



SEARCH TRAJECTORIES ILLUMINATED

Gabriela Ochoa

UNIVERSITY of
STIRLING

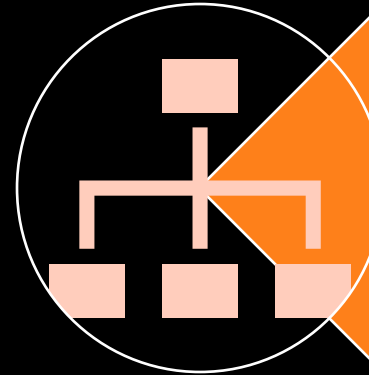


SEARCH IN COMPUTING SCIENCE



Stored Data

- Info in disk or memory
- Binary search, sequential search



Tree-like Structure

- Set of actions from start to goal states
- DFS, BFS, A*



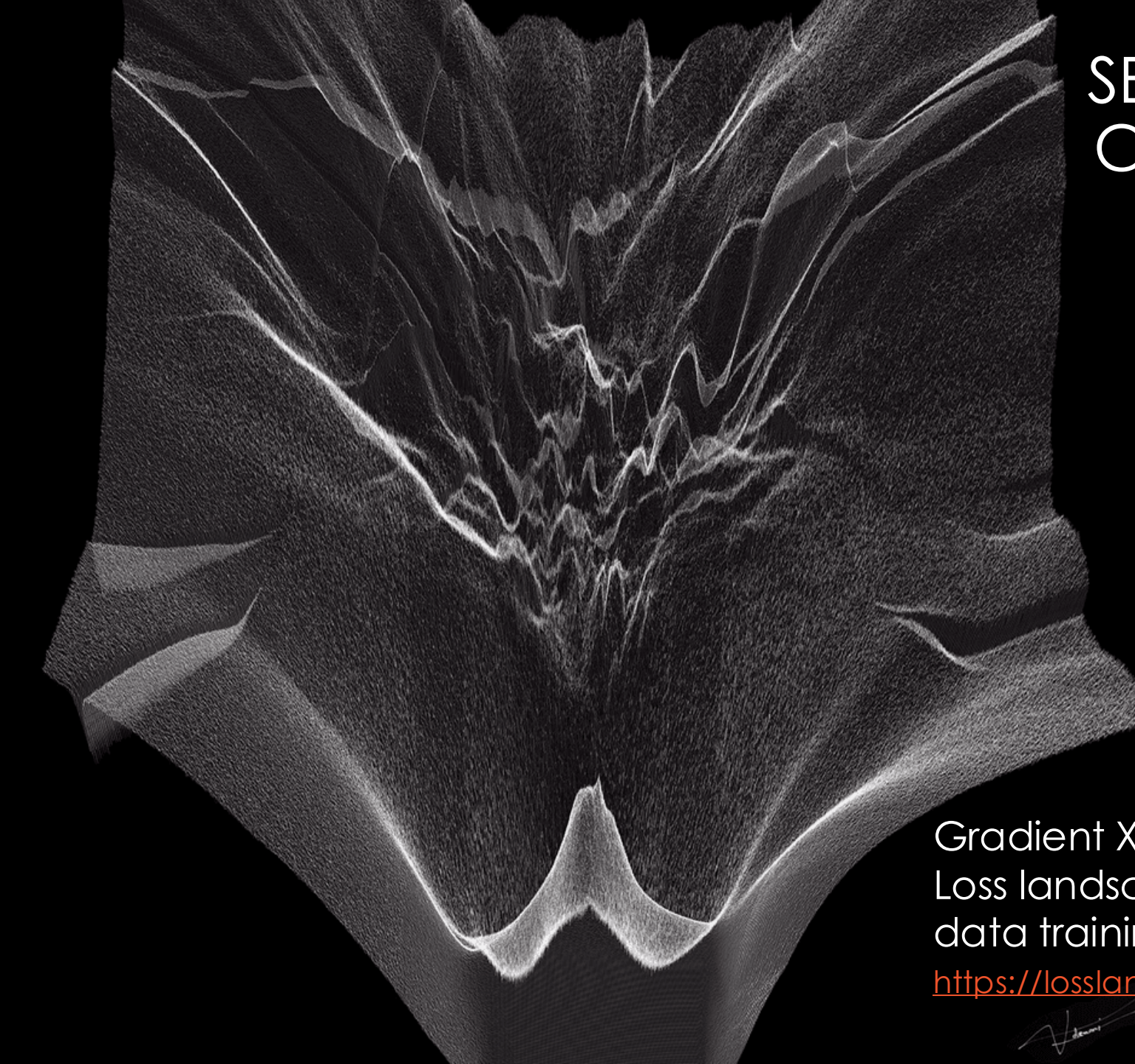
Web Documents

- Info on the WWW
- Web crawling



Solutions

- Solution in a large space
- EAs, metaheuristics



SEARCH FOR SOLUTIONS COMPLEX LANDSCAPES

- Vectors (Real, Integer, Binary)
- Permutations
- Grammars, Trees, Graphs

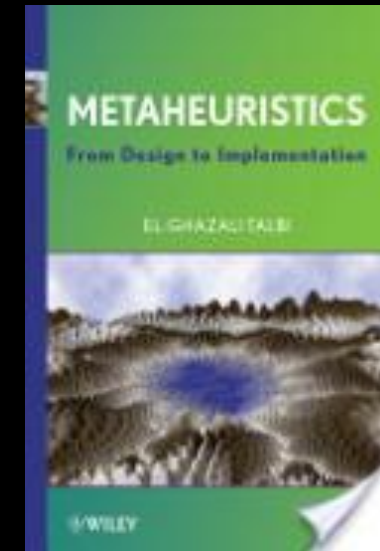
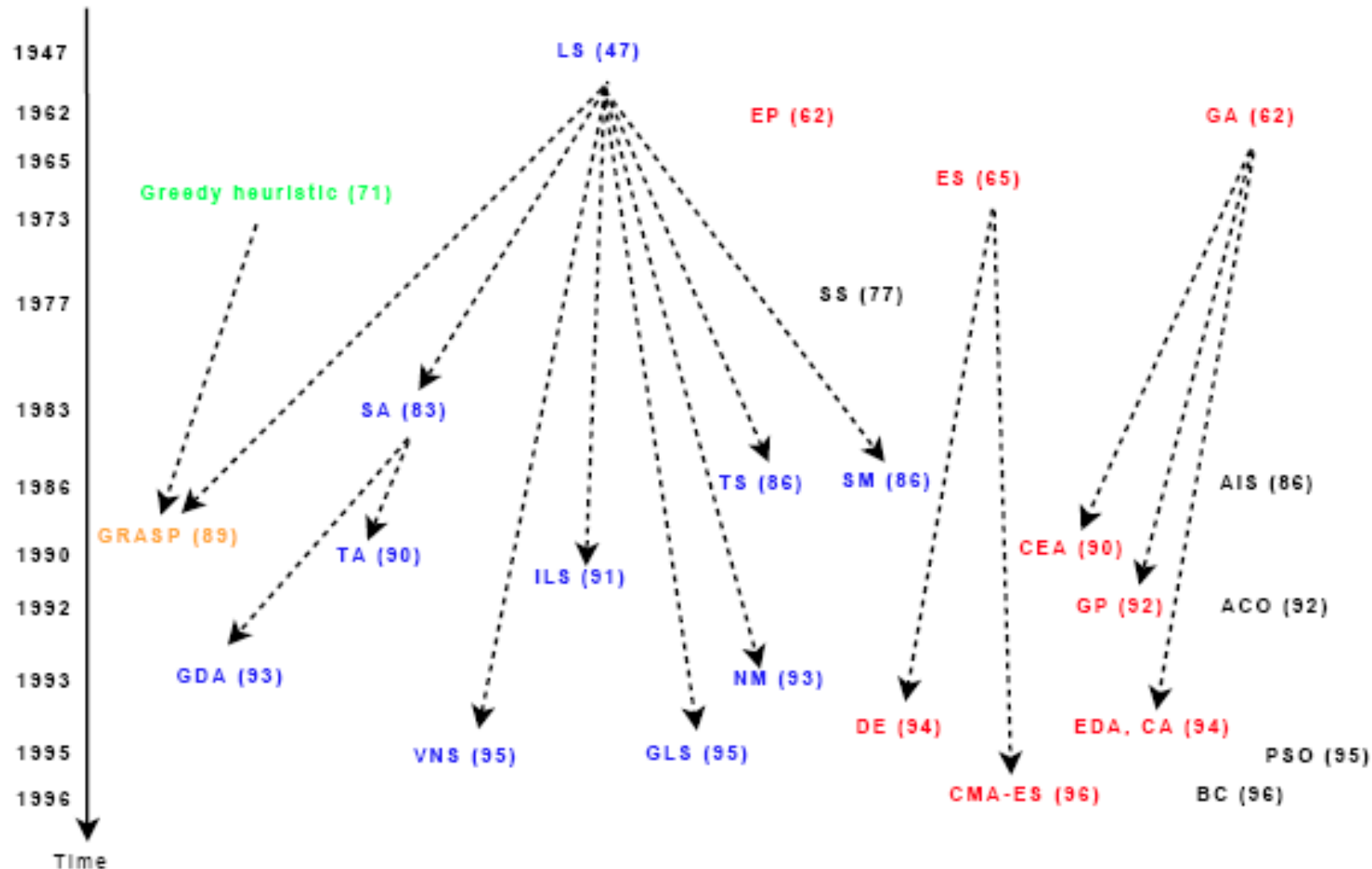
Wide applicability!

Gradient X-Ray ([Javier Ideami](#))

Loss landscape: from real
data training a deep NN

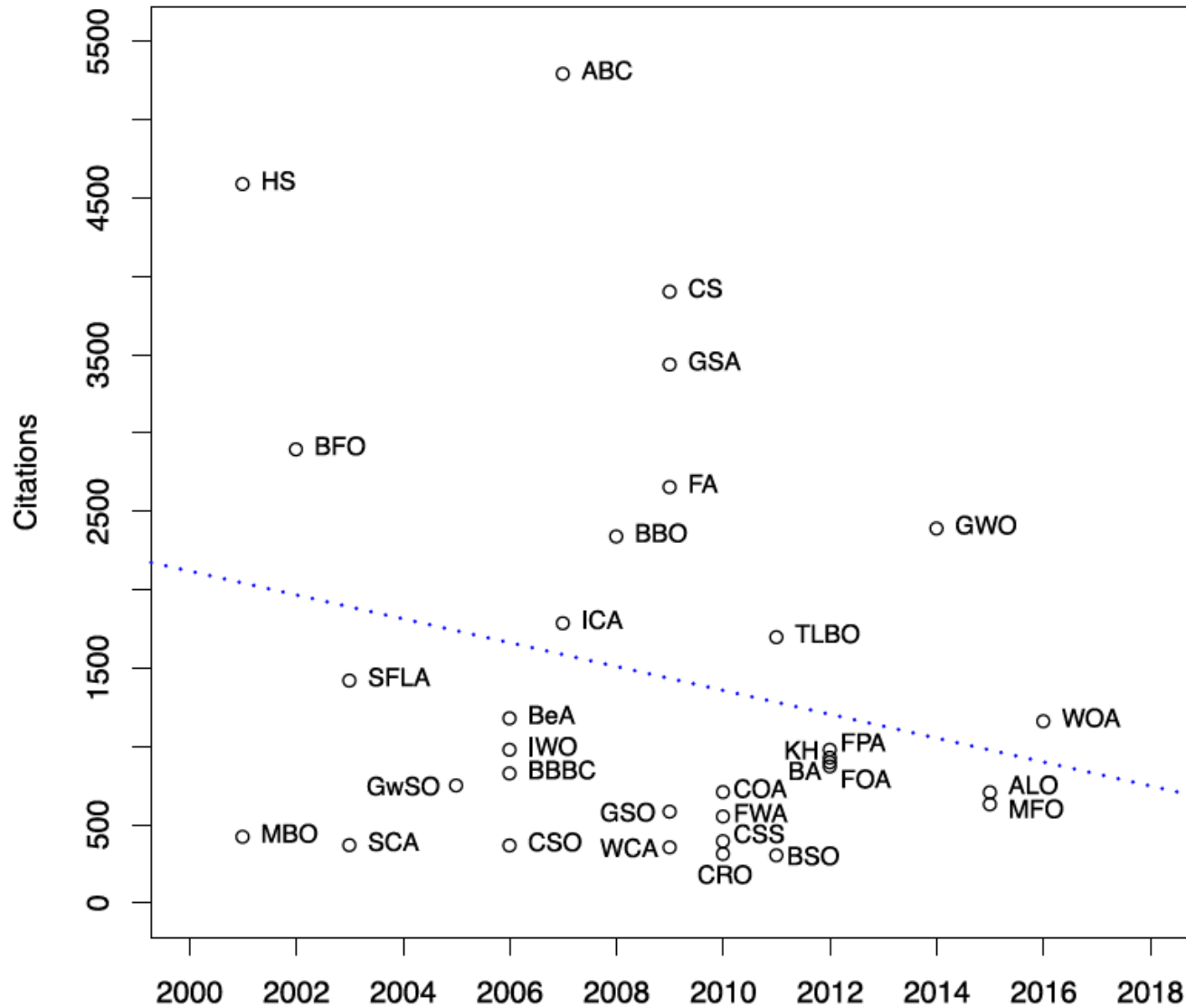
<https://losslandscape.com>

GENEALOGY OF METAHEURISTICS



E. Talbi (2009)

NATURE-INSPIRED ALGORITHMS: CITATIONS



ABC Artificial Bee Colony

HS Harmony Search

CS Cuckoo Search

GSA Gravitational Search Algorithm

BFO Bacterial Foraging Optimization

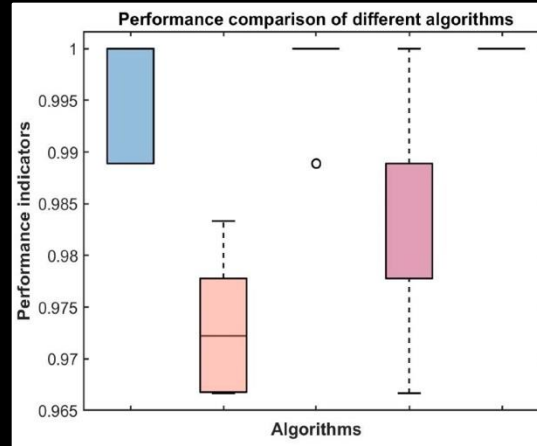
FA Firefly Algorithm

When the metaphor is stripped away, is the search process any different from the search process of existing established algorithms?

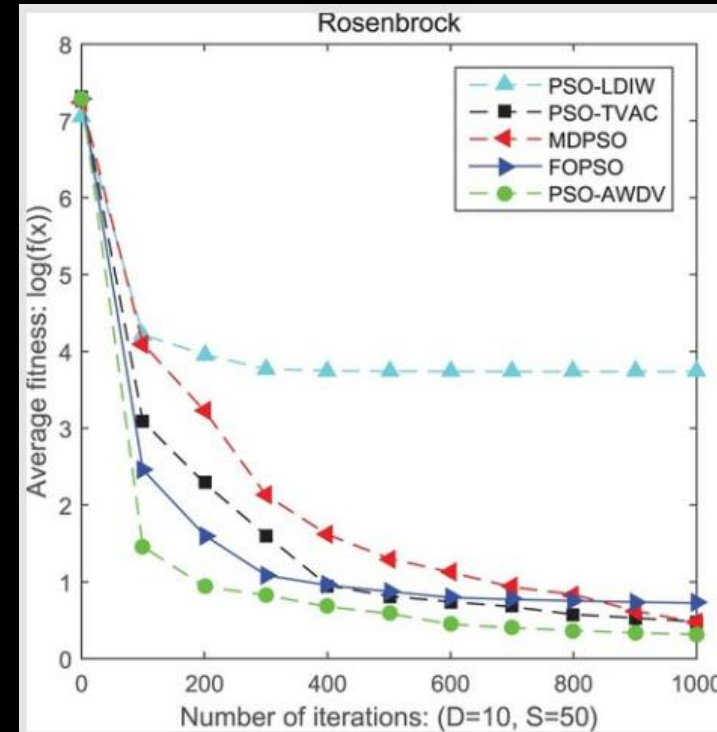
CONTRASTING ALGORITHMS

MOTIVATION FOR STNs

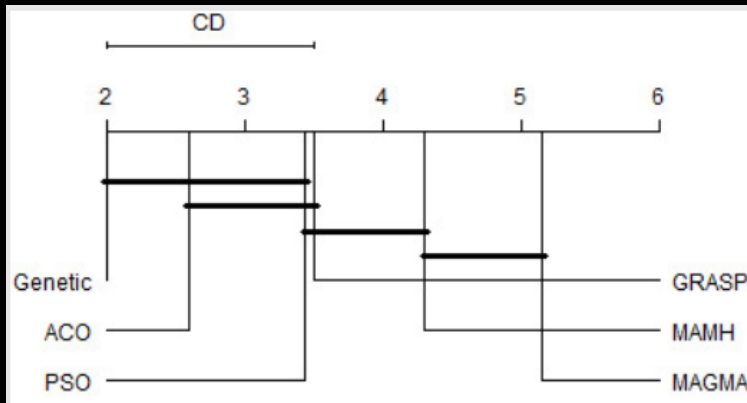
At the end of runs



During the run



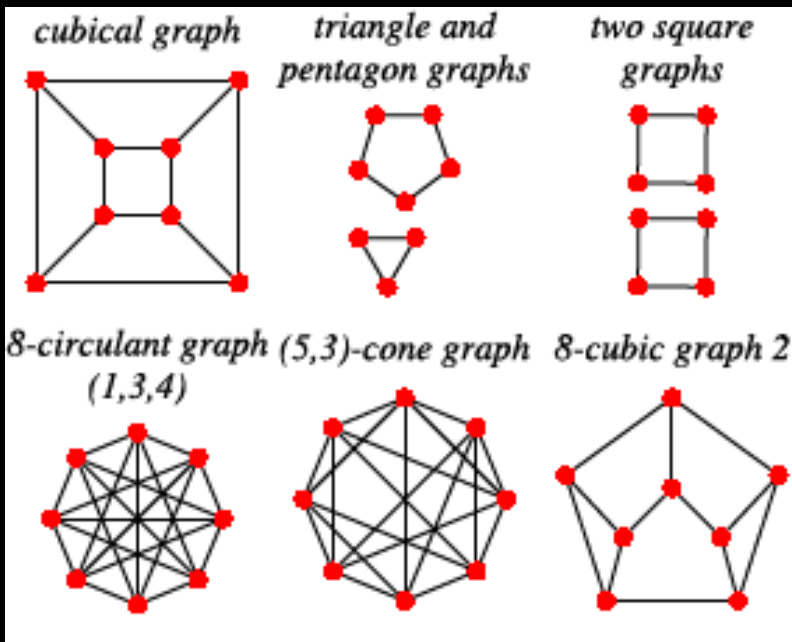
Convergence curves - show dynamics **only** on the objective space



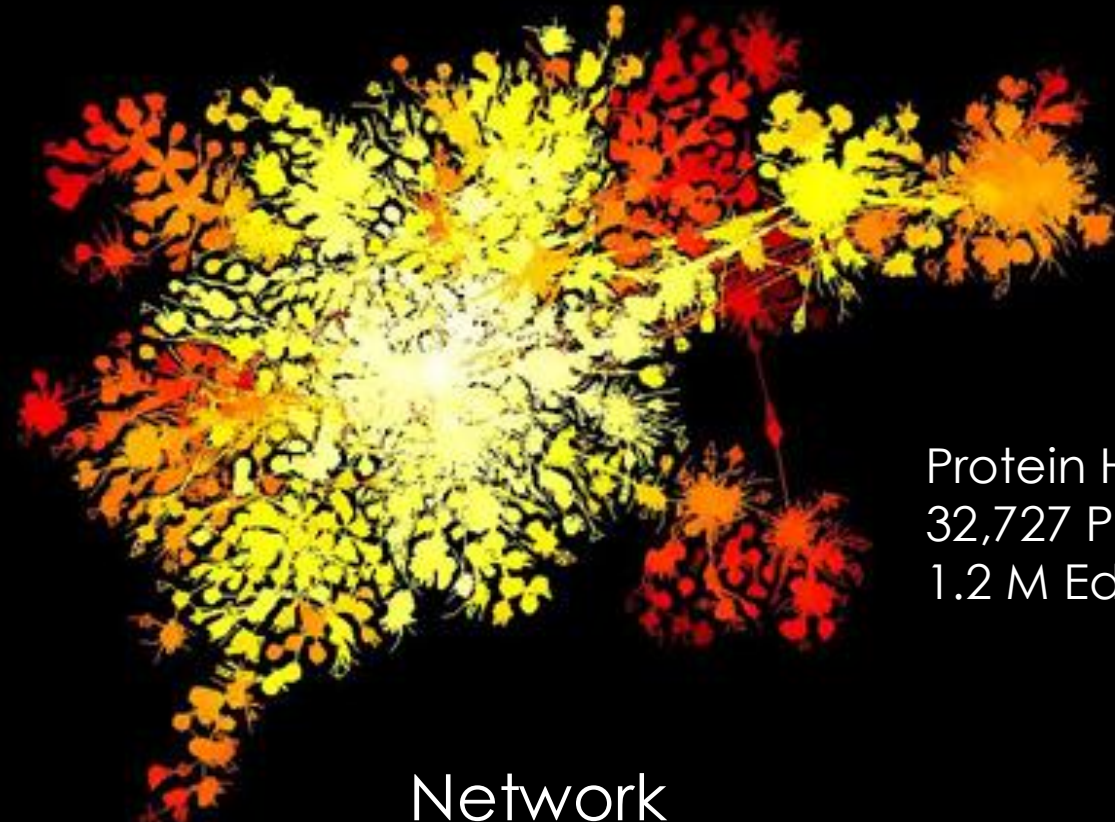
Critical difference plots

WHAT IS A (COMPLEX) NETWORK?

<https://mathworld.wolfram.com/WeaklyRegularGraph.html>



Graph
Mathematical Object



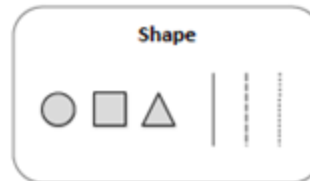
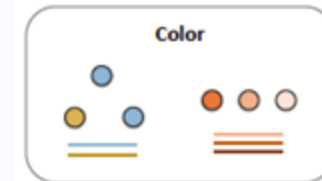
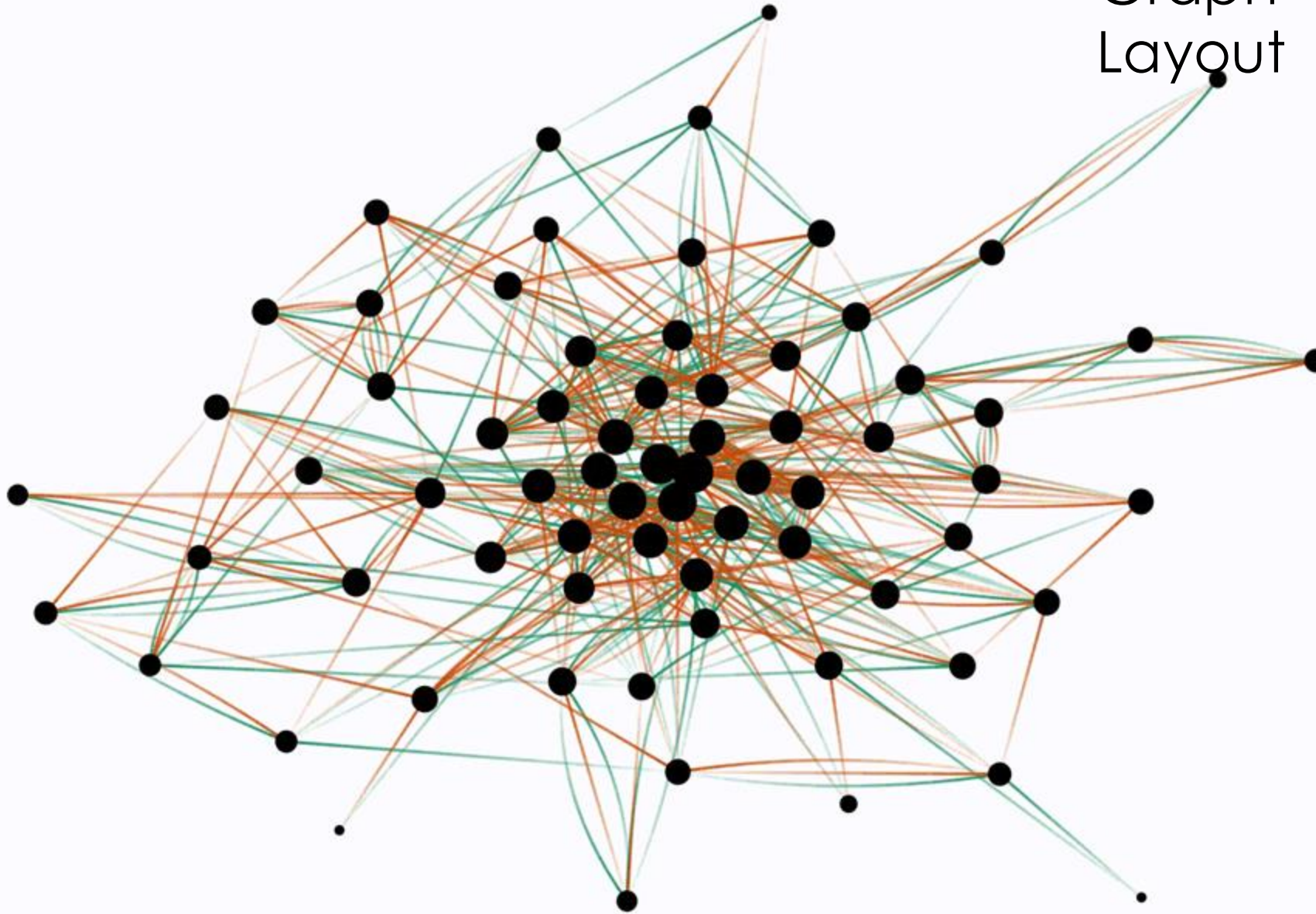
Protein Homology
32,727 Proteins
1.2 M Edges

Network
Data Driven Instantiation

Behind each complex system, there is an intricate network that encodes the interactions between the system's components. Albert-László Barabási, Network Science

Network Visualisation

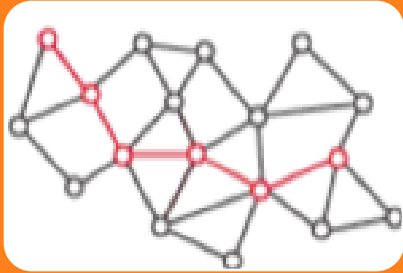
Graph Layout



<https://kateto.net/network-visualization>

<https://www.data-imaginist.com/2017/ggraph-introduction-layouts/>

NETWORK METRICS



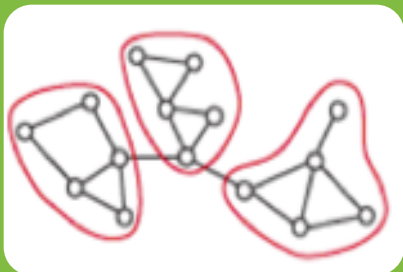
Distance

- Diameter
- Average shortest path



Topology

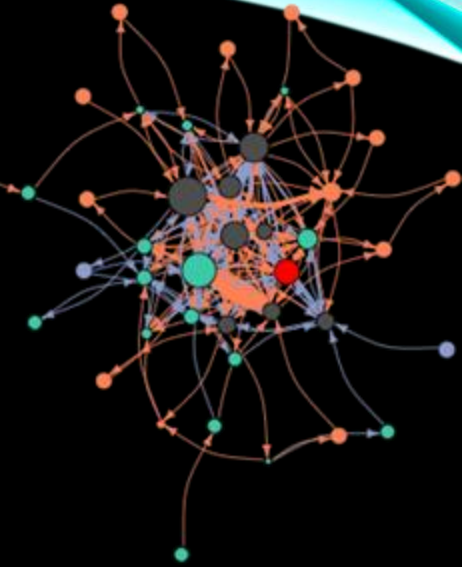
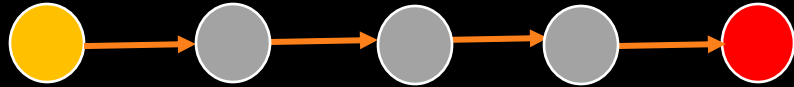
- Degree distribution
- Mean degree, Assortativity, disparity, centrality



Cohesion

- Clustering coefficient
- Community structure

SEARCH TRAJECTORY NETWORKS THE CONCEPT



Nodes (N)

*Locations of
representative
solutions*

Edges (E)

*Directed, connect
two consecutive
locations*

Representative
Solution

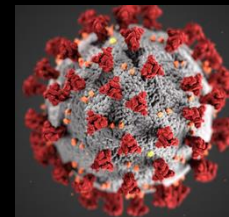
Location
(Partition)

Nodes

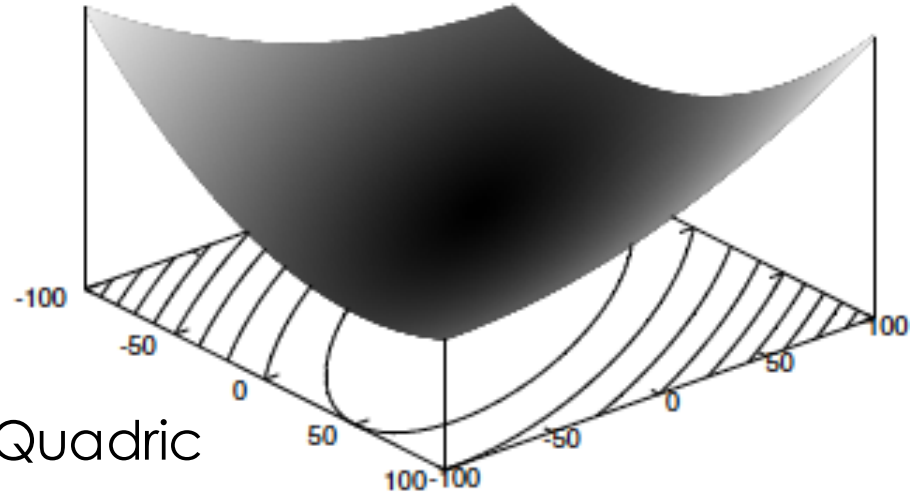
STN

*Directed graph
 $STN = (N, E)$*

(Ochoa, Malan, Blum,
EvoApps 2020,
Appl. Soft Comput. 2021)



CONTINUOUS BENCHMARK FUNCTIONS

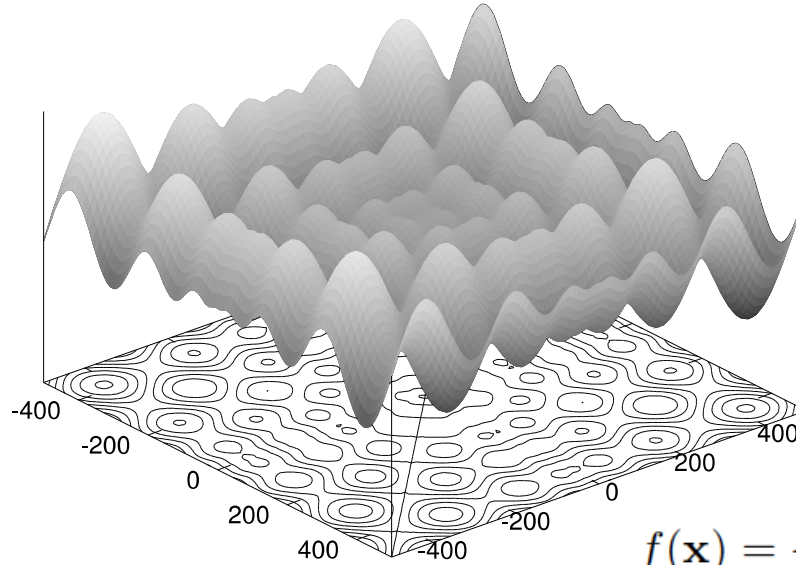


Quadric

$$f(\mathbf{x}) = \sum_{i=1}^D \left(\sum_{j=1}^i x_j \right)^2$$

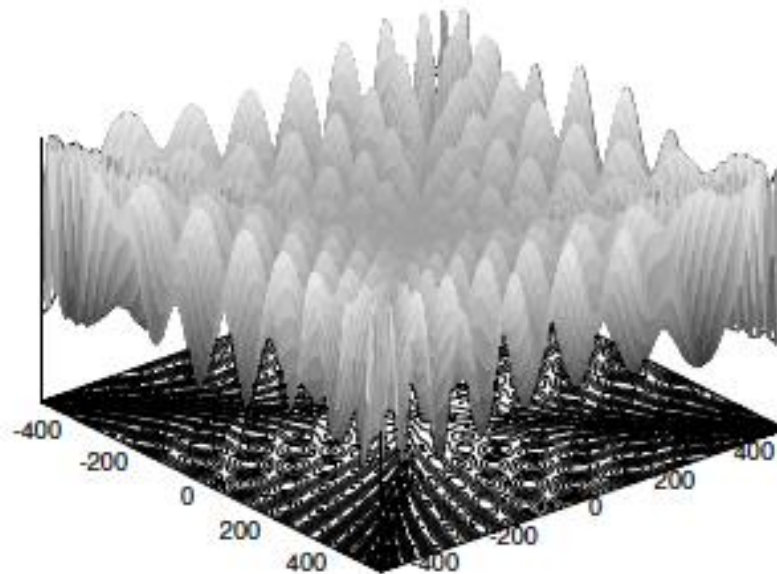
Rana

$$f(\mathbf{x}) = \sum_{i=1}^D x_i \sin(\alpha) \cos(\beta) + (x_{(i+1) \bmod D} + 1) \cos(\alpha) \sin(\beta),$$



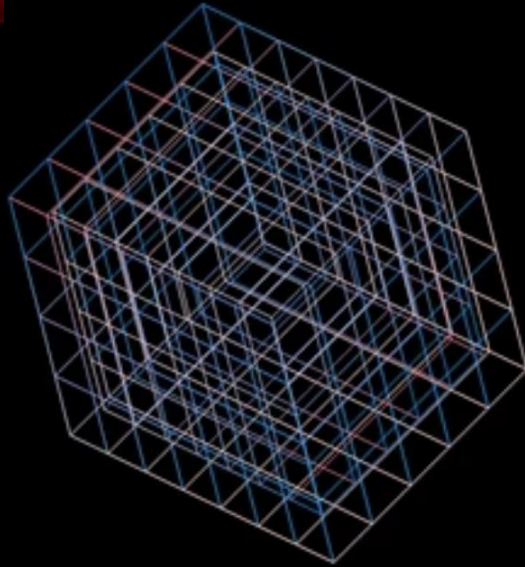
Schwefel

$$f(\mathbf{x}) = - \sum_{i=1}^D \left(x_i \sin(\sqrt{|x_i|}) \right)$$



MAPPING SOLUTIONS TO LOCATIONS

Solution space is divided into hypercubes



Example with
 $D = 3$

[0.170574,
0.83234,
1.016740]

Solution

Rounding

- Precision Factor PF = -1 (i.e 10^{-1} 0.1)
- [0.2, 0.8, 1.0]

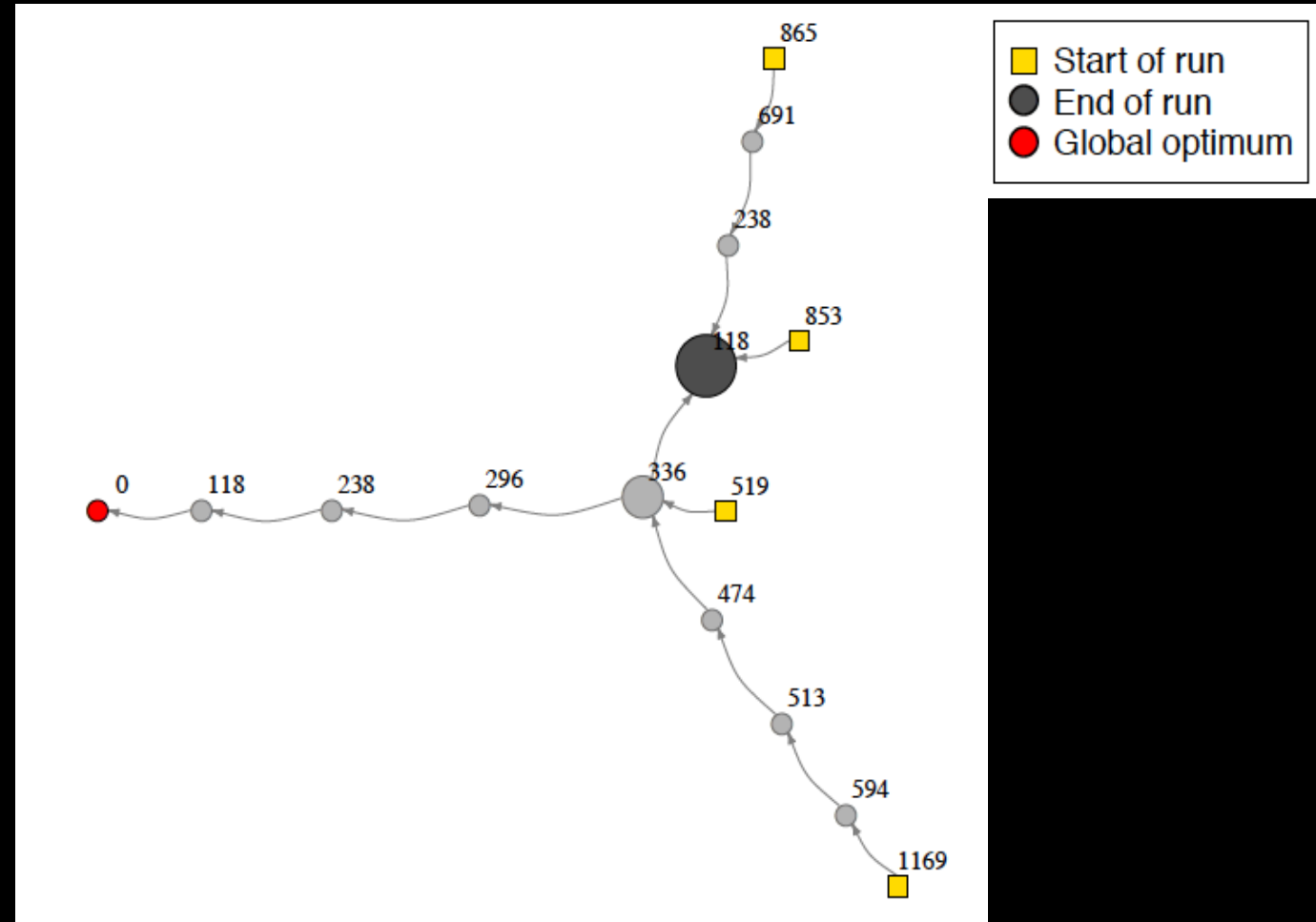
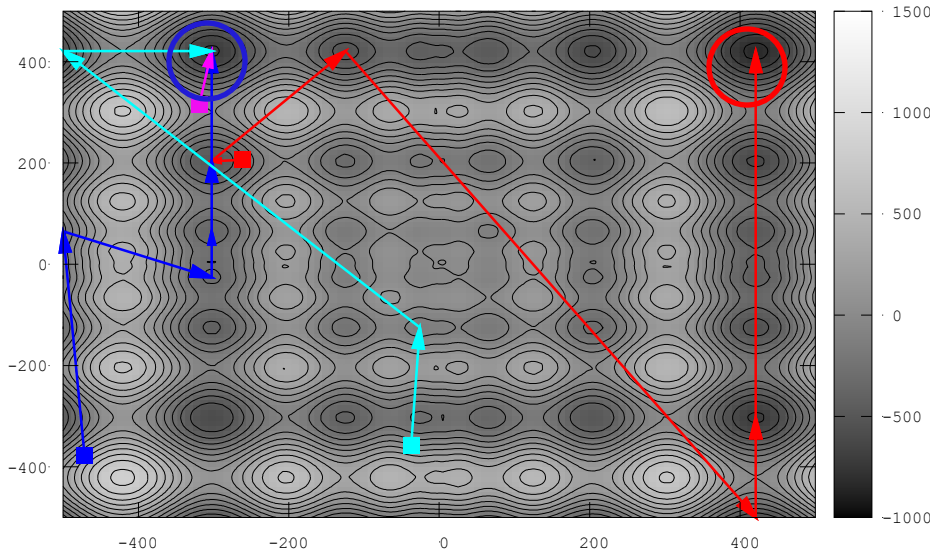
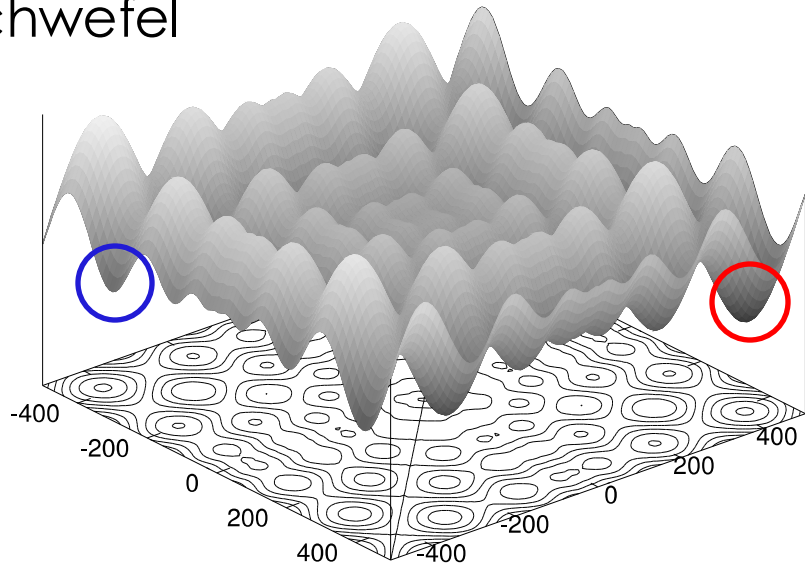
Example Input, Search Traces

Run Fitness Solution

1	12.079147	0.170574,0.832340,1.016740
1	9.693960	0.009483,0.788237,0.947641
1	6.600536	0.099082,1.102965,1.0443980
1	2.975199	0.005325,1.058486,0.0779451
2	22.757999	0.829453,1.129413,3.1201914
2	8.927973	1.018141,1.088751,0.1684573
2	5.947124	0.034037,1.042938,2.0281033
2	3.764063	0.973246,1.083225,0.0289796
...		

STN MODEL

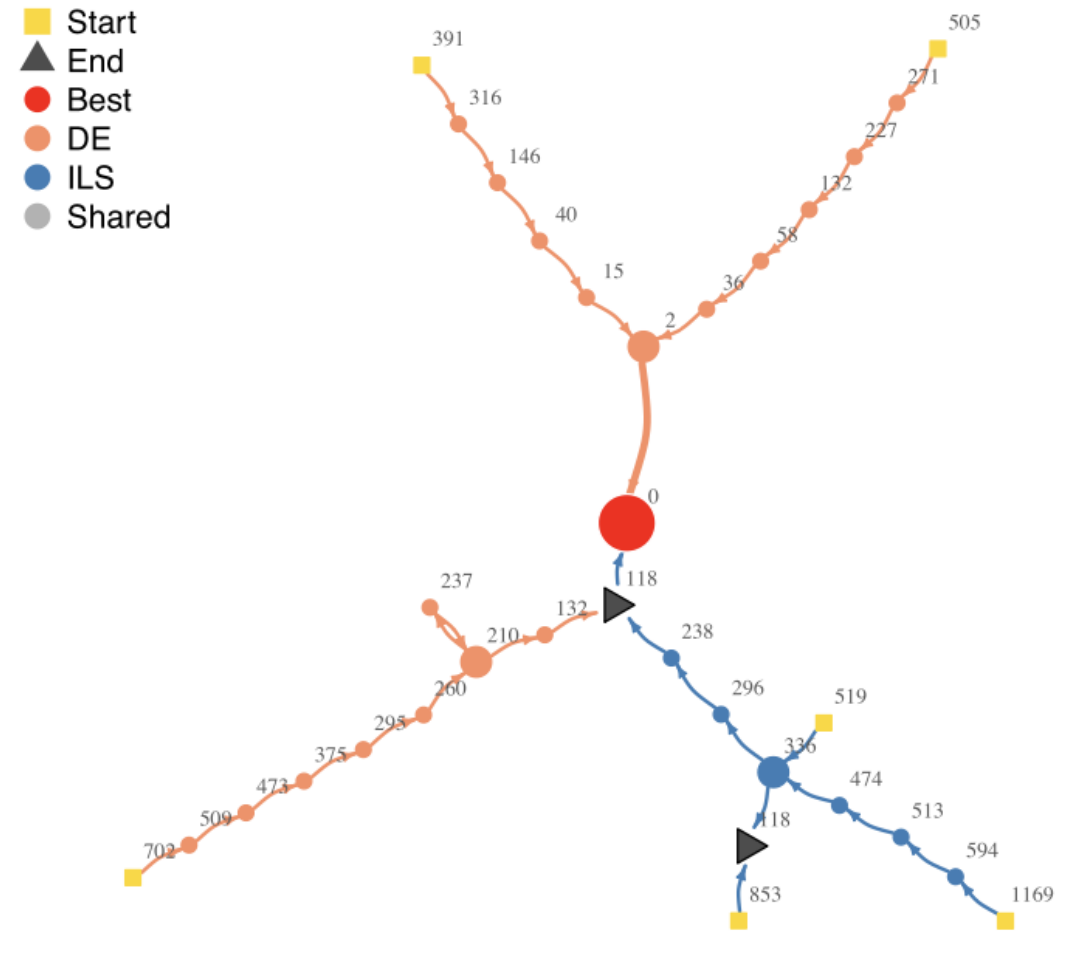
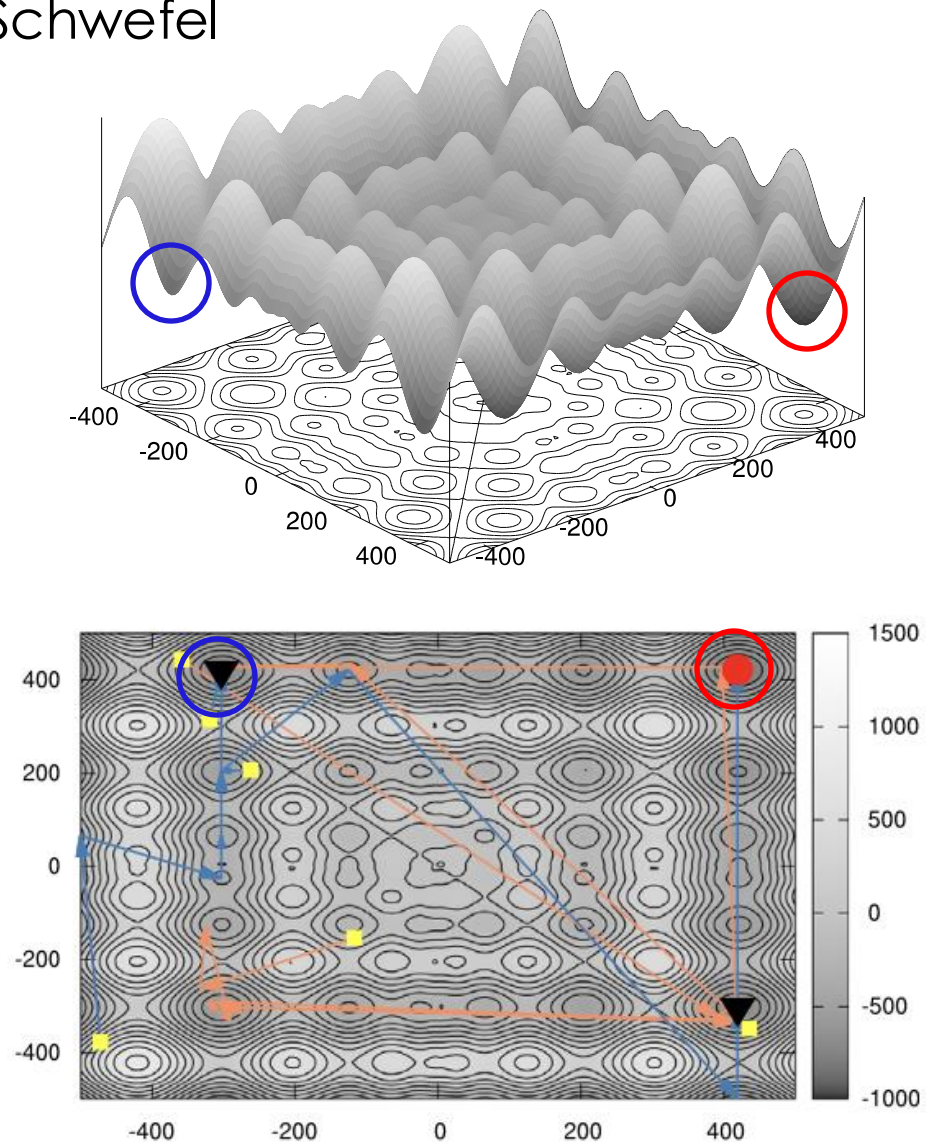
Schwefel



4 Runs
One Algorithm (ILS) It. Local Search

MERGED STN MODEL

Schwefel

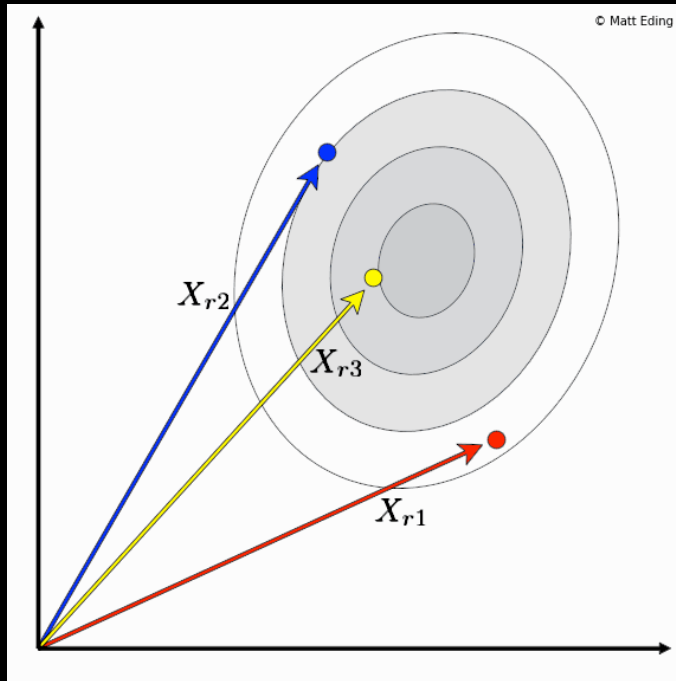


3 Runs

2 Algorithms: ILS and Differential Evolution (DE)

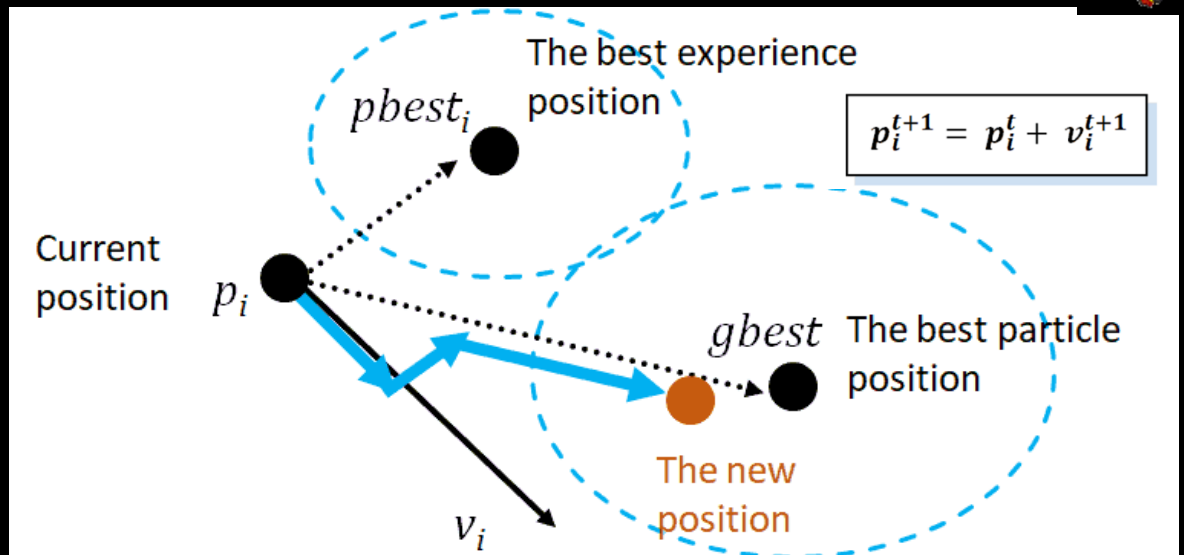
POPULATION-BASED ALGORITHMS

Differential Evolution (DE/rand/1)



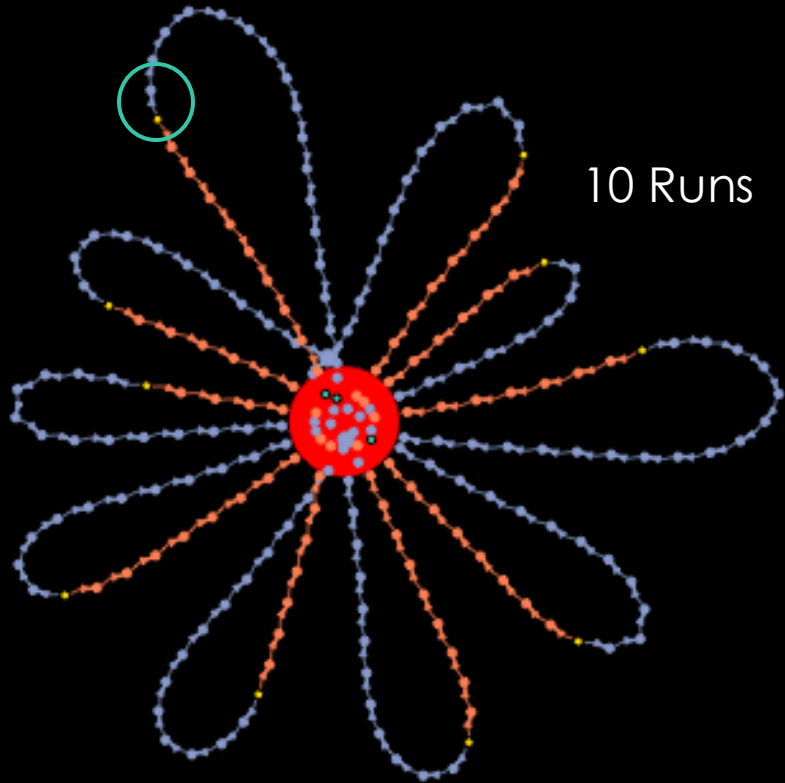
$$\vec{v}_i = \vec{x}_{r_1} + F_{xc}(\vec{x}_{r_2} - \vec{x}_{r_3})$$

Particle Swarm Optimisation (Global best PSO)

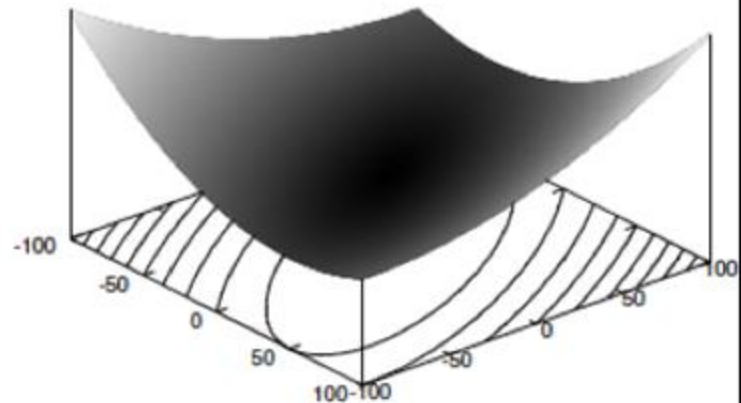
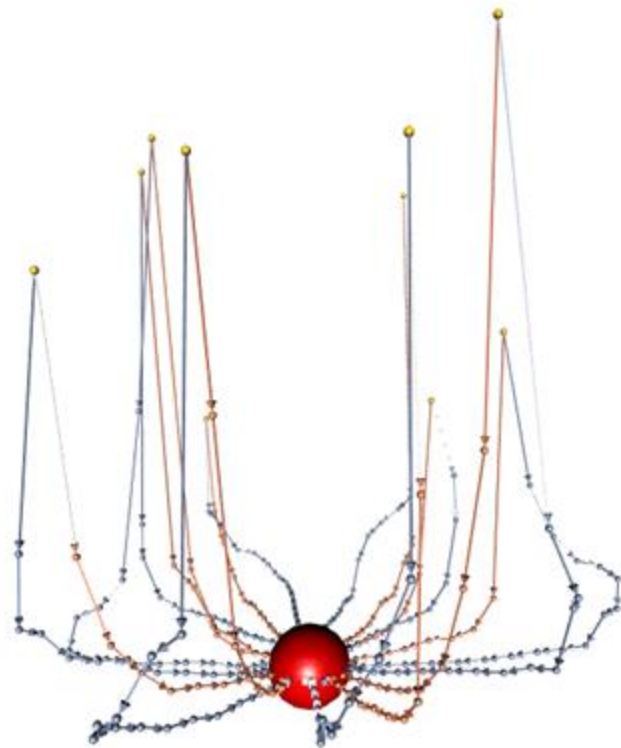


$$v_i^{t+1} = \underbrace{v_i^t}_{\text{Inertia}} + \underbrace{c_1 r_1 (pbest_i^t - p_i^t)}_{\text{Personal influence}} + \underbrace{c_2 r_2 (gbest^t - p_i^t)}_{\text{Social influence}}$$

QUADRIC, D = 10

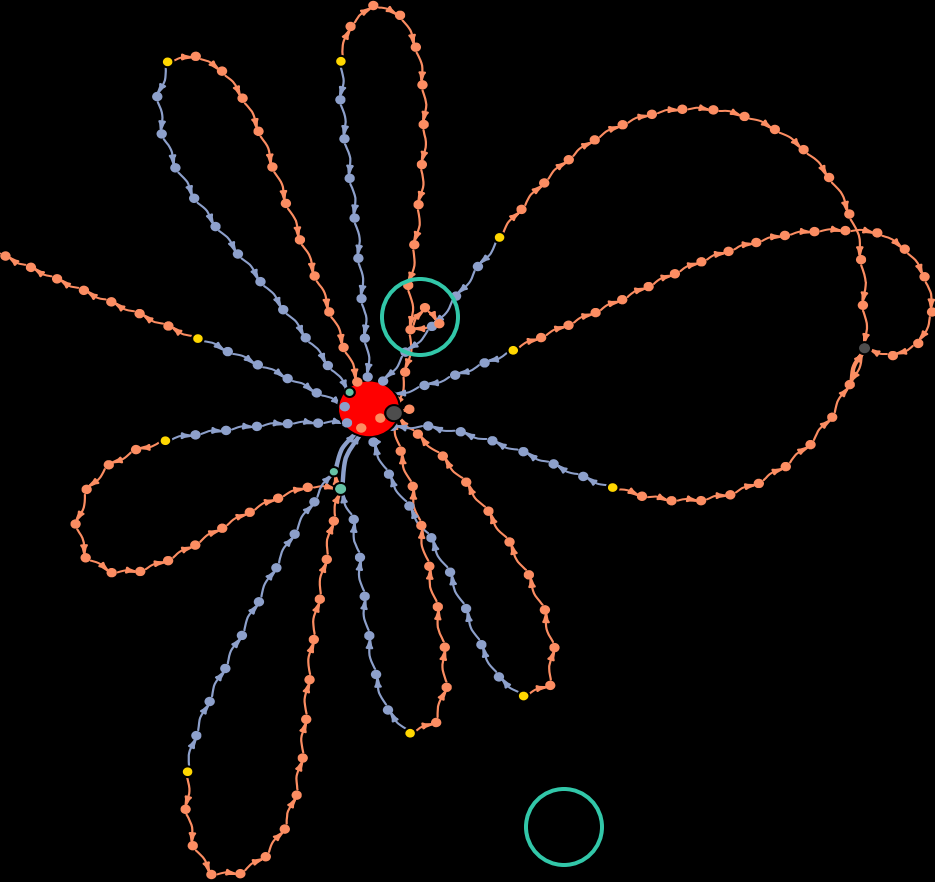


- Global
- PSO
- DE
- Both
- Start
- End

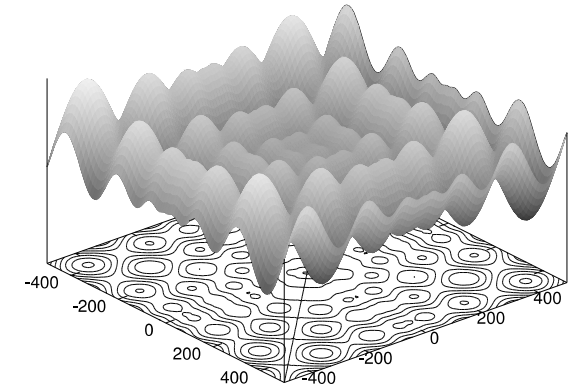
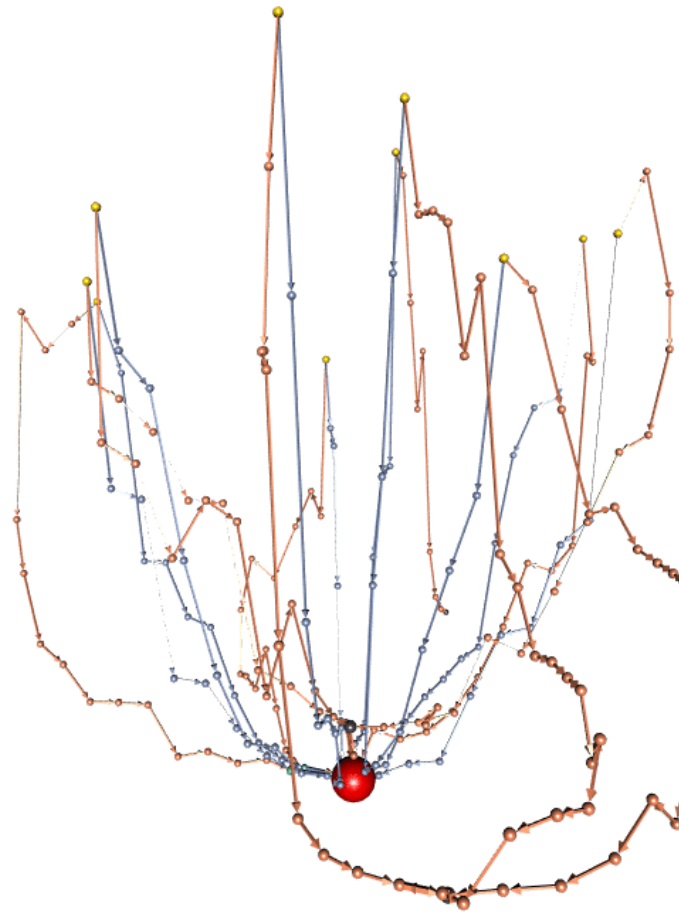


	PSO	DE
Nodes	93	154
Path length	9.2	15.1
Success	100%	100%

Schwefel, $D = 5$

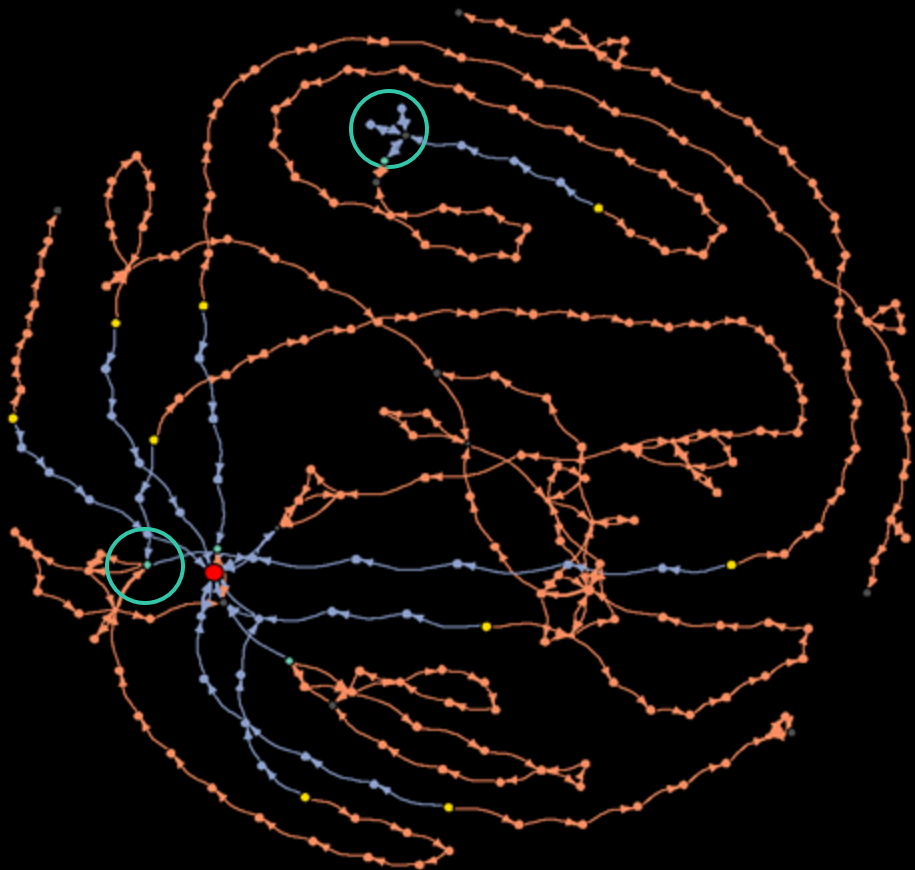


- Global
- PSO
- DE
- Both
- Start
- End

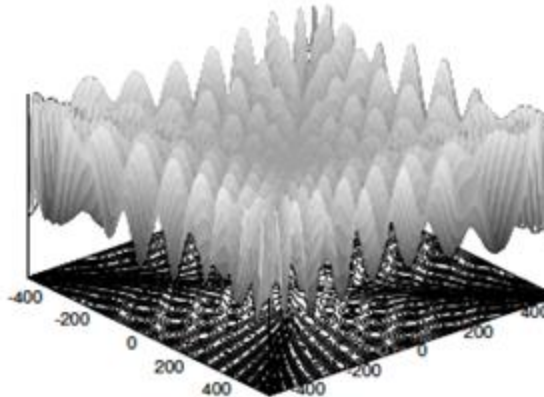
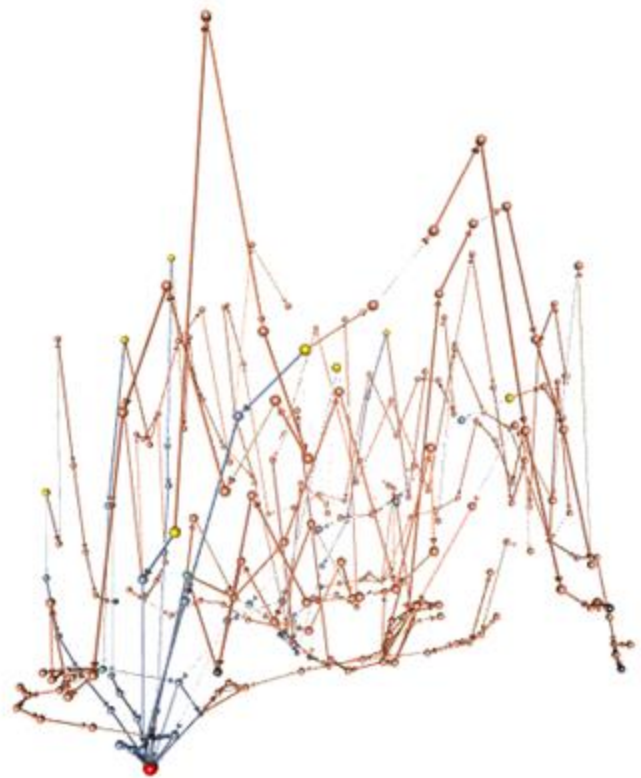


	PSO	DE
Nodes	138	81
Path length	12.6	8.0
Success	50%	100%

Rana, D = 3

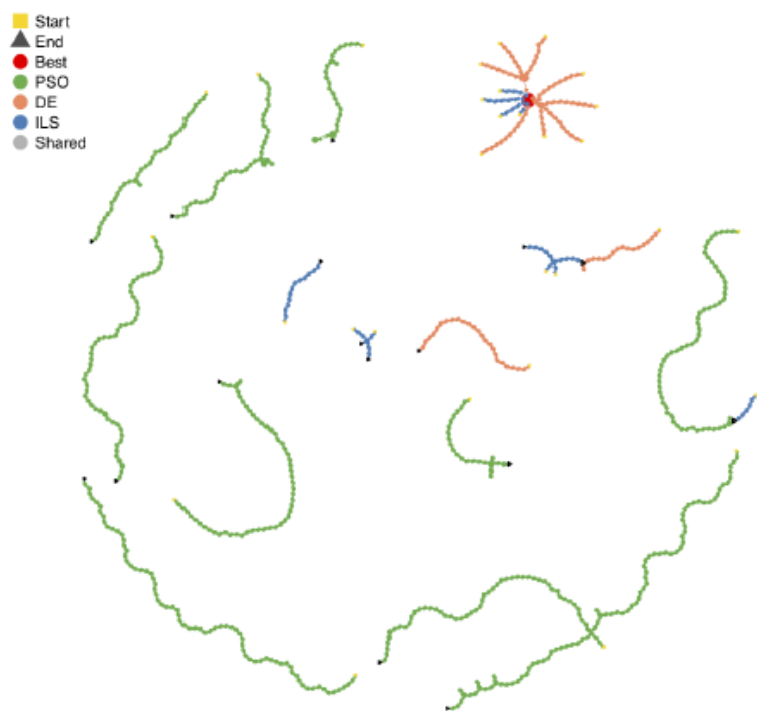
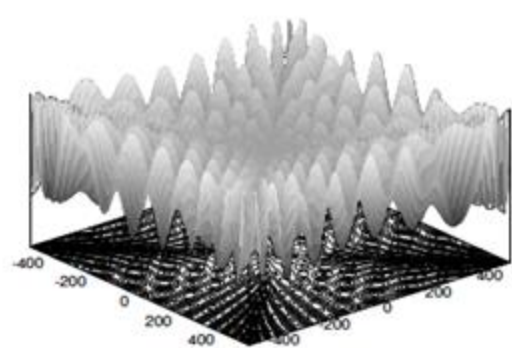


- Global
- PSO
- DE
- Both
- Start
- End

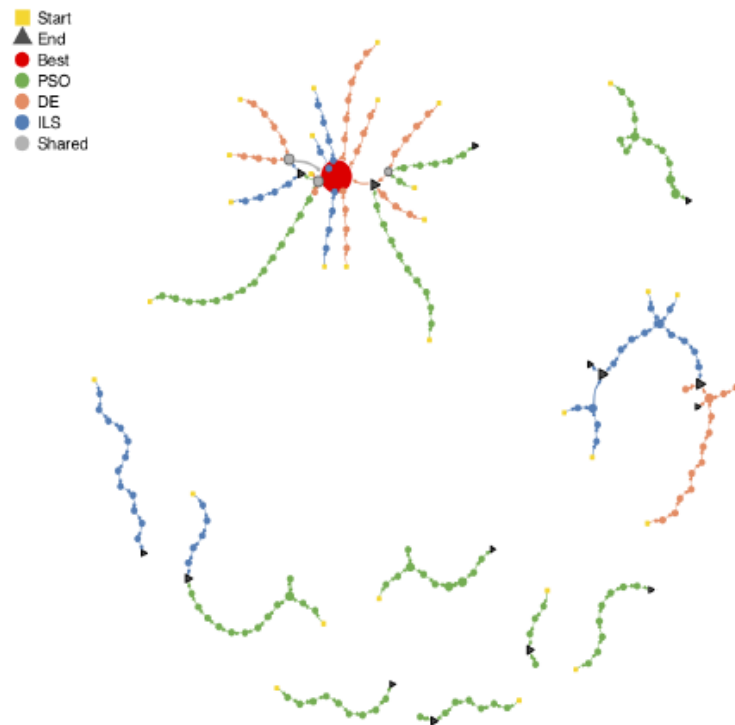


	PSO	DE
Nodes	211	49
Path length	13.5	4.7
Success	0%	90%

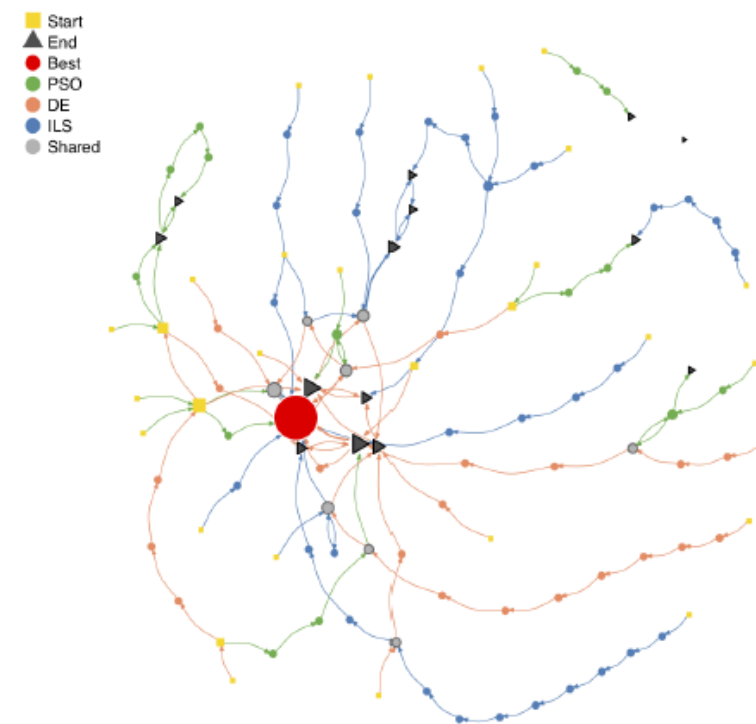
CHANGING PARTITIONING FACTOR



Fine partitioning $PF = -1$.



Medium partitioning, $PF = 1$.



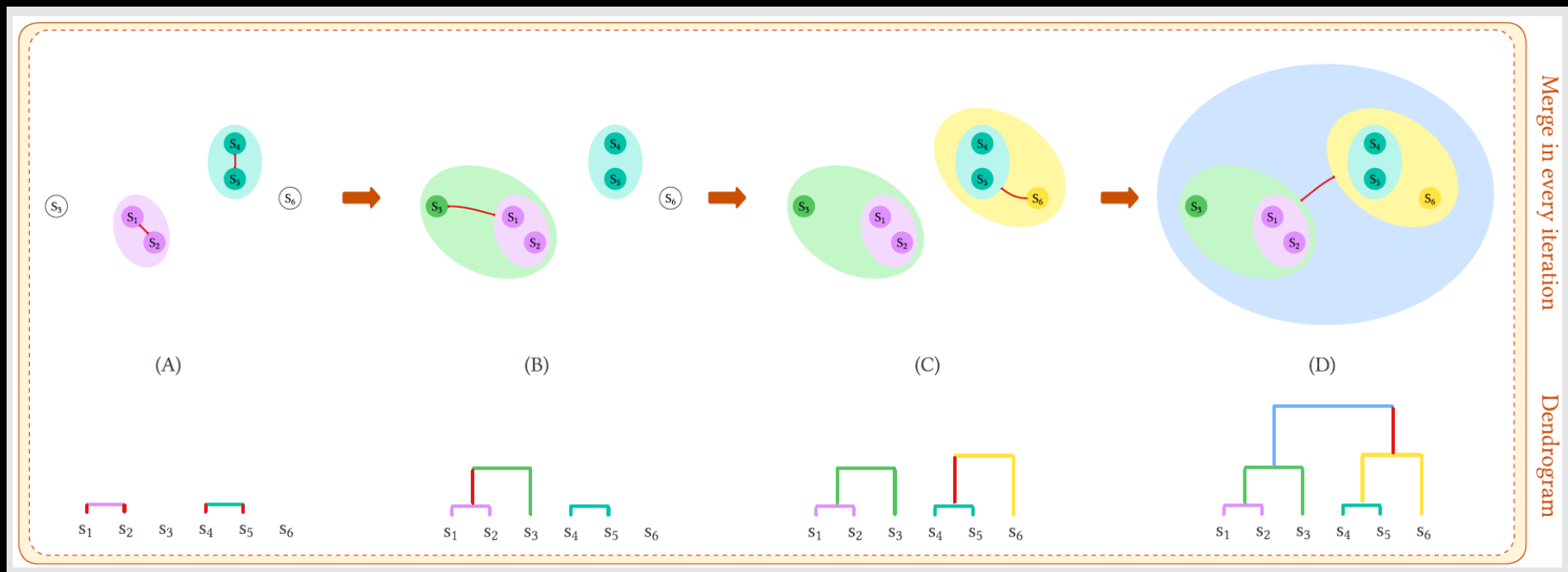
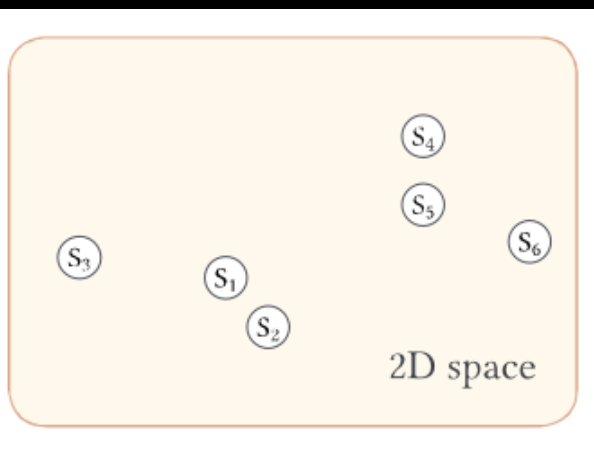
Coarse partitioning, $PF = 2$.

Rana function

Success rate: PSO (0%), DE (80%), ILS (40%)

ALTERNATIVE PARTITIONING METHOD

Hierarchical Agglomerative Clustering



At each step, the two cluster with minimum distance are merged

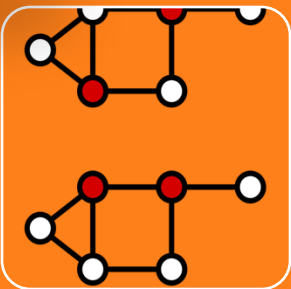
Modified to exclude clusters that are too large

(Chacon, Blum, Ochoa, GECCO'24)



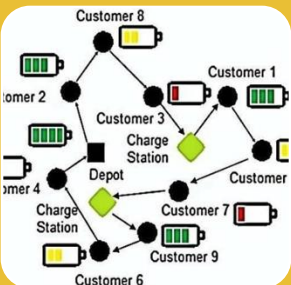
Christian Blum
IA Research Institute, Barcelona, Spain
<https://www.iiia.csic.es/~christian.blum/>

COMBINATORIAL OPTIMISATION: TWO CASE STUDIES



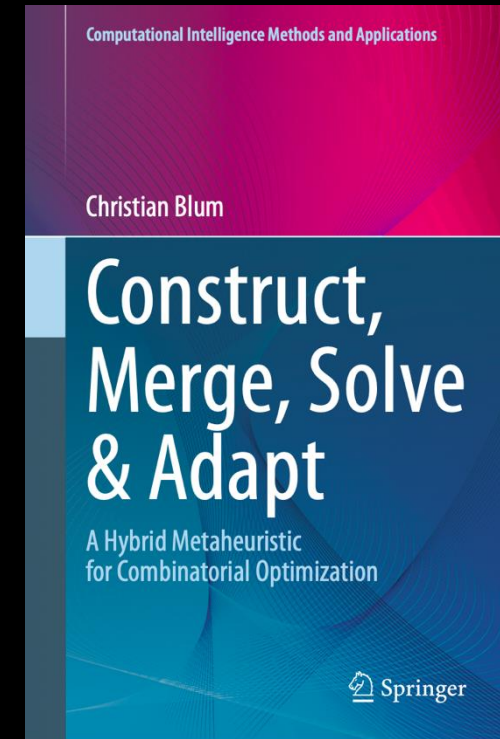
Dominating Set Problem

Minimum positive influence dominating set (MPIDS)



Electrical Vehicle Routing Problem

Two-Echelon Electric Vehicle Routing Problem with Simultaneous Pickup and Deliveries

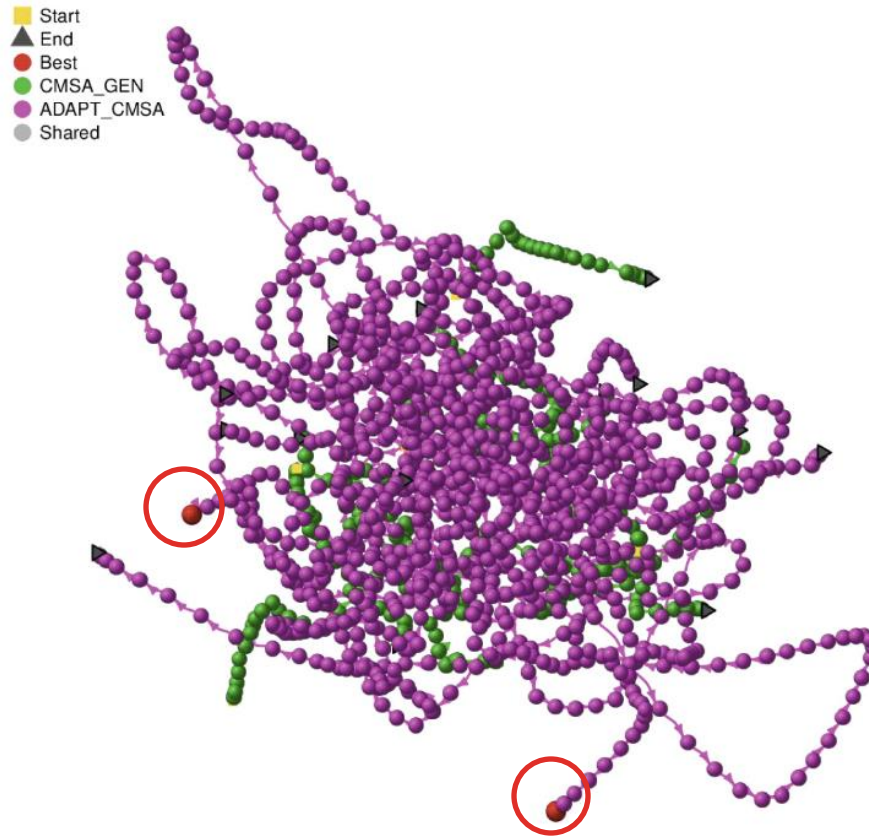


Akbay, M.A., Blum, C. (2024) Two Examples for the Usefulness of STNWeb for Analyzing Optimization Algorithm Behavior. Metaheuristics. MIC.

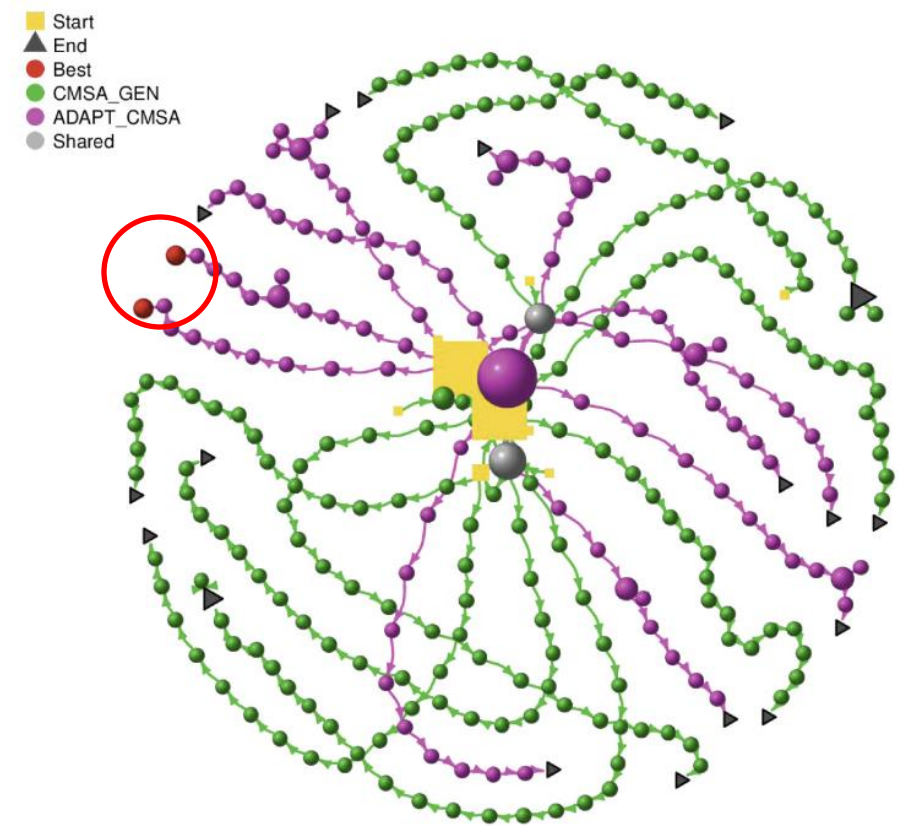
DOMINATING SET PROBLEM

Numerical Results

Algorithm	best	avg.
Green	3955	3958.9
Pink	3930	3934.2



(a) Complete STN



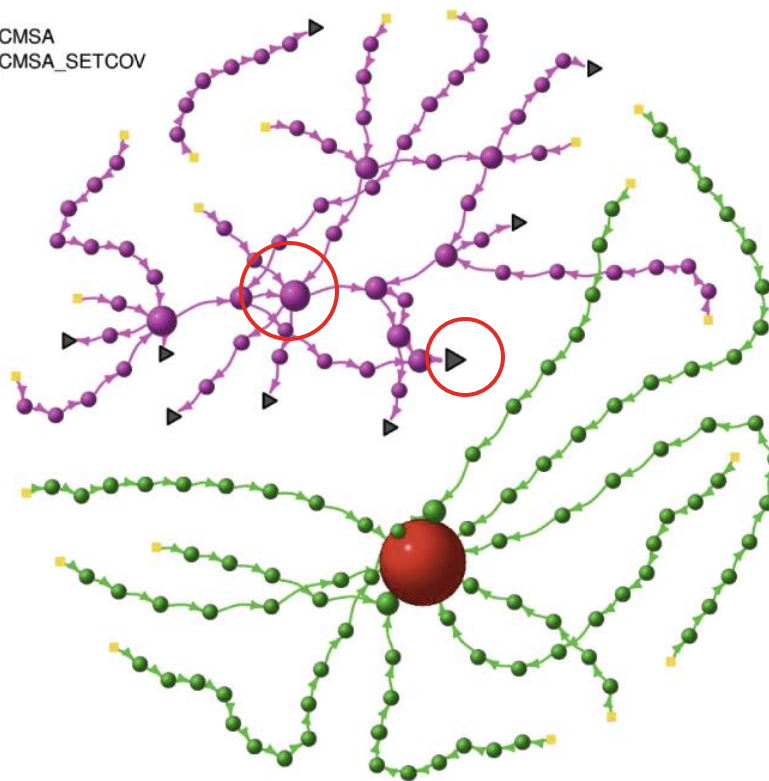
(b) STN after partitioning

ELECTRICAL VEHICLE ROUTING

Numerical Results

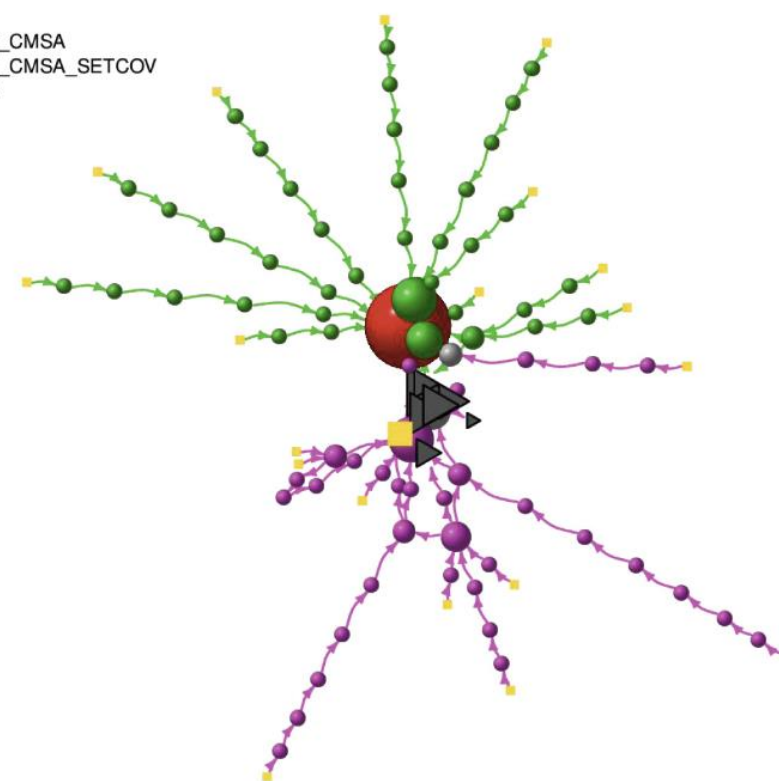
Algo.	best	avg.
Green	4629.95	4629.95
Pink	4678.37	4703.43

■ Start
▲ End
● Best
● ADAPT_CMSA
● ADAPT_CMSA_SETCOV
● Shared



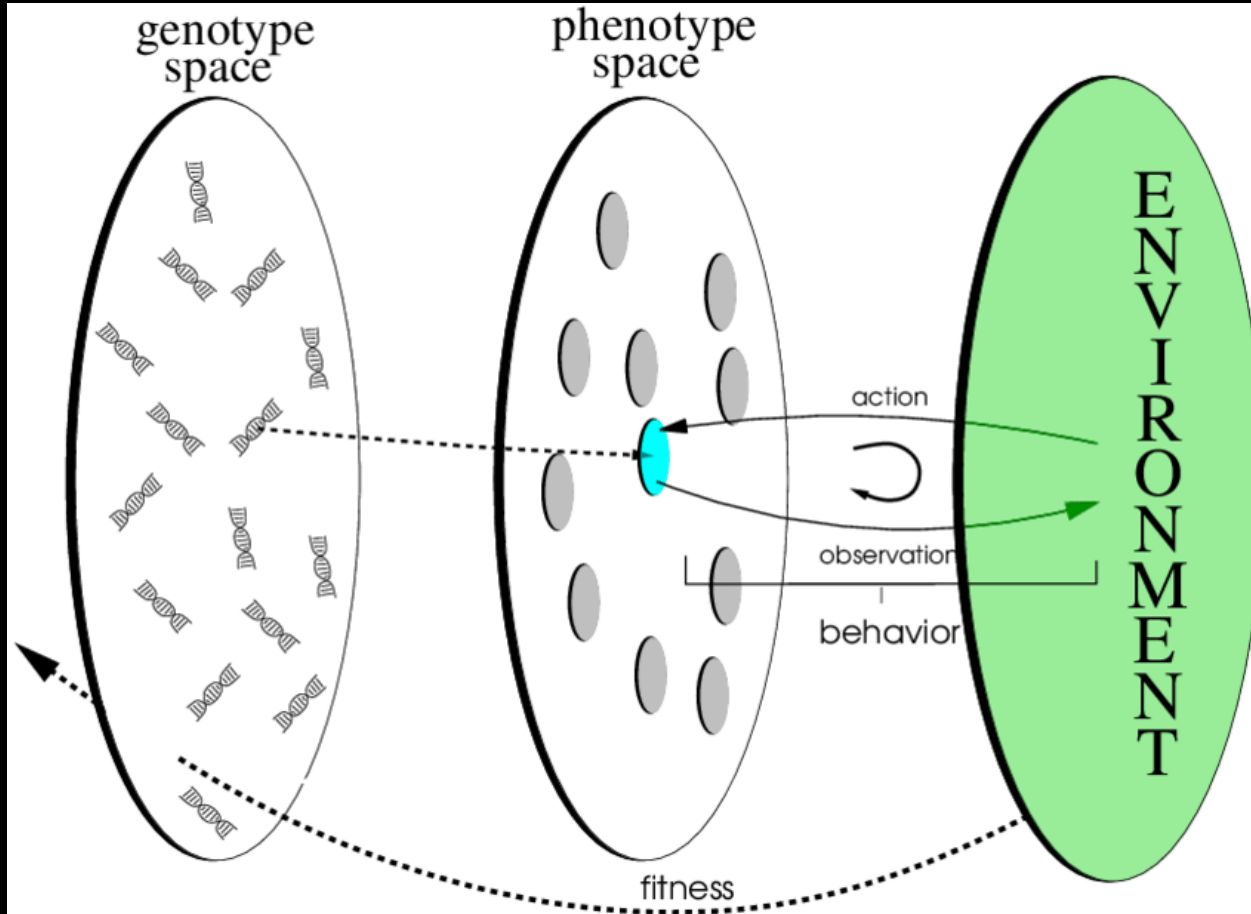
(a) Complete STN

■ Start
▲ End
● Best
● ADAPT_CMSA
● ADAPT_CMSA_SETCOV
● Shared

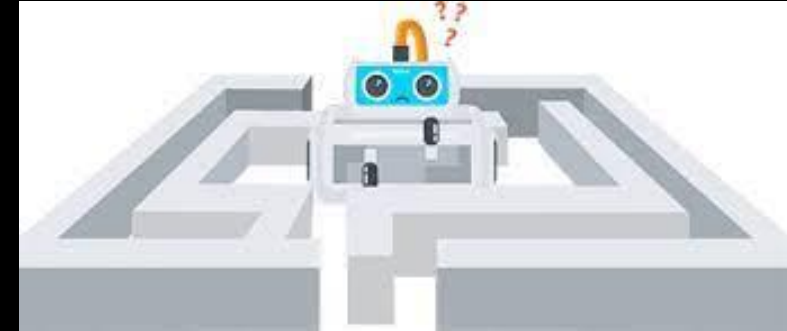


(b) STN after partitioning

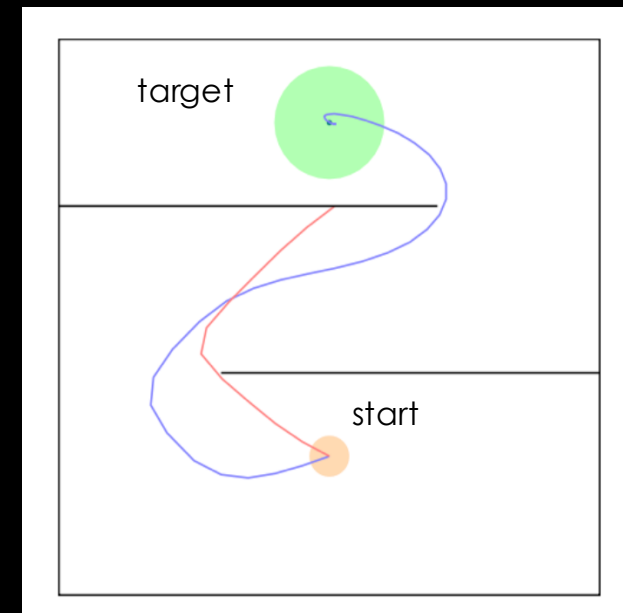
NEUROEVOLUTION & NAVIGATION TASKS



Genotype-Phenotype map.
(Gomez, Togelius, Schmidhuber; 2014)

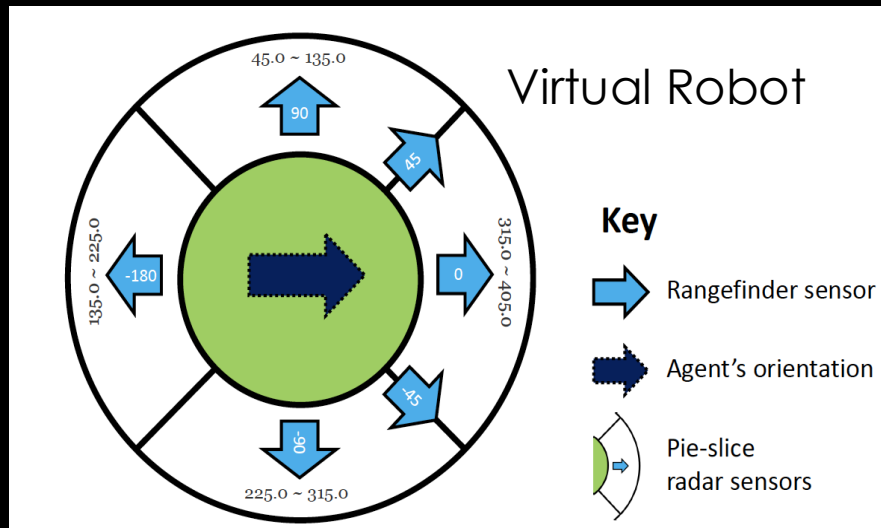


Sequential Decisions
Reinforcement Learning

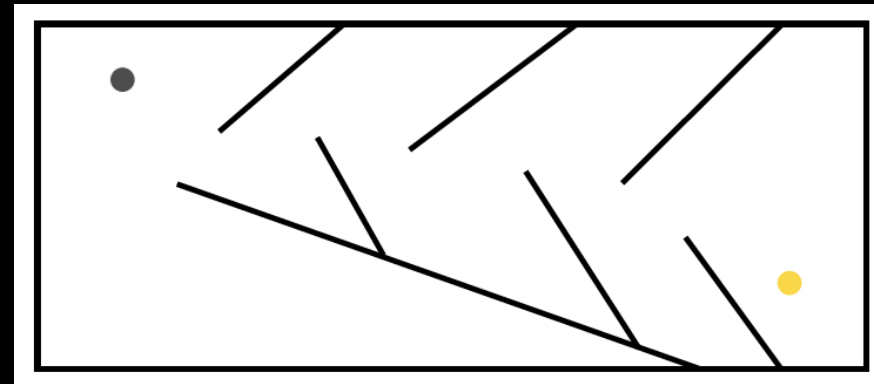


Evolving a
virtual robot
controller

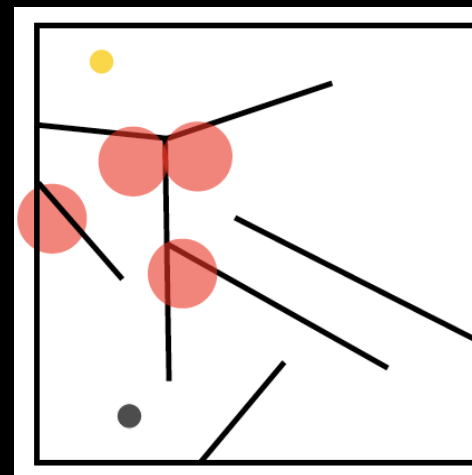
STNs FOR NEAT BENCHMARKS



S Sarti, J Adair, G Ochoa (2022) *Recombination and Novelty in Neuroevolution: A Visual Analysis*. *SN COMPUT. SCI.* 3, 185



Medium
Maze



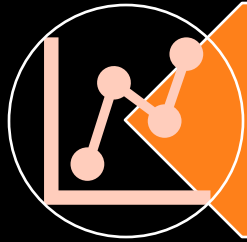
- Target
- Start
- Deceptive traps

Hard Maze
Deceptive problem

STNs FOR NEAT ALGORITHMS



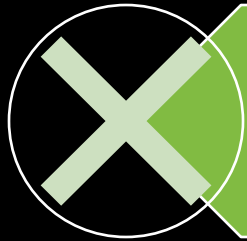
(Lehman Stanley, ECJ 2011)



Fitness-based
search



Novelty search



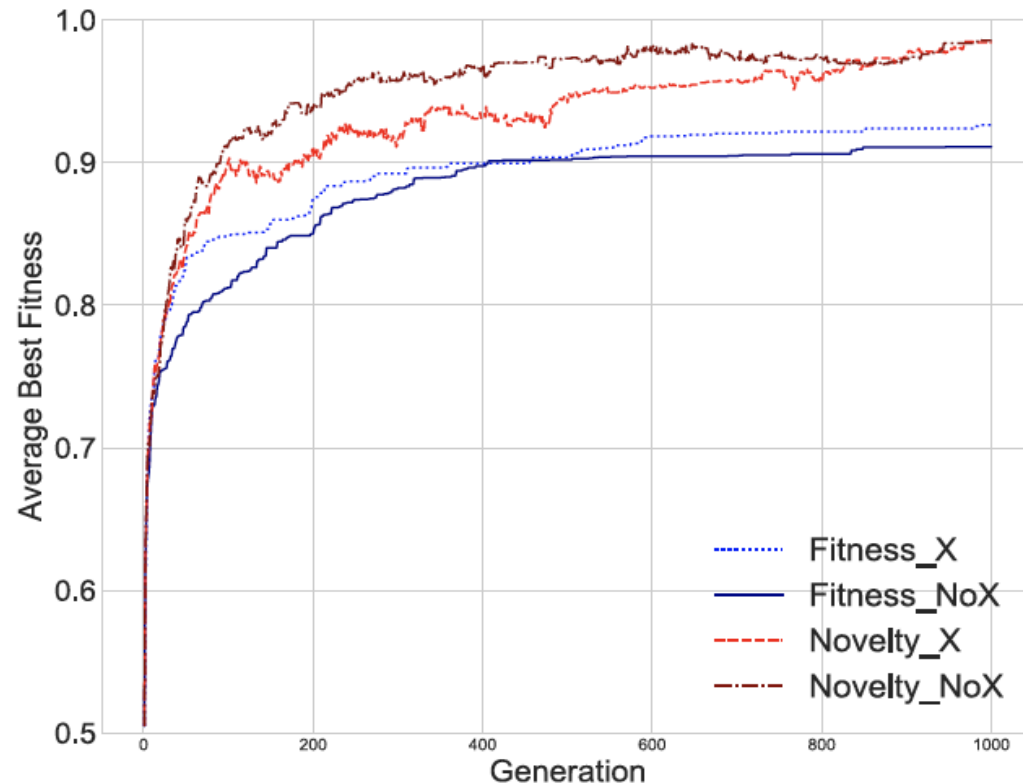
Crossover vs. no
Crossover

Novelty Search

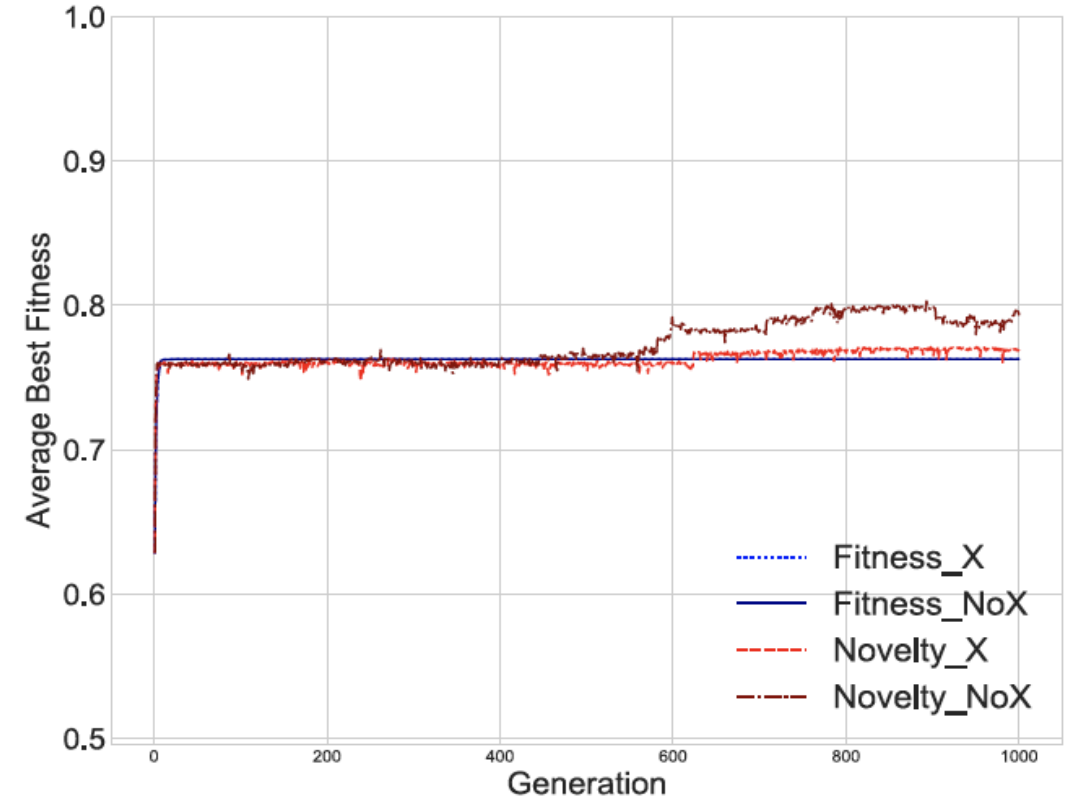
- Abandon objectives!
- Reward novel *behaviours*

NEAT PERFORMANCE CURVES

Average best fitness (30 runs) for the 4 NEAT variants



(a) Medium Maze Domain



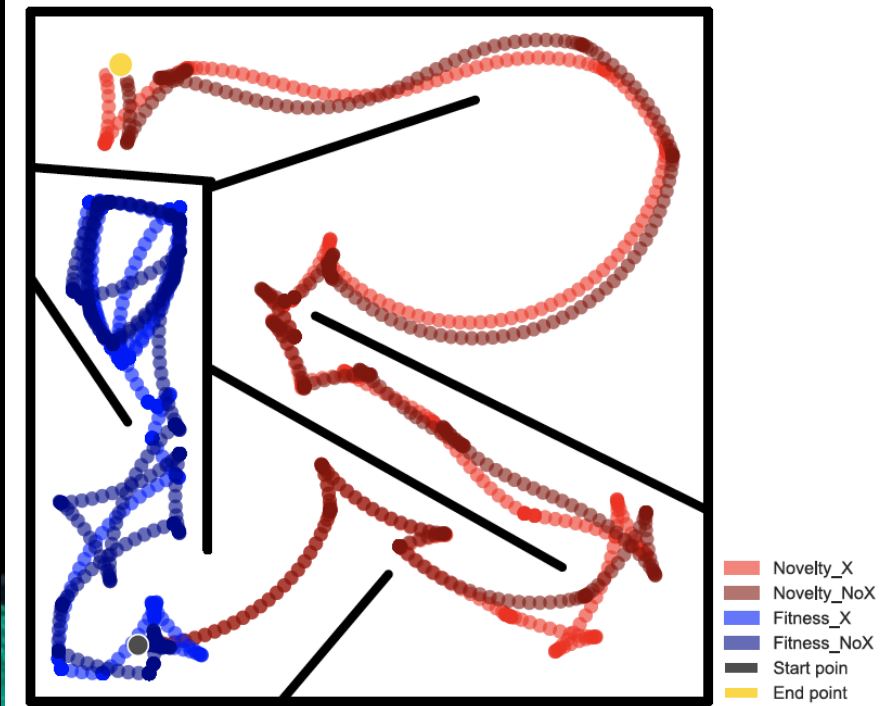
(b) Hard Maze Domain

Medium Maze

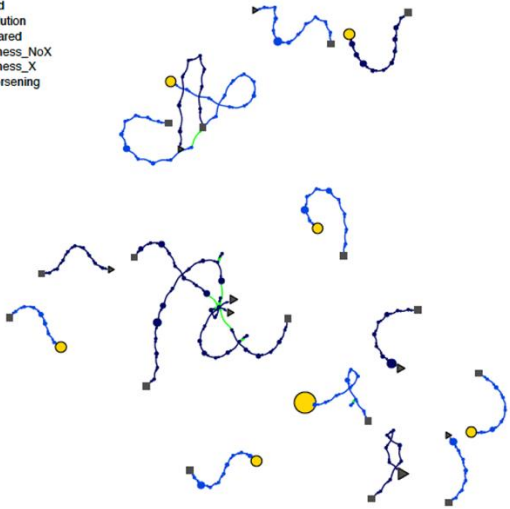
Hard Maze

NEAT STN ANALYSIS

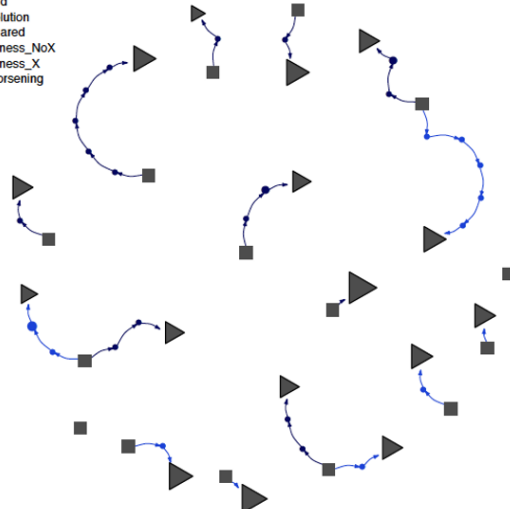
Hard Maze



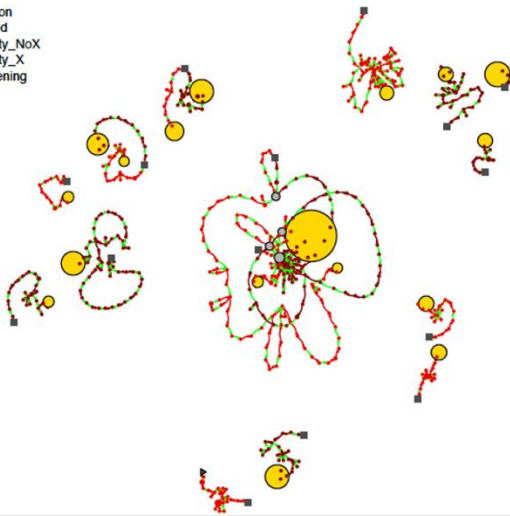
Start
End
Solution
Shared
Fitness_NoX
Fitness_X
Worsening



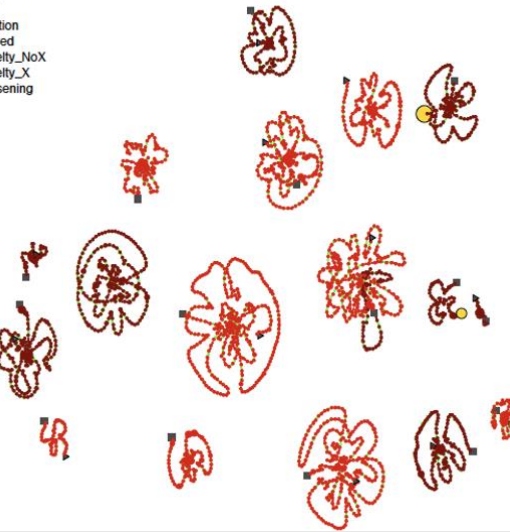
Start
End
Solution
Shared
Fitness_NoX
Fitness_X
Worsening



Start
End
Solution
Shared
Novelty_NoX
Novelty_X
Worsening



Start
End
Solution
Shared
Novelty_NoX
Novelty_X
Worsening

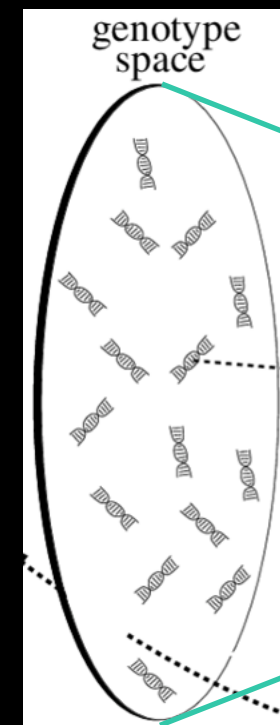
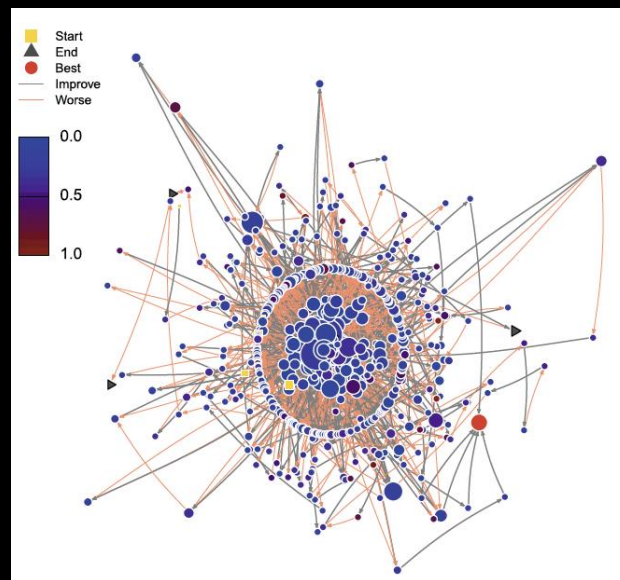
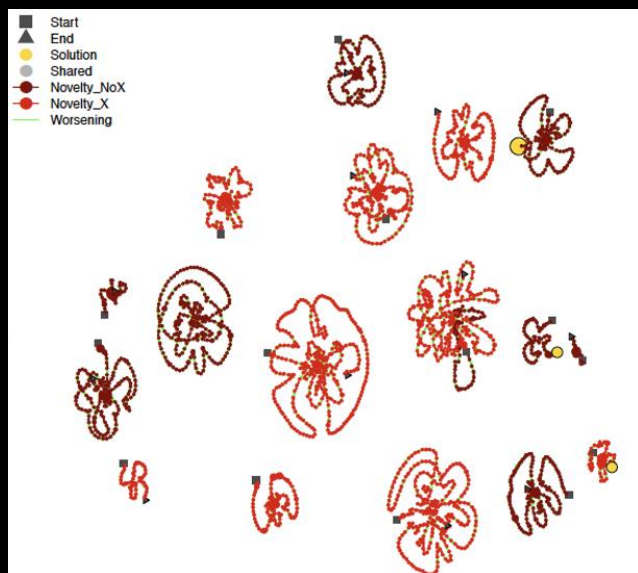
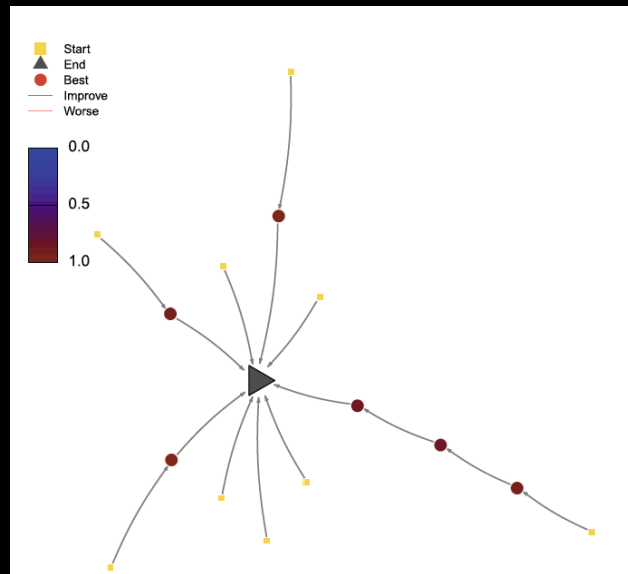
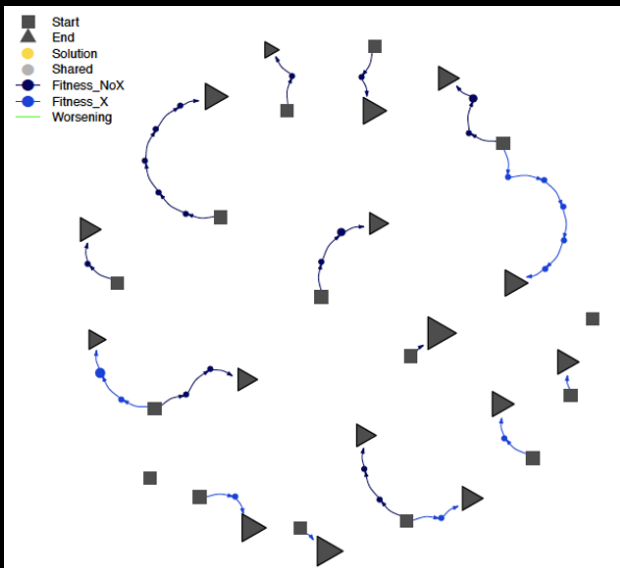


Genotype Space

Behaviour Space

STNs IN BEHAVIOUR SPACE

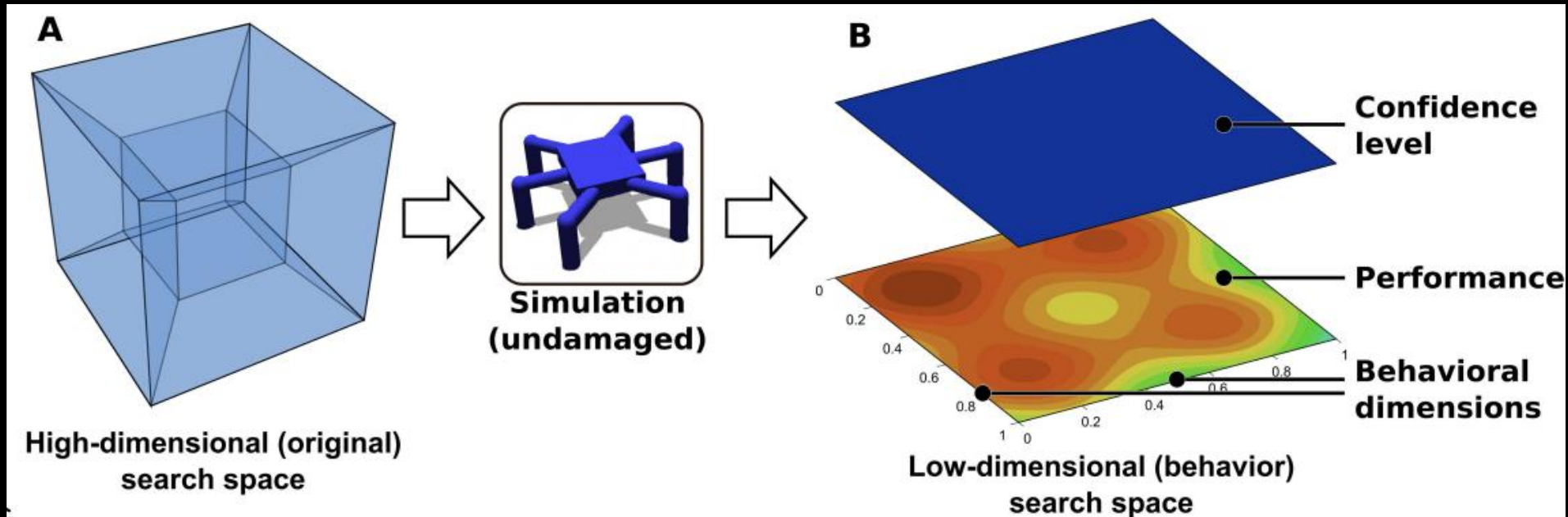
Behaviour Descriptor
(x, y) end of simulation



Neuroevolution trajectory networks of the behaviour space. Sarti, Ochoa, EvoApps 2022

MAP-ELITES & STEPPING STONES

MAP-Elites - Multi-dimensional Archive of Phenotypic Elites



J.-B Mouret, J. Clune (2015). Illuminating search spaces by mapping elites

A. Cully, J Clune, D Tarapore, J_B Mouret (2015) Robots that can adapt like animals. *Nature*,

FINDING STEPPING STONES WITH STNs: EXPERIMENTAL SETUP



Georgia Nadizar,
Univ. of Trieste, Italy

Ongoing Work

Point
Agent

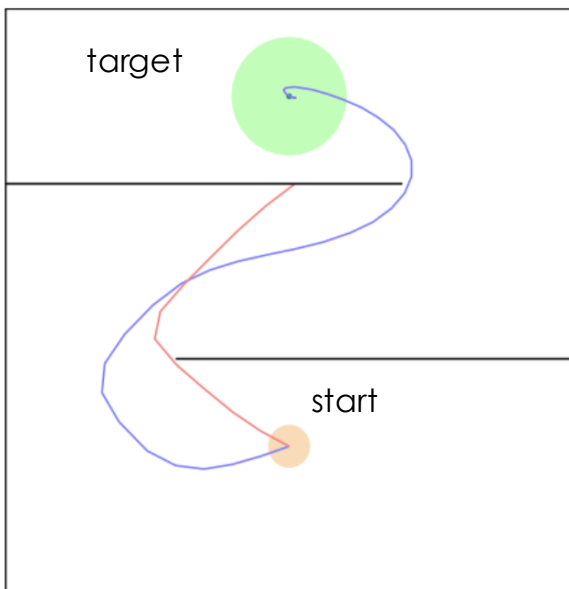
Controller
 $f(x, y) \rightarrow (s_x, s_y)$

Representations

1. Polynomial
2. ANN
3. Tree-based GP

Algorithms

1. Map-Elites
2. GA

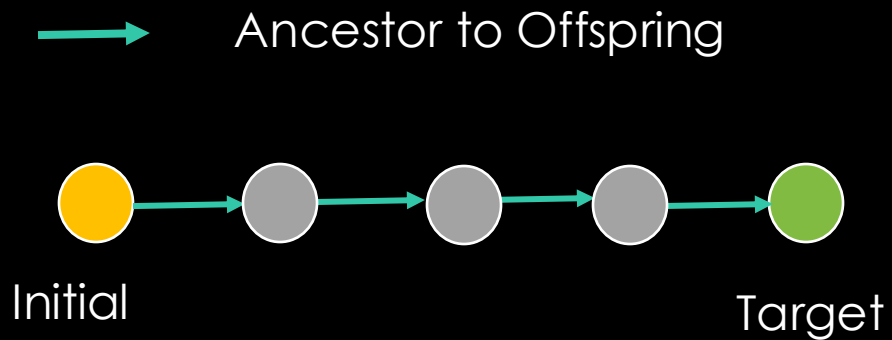


FINDING STEPPING STONES WITH STNs: DEFINITIONS & CONSTRUCTION

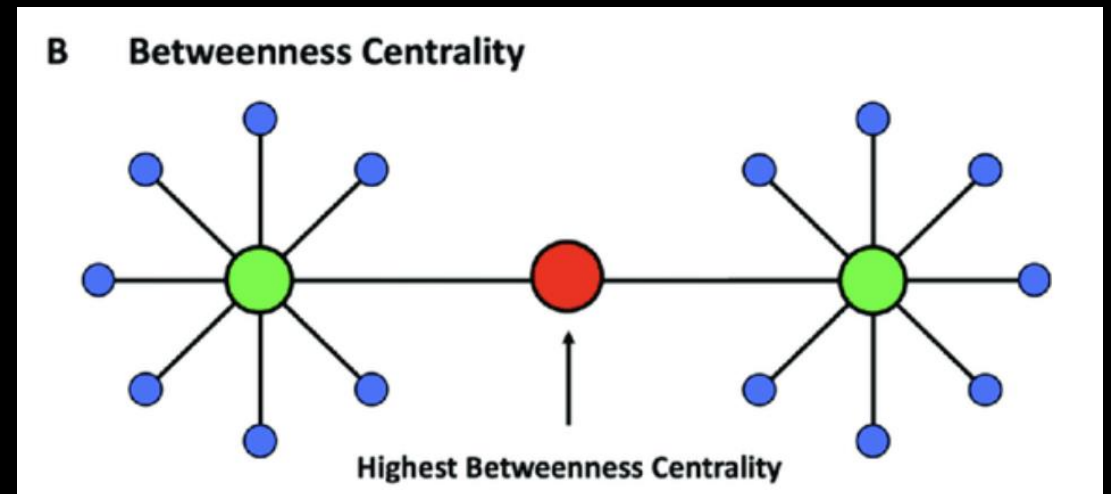
Representative
Solution
ancestors

Location
behaviour
descript. (x, y)

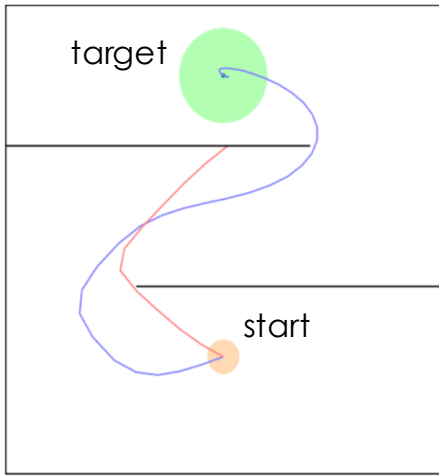
Nodes



Stepping Stones



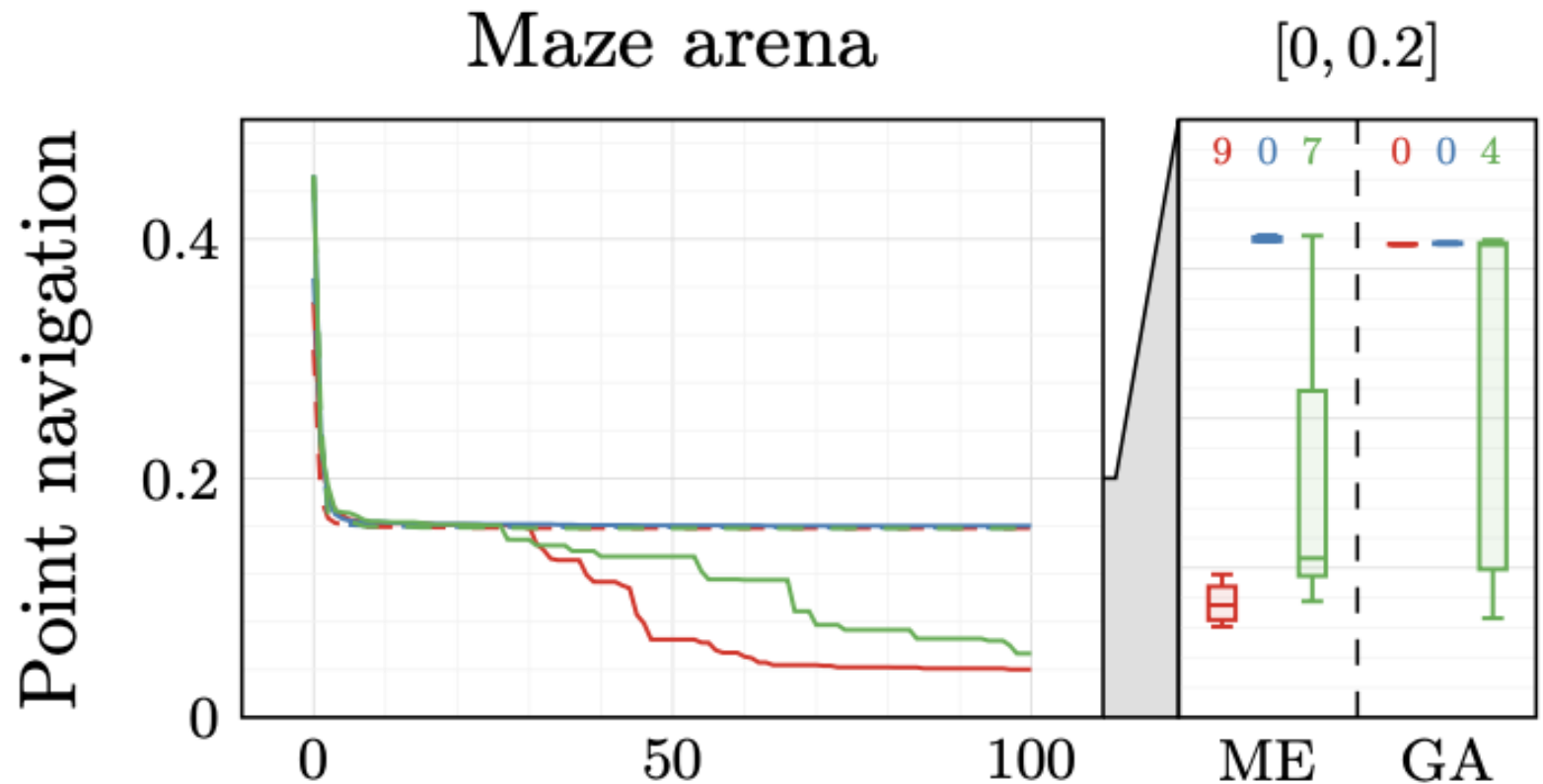
FINDING STEPPING STONES WITH STNs: PERFORMANCE RESULTS



Maze
Navigation

— ME — GA

— -- Polynomial — -- ANN — -- Tree-based



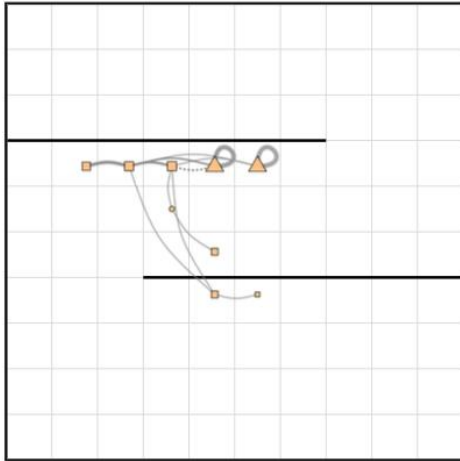
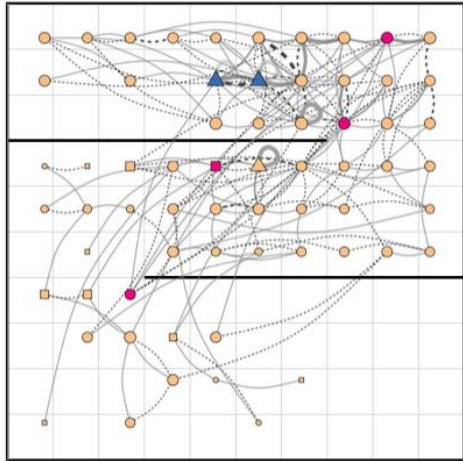
STN ANALYSIS

Nodes: ■ Start ● Medium ▲ End ○ Regular ● Stepping ● Target
Edges: - - - Worsening — Not-worsening

Polynomial

ME

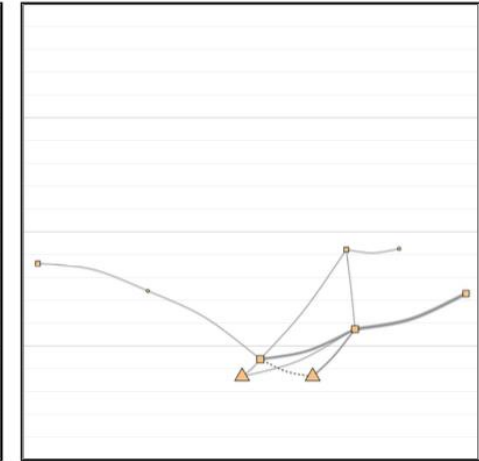
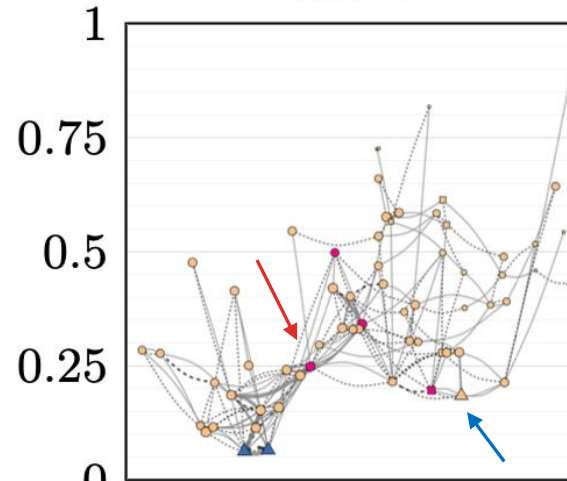
GA



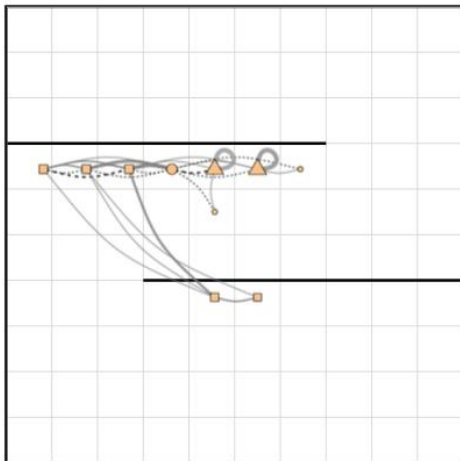
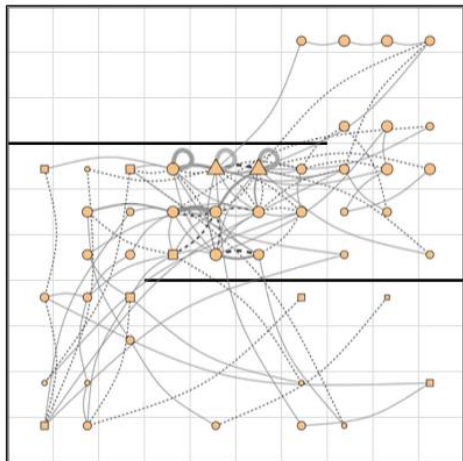
Fitness

ME

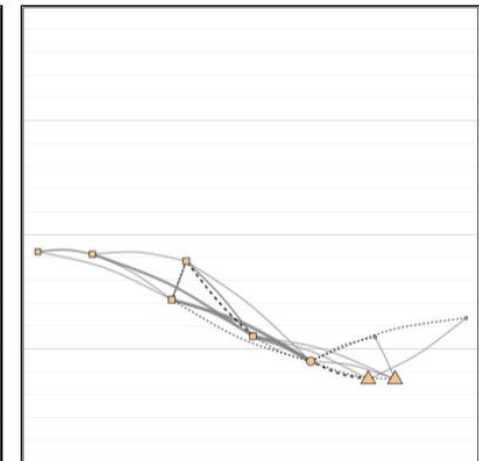
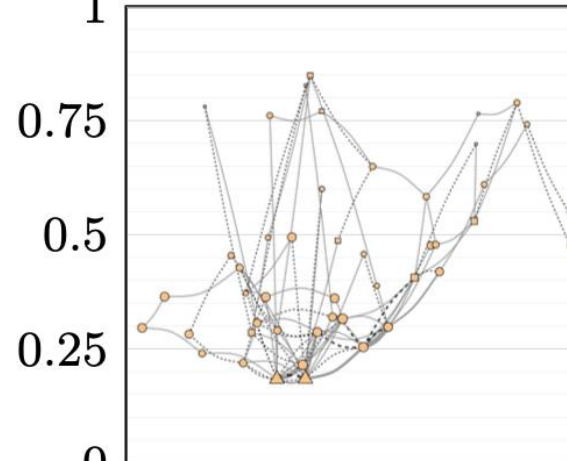
GA



ANN



Fitness



TAKE-HOME MESSAGE

Search Trajectory Networks - STNs

Visual, quantitative, accessible, versatile tool
to study the dynamics of algorithm behaviour

Nodes

Locations
Rep. solution/
Partition

Edges

iterations/genealogy

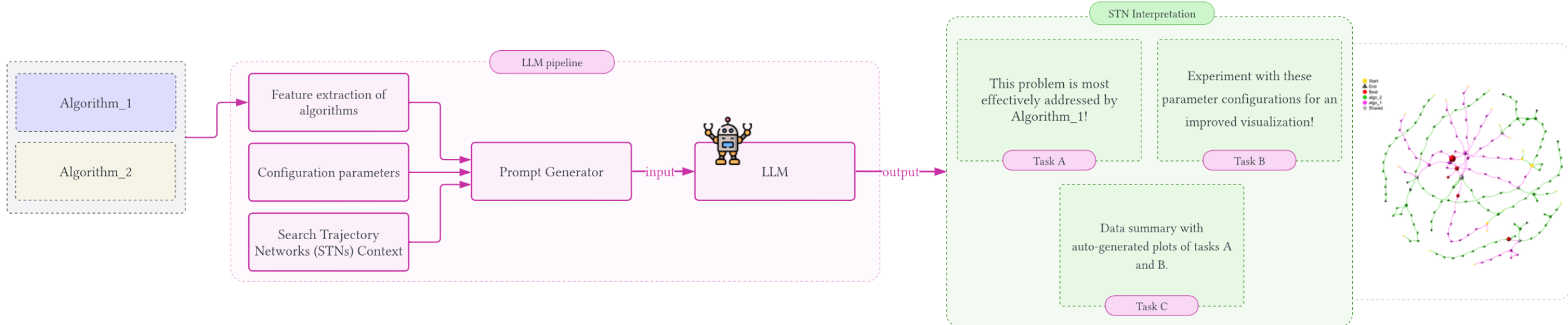




STNs & LLMs

PhD student: Camilo Chacón Sartori, Christian Blum & Gabriela Ochoa
Artificial Intelligence Research, Institute (IIA-CSIC), Barcelona

Large Language Models for the Automated Analysis of Optimization Algorithms (GECCO, 2024)



<https://arxiv.org/abs/2402.08472>

ACO

```

1,1050,110110100101010101
1,950,010110100101010101
1,931,010110100101010101
2,1120,010110100101010101
2,1100,010110100101010101
2,860,010110100101010101
3,1100,010110100101010101
3,999,010110100101010101
3,800,010110100101010101
3,790,010110100101010101

```

BRKGA

```

1,990,010111100101010101
1,950,010110100101010101
1,931,010110100101010101
2,1201,010110100101010101
2,1110,010110100101110101
2,860,010110100101010101
3,1100,010110100101010101
3,999,010110100101010101
3,800,010110100101010101
3,790,010110100101010101

```

Create files for each algorithm

1



Configuration

Strategy ⓘ Shannon Entropy

Partitioning ⓘ 0
(0% = no partitioning)

Advanced options ⓘ

Input files (algorithms)

Name #1

Color

No file chosen

Allowed file extensions: .csv, .txt, .tar.*

Add New Algorithm ⓘ

Generate

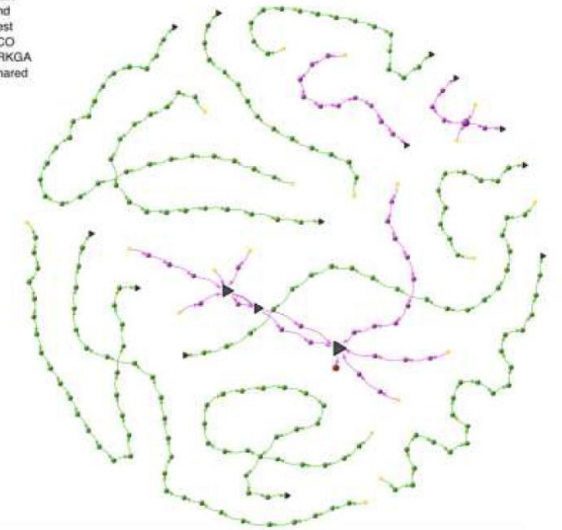
Complete the configuration and upload the files

2



FR layout

Start
 End
 Best
 ACO
 BRKGA
 Shared



View generated and download the PDF

3

stn-analytics.com

STNWeb: A new visualization tool for
analyzing optimization algorithms
CC Sartori, C Blum, G Ochoa

LONs & STNs R code
<https://github.com/gabro8a>