

Sometimes going from 1 to 2 can be difficult ...
... and going from 2 to 3 can be difficult, too!

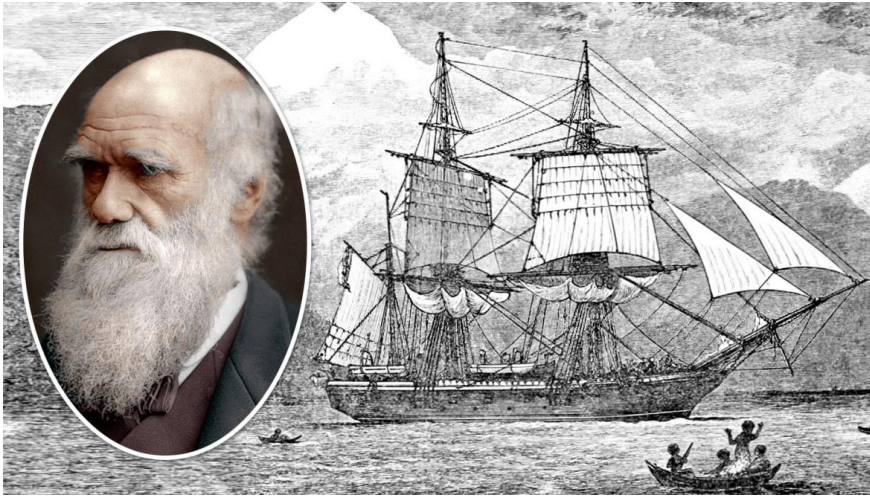
Generating Instances with Performance Differences for More Than Just Two Algorithms

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Code at <https://github.com/jakobbossek/GECCO2021-ECPERM-ttp-evolving>

200 years ago, Charles Darwin



Galápagos Islands

Islas Galápagos

4.6 ★★★★★ 2,344 reviews

Archipelago



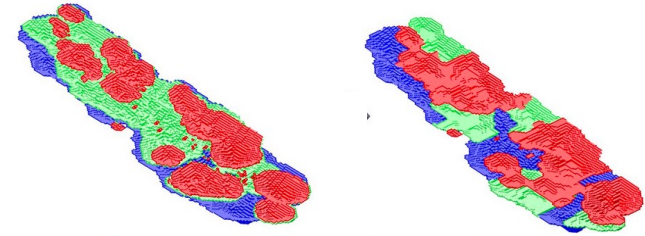
Four of Darwin's finches, clockwise (from top left):
Geospiza magnirostris, *Geospiza fortis*, *Certhidea fusca*, *Camarhynchus parvulus*

Each species is doing well
in its niche → “equally good”

Diversity nowadays: show alternatives

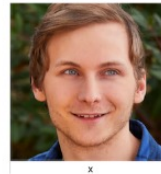
Mine planning:

optimize w.r.t. known objectives (money, time, ...) but then show alternative plans (e.g. sequences, ...)



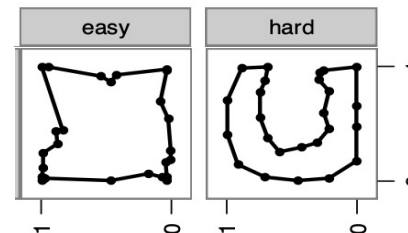
Inspirational image generation:

optimize quality & similarity (to a seed), but be diverse (search here via the latent space)



Algorithm understanding / algorithm tuning / algorithm portfolios / ...:

generate X instances (*diverse* w.r.t. Y features) on which Z algorithms perform as *differently* as possible



Algorithm footprint

[Background 1/4] Performance Diversity of instances for the Travelling Salesperson Problem

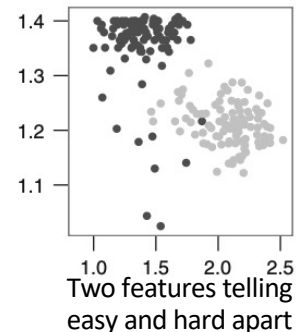
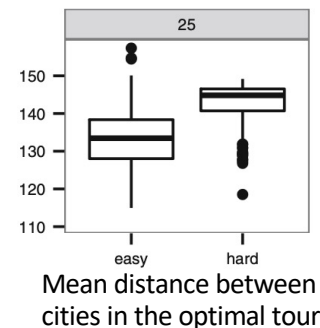
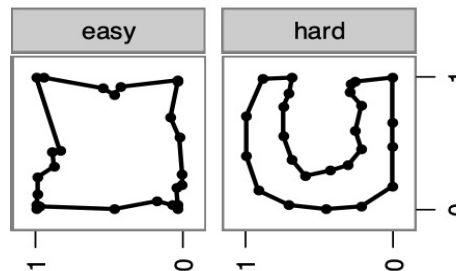
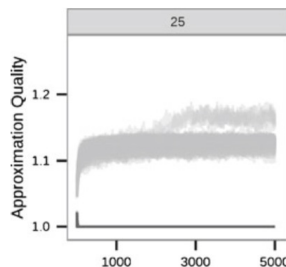
fundamental combinatorial problem: find the shortest tour across n cities

➔ In ~2010: we want to construct a set of TSP instances on which the performance of one algorithm varies

Examples:

- Diverse set where a certain algorithm is performing badly (high approximation ratio):
$$\alpha(I) = \frac{A(I)}{OPT(I)}$$
- Diverse set where two solvers A and B are performing differently (again: use performance ratios):
$$\alpha(I) = \frac{A(I)}{B(I)}$$

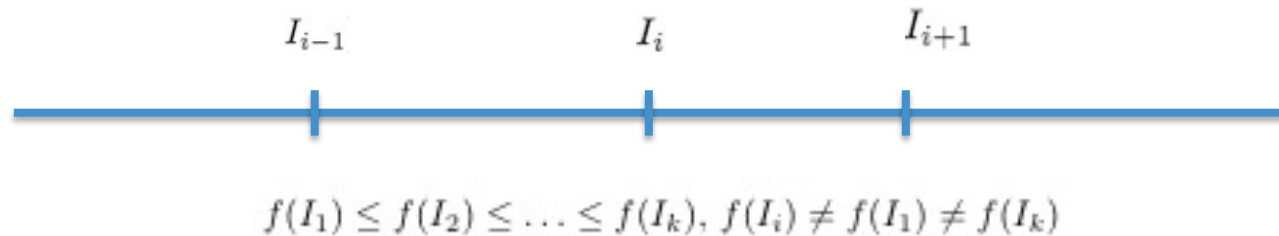
Here:
25 cities



[Background 2/4] Single-feature diversity measure

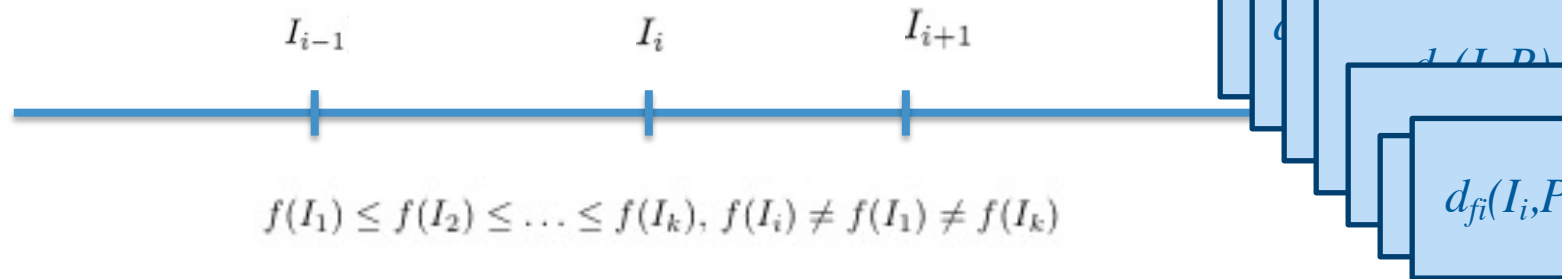
(also shows: going from 2 to 3+ can sometimes be challenging)

Feature f:



[Background 2/4] Single-feature diversity measure (also shows: going from 2 to 3+ can sometimes be challenging)

Feature f:



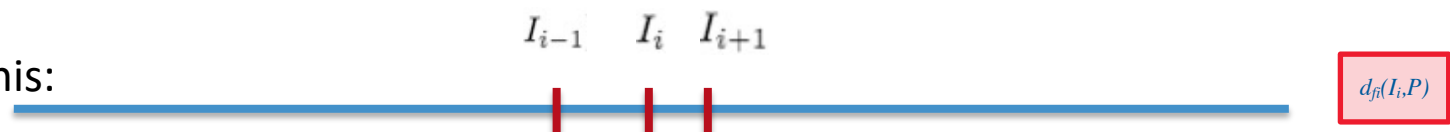
“Diversity” of
a single solution:

$$d_{f_i}(I_i, P) = (f(I_i) - f(I_{i-1})) \times (f(I_{i+1}) - f(I_i))$$

Diversity of a population: $d'(I, P) = \sum_{i=1}^k (w_i \times d_{f_i}(I, P))$

Maximum: if solutions are
equally spaced out, as this is
then the sum of squares

Compare with this:

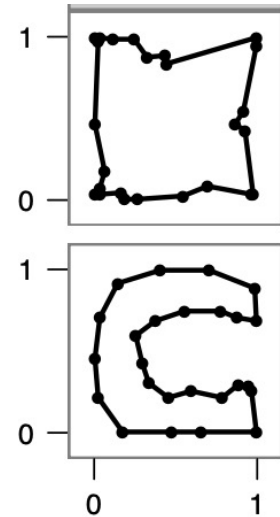


EA for evolving several diverse instances for the Traveling Salesperson Problem

(Gao, Nallaperuma, Neumann (PPSN 16))

$d(I, P)$ is the diversity contribution of instance I to the population P .
Diversity here: might be in difficulty, structure, feature, ...

Let I be an individual (tour).



Algorithm 1. $(\mu + \lambda)$ - EA_D

- 1 Initialize the population P with μ TSP instances of approximation ratio at least α_h .
 - 2 Let $C \subseteq P$ where $|C| = \lambda$.
 - 3 For each $I \in C$, produce an offspring I' of I by mutation. If $\alpha_A(I') \geq \alpha_h$, add I' to P .
 - 4 While $|P| > \mu$, remove an individual $I = \arg \min_{J \in P} d(J, P)$ uniformly at random.
 - 5 Repeat step 2 to 4 until termination criterion is reached.
-

Reminder: α is used here just as a quality constraint,
and survivor selection does not consider it, but only the diversity (contribution)

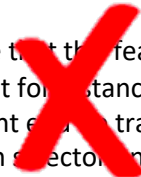
[Background 3/4] Features of “easy/hard” TSP instances for **2-opt** (with and without diversity optimization)

Feature values of evolved instances:

From left to right:

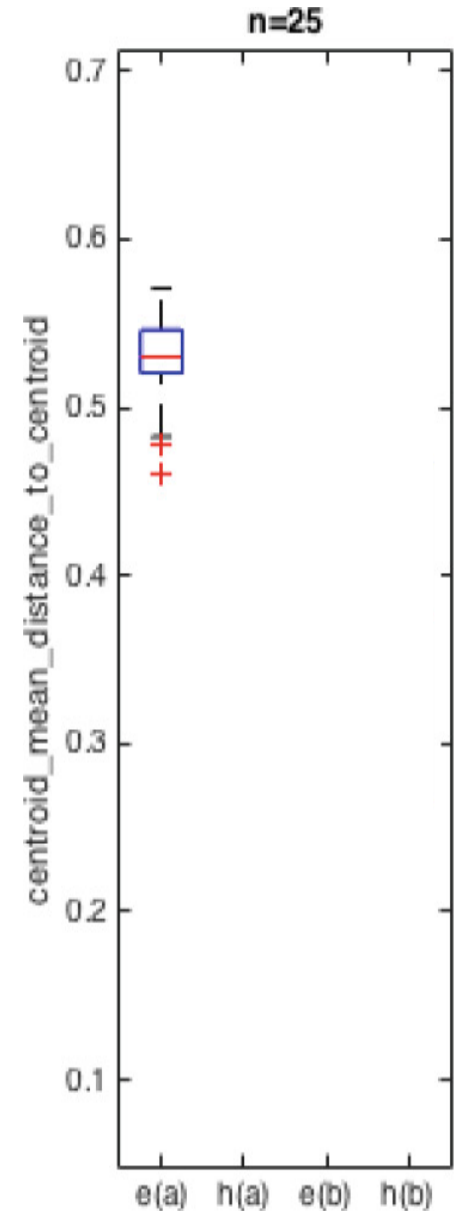
1. Easy instances / only using α
2. Hard instances / only using α
3. Easy instances / feature diversity (α as quality constraint)
4. Hard instances / feature diversity (α as quality constraint)

Conclude that the feature is important for instance difficulty (you might even be training an algorithm selector on this data)



Works for other features, too... but not for all.

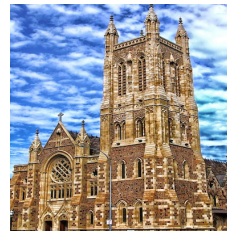
Long story short (here): old conclusions drawn re importance (for difficulty) invalidated by including feature diversity



[Background 4/4] Multi-feature diversity measure

(also shows: going from 1 to 2+ can sometimes be challenging)

- **Task:** evolve a diverse set of images that are close to a given image.
- Close means: RMSE to given image is less than 10.



On the right: either 1 feature as target, or a linear combination of two features

0.0342854



0.171715



0.343471



0.515221



0.686967



(0.613, 0.180)



(0.559, 0.265)



(0.541, 0.284)



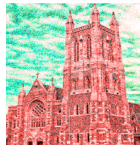
(0.577, 0.368)



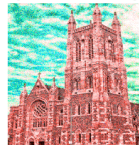
(0.595, 0.478)



(0.692, 0.116)



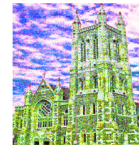
(0.680, 0.137)



(0.631, 0.528)



(0.649, 0.578)



(0.667, 0.654)

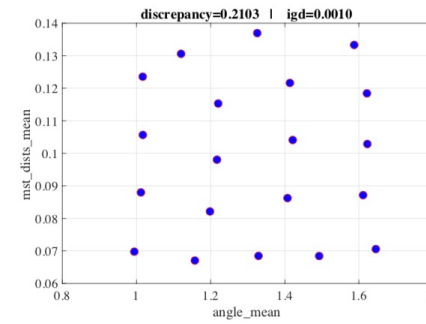


→ How to move to 2+ features in a less biased way? Related: what does “diversity” mean in the 2+D space?

[Background 4/4] Multi-feature diversity measure

(also shows: going from 1 to 2+ can sometimes be challenging)

- Feature diversity w.r.t. 2+ features
(GECCO'19 BPA nomination)
→ going from 1 to 2+ features has been challenging without favouring one feature (or value range or linear combination or ...) over another



Besides all of this: diversity-focused research is a hot field:

- Lots of theoretical runtime analyses by Frank Neumann et al. (GECCO'21 BPA nomination)
- More material: IEEE CEC 2021 tutorial
<https://cs.adelaide.edu.au/~optlog/EvolutionaryDiversityOptimisationTutorialCEC2021.php>

→ **The OPEN QUESTION this present talk aims to answer:**

How to evolve instances on which >2 algorithms perform as differently as possible?

For example: $I_1: A_1 > A_2 > A_3$ $I_2: A_3 > A_1 > A_2$ $I_3: A_3 > A_2 > A_1$

Approach

What shall our fitness function F be?

Algorithm 1: Outline of instance evolving $(1 + 1)$ -EA.

```
input : Fitness function  $F$ 
1 Initialize instance  $I$  randomly;
2 while budget not depleted do                                ▶ Often time-limit
3   |   Generate  $I'$  by applying mutation to  $I$ ;
4   |   if  $F(I') \geq F(I)$  then
5   |   |   Replace  $I$  with  $I'$ ;
6 return  $I$ ;
```

IDEA 1/3: Pairwise approach

Consider all $N(N-1)$ ordered pairs of algorithms and evolve for each pair in individual runs.



- Easy to formulate with existing tech (see [Background 1/4]):
maximise $A_1(I)/A_2(I)$, maximise $A_3(I)/A_2(I)$, ...
- But: a run ignores all other $N-2$ algorithms, e.g., a resulting instance might be easy for all of these.

Approach

What shall our fitness function F be?

IDEA 2/3: No order

Sort performances p_i and then maximise the crowding distance.



- Uses established technology (see [\[Background 2/4\]](#)):
maximise $F(x_x, p_y, p_z)$
- We need to get lucky to hit a desired permutation.

Algorithm 1: Outline of instance evolving $(1 + 1)$ -EA.

input: Fitness function F

- 1 Initialize instance I randomly;
- 2 **while** *budget not depleted* **do** ▷ Often time-limit
- 3 Generate I' by applying mutation to I ;
- 4 **if** $F(I') \geq F(I)$ **then**
- 5 Replace I with I' ;
- 6 **return** I ;

$$F(p_1, p_2, p_3) = \overbrace{(p_{(2)} - p_{(1)}) \cdot (p_{(3)} - p_{(2)})}^{(p_{(2)} - p_{(1)}) \quad (p_{(3)} - p_{(2)})}$$

$p_{(1)} \qquad \qquad \qquad p_{(2)} \qquad \qquad \qquad p_{(3)}$

Approach

What shall our fitness function F be?

Algorithm 1: Outline of instance evolving $(1 + 1)$ -EA.

input: Fitness function F

- 1 Initialize instance I randomly;
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IDEA 3/3: Explicit ranking

Use a three-tuple to implement two “pull”:

1. Pull: match the desired ranking
2. Pull: maximise the performance difference

Some details:

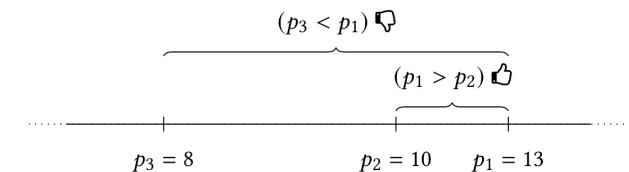
Let $p_1, \dots, p_N$ be the performance values of the algorithms, and let π be the desired ranking.

Good directions: $G = \{(i, i+1) \mid p_{\pi(i)} \geq p_{\pi(i+1)}\}$

Bad directions: $B = \{(i, i+1) \mid p_{\pi(i)} < p_{\pi(i+1)}\}$

→ Maximise lexicographically: $F(p_1, \dots, p_N; \pi) = (|G|, f_B, f_G)$

where f_B is the sum of the distances in the bad pairs, and f_G is the sum of the distances in the good pairs.*



Local sensitivity is necessary!

Case Study

Target problem: Travelling Thief Problem

(partly “find a permutation for the travelling” and partly “find a bitstring for a knapsack”)

Target algorithms:

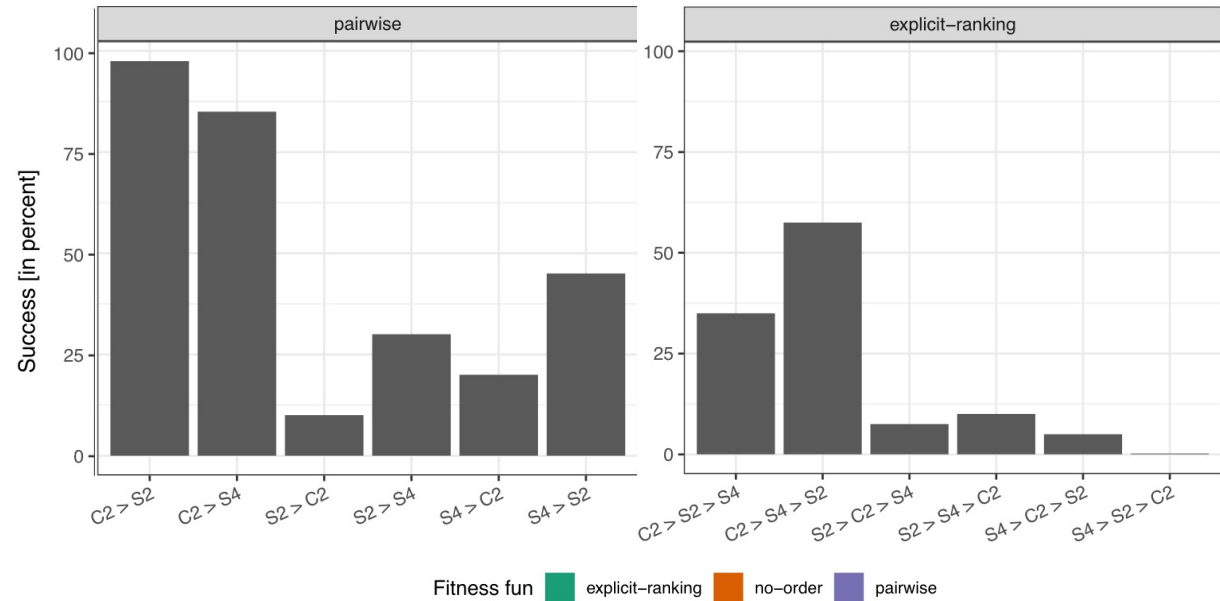
- **S2** (“simple”): targets bitstring
- **S4** (“simple”): targets permutation
- **C2** (“complex”): targets bitstring & permutation alternately

Instance evolution:

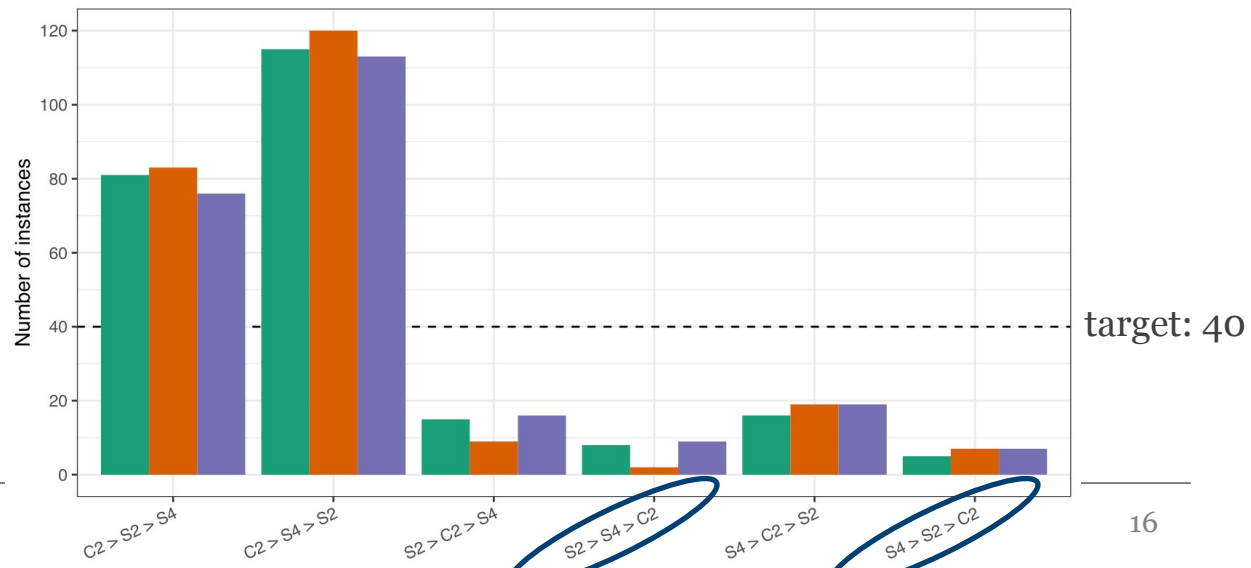
- simple (1+1)EA with disruptive operators
- instances with 200 nodes and with 200, ..., 2000 items
- performance on an instance:
 - During evolution: median of 5 runs
 - After evolution: run all three algorithms 30 times

Results: desired vs. actual rankings

% of successful jobs



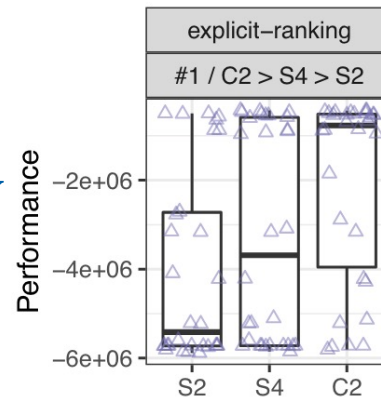
of instances evolved



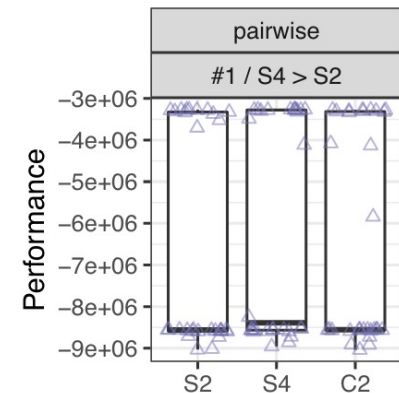
Results: Investigating issues

1) General noise...

(30*3=90 triangles show the raw performance)



... sometimes bi-modal behaviour

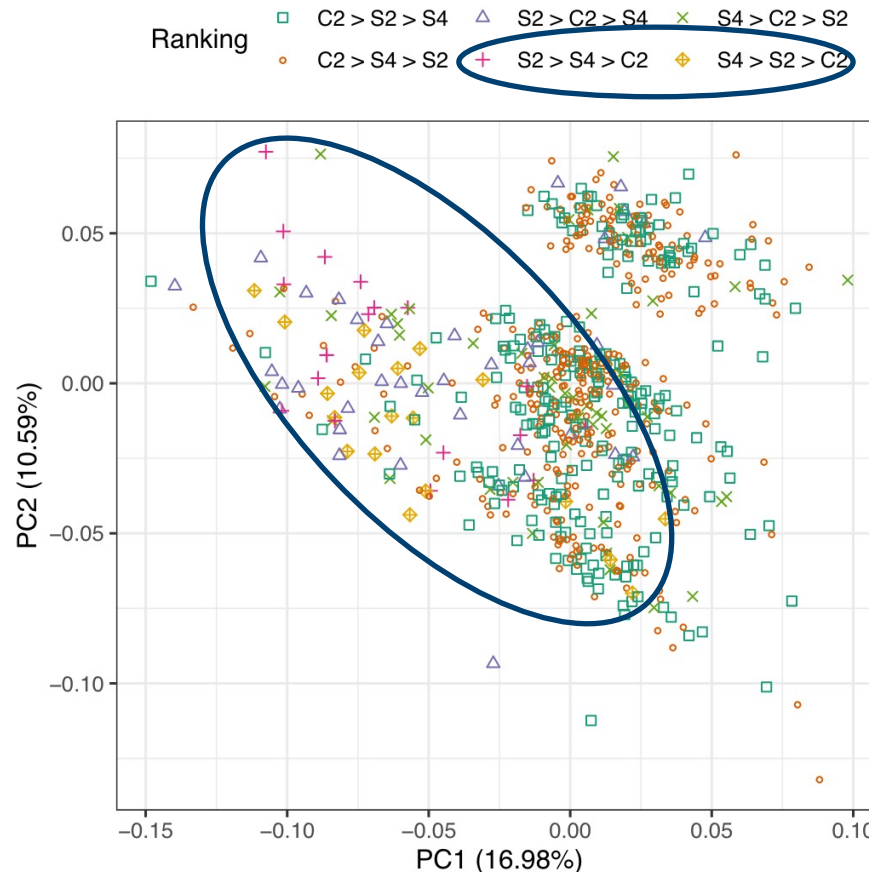


→ Address 1) and 2) by using more repetitions during evolution... but this costs computation time.

2) The complex **C2** heuristic is “more powerful” than the other two and tends to dominate.

Results: Properties of instances (1/2)

PCA in the “instance feature”-space



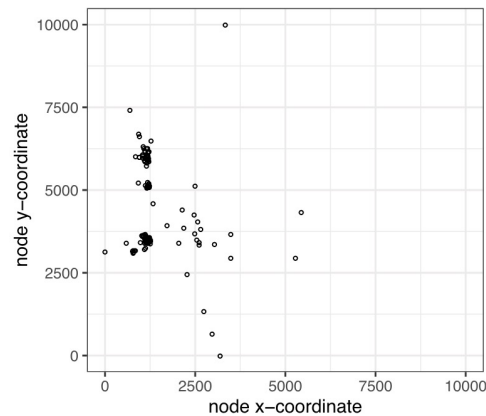
→ For some rankings: instances appear in distinct parts of the “instance feature”-space.
But remember [\[Background 3/4\]](#): we need to be careful when drawing conclusions from such observations, as we have *only* optimised performance rankings.

Results: Properties of instances (2/2)

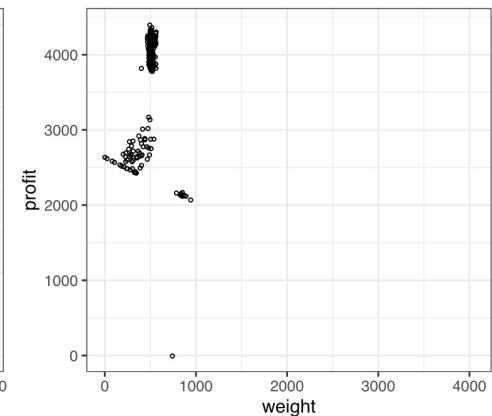
Two Examples

S2 > S4 > C2

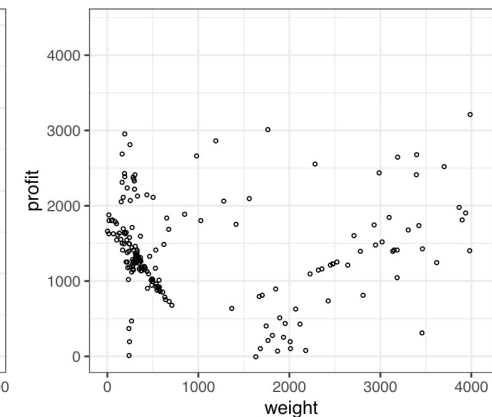
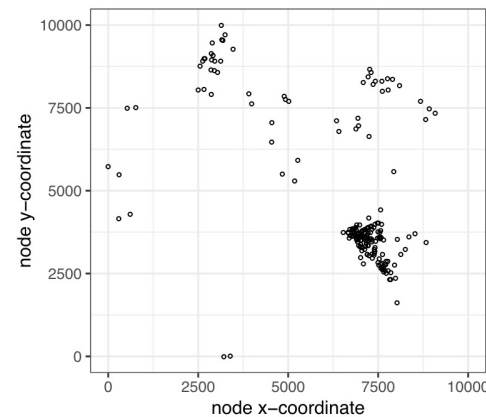
TSP: node
coordinates



knapsack items:
weight & profit



C2 > S4 > S2



Summary: **Diversity — when optimisation is not the goal**

10 years ago: “evolve *one* easy/hard instance for *one* algorithm”

Now: “evolve *sets* of solutions (== ‘actual’ solutions, instances, ...) that are *diverse in multi-dimensional spaces* (‘actual’ feature space, performance space, ...), and possibly subject to *minimum quality constraints*”

What is next???

- Optimisation: study custom variation operators [we learned that we have to be disruptive in the encoding space]
- Your solvers: how to change your state-of-the-art solvers to compute diverse sets of solutions (instead of a single one)? [beneficial to the end user, but maybe also during search?]
- Your domains: can ‘diversity’ be helpful to you, if so, why and how?

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Papers + code:

<http://www.jakobbossek.de/>

<https://cs.adelaide.edu.au/~markus/publications.html>

<https://cs.adelaide.edu.au/~frank/publications.html>