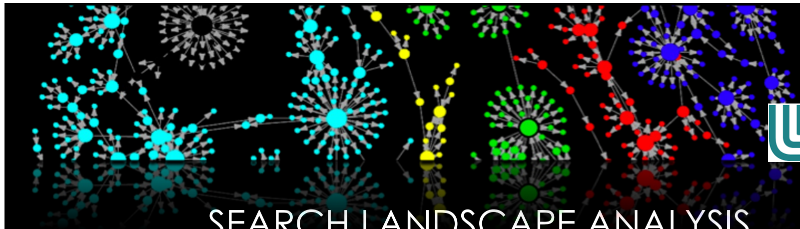

SSAAD 2023

Université de Lille

SEARCH LANDSCAPE ANALYSIS

PART 3 – LOCAL OPTIMA NETWORKS (LONS)

Gabriela Ochoa

UNIVERSITY of STIRLING

Thanks To
M Tomassini, S Verel
N Veerapen, F Daolio
S Thomson, S Herrmann
J Adair, M Contreraz
F Chicano, D Whitley

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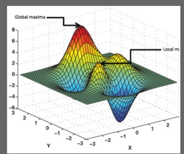
OUTLINE

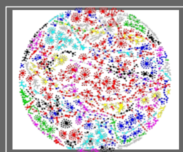


1932, ~2000

Landscape Analysis

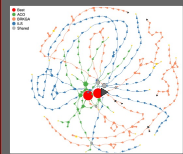
~2000

Complex Networks



2008

Local Optima Networks (LONs)



2020

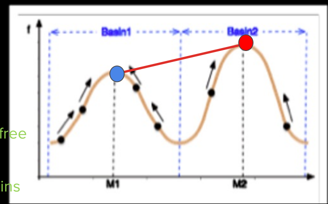
Search Trajectory Networks (STNs)

1

LOCAL OPTIMA NETWORKS (LONS)

Nodes - local optima according to a hill-climbing heuristic

Edges - transitions between optima (basin, escape, crossover)

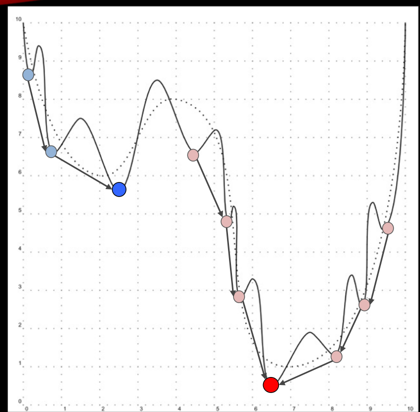


P. K. Doye. The network topology of a potential energy landscape: a static scale-free network. *Physical Review Letter*, 2002.

G. Ochoa, M. Tomassini, S. Verel, and C. Darabos. A study of NK landscapes' basins and local optima networks. GECCO 2008

2

Characterising Funnels with LONs



- Global minimum
- Sub-optimal sink
- Local minimum in optimal funnel
- Local minimum in sub-optimal funnel
- Monotonic edge

MLONs

Monotonic Sequence: a descending sequence of adjacent minima

Funnel: the aggregation of all monotonic sequences ending at the same point (or sink).

3

LON METHODS

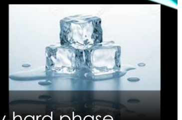
General

PROBLEM DOMAINS

- **Combinatorial**
  - **Binary**
    NK, Number Partitioning, MAX-SAT, UBQP, Multi Knapsack, String Partition
  - **Permutation**
    QAP, TSP, Flow shop, Cyclic Bandwidth
- **Continuous**
  - **Synthetic**
    Ackley, Griewank, Rana, Michalewicz, Rastrigin, Bi-rastrigin, Schwefel 2.26, ***UF***
  - **Engineering Design**
    Radar pulse modulation
- **ML & GI**
  - **Machine Learning**
    Feature Selection, Clustering, AutoML, Neuroevolution, NAS
  - **Genetic Improvement**
    Bug-fixing
- **More**
  - **Multi-hard problems**
    Traveling Thief
  - **Biotechnology**
    Protein Design
    Chemotherapy Scheduling

5

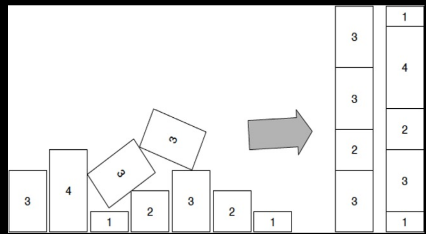
Number Partitioning (NPP)



Given a set of n positive integers $A=\{a_1, a_2, .., a_n\}$, drawn at random from the set $\{1, 2, .., M\}$, find a disjoint partition (S_1, S_2) of A such that the discrepancy D between their sums is minimised

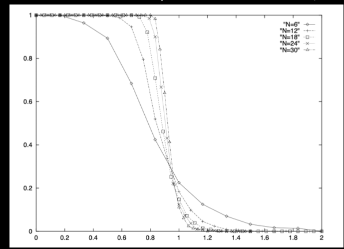
A partition is perfect if $D = 0$, where

$$D = | \Sigma_{S1}\, a_i - \Sigma_{S2}\, a_i \ |$$



Easy-hard phase transition, $k = \log_2(M)/n$

(Gent & Walsh, 1996)



$k < 1$ many partitions

$k > 1$ very few perfect partitions

$k = 1$ easy/hard phase transition

6

NPP Instance example N = 10, k = 0.4

Instance data, ten numbers: **10 7 10 4 14 14 11 3 9 6**

Worst solutions: when there is a maximal difference between the two sets.

This happens when all the elements are in one set

10 + 7 + 10 + 4 + 14 + 14 + 11 + 3 + 9 + 6 = 88

x = 0000000000 f(x)= 88 - 0 = 88

x = 1111111111 f(x)= 0 - 88 = 88

Best solutions: several solutions are optimal, here some examples

10 7 10 4 14 14 11 3 9 6

- 1 1 1 0 1 0 0 1 0 0 f(x)= (4+14+11+9+6) - (10+7+10+14+3) = 44 - 44 = 0
- 1 1 1 0 0 1 0 1 0 0 f(x)= (4+14+11+9+6) - (10+7+10+14+3) = 44 - 44 = 0
- 1 1 0 1 1 0 0 0 1 0 f(x)= (10+14+11+3+6) - (10+7+4+14+9) = 44 - 44 = 0
- 1 1 0 1 0 1 0 0 1 0 f(x)= (10+14+11+3+6) - (10+7+4+14+9) = 44 - 44 = 0

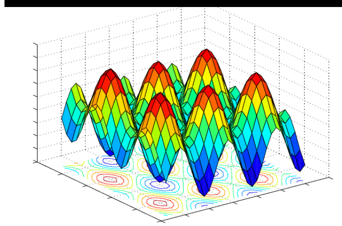
…

LON CONSTRUCTION

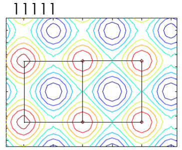
Binary representation

	2	1	3	2	3
Sol	1	1	0	1	0

Example with $N = 5$ $M = 3$



Full Enumeration
00000
00001 ...
11111



$N = \{10, 15, 20\}$ $2^{10} = 1024$, $2^{20} \cong 1M$
k in [0.4, 1.2] steps 0.1

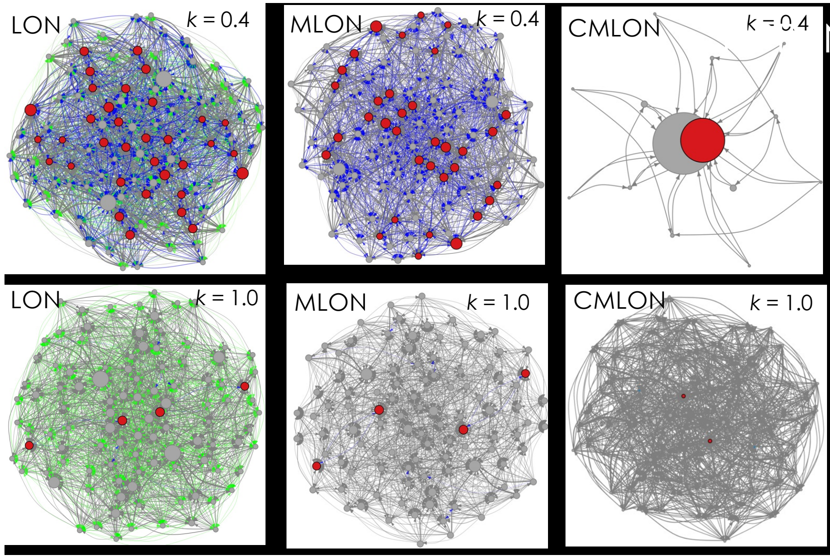
LON
- 1-flip local search, 2-flip perturbation

Monotonic LON (MLON)
- Worsening edges are pruned

Compressed MLON (CMLON)
- LON plateaus contracted into single nodes

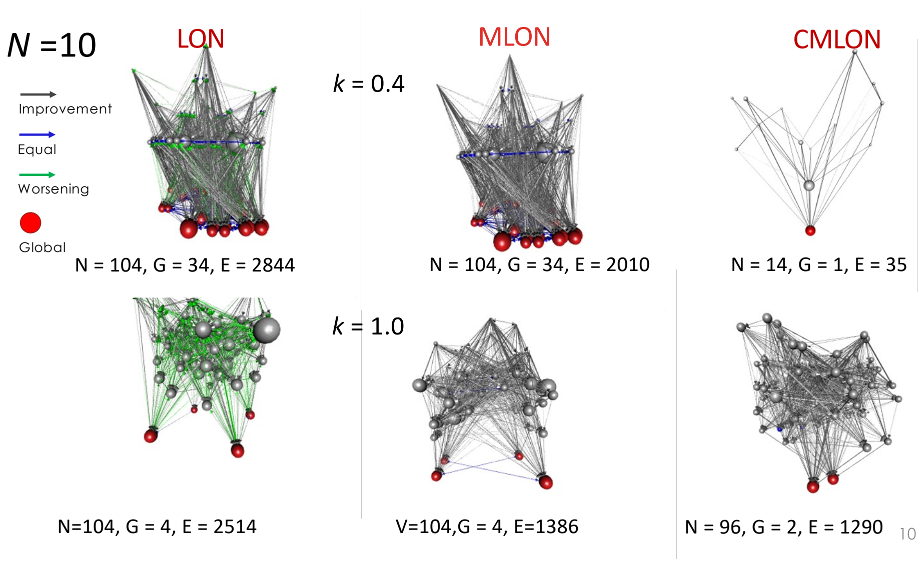
8

NPP
N = 10

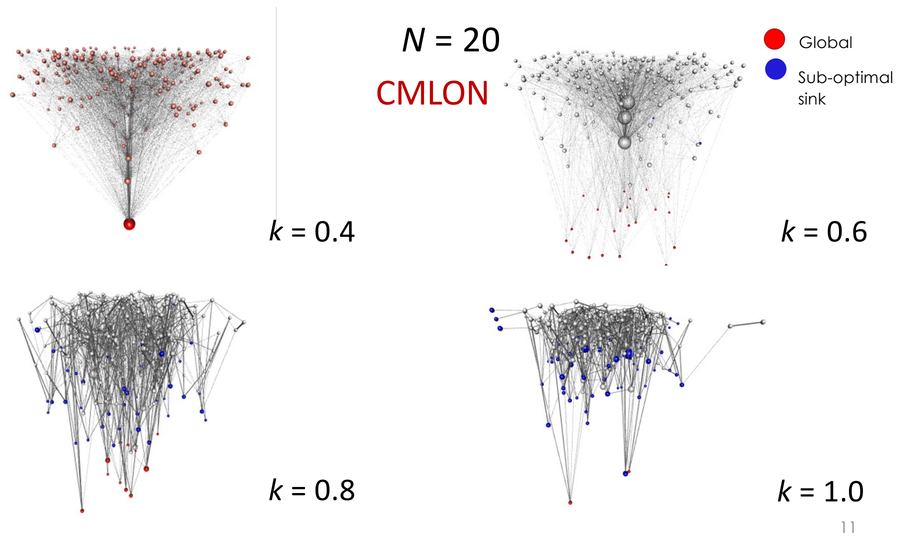


Improvement
Equal
Worsening
Global

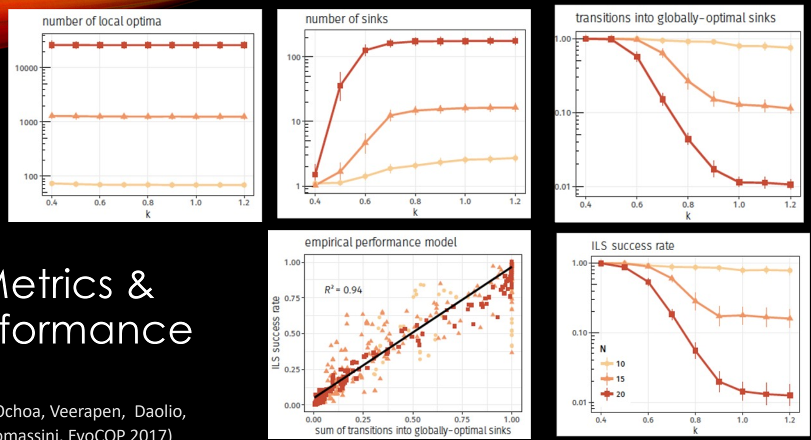
9



N =10
LON
MLON
CMLON
Improvement
Equal
Worsening
Global
k = 0.4
N = 104, G = 34, E = 2844
N = 104, G = 34, E = 2010
N = 14, G = 1, E = 35
k = 1.0
N=104, G = 4, E = 2514
V=104,G = 4, E=1386
N = 96, G = 2, E = 1290
10



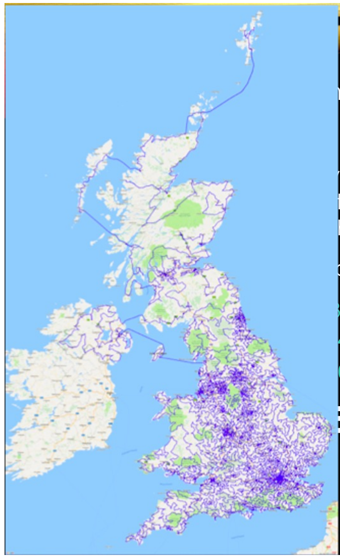
N = 20
CMLON
Global
Sub-optimal sink
k = 0.4
k = 0.6
k = 0.8
k = 1.0
11



Metrics & Performance

(Ochoa, Veerapen, Daolio, Tomassini. EvoCOP 2017)

12



mber of cities minimising the

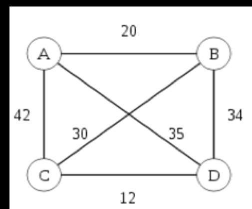
een each pair is given. We
te to visit each city exactly
he starting point.

ation (ordering) of cities.

0+12+35= 97
4+12+42=108
0+34+3

ESMAN

UK24727
A shortest-possible walking tour through the pubs of the United Kingdom.
http://www.math.uwaterloo.ca/tsp/pubs/index.html



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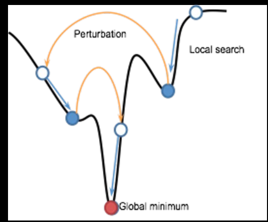
TRAVELLING SALESMAN (TSP)

Sampling and constructing LONs with escape edges

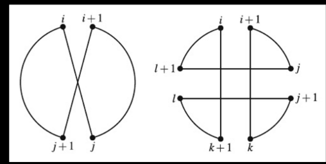
Algorithm 1 ILS sampling

$L \leftarrow \{\}$; $E \leftarrow \{\}$ (initialise LON data)
repeat
  $s_0 \leftarrow \mathrm{RandomInitialSolution}$
  $s^* \leftarrow \mathrm{HillClimber}(s_0)$
  $L \leftarrow L \cup \{s^*\}$ (record LON data)
  repeat
    $s' \leftarrow \mathrm{RandomMutation}(s^*)$
    $s'^* \leftarrow \mathrm{HillClimber}(s')$
    if $f(s'^*) \leq f(s^*)$ **then**
      $L \leftarrow L \cup \{s'^*\}$ (record LON data)
      $E \leftarrow E \cup \{(s^*, s'^*)\}$ (record LON data)
      $s^* \leftarrow s'^*$
    end if
  until *ILS termination condition is met*
until *sampling termination condition is met*

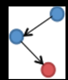


Chained Lin-Kernighan
(Martin, Otto, Felten, 1992)

- Form of Iterated Local Search
- Diversification & Intensification



2-exchange double-bridge



Nodes: LK local optima
Edges: double-bridge escapes

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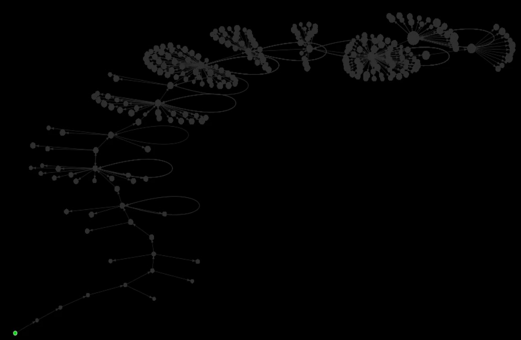
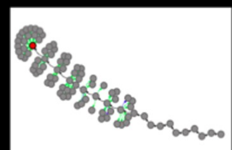


A Chained-LK run on instance lin318
318 points, drilling application



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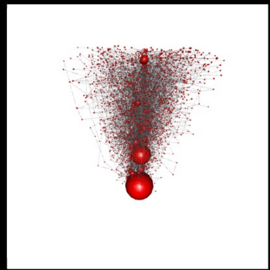
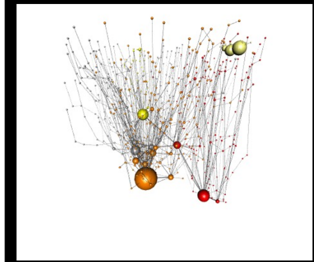
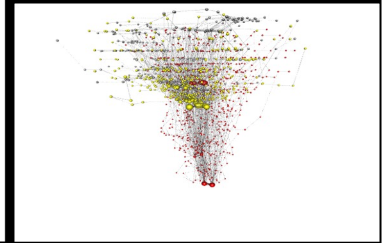
TSP INSTANCES



c755 Clustered Cities
Funnels: 1, Success: 100%



E755 Uniform Cities
Funnels: 4, Success: 13%



att532 (cities in the US)
Funnels: 2, Success: 44%

(Ochoa & Veerapen, JoH, 2018)

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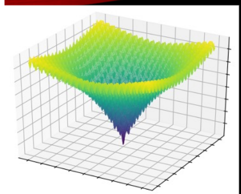
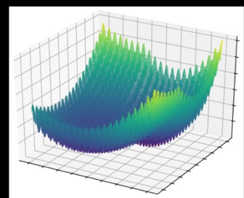
NUMERICAL OPTIMISATION BENCHMARK FUNCTIONS



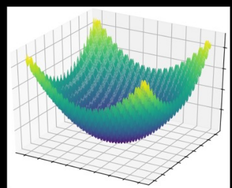
$$f(x,y) = -20\exp\left[-0.2\sqrt{0.5\left(x^2+y^2\right)}\right] - \exp\left[0.5\left(\cos 2\pi x + \cos 2\pi y\right)\right] + e + 20$$

Ackley
[−32.768, 32.768]



$$f(\mathrm{x}) = f(x_1, \ldots, x_n) = 10\sum_i^n (1 - \cos 2\pi(x_i - \mu_1)) + \min\left(\sum_i^n (x_i - \mu_1)^2, \quad d \cdot n + s \cdot \sum_i^n (x_i - \mu_2)^2\right)$$

Birastrigin



Rastrigin
[−5.12, 5.12]

$$f(\mathrm{x}) = f(x_1, \ldots, x_n) = 10n + \sum_{i=1}^n \left(x_i^2 - 10\cos(2\pi x_i)\right)$$

LONs for continuous optimisation - Methodology

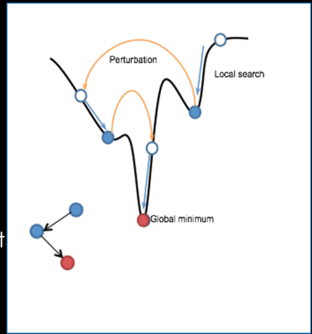
Sampling with *Basin-Hopping* - 100 runs

- Local minimiser: L-BFGS
- Perturbation operator (step size *pstep*)

  $x_i = x_i + pstep \times$ uniform random [-1, 1]

  pstep: empirically determined (50% escape)
- Stopping condition: 1,000 iterations without improvement

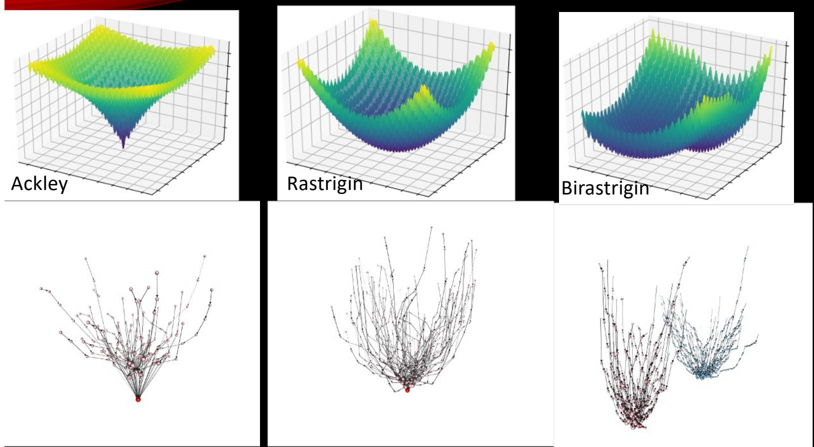
MLON. Monotonic LON – non deteriorating edges



David J. Wales and Jonathan P. K. Doye (1997) Global Optimization by Basin-Hopping and the Lowest Energy Structures of Lennard-Jones Clusters Containing up to 110 Atoms. *The Journal of Physical Chemistry A 101, 28*

(Adair, Malan, Ochoa, GECCO C 2019)

CONTINUOUS OPTIMISATION



2 variables

5 variables!

Basin-hoping

(Adair, Malan, Ochoa, GECCO C 2019)

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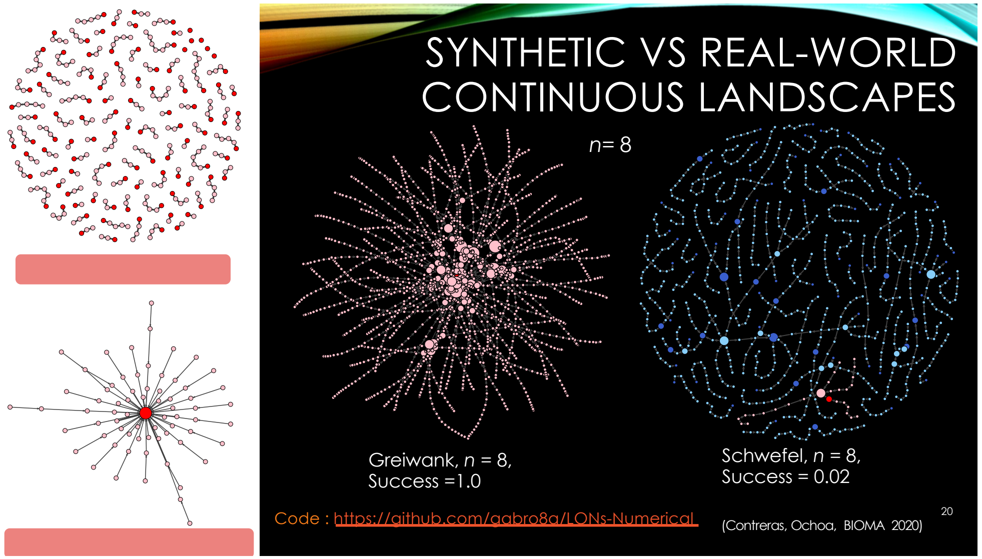
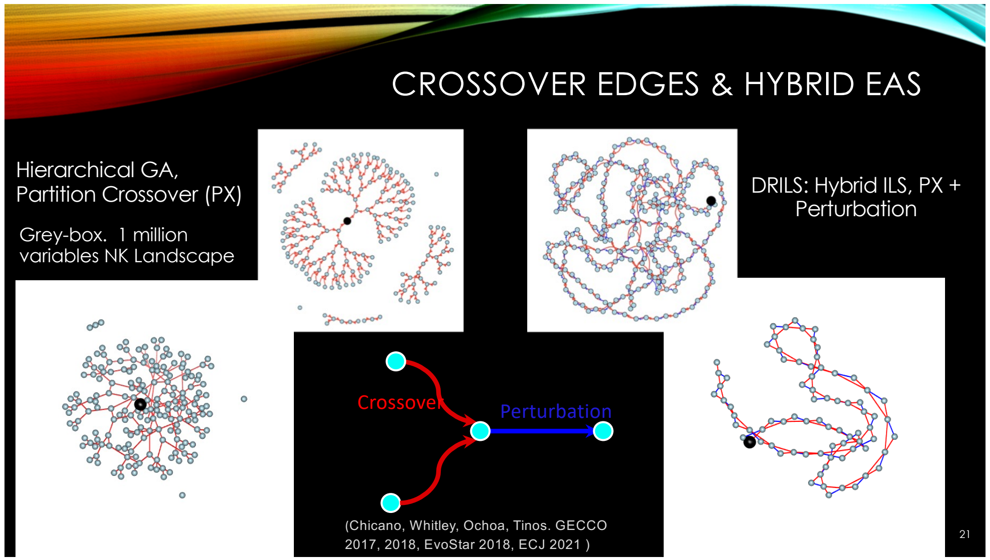


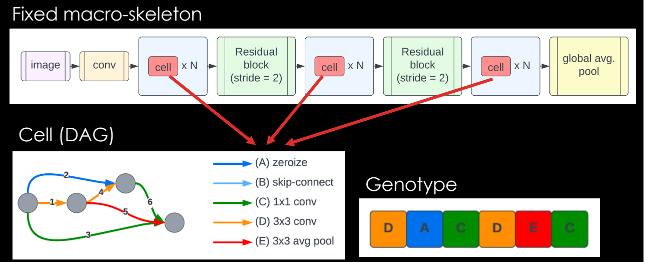
SYNTHETIC VS REAL-WORLD CONTINUOUS LANDSCAPES
n= 8
Greiwank, n = 8,
Success =1.0
Schwefel, n = 8,
Success = 0.02
Code : https://github.com/gabro8a/LONs-Numerical
(Contreras, Ochoa, BIOMA 2020)
20



CROSSOVER EDGES & HYBRID EAS
Hierarchical GA,
Partition Crossover (PX)
Grey-box. 1 million
variables NK Landscape
DRILS: Hybrid ILS, PX +
Perturbation
Crossover
Perturbation
(Chicano, Whitley, Ochoa, Tinos. GECCO
2017, 2018, EvoStar 2018, ECJ 2021)
21

CASE STUDY: NAS BENCHMARK

- Tabular benchmark (NATS-Bench - Image classification)
- Cell-based search space
- Fitness Landscape Analysis (DOS, FDC, LONS)
- Impact of noise in performance estimation



Discrete optimisation problem
max $a \in A$ $f(a)$
$f(a)$ validation accuracy

- DAG with 6 edges.
- Each edge can be one of 5 operations
- Size of the search space is $5^6 = 15,625$

Dong, X. et. al. (2021) NATS-Bench: Benchmarking NAS algorithms for architecture topology and size. *IEEE Trans. Pattern Analysis and Machine Intelligence*

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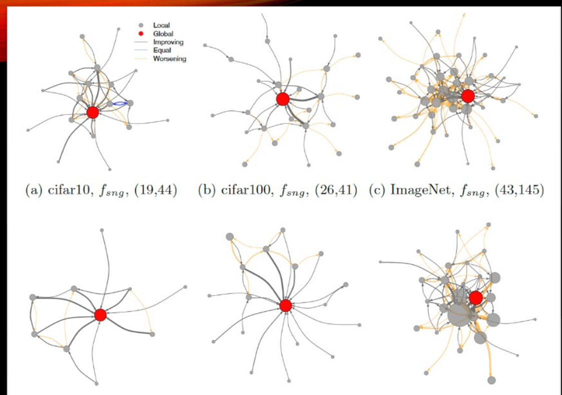
NAS LANDSCAPES LONS



(a) cifar10, f_{sng}, (19,44) (b) cifar100, f_{sng}, (26,41) (c) ImageNet, f_{sng}, (43,145)

(d) cifar10, f_{avg}, (10,18) (e) cifar100, f_{avg}, (18,27) (f) ImageNet, f_{avg}, (28,98)

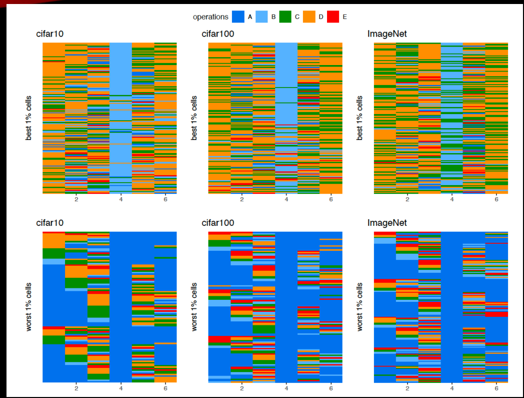
Local optima networks (**LONs**) for all datasets and the two fitness functions.

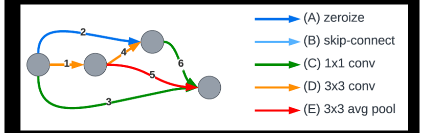
The number of nodes n and edges e are indicated as (n, e).

Size of nodes: proportional to incoming degree

Neural Architecture Search: A Visual Analysis (2022) G Ochoa & N Veerapeen, PPSN

NAS LANDSCAPES GENOTYPE MAPS





Genotype maps of the best 1% (top), and worst 1% (bottom) performing cells, sorted according to *f_avg*.

Each line visualises a cell. Positions are coloured according to the respective operation.

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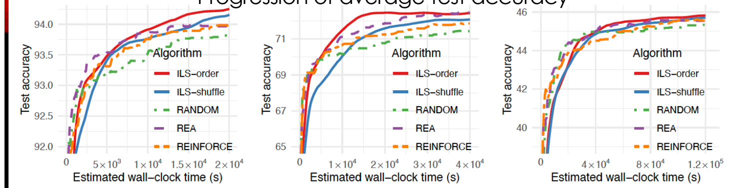
NAS ALGORITHM PERFORMANCE

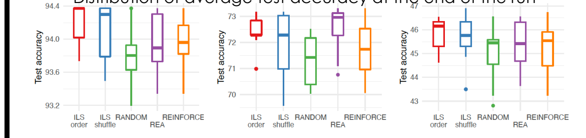
Progression of average test accuracy



(a) cifar10 (b) cifar100 (c) ImageNet

- 30 Runs
- 5 Search strategies

Distribution of average test accuracy at the end of the run



(a) cifar10 (b) cifar100 (c) ImageNet

- Two versions of Iterated Local Search (ILS) (order shuffle) – order to explore neighbours
- Random Search, Regularized Evolutionary Algorithm, Reinforcement Learning

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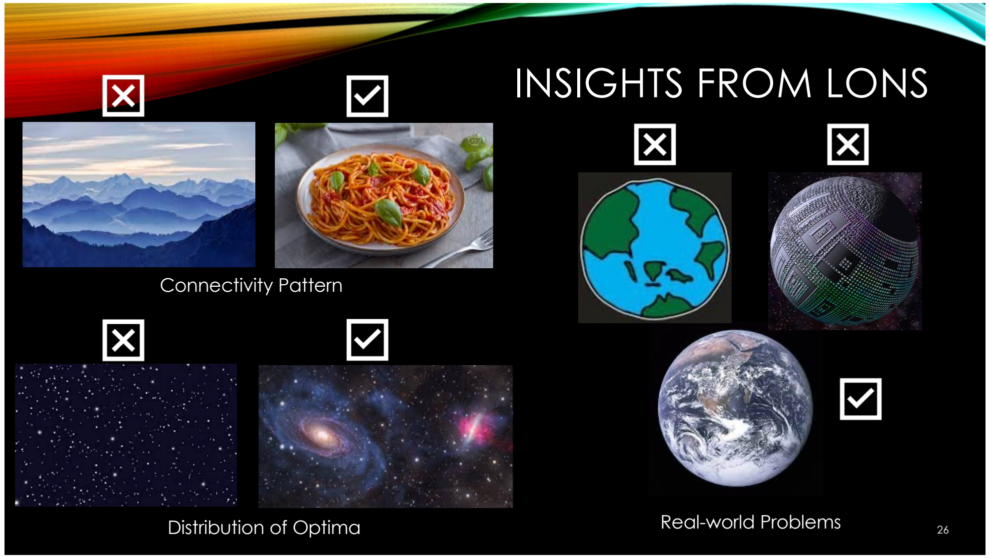

REFERENCES (LONS)

Inspiration from Energy Landscapes

- J P K Doye (2002) Network Topology of a Potential Energy Landscape: A Static Scale-Free Network, *Phys. Rev. Lett.*, vol. 88, no. 23, p. 238701
- J P K Doye, M A Miller, and D J Wales (1999) The double-funnel energy landscape of the 38-atom Lennard-Jones cluster, *The Journal of Chemical Physics*, vol. 110, no. 14, pp. 6896–6906

Original/Early Papers

- G Ochoa, M Tomassini, S Vérel, and C. Darabos (2008) A Study of NK Landscapes' Basins and Local Optima Networks, Conference on Genetic and Evolutionary Computation, GECCO, 2008, pp. 555–562.
- S Vérel, G Ochoa, M Tomassini (2011) Local Optima Networks of NK Landscapes With Neutrality. *IEEE Trans. Evol. Comput.* 15(6): 783-797

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REFERENCES (LONS)

- Jason Adair, Gabriela Ochoa, Katherine M. Malan (2019) Local optima networks for continuous fitness landscapes. GECCO (Companion) 2019: 1407-1414
- F Chicano, D Whitley, G. Ochoa, R. Tinos (2017 Optimizing One Million Variables NK Landscapes by Hybridizing Deterministic Recombination and Local Search. Genetic and Evolutionary Computation Conference, GECCO 2017: 753-760
- M Contreras-Cruz, G Ochoa, J Ramirez-Paredes (2020) Synthetic vs. Real-World Continuous Landscapes: A Local Optima Networks View. BIOMA 2020: 3-16
- S Herrmann, G Ochoa, F Rothlauf (2018)PageRank centrality for performance prediction: the impact of the local optima network model. *J. Heuristics* 24(3): 243-264
- G Ochoa, N Veerapen (2022) Neural Architecture Search: A Visual Analysis. PPSN 2022: 603-615
- G Ochoa, NVeerapen, F Daolio, and M Tomassini (2017) Understanding Phase Transitions with Local Optima Networks: Number Partitioning as a Case Study, EvoCOP, Springer vol. 10197, pp. 233–248.
- G Ochoa, N Veerapen (2018) Mapping the global structure of TSP fitness landscapes. *J. Heuristics* 24(3): 265-294 (2018)
- G Ochoa, S Herrmann (2018) Perturbation Strength and the Global Structure of QAP Fitness Landscapes. PPSN: 245-256
- S L Thomson, G Ochoa, Vérel, N Veerapen (2020) Inferring Future Landscapes: Sampling the Local Optima Level. *Evol. Comput*. 28(4): 621-641 (2020)