i) \neq f(I_\mu)$. Then we set the *feature-based diversity contribution* as

$$d(I_i, P) = (f(I_i) - f(I_{i-1})) \cdot (f(I_{i+1}) - f(I_i))$$



TSP Feature Diversity - Results

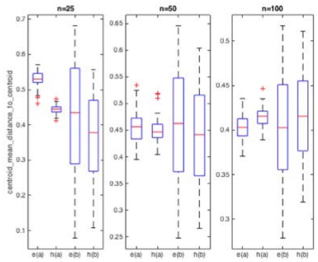


Figure 2: Distribution of feature `centroid_mean_distance_to_centroid` feature values of a population consisting of 100 different hard or easy TSP instances. e=easy, h=hard, a=classical, b=diversity.

More TSP Diversity: A Different Approach

Problem

Evolved instances, though different in feature space, "look" very similar.[6]

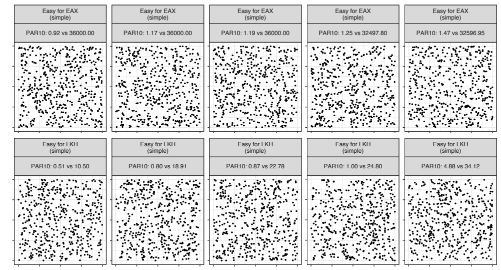


Figure 3: Each 5 instances that are easy for EAX and hard for LKH (top) and vice versa (bottom).

[6] In fact they look more or less random uniform.

More TSP Diversity: A Different Approach

Creative Mutation Operators [Bos+19]

No explicit diversity preservation / focus in the EA at all. Instead, modify the mutation operators such that they have a much higher impact on the points.

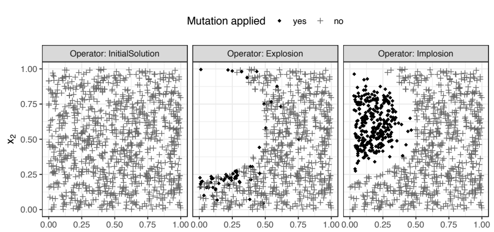


Figure 4: Explosion and implosion operators.

More TSP Diversity: A Different Approach (cont.)

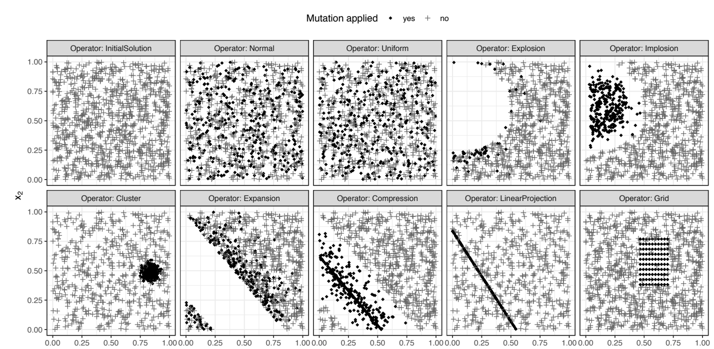


Figure 5: All operators proposed in [Bos+19].

A Different Approach: Some Results

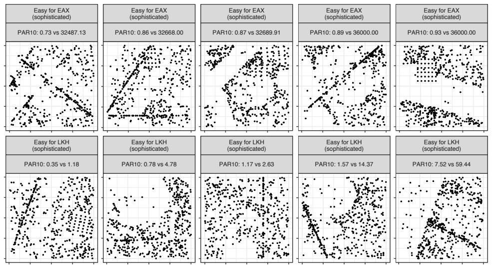


Figure 6: Each 5 instances that are easy for EAX and hard for LKH (top) and vice versa (bottom) evolved by using the new mutation operators.

EDO for Images

A Different Approach: Some Results

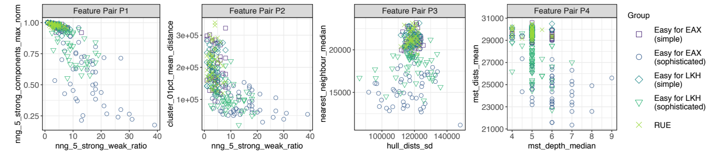
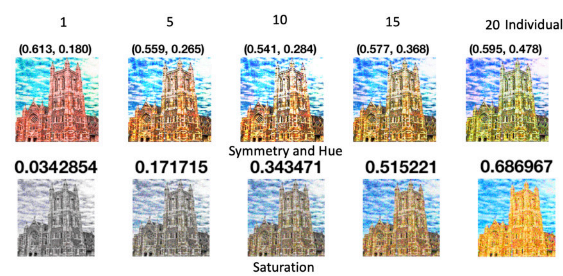


Figure 7: Evolved instances in different feature spaces spanned by each two features with classical operators (simple) and new operators (sophisticated).

EDO for Images: Key Idea

- Produce diverse image sets using evolutionary computation methods [AKN17].
- Use a $(\mu + \lambda)$-EA_D for evolving image instances.
- Select the individuals based on their contribution to diversity of the image.



EDO for Images

- We use a $(\mu + \lambda)$-EA_D for evolving image instances.
- Knowledge on how we can combine different image features to produce interesting image effects.
- Study how different combinations of image features correlate when images are evolved to maximize diversity.

The $(\mu + \lambda$-EA_D

Algorithm: Diversity maximizing $(\mu + \lambda)$ EA_D [AKN17]

```
Input: An image S
Output: A population P = {I_1, ..., I_μ} of image variants.
P ← {mutate(S), ..., mutate(S)};
;                                  // μ mutated copies of source
repeat
    Randomly select C ⊆ P where |C| = λ;
    for I ∈ C do
        Produce I' = mutate(I);
        if valid(I') then
            add I' to P;
    while |P| > μ do
        Remove an individual I = arg min_{J∈P} d(J, P);
until termination condition reached;
```

Feature Diversity Measure

Measuring Diversity [GNN16]

Let $I_1, \ldots, I_\mu$ be the elements of the population and $f(I_1), \ldots, f(I_k) \in [0, R]$ their feature values. Further assume that $f(I_1) \leq f(I_2) \leq \ldots \leq f(I_\mu)$. Let I_i be such that $f(I_i) \neq f(I_1)$ and $f(I_i) \neq f(I_\mu)$. Then we set the *feature-based diversity contribution* as

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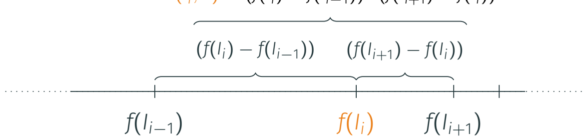
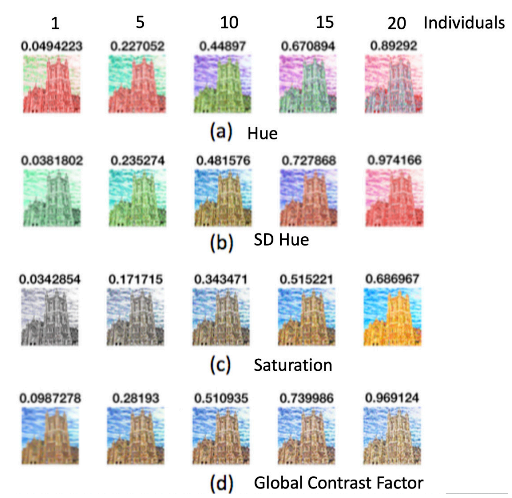
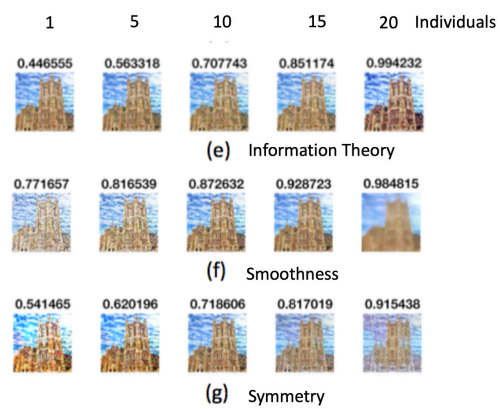


Single-Dim. Feature Experiments



Single-Dim. Feature Experiments



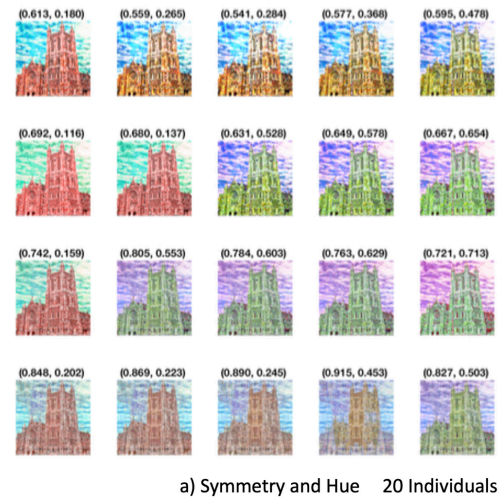
Multiple Features

- For 2 or more features, weightening of diversity contributions might not lead to good diversity.
- Results depend on chosen weightening.

Questions

- What is a good diversity measure?
- What is the diversity optimization goal?

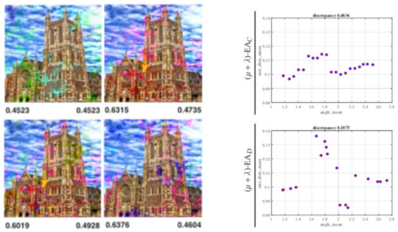
Two-Dim. Feature Experiments



Discrepancy-Based EDO

Discrepancy-Based EDO: Goal and Key Idea

- Design new approach of discrepancy-based EDO [Neu+18].
- Construct sets of solutions for evolved images and instances of the TSP.



Discrepancy-Based EDO

- New approach for discrepancy-based evolutionary diversity optimization.
- Investigate the use of the star discrepancy measure for diversity optimization for images.
- Introduce an adaptive random walk mutation operator based on random walks.
- Compare to other approaches for images [AKN17].

Discrepancy-Based EDO: Example Runs

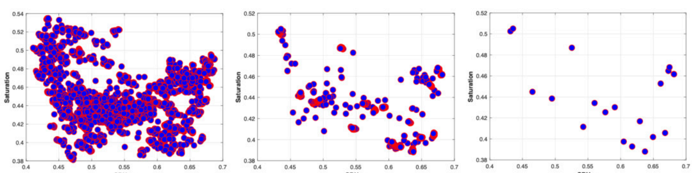


Figure 3: All feature vectors generated in 10 runs of $(\mu + \lambda)$-EA_T with 1000 iterations each (left), one run with 1000 iterations (middle), the final population after 1000 iteration with discrepancy 0.22637 (right).

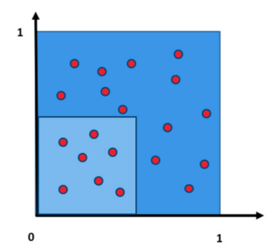
Star Discrepancy

Given a set for points $X = \{s^1, \dots, s^n\} \subseteq S$ with $S = [0,1]^d$. Let

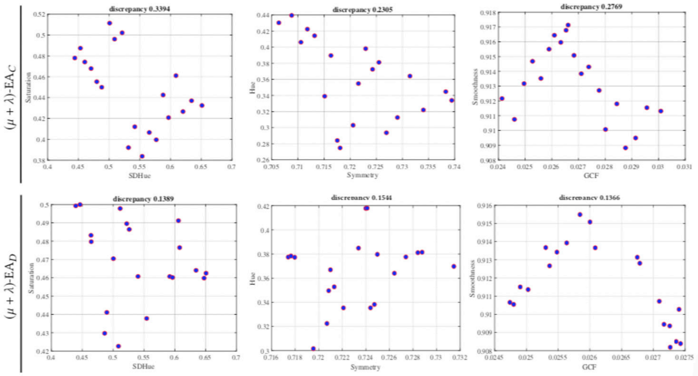
$$, [a,b] := [a_1, b_1] \times \dots \times [a_d, b_d].$$

Then, the *star discrepancy* is defined as

$$D(X, \mathcal{B}) := \sup\{\mathrm{Vol}([a,b]) - |X \cap [a,b]|/n \mid a \leq b \in [0,1]^d\}$$



Discrepancy-Based EDO for Images



Discrepancy-Based EDO for Images

	$(\mu+\lambda)$-EA_C(1)				$(\mu+\lambda)$-EA_D (2)				$(\mu+\lambda)$-EA_T(3)			
	min	mean	std	stat	min	mean	std	stat	min	mean	std	stat
(f1, f2)	0.2014	0.3234	0.0595	$2^{(-)},3^{(-)}$	0.1272	0.2038	0.1157	$1^{(+)}$	0.1119	0.1530	0.0269	$1^{(+)}$
(f3, f4)	0.1964	0.2945	0.0497	$2^{(-)},3^{(-)}$	0.1574	0.2280	0.0592	$1^{(+)},3^{(-)}$	0.1051	0.1417	0.0179	$1^{(+)},2^{(+)}$
(f5, f6)	0.1997	0.2769	0.0344	$2^{(-)},3^{(-)}$	0.1363	0.2025	0.0538	$1^{(+)}$	0.1457	0.1800	0.0234	$1^{(+)}$
(f1, f2, f3)	0.3389	0.4327	0.0613	$2^{(-)},3^{(-)}$	0.1513	0.3335	0.1062	$1^{(+)}$	0.2253	0.2814	0.0422	$1^{(+)}$
(f1, f4, f3)	0.2754	0.3395	0.0483	$2^{(-)},3^{(-)}$	0.2100	0.3118	0.1309	$1^{(+)}$	0.2224	0.2600	0.0123	$1^{(+)}$
(f5, f4, f2)	0.4775	0.6488	0.0841	$2^{(-)},3^{(-)}$	0.2021	0.3007	0.1467	$1^{(+)}$	0.1983	0.2229	0.0125	$1^{(+)}$

Discrepancy-Based EDO for TSP

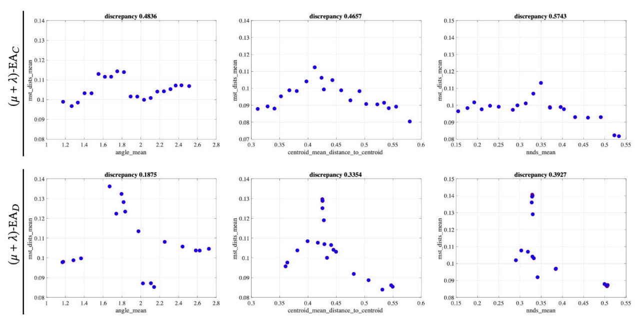


Figure 5: Feature vectors for final population of $(\mu+\lambda)$-EA$_C$ (top) and $(\mu+\lambda)$-EA$_D$ (bottom) for TSP based on two feature from left to right: (angle_mean, mst_dists_mean), (centroid_mean_distance_to_centroid, mst_dists_mean), (nnds_mean, mst_dists_mean)

Discrepancy-Based EDO for TSP

	$(\mu+\lambda)$-EA_C				$(\mu+\lambda)$-EA_D				$(\mu+\lambda)$-EA_T			
	min	mean	std	stat	min	mean	std	stat	min	mean	std	stat
(f1,f4)	0.4836	0.5535	0.0362	$2^{(-)},3^{(-)}$	0.2229	0.2942	0.0512	$1^{(+)},3^{(-)}$	0.2013	0.2354	0.0252	$1^{(+)},2^{(+)}$
(f2, f4)	0.4657	0.5192	0.0256	$2^{(-)},3^{(-)}$	0.3229	0.3708	0.0414	$1^{(+)},3^{(-)}$	0.2816	0.3363	0.0435	$1^{(+)},2^{(+)}$
(f3, f4)	0.5743	0.6296	0.0219	$2^{(-)},3^{(-)}$	0.3590	0.4422	0.0534	$1^{(+)}$	0.3831	0.4113	0.0175	$1^{(+)}$
(f1, f3, f4)	0.7765	0.7997	0.0204	$2^{(-)},3^{(-)}$	0.4303	0.4585	0.0183	$1^{(+)}$	0.4372	0.4604	0.0422	$1^{(+)}$
(f2, f3, f4)	0.7641	0.7962	0.0198	$2^{(-)},3^{(-)}$	0.4197	0.4563	0.0215	$1^{(+)}$	0.3730	0.4514	0.0327	$1^{(+)}$
(f1, f2, f3)	0.7593	0.7836	0.0111	$2^{(-)},3^{(-)}$	0.3900	0.4095	0.0160	$1^{(+)}$	0.3547	0.3988	0.0217	$1^{(+)}$

Table 2: Statistics of discrepancy values for TSP. f1, f2, f3, f4 denote the feature angle_mean, centroid_mean_dist_centroid, nnds_mean, mst_dists_mean respectively.

Multi-Objective Indicator-Based EDO

Multi-Objective Performance Indicators

Popular indicators in the field are given an approximation set S and a reference set R / reference point r:

- **Dominated Hypervolumne** (HYP):

$$\text{HYP}(S, r) := \text{VOL}\left(\bigcup_{s \in S} [r_1, s_1] \times \ldots \times [r_d, s_d]\right)$$

- **Inverted Generational Distance** (IGD):

$$\text{IGD}(S, R) := \frac{1}{|R|} \sum_{r \in R} \min_{s \in S} d(r, s)$$

- **Additive ε-Indicator** (EPS):

$$\text{EPS}(S, R) := \max_{r \in R} \min_{s \in S} \max_{1 \le i \le d} (s_i - r_i)$$

Indicator-Based MOO

- Let I be a search point
  - Let $f : \mathcal{X} \to \mathbb{R}^d$ be a function that assigns to each search point $I \in \mathcal{X}$ an objective vector.
  - Let $q : \mathcal{X} \to \mathbb{R}$ be a function that measures constraint violations.
  - We require $q(I) \ge \alpha$ for all ”good” solutions.
- A multi-objective (MO) indicator $D : 2^{\mathcal{X}} \to \mathbb{R}$ measures the quality of a given set of search points.

Goal

Compute set $P = \{I_1, \ldots, I_\mu\}$ of μ solutions maximizing (minimizing) D among all sets of μ solutions under the condition that $q(I) \ge \alpha$ holds for all $I \in P$, where α is a given quality threshold.

Idea: How to Use MO-Indicators for EDO?

- Diversity optimization aims to compute a diverse set of solutions for a given single-objective problem.
- Multi-objective indicators guide the search towards a diverse set of Pareto-optimal solutions.

Use of multi-objective indicators [Neu+19]:

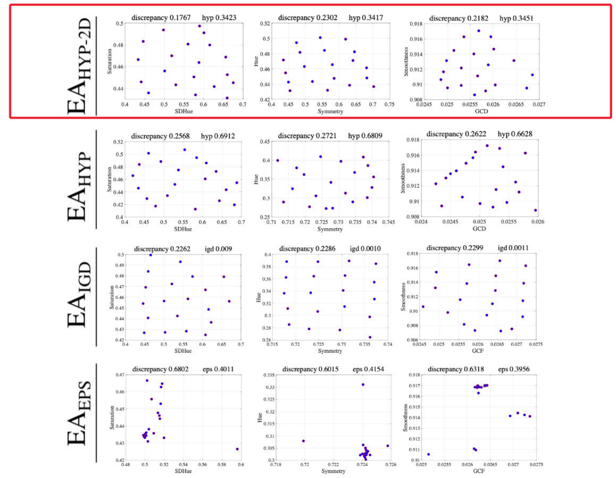
- Transform feature vectors of search points to make them (artificially) incomparable.
- Apply multi-objective indicators after transformation has occurred.

Generic Algorithm

Algorithm 3: Diversity maximizing $(\mu + \lambda)$ EA [Neu+19]

1. Initialize the population P with μ instances of quality at least α;
2. Let $C \subseteq P$ where $|C| = \lambda$;
3. For each $I \in C$, produce an offspring I' of I by mutation. If $q(I') \geq \alpha$, add I' to P;
4. While $|P| > \mu$, remove the individual with the smallest loss to the diversity indicators D;
5. Repeat steps 2 to 4 until a termination criterion is reached;

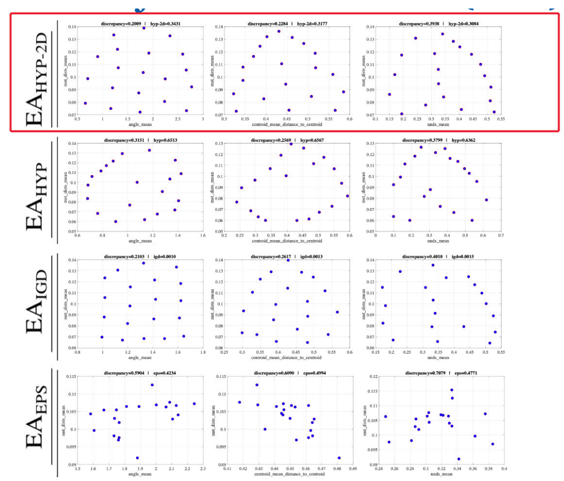
MO-Indicator-Based EDO for Images



MO-Indicator-Based EDO for Images

		$EA_{HYP\text{-}2D}$ (1)			EA_{HYP} (2)			EA_{IGD} (3)			EA_{EPS} (4)			EA_{DIS} (5)		
		mean	st	stat	mean	st	stat	mean	st	stat	mean	st	stat	mean	st	stat
HYP-2D	f_1,f_2	0.347	0.004	$4^{(+)},5^{(+)}$	0.382	0.007	$3^{(+)},4^{(+)},5^{(+)}$	0.335	0.003	$2^{(-)},5^{(+)}$	0.198	0.019	$1^{(-)},2^{(-)}$	0.112	0.030	$1^{(-)},2^{(-)},3^{(-)}$
	f_3,f_4	0.344	0.004	$2^{(+)},4^{(+)},5^{(+)}$	0.268	0.014	$1^{(-)},3^{(-)},4^{(+)},5^{(+)}$	0.339	0.004	$2^{(+)},4^{(+)},5^{(+)}$	0.221	0.015	$1^{(-)},2^{(-)},3^{(-)}$	0.105	0.025	$1^{(-)},2^{(-)},3^{(-)}$
	f_5,f_6	0.350	0.007	$2^{(+)},3^{(+)},4^{(+)},5^{(+)}$	0.342	0.004	$1^{(-)},4^{(+)},5^{(+)}$	0.332	0.004	$1^{(-)},4^{(+)},5^{(+)}$	0.220	0.045	$1^{(-)},2^{(-)},3^{(-)}$	0.134	0.016	$1^{(-)},2^{(-)},3^{(-)}$
HYP	f_1,f_2	0.525	0.012	$3^{(+)},4^{(+)},5^{(+)}$	0.693	0.013	$3^{(+)},4^{(+)},5^{(+)}$	0.374	0.006	$1^{(-)},2^{(-)},4^{(+)}$	0.344	0.003	$1^{(-)},2^{(-)},3^{(-)}$	0.363	0.014	$1^{(-)},2^{(-)}$
	f_3,f_4	0.500	0.007	$3^{(+)},4^{(+)},5^{(+)}$	0.681	0.010	$3^{(+)},4^{(+)},5^{(+)}$	0.268	0.072	$1^{(-)},2^{(-)},4^{(+)},5^{(+)}$	0.280	0.010	$1^{(-)},2^{(-)},3^{(-)}$	0.267	0.014	$1^{(-)},2^{(-)},3^{(-)}$
	f_5,f_6	0.518	0.012	$2^{(-)},4^{(+)},5^{(+)}$	0.663	0.010	$1^{(+)},3^{(+)},4^{(+)},5^{(+)}$	0.335	0.004	$2^{(-)},4^{(+)}$	0.317	0.006	$1^{(-)},2^{(-)},3^{(-)}$	0.327	0.008	$1^{(-)},2^{(-)}$
IGD	f_1,f_2	0.001	0.335	$2^{(+)},4^{(+)},5^{(+)}$	0.003	0.000	$1^{(-)},3^{(-)}$	0.001	0.000	$2^{(+)},4^{(+)},5^{(+)}$	0.003	0.000	$1^{(-)},3^{(-)},5^{(+)}$	0.005	0.001	$1^{(-)},3^{(-)},4^{(-)}$
	f_3,f_4	0.001	0.339	$2^{(+)},4^{(+)},5^{(+)}$	0.004	0.000	$1^{(-)},3^{(-)},5^{(+)}$	0.001	0.000	$2^{(+)},4^{(+)},5^{(+)}$	0.003	0.000	$1^{(-)},3^{(-)},5^{(+)}$	0.005	0.001	$1^{(-)},2^{(-)},3^{(-)},4^{(-)}$
	f_5,f_6	0.002	0.332	$2^{(+)},5^{(+)}$	0.007	0.000	$1^{(-)},3^{(-)},4^{(-)},5^{(-)}$	0.001	0.000	$2^{(+)},4^{(+)},5^{(+)}$	0.003	0.001	$2^{(+)},3^{(-)}$	0.004	0.001	$1^{(-)},2^{(+)},3^{(-)}$
EPS	f_1,f_2	0.190	0.198	$2^{(+)},4^{(+)},5^{(+)}$	0.498	0.011	$1^{(-)}, 3^{(-)}$	0.194	0.032	$2^{(+)},4^{(+)},5^{(+)}$	0.402	0.039	$1^{(-)},3^{(-)},5^{(+)}$	0.600	0.106	$1^{(-)},3^{(-)},4^{(-)}$
	f_3,f_4	0.198	0.221	$2^{(+)},4^{(+)},5^{(+)}$	0.569	0.016	$1^{(-)},3^{(-)}$	0.208	0.035	$2^{(+)},4^{(+)},5^{(+)}$	0.418	0.036	$1^{(-)},3^{(-)},5^{(+)}$	0.615	0.069	$1^{(-)},3^{(-)},4^{(-)}$
	f_5,f_6	0.125	0.220	$2^{(+)},4^{(+)},5^{(+)}$	0.946	0.001	$1^{(-)},3^{(-)},4^{(-)}$	0.225	0.064	$2^{(+)},4^{(+)},5^{(+)}$	0.397	0.110	$1^{(-)},2^{(+)},3^{(-)}$	0.587	0.063	$1^{(-)},3^{(-)}$
DIS	f_1,f_2	0.171	0.018	$2^{(+)},4^{(+)},5^{(+)}$	0.257	0.010	$1^{(-)},4^{(+)}$	0.201	0.031	$4^{(+)},5^{(+)}$	0.686	0.064	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.204	0.116	$1^{(-)},3^{(-)},4^{(+)}$
	f_3,f_4	0.234	0.031	$4^{(+)}$	0.273	0.041	$3^{(-)},4^{(+)},5^{(-)}$	0.198	0.017	$2^{(+)},4^{(+)}$	0.606	0.054	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.228	0.059	$2^{(+)},4^{(+)}$
	f_5,f_6	0.221	0.026	$4^{(+)}$	0.263	0.070	$3^{(-)},4^{(+)},5^{(-)}$	0.205	0.055	$2^{(+)},4^{(+)}$	0.633	0.158	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.203	0.054	$2^{(+)},4^{(+)}$

MO-Indicator-Based EDO for TSP



MO-Indicator-Based EDO for TSP

		$EA_{HYP\text{-}2D}$ (1)			EA_{HYP} (2)			EA_{IGD} (3)			EA_{EPS} (4)			EA_{DIS} (5)		
		mean	st	stat	mean	st	stat	mean	st	stat	mean	st	stat	mean	st	stat
HYP-2D	f_1,f_4	0.338	2E-3	$2^{(+)},4^{(+)},5^{(+)}$	0.309	4E-3	$1^{(-)},4^{(+)}$	0.331	3E-3	$4^{(+)},5^{(+)}$	0.190	1E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.256	1E-2	$1^{(-)},3^{(-)}$
	f_2,f_4	0.317	3E-3	$2^{(+)},4^{(+)},5^{(+)}$	0.303	5E-3	$1^{(-)},3^{(-)},4^{(+)}$	0.316	3E-3	$2^{(+)},4^{(+)},5^{(+)}$	0.178	1E-7	$1^{(-)},2^{(-)},3^{(-)}$	0.252	1E-2	$1^{(-)},3^{(-)}$
	f_3,f_4	0.303	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.296	5E-3	$1^{(-)},3^{(-)},4^{(+)},5^{(+)}$	0.304	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.190	2E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.238	2E-2	$1^{(-)},2^{(-)},3^{(-)}$
HYP	f_1,f_4	0.645	5E-3	$4^{(+)},5^{(+)}$	0.638	7E-3	$4^{(+)},5^{(+)}$	0.639	6E-3	$4^{(+)},5^{(+)}$	0.424	2E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.529	3E-2	$1^{(-)},2^{(-)},3^{(-)}$
	f_2,f_4	0.609	7E-3	$2^{(-)},4^{(+)},5^{(+)}$	0.632	1E-2	$1^{(+)},4^{(+)},5^{(+)}$	0.621	6E-3	$4^{(+)},5^{(+)}$	0.398	1E-6	$1^{(-)},2^{(-)},3^{(-)}$	0.505	2E-2	$1^{(-)},2^{(-)},3^{(-)}$
	f_3,f_4	0.584	3E-2	$2^{(-)},4^{(+)}$	0.621	9E-3	$1^{(+)},3^{(+)},4^{(+)},5^{(+)}$	0.595	4E-2	$2^{(-)},4^{(+)},5^{(+)}$	0.410	2E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.485	3E-2	$2^{(-)},3^{(-)}$
IGD	f_1,f_4	0.001	2E-5	$4^{(+)},5^{(+)}$	0.001	6E-5	$3^{(-)},4^{(+)}$	0.001	4E-5	$2^{(+)},4^{(+)},5^{(+)}$	0.003	2E-5	$1^{(-)},2^{(-)},3^{(-)}$	0.002	2E-4	$1^{(-)},3^{(-)}$
	f_2,f_4	0.001	3E-5	$2^{(+)},4^{(+)},5^{(+)}$	0.002	6E-5	$1^{(-)},3^{(-)},4^{(+)}$	0.001	3E-5	$2^{(+)},4^{(+)},5^{(+)}$	0.003	2E-10	$1^{(-)},2^{(-)},3^{(-)}$	0.002	2E-4	$1^{(-)},3^{(-)}$
	f_3,f_4	0.002	3E-4	$4^{(+)},5^{(+)}$	0.002	6E-5	$3^{(-)},4^{(+)},5^{(+)}$	0.002	3E-4	$2^{(+)},4^{(+)},5^{(+)}$	0.003	3E-5	$1^{(-)},2^{(-)},3^{(-)}$	0.003	3E-4	$1^{(-)},2^{(-)},3^{(-)}$
EPS	f_1,f_4	0.196	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.249	2E-2	$1^{(-)},3^{(-)},4^{(+)}$	0.189	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.423	1E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.345	4E-2	$1^{(-)},3^{(-)}$
	f_2,f_4	0.226	8E-3	$2^{(+)},4^{(+)},5^{(+)}$	0.256	2E-2	$1^{(-)},3^{(-)},4^{(+)},5^{(+)}$	0.228	1E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.499	2E-16	$1^{(-)},2^{(-)},3^{(-)}$	0.360	5E-2	$1^{(-)},2^{(-)},3^{(-)}$
	f_3,f_4	0.260	4E-2	$4^{(+)},5^{(+)}$	0.278	2E-2	$4^{(+)},5^{(+)}$	0.265	4E-2	$4^{(+)},5^{(+)}$	0.477	3E-3	$1^{(-)},2^{(-)},3^{(-)}$	0.368	5E-2	$1^{(-)},2^{(-)},3^{(-)}$
DIS	f_1,f_4	0.222	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.353	2E-2	$1^{(-)},3^{(-)},4^{(+)}$	0.249	2E-2	$2^{(+)},4^{(+)}$	0.589	4E-3	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.292	5E-2	$1^{(-)},4^{(+)}$
	f_2,f_4	0.230	2E-2	$2^{(+)},4^{(+)},5^{(+)}$	0.274	2E-2	$1^{(-)},4^{(+)},5^{(+)}$	0.252	1E-3	$4^{(+)},5^{(+)}$	0.609	1E-16	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.336	4E-2	$1^{(-)},2^{(-)},3^{(-)},4^{(+)}$
	f_3,f_4	0.418	6E-2	$4^{(+)}$	0.416	3E-2	$4^{(+)}$	0.401	7E-2	$4^{(+)},5^{(+)}$	0.719	6E-3	$1^{(-)},2^{(-)},3^{(-)},5^{(-)}$	0.448	9E-2	$3^{(-)},4^{(+)}$

Questions

- What type of features are good to characterize problem instances of a given problem (e.g. TSP) for a particular algorithm.
- What is a good diversity measure?
- What is the runtime behavior of EAs maximizing search-space/feature diversity?
- How do we compute diverse sets of high quality solutions for important combinatorial optimization problems?
- How do we adjust state of the art solver to compute diverse sets of solutions (instead of a single one)

Results

- We proposed a new approach for EDO.
- We demonstrated that multi-objective performance indicators can be used to achieve a good diversity of sets of solutions according to a given set of features.
- The advantages of our approaches are (i) their simplicity and (ii) the quality of diversity achieved as measured by the respective indicators.
- We have shown that the best performing approaches use HYP or IGD as indicators, and often even outperform the discrepancy-based approach.

Diversity Optimization for TSP Tours

TSP Tour Diversity

Motivation

- We already investigated feature-diversity of TSP instances.
- Now, we study the TSP in the context of diversity optimization by focusing on the diversity of tours themselves, not their qualities [Do+20].

Problem Formulation

We are given a (complete) edge-weighted graph $G = (V, E, c)$ with cost function $c : E \to \mathbb{R}^+$. Let $n = |V|, m = |E| = n(n-1)/2$. Given parameters $\mu \geq 2$ and $\alpha > 0$ find a population $P, |P| = \mu$, such that

$$c(T) \leq (1+\alpha)\text{OPT} \; \forall T \in P$$

and P is maximally diverse with respect to some diversity measure D.

Diversity maximizing $(\mu + 1)$ EA

Algorithm 4: Diversity maximizing $(\mu + 1)$ EA [Do+20]

1 Initialize the population P with μ TSP tours such that $c(T) \leq (1+\alpha) \cdot OPT$ for all $T \in P$;
2 Choose $T \in P$ uniformly at random and produce an offspring T' of T by mutation;
3 If $c(T') \leq (1+\alpha) \cdot OPT$, add T' to P;
4 If $|P| = \mu + 1$, remove exactly one individual T, where $T = \arg\min_{J \in P} D(P \setminus \{J\})$, from P;
5 Repeat steps 2 to 4 until a termination criterion is reached;

Maximizing Edge Diversity

Intuitively: Each edge should be used in as few tours as possible (in at most one tour if possible).

- **Edge Diversity (ED)**: Equalize frequencies of edges.

$$ED(P) = \sum_{T_1 \in P} \sum_{T_2 \in P} |E(T_1) \setminus E(T_2)| = \mu(\mu-1)n + \sum_i n_i - \sum_i n_i^2.$$

- **Pairwise Distances (PD)**: Equalizing pairwise edge distances between tours.

Theorem

For every pair of integers $\mu \geq 1$ and $n \geq 3$, given a complete graph $G = (V, E)$ where $|V| = n$, there is a μ-size population P of tours such that

$$\max_{e \in E}\{n(e, P)\} - \min_{e \in E}\{n(e, P)\} \leq 1.$$

Unconstrained Case

All tours meet the quality criterion ($\alpha = \infty$).

Table 1: Comparison in terms of diversity (gtype), the number of iterations (#iter) and results of statistical testing (stat) between variants with ED approach in unconstrained cases. The Kruskal-Wallis test and the Bonferroni correction method [4] are used on #iter. X^+ means the measure is larger than the one for variant X, X^- means smaller and X^* means no difference.

n	μ	2-OPT(1)					3-OPT(2)					4-OPT(3)				
		gtype	std	# iter	std	stat	gtype	std	# iter	std	stat	gtype	std	# iter	std	stat
50	3	100.00%	0.00	104.50	59.19	$2^+, 3^+$	100.00%	0.00	68.60	35.67	$1^-, 3^*$	100.00%	0.00	**54.37**	24.28	$1^-, 2^*$
	10	100.00%	0.00	**1635.80**	485.88	$2^*, 3^*$	100.00%	0.00	1808.43	484.96	$1^*, 3^*$	100.00%	0.00	1736.60	545.36	$1^*, 2^*$
	20	100.00%	0.00	**25383.03**	8594.81	$2^-, 3^-$	99.97%	0.02	49881.60	471.00	$1^+, 3^*$	99.93%	0.02	50000.00	0.00	$1^+, 2^*$
	50	99.99%	0.00	**125000.00**	0.00	$2^*, 3^*$	99.95%	0.00	**125000.00**	0.00	$1^*, 3^*$	99.93%	0.01	**125000.00**	0.00	$1^*, 2^*$
100	3	100.00%	0.00	170.83	98.50	$2^*, 3^+$	100.00%	0.00	137.53	69.76	$1^*, 3^*$	100.00%	0.00	**102.13**	58.69	$1^-, 2^*$
	10	100.00%	0.00	1901.73	632.60	$2^*, 3^+$	100.00%	0.00	1598.80	386.85	$1^*, 3^+$	100.00%	0.00	**1305.63**	343.38	$1^-, 2^-$
	20	100.00%	0.00	**8422.40**	1742.96	$2^-, 3^*$	100.00%	0.00	9902.63	1984.39	$1^+, 3^*$	100.00%	0.00	9414.27	2018.82	$1^*, 2^*$
	50	99.95%	0.00	**500000.00**	0.00	$2^*, 3^*$	99.86%	0.00	**500000.00**	0.00	$1^*, 3^*$	99.82%	0.01	**500000.00**	0.00	$1^*, 2^*$
200	3	100.00%	0.00	401.03	213.80	$2^+, 3^+$	100.00%	0.00	254.80	111.06	$1^-, 3^*$	100.00%	0.00	**197.60**	78.85	$1^-, 2^*$
	10	100.00%	0.00	3350.47	958.53	$2^+, 3^+$	100.00%	0.00	2261.10	570.16	$1^-, 3^*$	100.00%	0.00	**1888.87**	510.91	$1^-, 2^*$
	20	100.00%	0.00	10189.73	2233.72	$2^+, 3^+$	100.00%	0.00	8959.07	2242.66	$1^-, 3^*$	100.00%	0.00	**7901.73**	1286.07	$1^-, 2^*$
	50	100.00%	0.00	**76856.37**	14056.12	$2^-, 3^-$	100.00%	0.00	102039.53	17118.06	$1^+, 3^-$	100.00%	0.00	132837.73	25315.99	$1^+, 2^+$
500	3	100.00%	0.00	974.33	509.02	$2^+, 3^+$	100.00%	0.00	631.20	267.24	$1^-, 3^*$	100.00%	0.00	**560.77**	332.16	$1^-, 2^*$
	10	100.00%	0.00	6608.33	2298.31	$2^*, 3^+$	100.00%	0.00	5281.23	1729.61	$1^*, 3^+$	100.00%	0.00	**3537.07**	965.71	$1^-, 2^-$
	20	100.00%	0.00	20888.53	5343.92	$2^+, 3^+$	100.00%	0.00	15007.67	3265.35	$1^-, 3^+$	100.00%	0.00	**11821.93**	3388.06	$1^-, 2^-$
	50	100.00%	0.00	93280.70	17697.95	$2^+, 3^+$	100.00%	0.00	67817.73	13010.55	$1^-, 3^*$	100.00%	0.00	**64425.13**	9267.66	$1^-, 2^*$

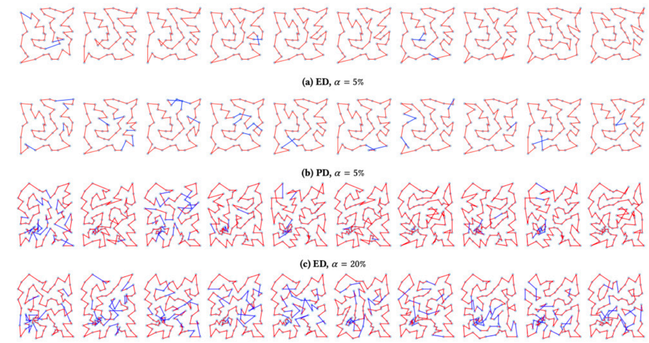
Constrained Case

Table 3: Comparison in terms of diversity (gtype) and pairwise edge distances ranges (ς) among all variants of the EA on TSPlib instances. Better values with statistical significance (based on Wilcoxon rank sum tests with 95% confidence threshold) between ED and PD are bold-faced.

			ED						PD					
	μ	α	2-OPT		3-OPT		4-OPT		2-OPT		3-OPT		4-OPT	
			gtype	ς	gtype	ς	gtype	ς	gtype	ς	gtype	ς	gtype	ς
eil51	3	0.05	34.27%	68.37%	36.23%	67.78%	28.95%	74.05%	32.07%	69.54%	35.95%	66.14%	29.78%	71.96%
		0.2	70.78%	31.83%	67.93%	35.03%	63.68%	40.46%	71.11%	30.20%	65.95%	35.75%	63.12%	38.56%
		0.5	93.83%	8.43%	90.85%	11.05%	90.78%	11.37%	93.62%	**7.12%**	90.26%	11.18%	90.37%	10.59%
		1	99.89%	0.13%	99.83%	0.26%	99.80%	0.33%	99.80%	0.33%	99.74%	0.65%	99.76%	0.52%
	10	0.05	**31.82%**	79.67%	**33.64%**	78.43%	27.79%	82.88%	29.37%	78.24%	31.60%	**75.95%**	27.65%	**79.61%**
		0.2	**63.04%**	70.39%	**60.60%**	67.12%	**57.78%**	63.40%	60.99%	**44.90%**	59.23%	**47.39%**	55.99%	**51.31%**
		0.5	**83.14%**	30.85%	**81.34%**	36.67%	**81.29%**	37.58%	82.00%	**20.33%**	80.12%	**23.01%**	79.87%	**23.99%**
		1	**95.06%**	10.26%	**94.14%**	11.76%	**94.19%**	11.63%	94.57%	**7.58%**	93.30%	**8.50%**	93.16%	**8.50%**
	20	0.05	**32.52%**	95.23%	**32.86%**	91.37%	**27.89%**	90.85%	29.20%	**82.42%**	31.23%	**79.08%**	26.45%	**83.53%**
		0.2	**62.32%**	92.09%	**59.98%**	91.57%	**57.46%**	91.70%	59.30%	**49.15%**	57.84%	**51.37%**	54.53%	**55.29%**
		0.5	**80.95%**	59.02%	**79.24%**	63.27%	**79.60%**	64.84%	79.03%	**25.29%**	77.69%	**27.84%**	77.32%	**29.08%**
		1	**92.17%**	19.87%	**91.41%**	22.42%	**91.58%**	21.31%	90.97%	**11.83%**	90.28%	**12.42%**	90.24%	**12.75%**
	50	0.05	**32.66%**	100.00%	**33.23%**	100.00%	**28.01%**	100.00%	29.81%	**85.88%**	31.75%	**82.48%**	26.93%	**85.95%**
		0.2	**63.26%**	99.48%	**61.52%**	97.78%	**58.92%**	96.99%	59.68%	**53.59%**	58.36%	**57.12%**	55.04%	**59.80%**
		0.5	**80.74%**	92.35%	**79.56%**	90.59%	**79.80%**	88.76%	79.15%	**29.67%**	78.12%	**32.29%**	77.94%	**33.66%**
		1	**91.65%**	48.95%	**91.25%**	52.68%	**91.33%**	48.37%	90.60%	**15.69%**	90.42%	**15.75%**	90.42%	**16.67%**

Outlook and Conclusions

Exemplary Populations



(a) ED, α = 5%

(b) PD, α = 5%

(c) ED, α = 20%

(d) PD, α = 20%

Figure 8: Visualized tour populations from resulted populations in eil51 cases with $\mu = 10$ and 2-OPT as mutation operator. Red edges are shared by at least two tours in the population, and blue ones are unique to the tour.

Outlook: runtime complexity

Theory: Runtime Results ☹

So far pretty sparse list of results:

- [GN14] study the maximization of population diversity on OneMax and LeadingOnes, [DGN16] for OneMinMax.
- [Do+21] studies EDO on permutation problem TSP and QAP, [BN21] on MSTs. More results on well-known combinatorial optimization problems desirable.
- One of the major challenges: given a diversity measure, how does a maximally diverse population of size μ look like?
- Call for participation ☺

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