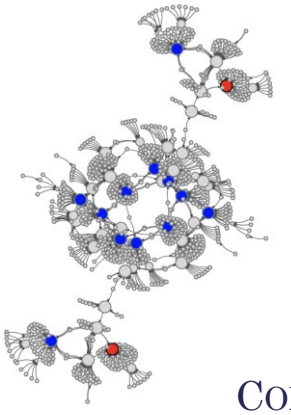


EPSRC
Engineering and Physical Sciences Research Council

The Leverhulme Trust

THE CARTOGRAPHY OF COMPUTATIONAL SEARCH SPACES

On Funnels, Tunnels, and Snakes!

Gabriela Ochoa

UNIVERSITY OF STIRLING

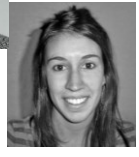
UNIVERSITY OF STIRLING

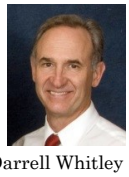

Nadarajen Veerapen


Fabio Daolio


Sarah Thomson


Bill Langdon


Leticia Hernando


Darrell Whitley


Renato Tinos


Sebastian Herrmann


Marco Tomassini

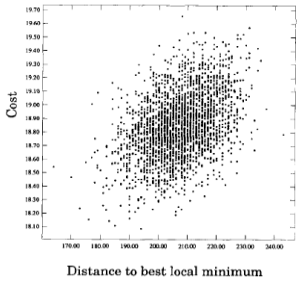

Sebastien Verel


Francisco Chicano

2

Travelling Salesman Problem (TSP)

TSP: The Big-valley Structure. Local optima confined to a small region



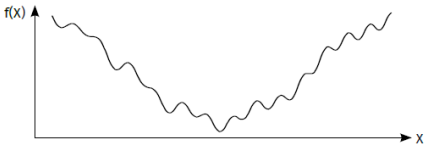


Fig. 1: Depiction of the 'big-valley' structure.

3

WHAT IS A FUNNEL?

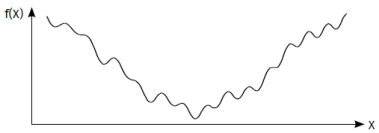


Fig. 1: Depiction of the 'big-valley' structure.

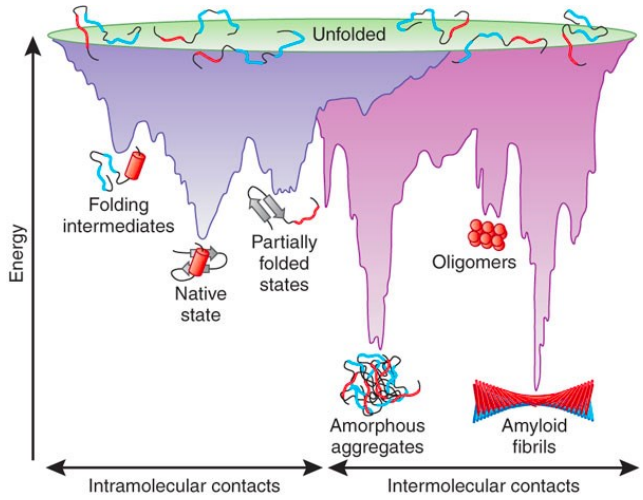
- Term from the protein folding community

"*a region of configuration space that can be described in terms of a set of downhill pathways that converge on a single low-energy structure or a set of closely-related low-energy structures*" (Doye et al 1999)

- Related to the notion of the "big-valley" in COP
- Studied mainly in the context of continuous optimisation (Global structure)

4

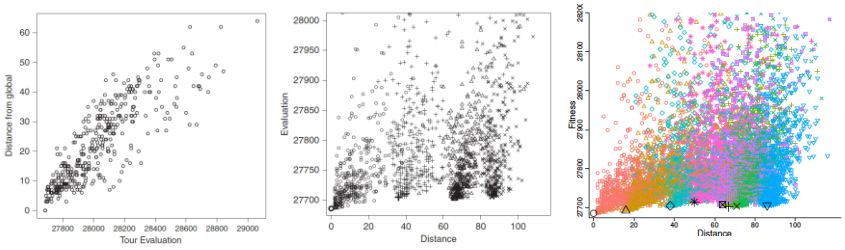
Protein Folding Energy Landscape



5

THE TSP BIG-VALLEY STRUCTURE REVISITED

- Big valley structure breaks down around solutions close to the global optimum. Multiple funnels appear!
- Explains why: ILS can quickly find high-quality solutions, but fail to consistently find the global optimum.



- D. Hains, D. Whitley, A. Howe. 2011. Revisiting the Big Valley Search Space Structure in the TSP. *Journal of the Operational Research Society*.
- G. Ochoa, N. Veerapen, D. Whitley and E. K.Burke. The Multi-Funnel Structure of TSP Fitness Landscapes: A Visual Exploration, *Artificial Evolution, EA 2015*

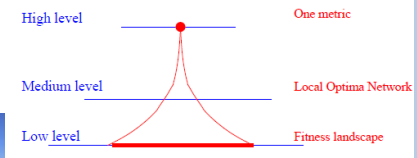
6

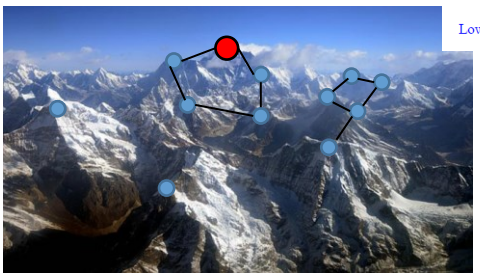
NETWORKS ARE EVERYWHERE!

The Internet: global computer network providing a variety of information and communication facilities, consisting of interconnected networks using standardized communication protocols.

Social networks: collections of people, each of whom is acquainted with some subset of the others

LOCAL OPTIMA NETWORKS (LON MODEL)





Mount Everest (centre) and the Himalayan mountain range

Nodes: local optima
Edges: transitions

P. K. Doye. The network topology of a potential energy landscape: a static scale-free network. *Physical Review Letter*, 88:238701, 2002.

G. Ochoa, M. Tomassini, S. Verel, and C. Darabos. A study of NK landscapes' basins and local optima networks. GECCO' 08, pages 555-562. ACM, 2008.

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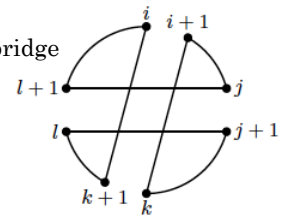
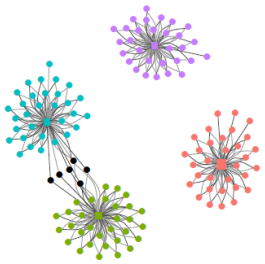
DEFINITIONS

Double bridge move



- Nodes: local optima, *LO*
  - A tour is a *local optimum* if no tour in its neighbourhood is shorter than it
  - Neighbourhood: LK-search, which has variable values of k.
- Escape Edges: Directed and based on the double-bridge operator. E_{esc}
  - A ➔ B if B can be obtained after applying a double-bridge kick to A followed by LK.
- Local Optima Network
  - Graph $LON = (LO, E_{esc})$



Data: I, TSP instance
Result: L, set of local optima,
E, set of escape edges

```
L ← {}; E ← {}
for i ← 1 to 1000 do
    s_start ← initialSolution()
    s_start ← LK(s_start)
    L ← L ∪ {s_start}
    while j < 10000 do
        s_end ← applyKick(s_start)
        s_end ← LK(s_end)
        j ← j + 1
        if fitness(s_end) ≤ fitness(s_start) then
            L ← L ∪ {s_end}
            E ← E ∪ {(s_start, s_end)}
            s_start ← s_end
            j ← 0
        end
    end
end
```

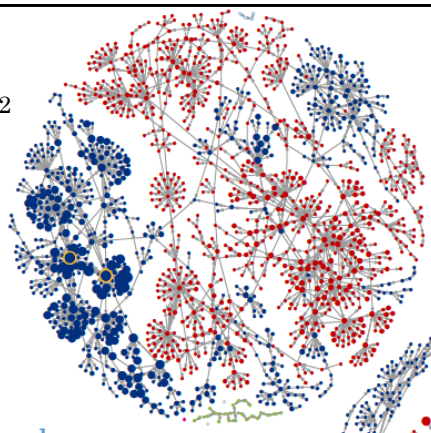
Nodes: LK optima
Edges: Double-bridge move

- Lin-Lin-Kernighan (1975)
- Chained Lin-Kernighan (Martin, Otto, Felten, 1991)

10

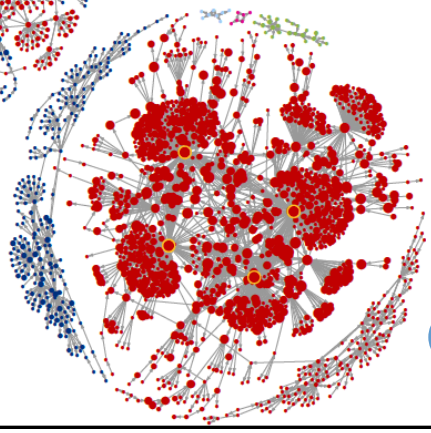
GATHERING LANDSCAPE DATA

att532



Node in largest component
Node in 2nd largest component
Node in 3rd largest component
Node in 4th largest component
Node in 5th largest component
Global Optimum

u574



R, igraph

Fruchterman & Reingold Layout (force-directed method)

- Position nodes in 2D
- Edges of similar length
- Minimise crossings
- Exhibit symmetries

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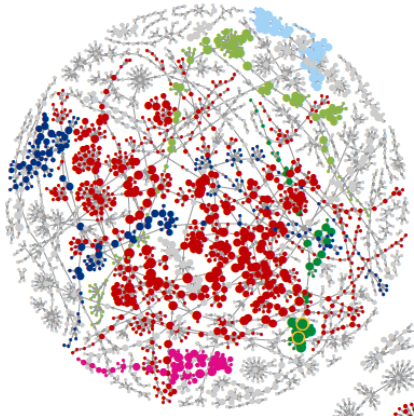
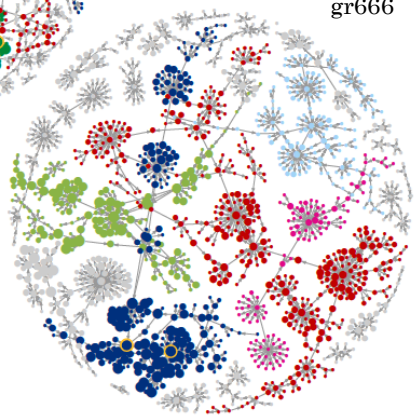
rat575



Node in largest component
Node in 2nd largest component
Node in 3rd largest component
Node in 4th largest component
Node in 5th largest component
Node in a smaller component containing global optimum
Node in any remaining component
Global Optimum

gr666



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Characterising Funnels

- **Funnel Floors**: High quality optima conjectured to be at the bottom of a funnel

1. Empirically: end of a CLK run for a large enough effort (10,000 without an improvement)
2. *Sinks* of the induced sub-graph of the funnel floors

- **Funnel Basins**: Local optima belonging to ta funnel

1. Connected components
2. Communities?
3. 3D visual inspection
4. *Monotonic sequences* (MLON)
   - Sequence of local optima where the fitness is non-deteriorating.
   - Compute all downhill paths to funnel *sinks*

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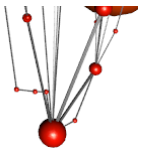
Identifying Funnel Structures

- Adapt notion of *monotonic sequences:* sequence of local optima where fitness is always improving
- The set of monotonic sequences leading to a particular minimum is a *funnel* or *super-basin*
- A solution may belong to more than one funnel!

S: set of *sinks*. Nodes without outgoing edges

$i \leftarrow 0$
for $s \in S$ **do**
  $fbasin[i] \leftarrow \text{breadthFirstSearch}(LON, s)$
  $fbsize[i] \leftarrow \text{length}(fbasin[i])$
  $i \leftarrow i + 1$
end



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TSP INSTANCES & METRICS

Name	CLK	*go*	*n*	*fit*	*n/fit*	*f*
C755	1.0	1	32,040	28,937	1.11	1
C1243	0.136	1	59,894	52,929	1.13	9
E755	0.128	1	24,774	23,569	1.05	10
E1243	0.030	1	50,779	46,366	1.10	148
att532	0.437	2	23,851	827	28.8	2
u574	0.442	4	28,115	1,230	22.9	2
u1060	0.214	163,569	1.4 million!	5,579	250.2	90

DIMACS Random Generator & TSBLIB

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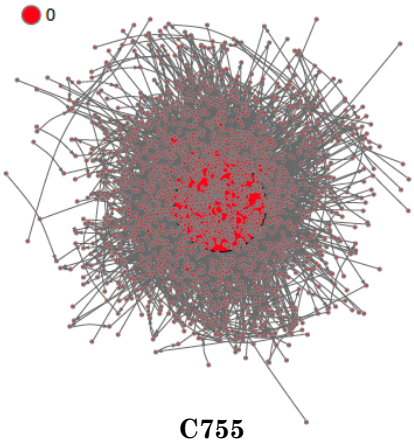
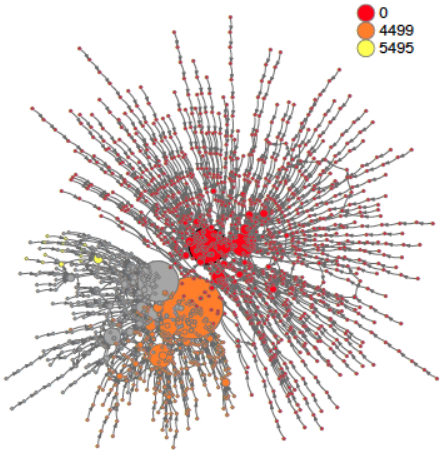
CLUSTERED RANDOM INSTANCES



C755
0.1% , 1 funnel, CLKs: 1.0



C1243
0.05% , 3 funnels, CLKs: 0.14

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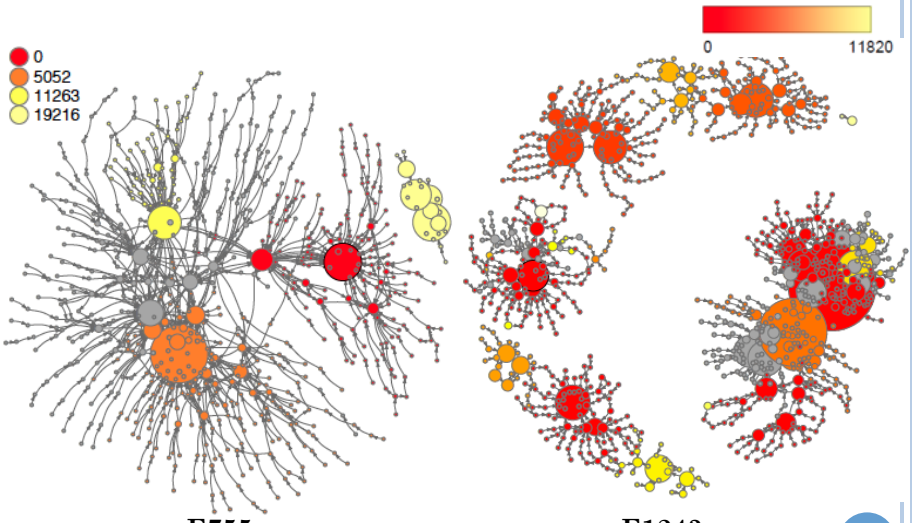
UNIFORM RANDOM INSTANCES



E755
0.1% , 4 funnels, CLKs: 0.13

E1243
0.05% , 19 funnels, CLKs: 0.03

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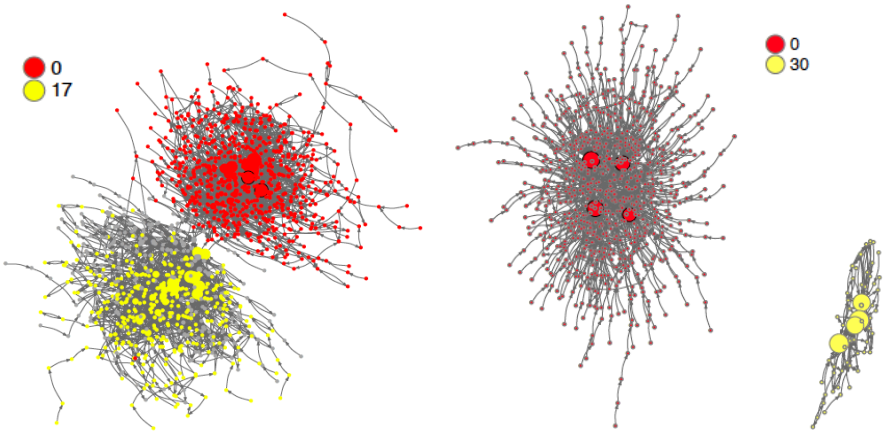
STRUCTURED INSTANCES



att532
0.1% , 2 funnels, CLK: 0.44

u574
0:1%, 2 funnels, CLK: 0.44

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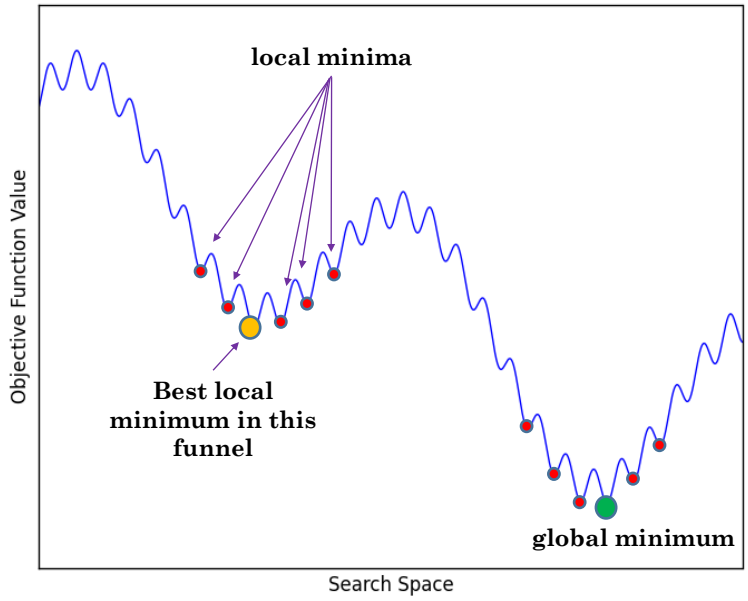
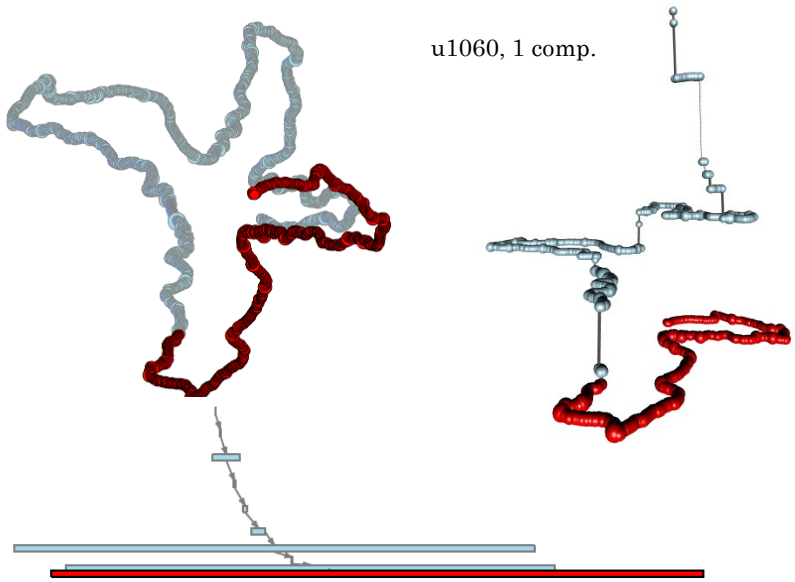
Main Finding 1: More than one valley on TSP lsndscapes



Main Finding 2: Presence of Neutrality (large plateaus)



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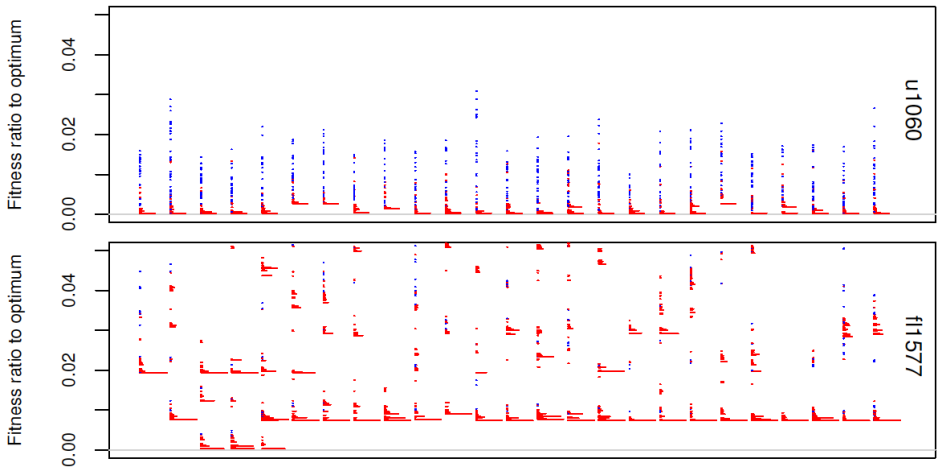
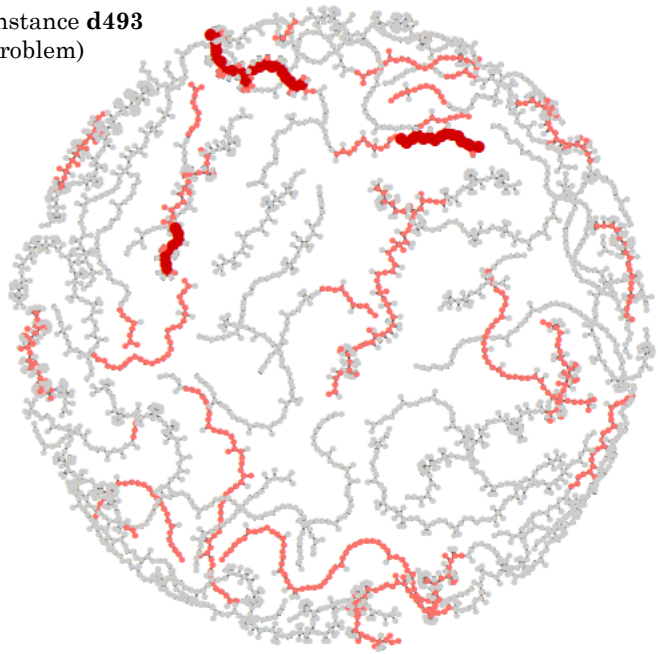
Main Finding 2: Presence of Neutrality (large plateaus)



CLK Success rate u1060: 0.214, fl1577: 0.012

TSPLIB instance **d493** (drilling problem)



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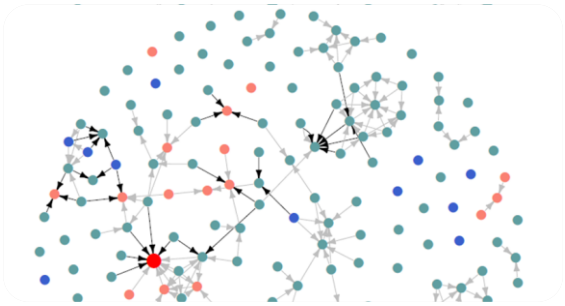


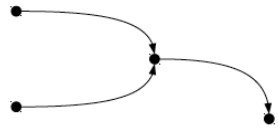
TUNNELLING CROSSOVER NETWORKS

- NK landscapes
- Asymmetric TSP

EXTENDING LONS TO EAS AND HYBRID EAS

```
P ← popInit()
while termination condition is not satisfied do
    Q(1) ← bestSolution(P)
    for i ← 2 to maxPop do
        (p1, p2) ← selection(P)
        Q(i) ← crossover(p1, p2); s ← 3opt(Q(i))
        LO ← LO ∪ {s}; E ← E ∪ {(p1, s), (p2, s)}
        if crossover did not improve the solutions then
            best ← chooseBest(p1, p2)
            Q(i) ← doubleBridgeMutation(best); s ← 3opt(Q(i))
            LO ← LO ∪ {s}; E ← E ∪ {(best, s)}
        end
    end
    if best sol. did not improve in last 20 gen. then Q ← immigration(P)
    P ← Q
end
```

Algorithm 1: Local optima network sampling in evolutionary algorithm.



Two types of Edges

- Perturbation
- Crossover

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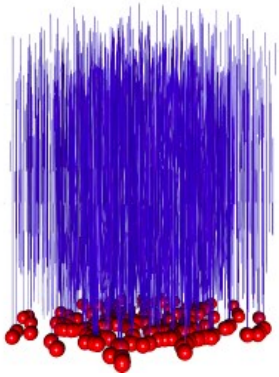
Instance rbg323
LONs, 20 Runs



Hybrid GA

Local search
(Chained-LK)

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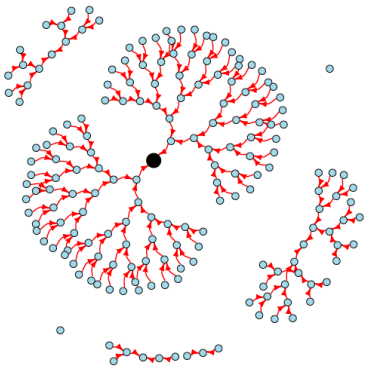
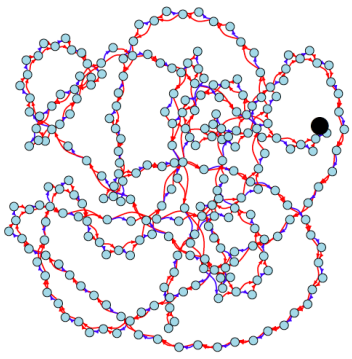
VISUALISING GREY-BOX BASED HYBRID EAS



PX-based Algorithms



PX + perturbation

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Conclusions

- More accessible (visual) approach to heuristic understanding
- Global structure characterisation is challenging!
- Model extended: XLON, MLON, CMLON
- Big valley de-constructs into several valleys, also called *funnels* in theoretical chemistry
- Search difficulty relates to the global structure
  - Easy: global optimum in dominant funnel
  - Hard: global optimum in small funnel
- Presence of *neutrality* on structured instances
- Crossover may help to escape funnels

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- N. Veerapen, G. Ochoa, R. Tinós, D. Whitley. Tunnelling Crossover Networks for the Asymmetric TSP. PPSN 2016, LNCS, vol. 9921. Springer, 2016.
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