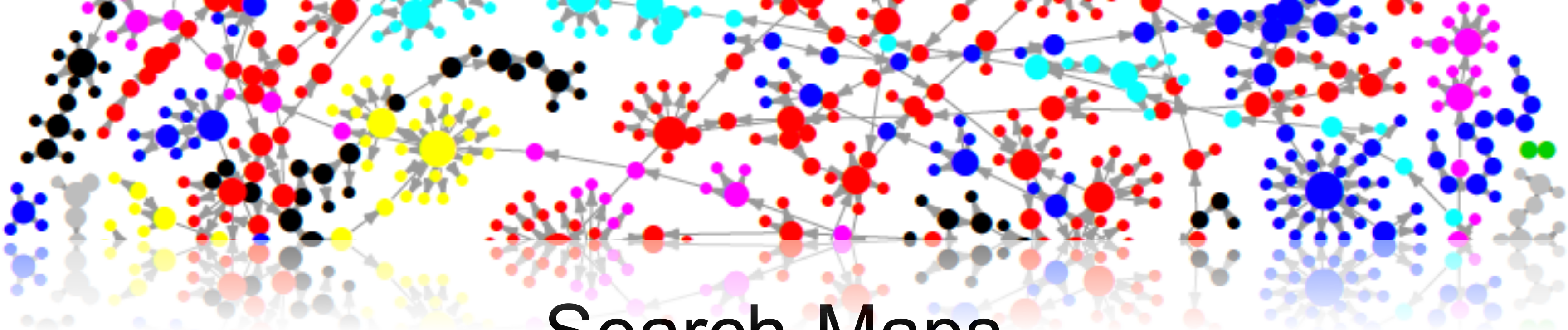

Search-Maps

Visualising and Exploiting the Global Structure of Computational Search Spaces

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Stirling

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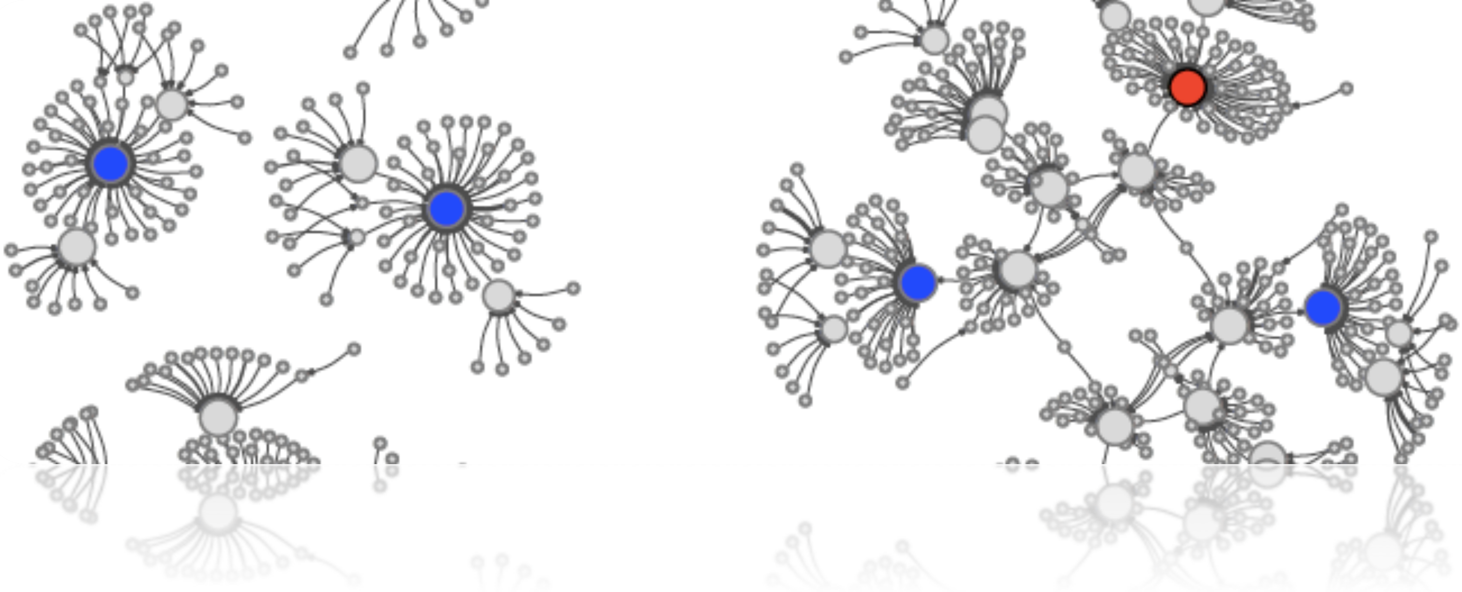
Outline

- Motivation and Background
  - Fitness landscapes
  - The notion of funnels
  - Complex networks
- Local Optima Networks
  - Definition of Nodes & Edges
  - Visualisation & Metrics
- Case Studies
  - Combinatorial optimisation
    - Binary: NK landscapes, number partitioning (NPP)
    - Permutation: TSP
  - Genetic Improvement
- Closing

Practical Sessions

- Sampling
- Constructing LONs
- Visualisation
- Metrics

Download Materials
lonmaps.com see Resources



- Overall goal
- Fitness landscapes
- The notion of funnels
- Complex networks

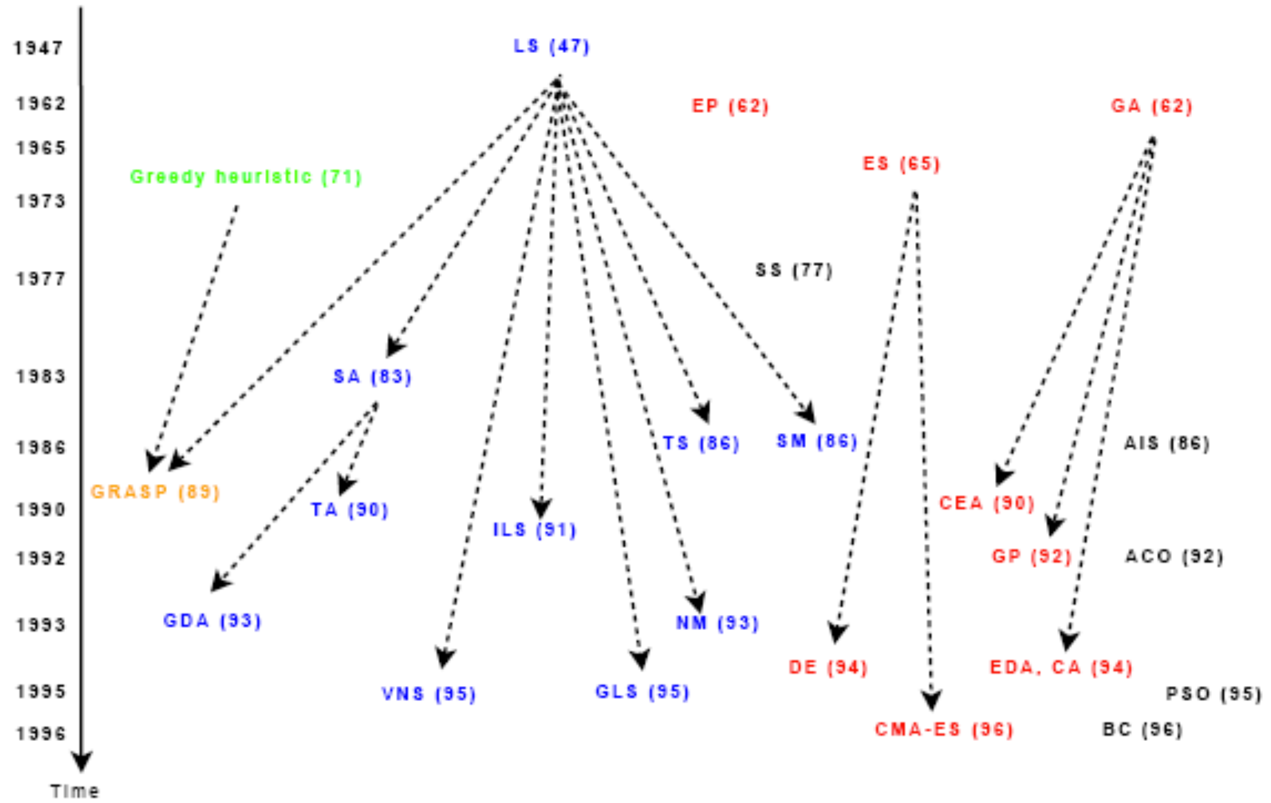
MOTIVATION AND BACKGROUND

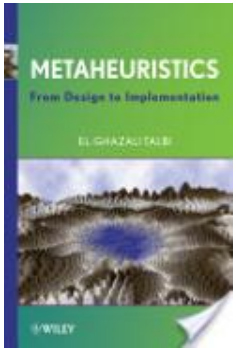
Overall goal

- To develop and establish a set of sampling methodologies, visualisation techniques and metrics to thoroughly characterise the *global structure* of computational search spaces.

- To lay the foundations for a new perspective to understand problem structure and improve heuristic search algorithms: *The Cartography of Computational Search Spaces*

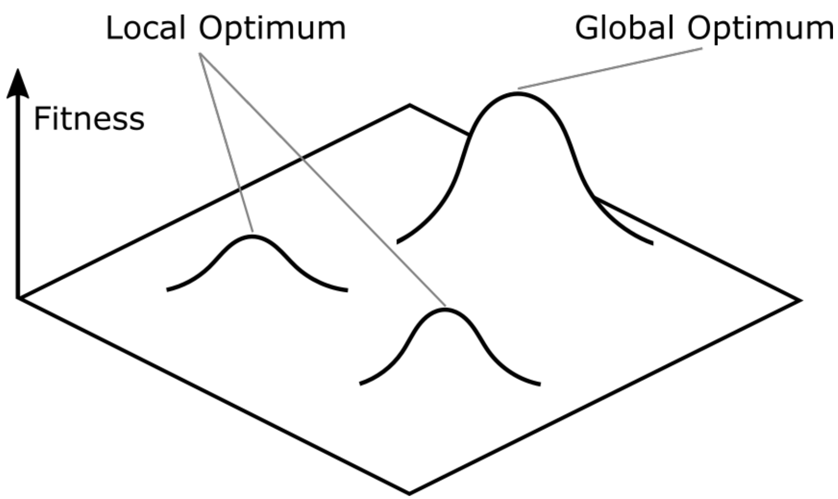
Genealogy of metaheuristics





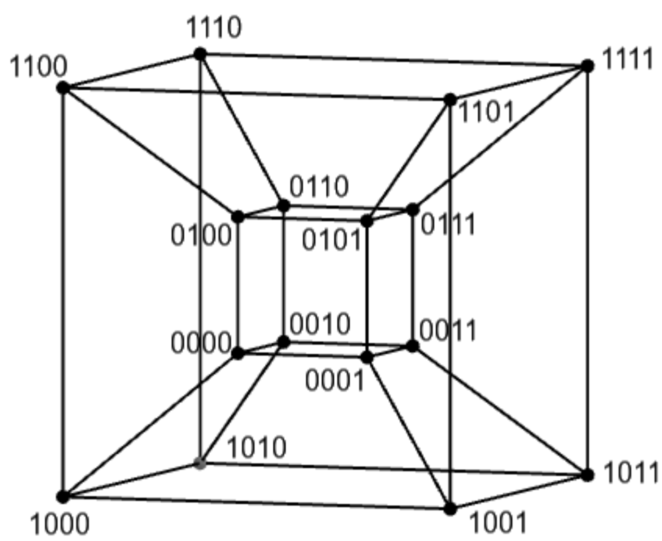
Metaheuristics: From Design to Implementation
El-Ghazali Talbi (2009)

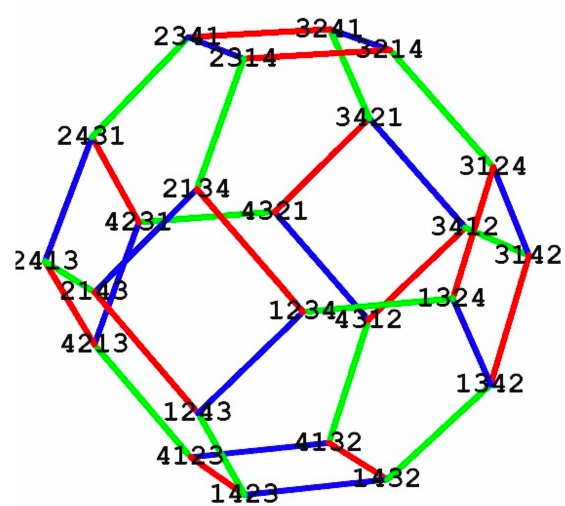
Fitness landscapes



(S, N, f)

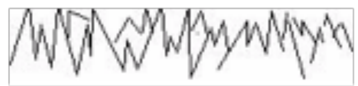
S Search space
N Neighbourhood structure
f Fitness function





Features of landscapes

M. Fuji, Japan



Aiguille du Midi: the Mont Blanc massif in the French Alps

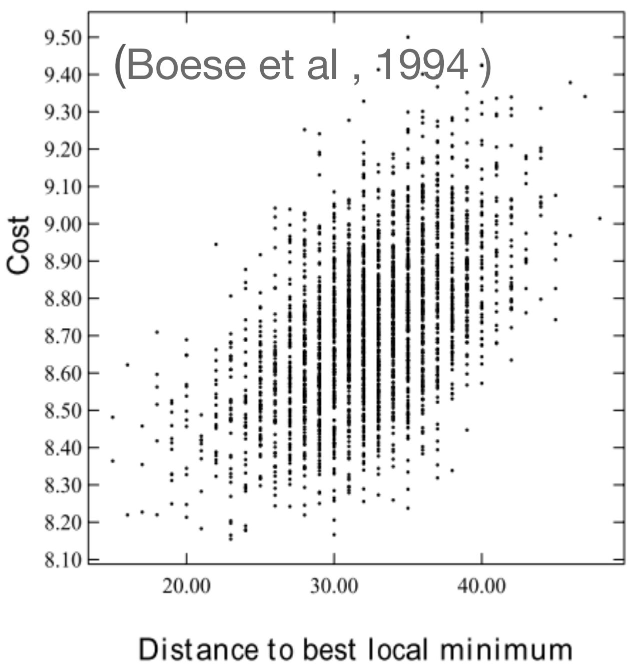
M. Auyantepui, Venezuela (Angel Falls, Highest Waterfall)

Multimodality, ruggedness, deceptiveness & neutrality

- No. of local optima
- Avg. size of local basins
- Avg. size of global basin
- Fitness-distance correlation
- Auto-correlation length
- Neutral degree
- …

The *big-valley* structure in combinatorial optimisation

- Several studies in the 90s. TSP (Boese et al, 1994), NK landscapes (Kauffman, 1993), graph bipartitioning (Merz & Freisleben, 1998) flowshop scheduling (Reeves, 1999)
- Distribution of local optima is not uniform. Clustered in a big-valley (*globally convex)* structure
- Many local optima, but easy to escape. Gradient at the coarse level leads to the global optimum.



100 cities TSP instance, 2,500 2-opt local optima

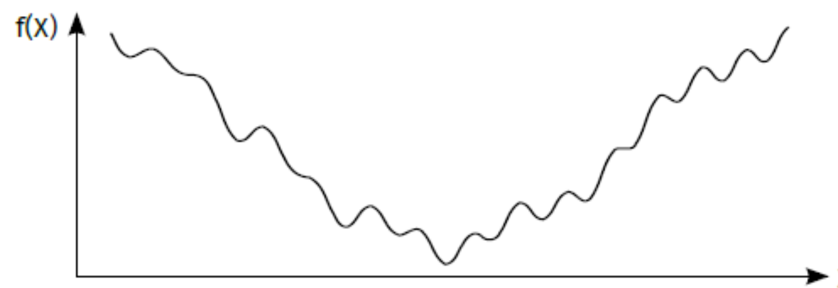


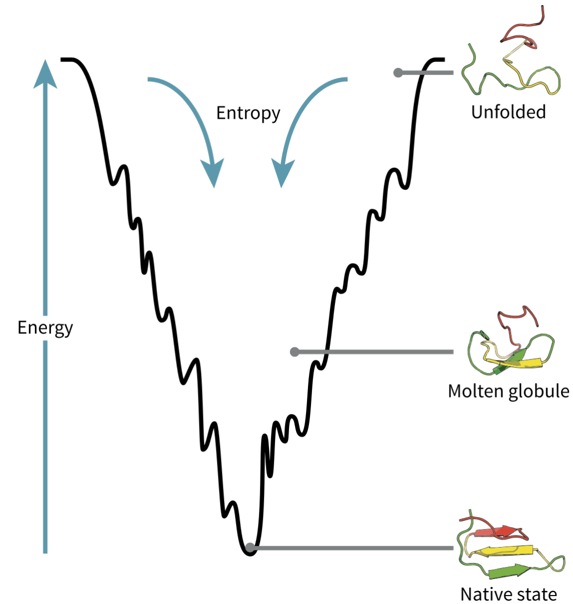
Fig. 1: Depiction of the 'big-valley' structure.

TSP: big-valley. Local optima confined to a small region

What is a Funnel?

"A key concept that has arisen within the protein folding community is that of a *funnel* consisting of a set of downhill pathways that converge on a single low-energy minimum."

Doye, J. P. K., Miller, M. A., & Wales, D. J . The double-funnel energy landscape of the 38-atom Lennard-Jones cluster. *Journal of Chemical Physics*, 1999



By Thomas Splettstoesser (link) (www.scistyle.com) - Own work

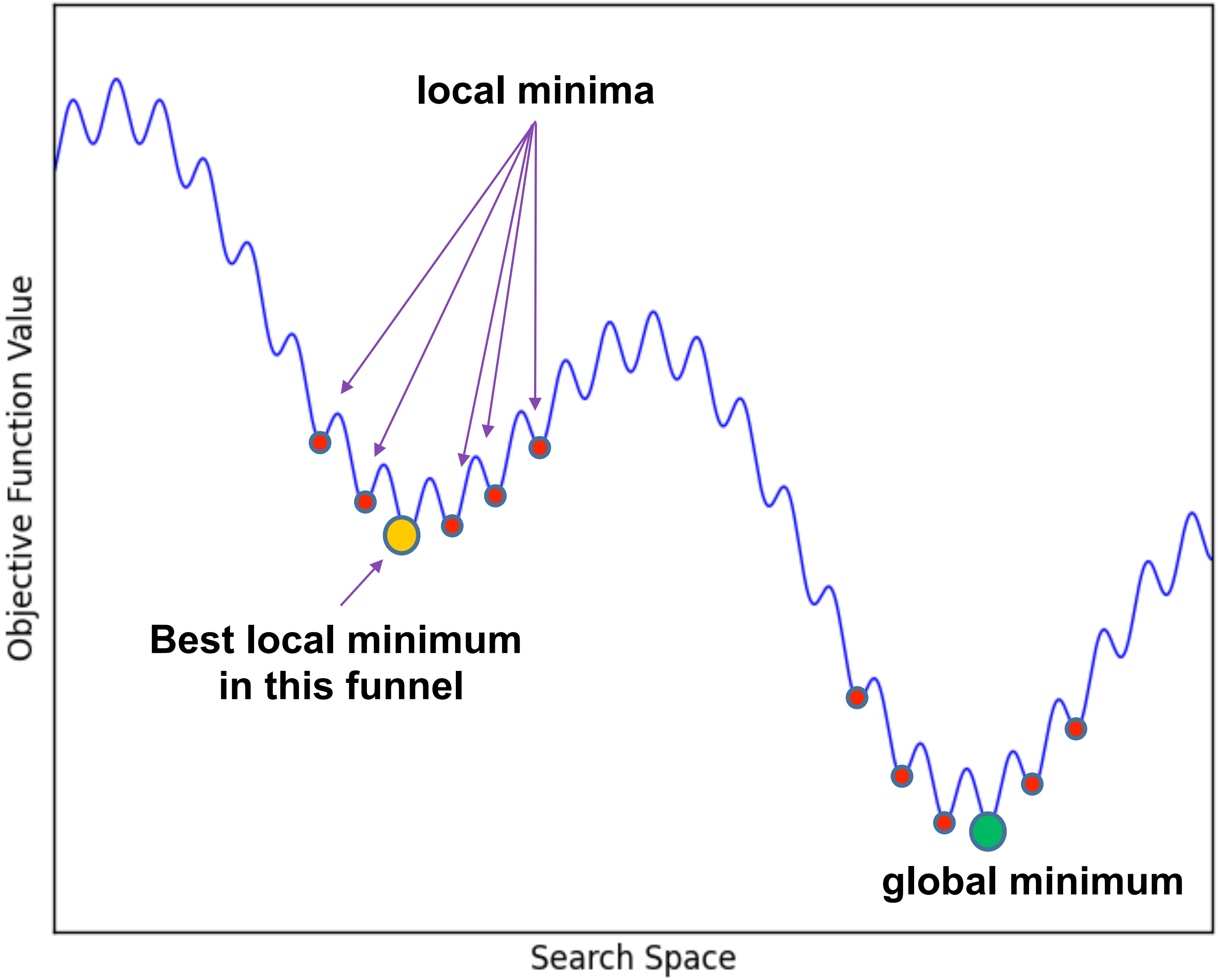
Funnels in continuous optimisation

- Multilevel global structure (Locatelli, 2005)
- *Dispersion* metric (Lunacek &Whitley, 2006, 2008)
- Feature-based detection of (single) funnel structure (Kerschke et al., 2015)

Funnels in combinatorial optimisation

- Related to the big-valley (central-massif) hypothesis (previous slide)
- The big-valley re-visited (Hains, Whitley & Howe, 2011)
- Characterisation of funnels with Local Optima Networks (our contribution)

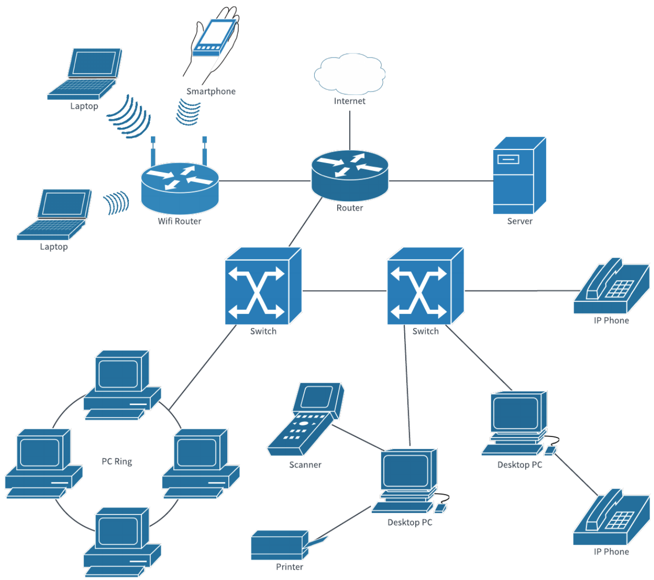
What is a Funnel?



Complex networks are everywhere!

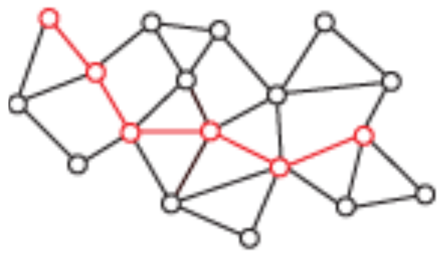
Social
Networks

Technological
Networks



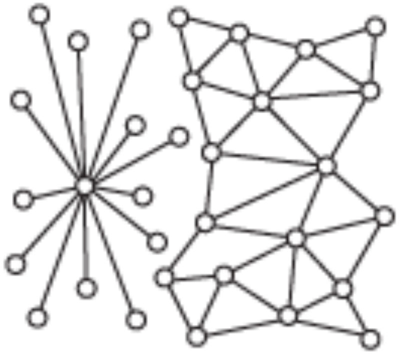
"Behind each complex system, there is an intricate network that encodes the interactions between the system's components."
Albert-László Barabási, Network Science

Features of networks



Distance

- Number of links that make up the path between two points
- "Geodesic" = shortest path



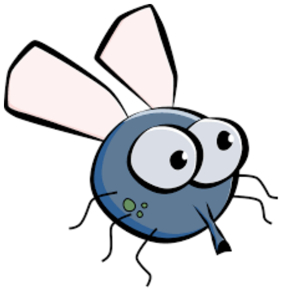
Topology (Degree distribution)

- Gives an idea of the spread in the number of links the nodes have
- $p(k)$ is the probability that a randomly selected node has k links

Cohesion

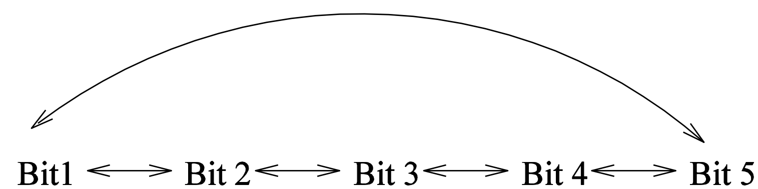
- Local: clustering coefficient or transitivity
- Global: components, community structure

NK landscapes (Kauffman, 93), NKq (Newman, 98)



- Binary strings of length N
- Fitness function $f: \mathrm{B}^N \to \mathrm{R}^+$
- K $(0 \leq K < N)$ determines how many other bits in the string influence a given bit x_i
- Interacting bits can be Adjacent or Random
- Fitness contribution of each bit is:
  - Standard *NK* model: random real numbers [0,1]
  - Quantized *NKq* model: integer numbers [0,q) (plateaus and neutrality)

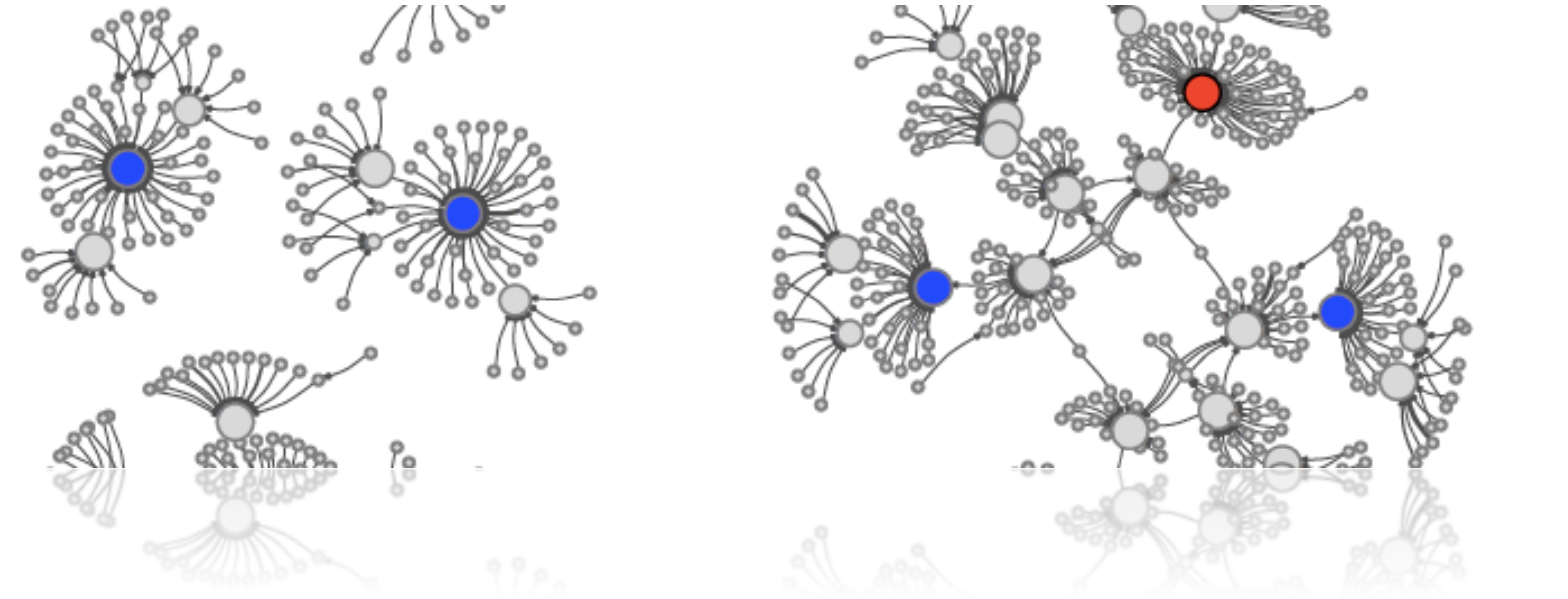
$$f(x) = \sum_{i=1}^{N} f_i(x|_{mask_i})$$



N=5, K = 2, Adjacent interaction

Sum of sub-functions.

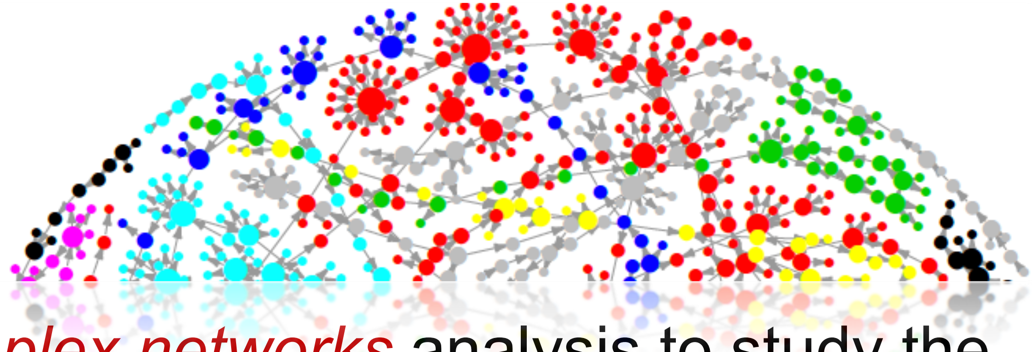
$mask_i$: selects the K+1 bits that will be accessed by sub-function f_i



- Overview
- Definition of Nodes
- Definition of Edges: basin, escape, monotonic, crossover
- Visualisation & Metrics

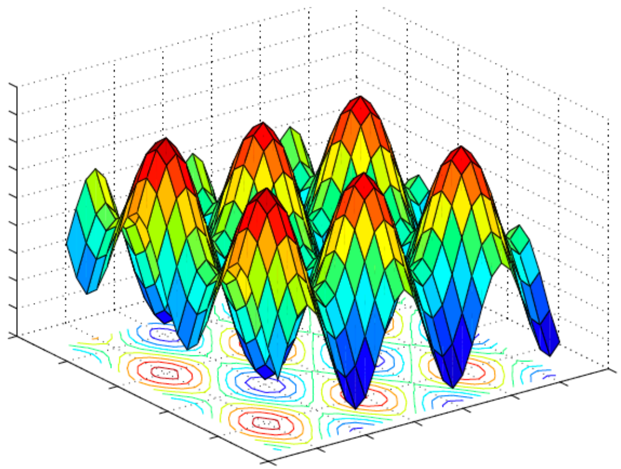
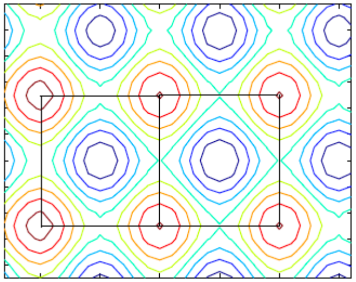
LOCAL OPTIMA NETWORKS

Overview



- Bring the tools of *complex networks* analysis to study the structure of combinatorial fitness landscapes
- Goal. Understand problem difficulty, design effective heuristic search algorithms
- Methodology. Extract a network that represents the landscape
  - Nodes. Local optima
  - Edges. Notion of adjacency/transition among local optima
- Conduct a network analysis
- Relate network features to search difficulty
- Exploit knowledge to design better algorithms

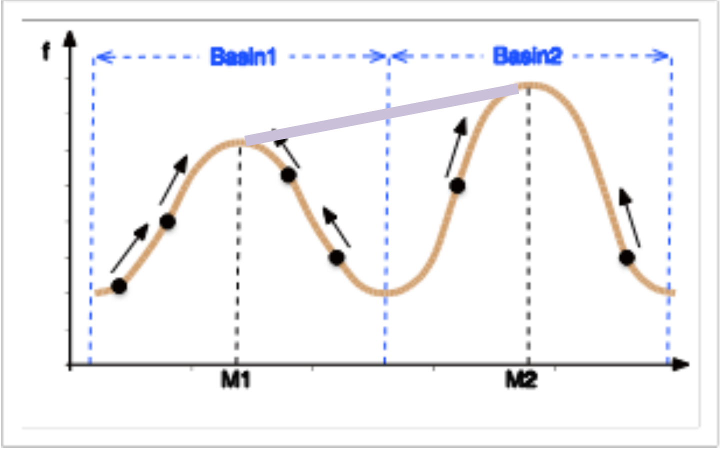
Local Optima Networks (LONs)

- Nodes. Local optima according to a hill-climbing heuristic
- Edges. Adjacency of basins. Transitions among optima.

2D function landscape (left), and a contour plot of the local optima partition of space into basins of attraction (right). A simple regular network of six local maxima can be observed.

- 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

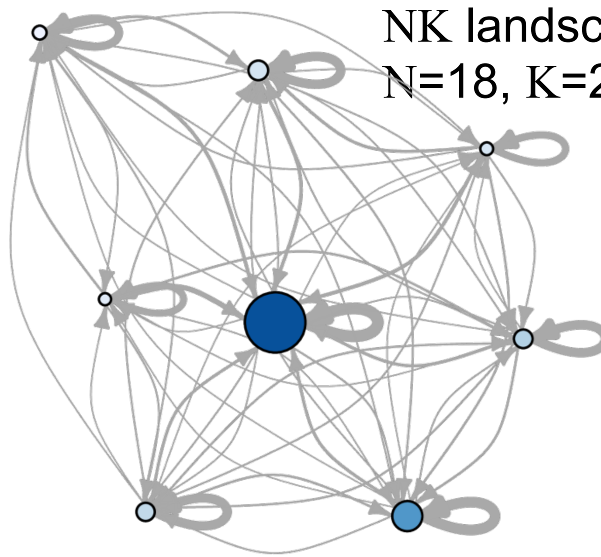


LON original model

- Space S, Neigborhood $N(s)$, fitness $f(s)$
- LON Model. Directed graph $\text{LON} = (L, E)$
- $h(s)$ stochastic operator that associates each solution s to its local optimum (Alg. 1)
- The basin of attraction of a local optimum $l_i \in L$ is the set $B_i = \{s \in S \mid h(s) = l_i\}$
- Nodes (L). A local optima is a solution l such that $\forall\ s \in N(s), f(s) \leq f(l)$
- Basin Edges (E). Two local optima are connected if their basins of attraction intersect. At least one solution within a basin has a neighbour within the other basin.

Algorithm 1: Best-improvement local search

Choose initial solution $s \in S$
repeat
  choose $s' \in N(s)$, $f(s') = max_{x \in N(s)} f(x)$
  if $f(s) \leq f(s')$ **then**
    $s \leftarrow s'$
  end if
until s is a Local optimum



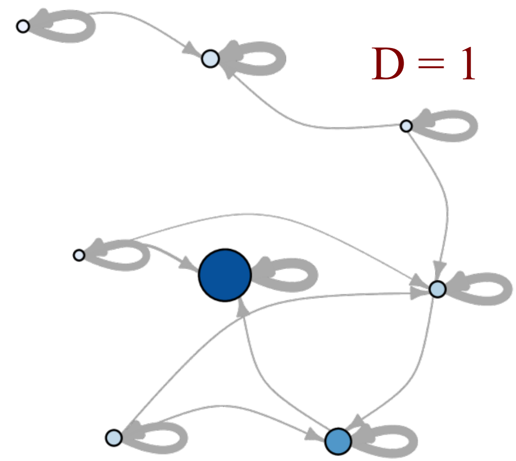
NK landscape
N=18, K=2

w_{ij} proportion of transitions from solutions $s \in Bi$ to solutions $s' \in Bj$

Escape edges

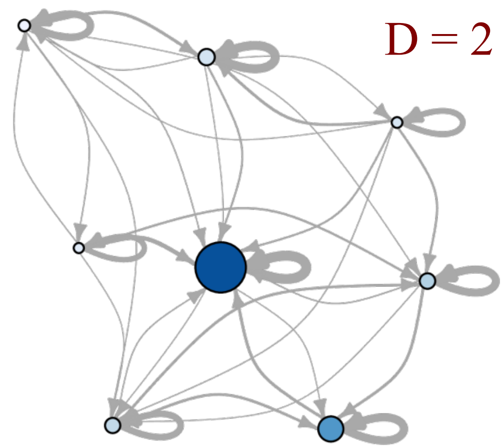
NK landscape
N=18, K=2

- Account for the chances of escaping a local optimum after a controlled mutation (e.g. 1 or 2 bit-flips in binary space) followed by hill-climbing



- Given a distance function d and integer value D, there is and edge e_{ij} between l_i and l_j f a solution s exists such that $d(s,l_i) \leq D$ and $h(s) = l_j$

- w_{ij} cardinality of $\{s \in S \mid d(s,l_i) \leq D \text{ and } h(s) = l_j\}$



- Sampled networks. There is an edge e_{ij} between l_i and l_j if l_j can be obtained after applying a *perturbation* to l_i followed by hill-climbing. Weights are estimated by the sampling process.

Complex network tools

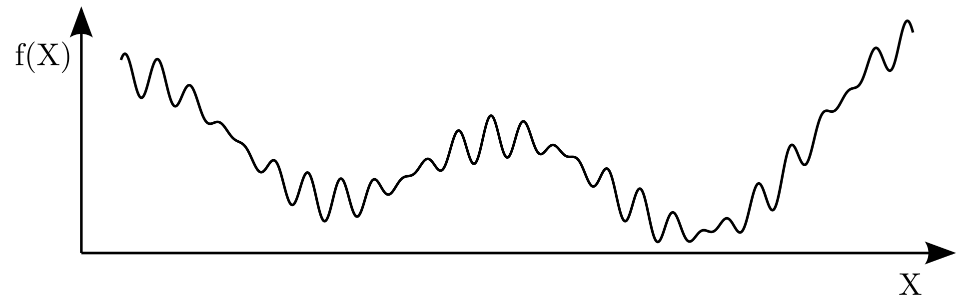
Visualisation

- **Force directed layout**
  - Position nodes in 2D
  - Edges of similar length
  - Minimise crossings
  - Exhibit symmetries
- **Example algorithms**
  - Fruchterman & Reingold
  - Kamada & Kawai
- **Software packages**
  - R igraph
  - Gephi

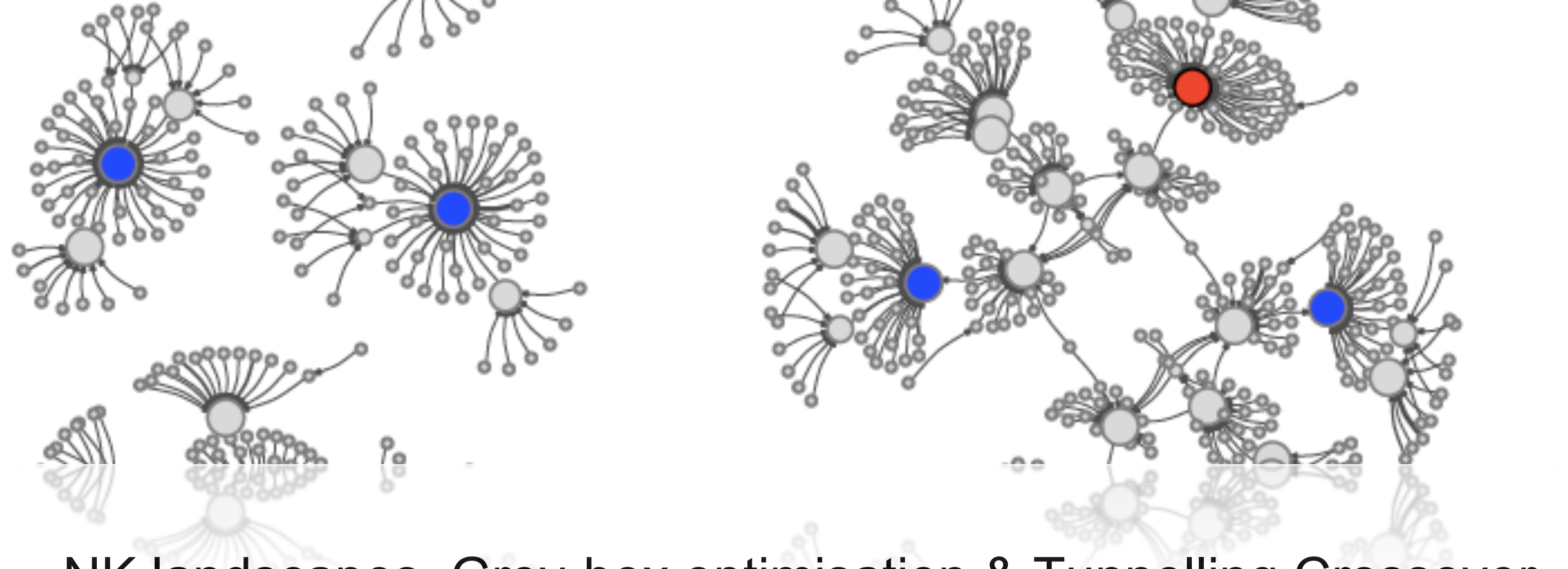
Metrics

- **Network metrics**
  - Number of nodes
  - Number of edges (density)
  - Number of global optima
  - Weight of self-loops
  - Avg. fitness of local optima
  - Number of connected components
  - Avg. path length to a global optimum
  - Centrality (PageRank) of global optima
  - Clustering coefficient
- **Funnel metrics**
  - Number of funnels (sinks)
  - Normalised size of global funnel(s)
  - Normalised incoming strength (weighted degree) of global sink(s)

Characterisation of funnels



- Funnels can be loosely defined as groups of local optima, which are close in configuration space within a group, but well-separated between groups.
- A funnel conforms a coarse-grained gradient towards a low cost optimum.
- How to characterise funnels more rigorously using LONs?
  - Connected components. Funnels are sub-graphs, connected components within LONs. (EvoCOP, 2016)
  - Communities. Funnels are *communities* within LONs. (GECCO, 2016, 2017)
  - Monotonic sequences. Concept from energy landscapes. Conceptually sound characterisation, incorporating both grouping and coarse-grained gradient. (EvoCOP 2017, 2018; JoH 2017)

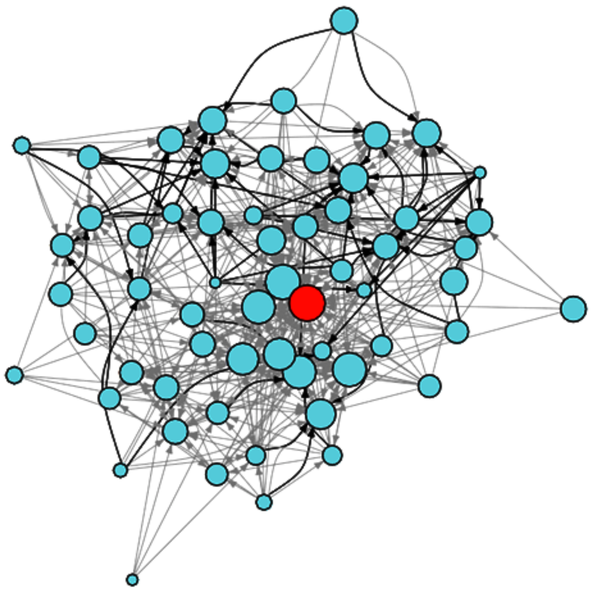


- NK landscapes, Grey-box optimisation & Tunnelling Crossover
- Number partitioning phase transition & multiple funnels
- TSP and multiple funnels
- Exploiting knowledge of the global structure
- Genetic improvement landscapes

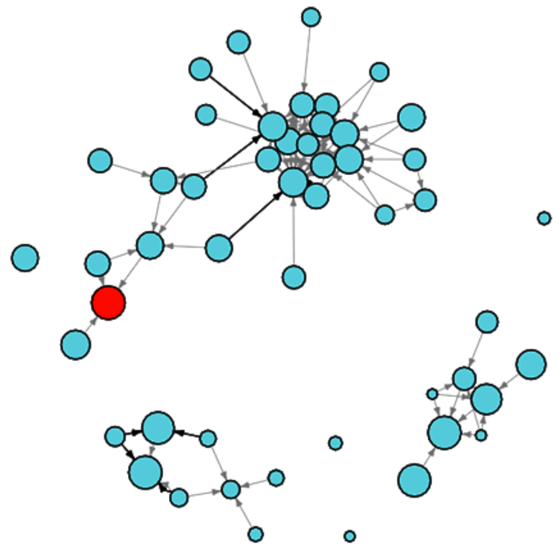
CASE STUDIES

Crossover network model (XLON)

- Partition Crossover (PX), deterministic and greedy
- NKq landscapes q=100; K={2, 3} and N ={20, 25, 30}
- Fast extraction of all local optima using Grey-box optimisation (*k*-bounded additive functions).



Adjacent: 60 nodes, 1 component



Random: 50 nodes, 7 components

Example XLON:

- N = 20, K = 2
- 2^{20} = 1,048,576

(Ochoa, Chicano, Tinos, Whitley. GECCO 2015)

XLON

Definition

Graph (V,E_{PX}) where nodes are local optima end edges link parents to offspring via partition crossover

Construction

Output: V (set of local optima)

$V \leftarrow \emptyset$
for $x \in \mathbb{B}^n$ **do**
  if $S_i(x) \leq 0$ for all $1 \leq i \leq n$ **then**
    $V \leftarrow V \cup \{x\}$
  end if
end for

1. Local optima identification

- *Score* $S_i(x)$ is the change in fitness from x to solution flipping bit i
- x is a local optimum if all $S_i(x)$ are lower than or equal to zero
- Efficient incremental calculation of *Score*. Overall complexity $O(2^N)$

Input: V
Output: $XLON = G(V, E_{PX})$

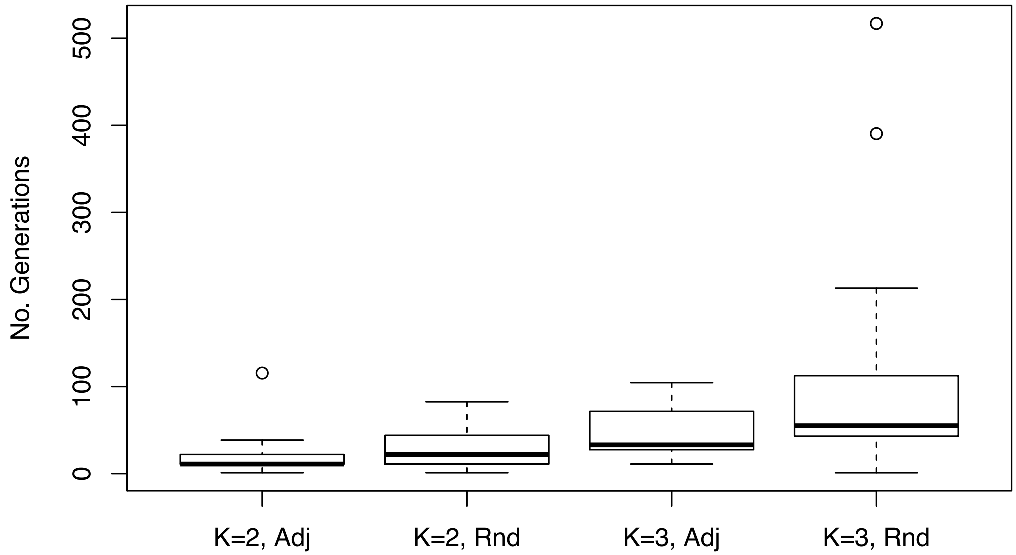
for $\{x, y\} \subseteq V$ **do** {All pairs of local optima}
  $w \leftarrow$ PartitionCrossover(x,y)
  $z \leftarrow$ HillClimber (w)
  if $z \neq x$ and $z \neq y$ **then**
    $E_{PX} \leftarrow E_{PX} \cup \{(x, z), (y, z)\}$
  end if
end for

2. Network construction

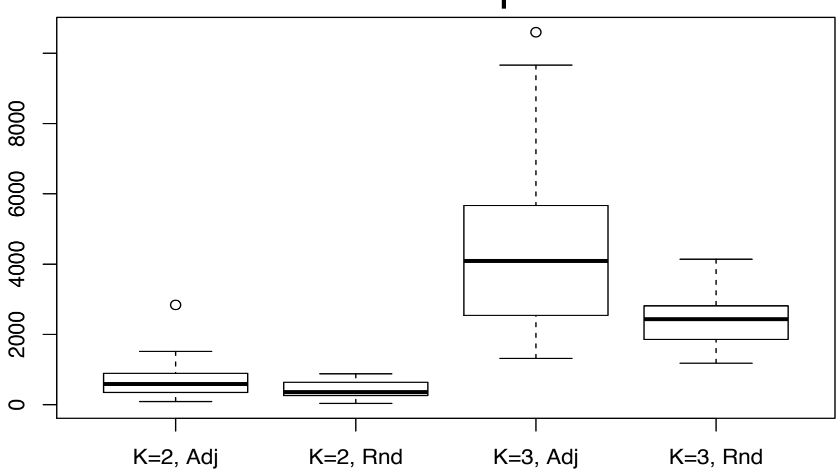
- All *x, y* pairs $nv*(nv-1)/2$
- PX and fast deterministic HC
- If z different to parents, two edges (x,z) and (y,z) are added to the network

Results N = 30, q=100, 30 replicas

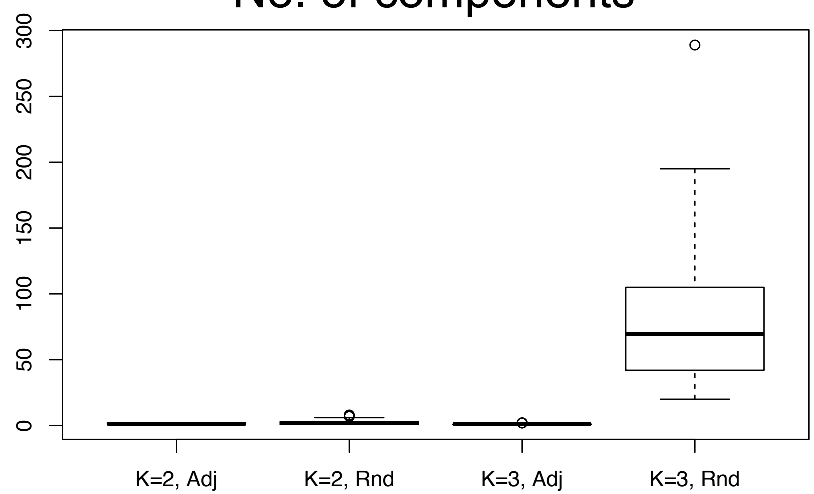
Search difficulty
number of generations to global optimum with a GA



No. of local optima



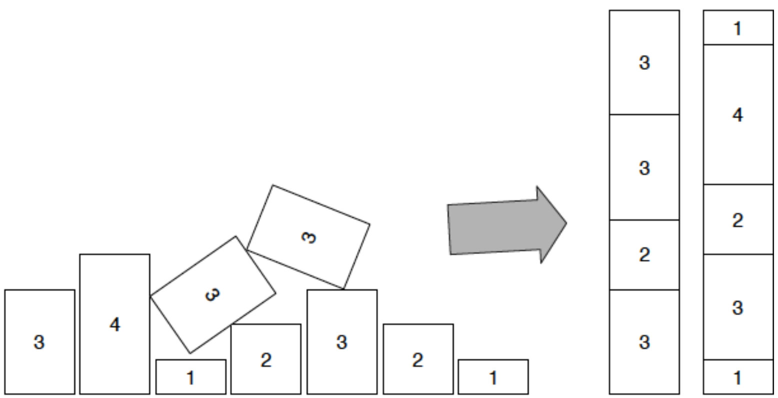
No. of components



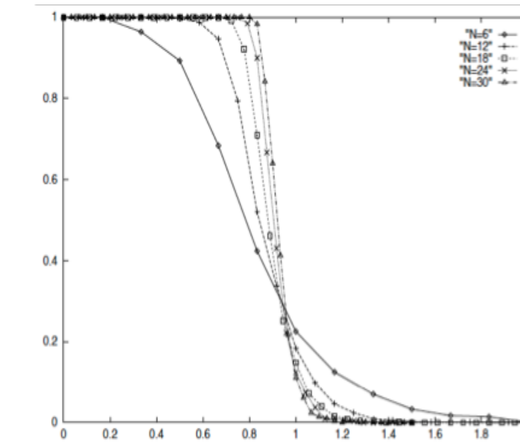
Number Partitioning (NPP)

- 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, $k = \log_2(M)/n$



Probability of an NPP instance having a perfect partition



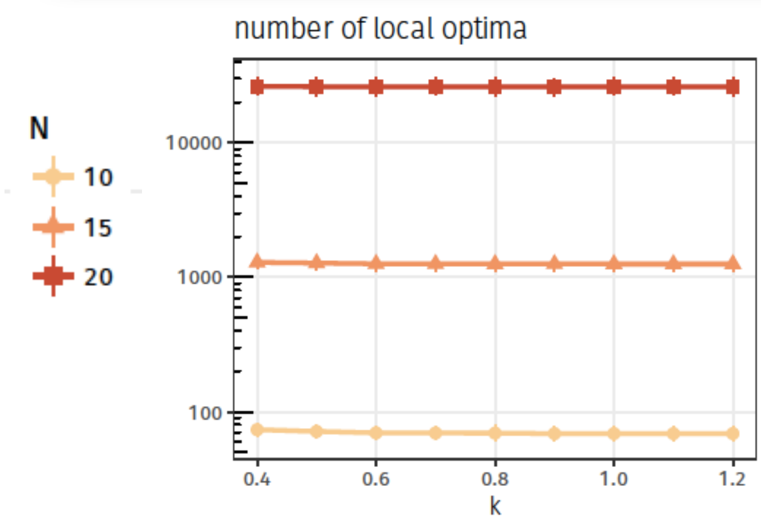
(Gent & Walsh, 1996)

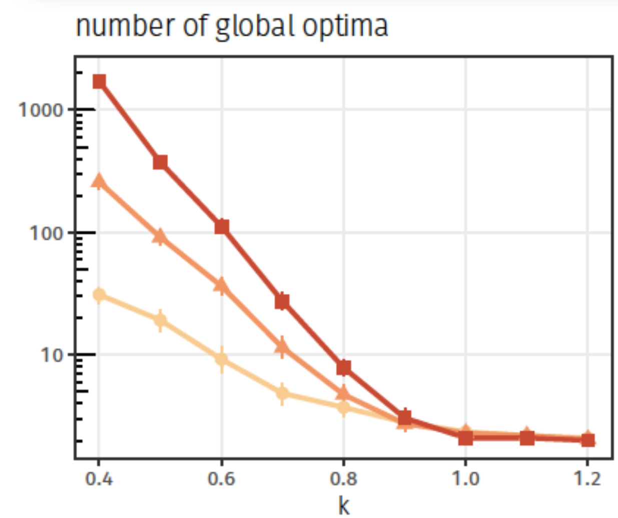
$k < 1$ many perfect partitions
$k > 1$ very few perfect partitions
$k = 1$ easy/hard phase transition

NPP fitness landscape

What features of the fitness landscape are responsible for the widely different behaviours?

Most fitness landscape metrics are insensitive/oblivious to the easy/hard phase transition!





- Stadler, P., Hordijk, W., & Fontanari, J. (2003). Phase transition and landscape statistics of the number partitioning problem. *Physical Review E*
- K. Alyahya, J. Rowe (2014). Phase Transition and Landscape Properties of the Number Partitioning Problem. *EvoCOP*.

Characterisation of funnels with LONs

- Monotonic edges. Keep only non-deteriorating edges $l_1 \rightarrow l_2$, if $f(l_2) \leq f(l_1)$
- Monotonic sequence. Path of connected local optima $l_1 \rightarrow l_2 \rightarrow l_3 \ldots \rightarrow l_s$,$f(l_i) \leq f(l_{i\text{-}1})$
- Sink. Natural end of the sequence, when there is no adjacent improving local optima
- Funnel.
  - Aggregation of all monotonic sequences ending at the same point (sink).
  - Basin of attraction level of local optima

Sink. Node without outgoing edges

S set of sinks

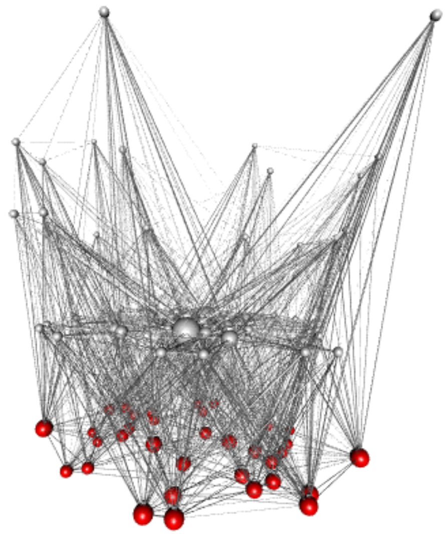
$i \leftarrow 0$
for $s \in S$ **do**
  $fbasin[i] \leftarrow \text{breadthFirstSearch}(LON, s)$
  $fbsize[i] \leftarrow \text{length}(fbasin[i])$
  $i \leftarrow i + 1$
end

Methodology

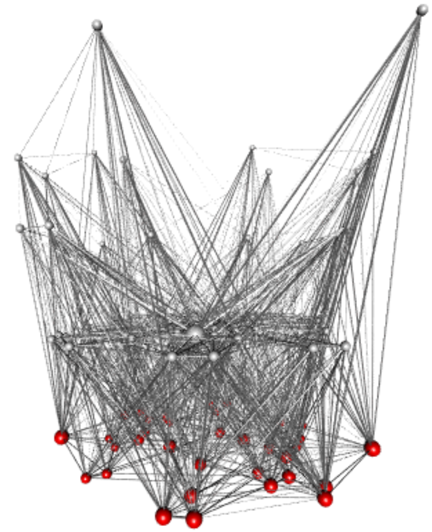
- Full enumeration and extraction of LONs
- $N = \{10, 15, 20\}$, k in $[0.4, 1.2]$ step 0.1
- 30 instances for each N and k
- LON. 1-flip local search, 2-flip perturbation $(D = 2)$
- MLON. Monotonic LON, worsening edges pruned
- CMLON. compressed MLON, LON plateaus contracted in a single node
- Empirical search performance: ILS success rate

$N = 10$

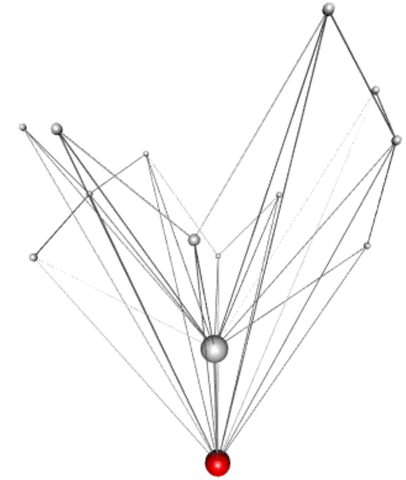
$k = 0.4$



LON V = 104, E = 2844

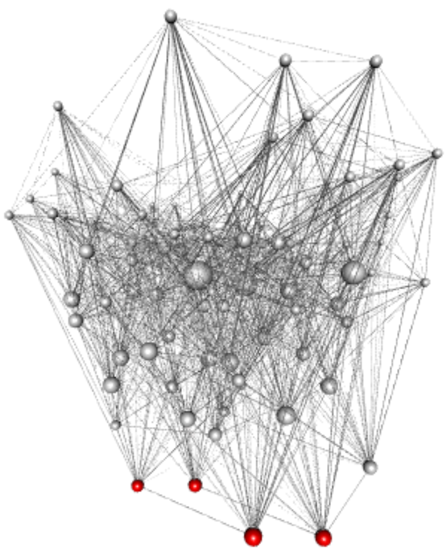


MLON V = 104, E = 2010

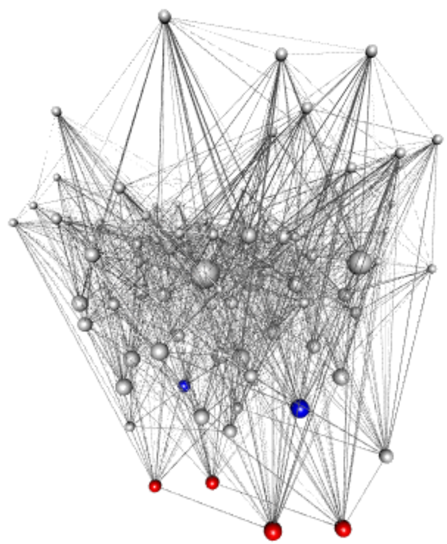


CMLON V = 14, E = 35

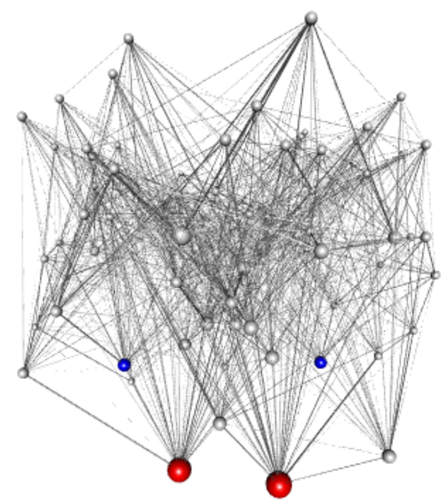
$k = 1.0$



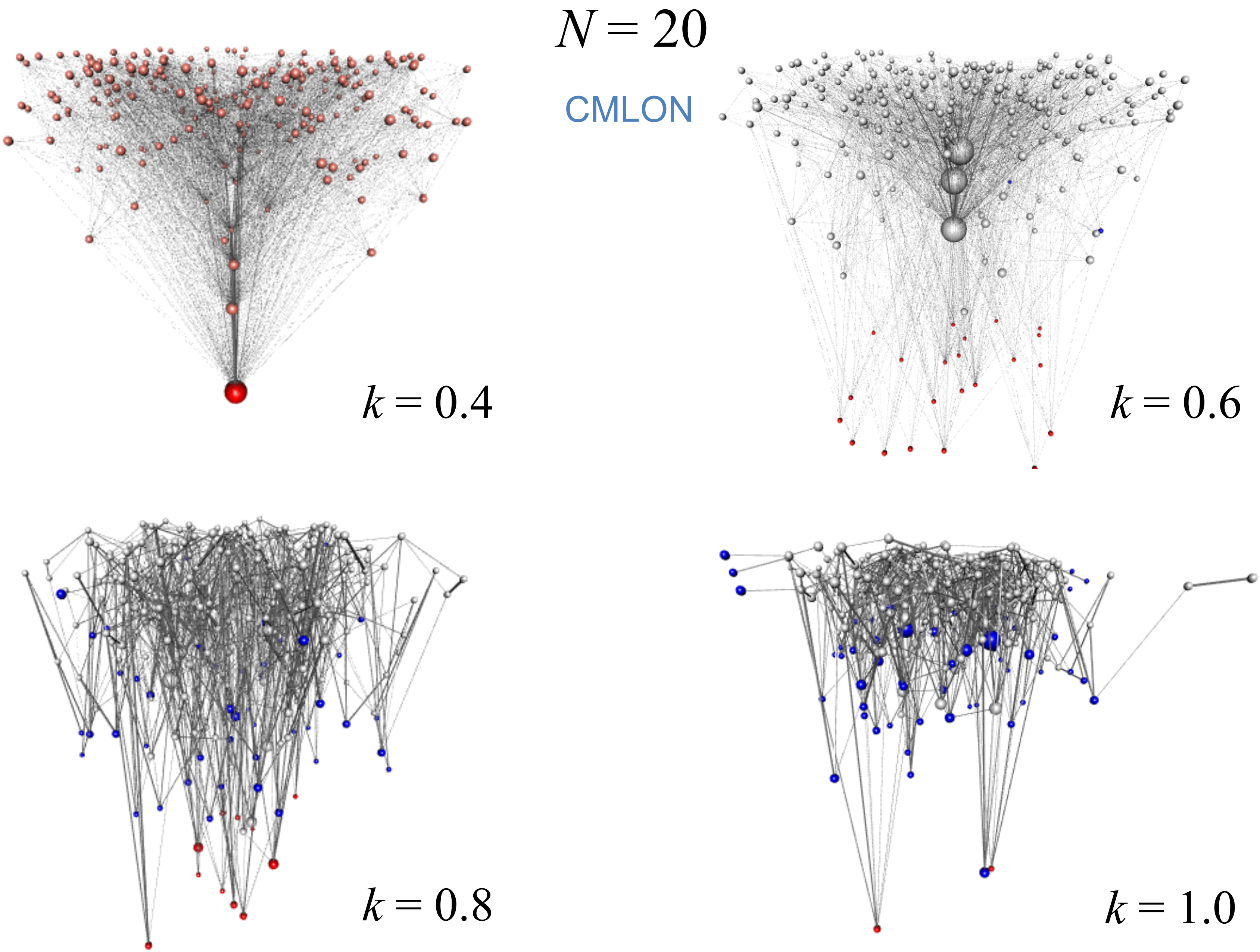
LON V=104, E=2514



MLON: V=104, E=1386

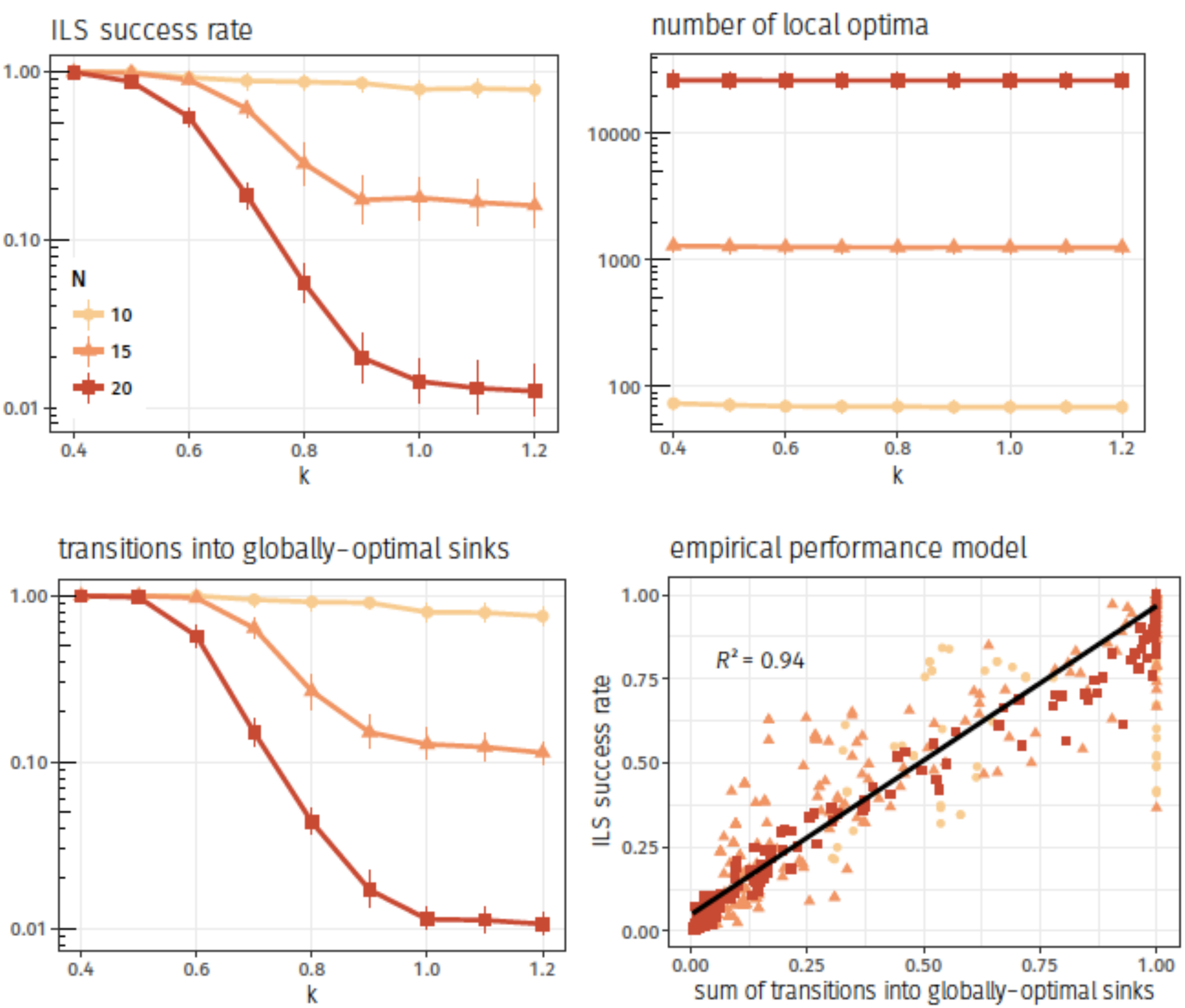


CMLON: V = 96, E = 1290



$N = 20$
CMLON
$k = 0.4$
$k = 0.6$
$k = 0.8$
$k = 1.0$

LON metrics & Search Performance



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

Travelling Salesman Problem (TSP)

- A prominent combinatorial optimisation problem
- Given n cities and the pairwise distance between them: what is the shortest possible route that visits each city and returns to the origin city?
- After over 50 years of intense study maintains its theoretical and practical relevance
- Successful exact solver: Concorde (Applegate et al., 2006)
- Successful heuristic solvers
  - Chained-LK. Iterated local search using Lin-Kernighan heuristic and *double-bridge* perturbation (Martin, Otto, Felten, 1992)
  - LKH. Improved implementation of Lin-Kernighan heuristic (Helsgaun, 2000,2009)
  - EAX. Evolutionary algorithm with edge exchange crossover (Nagata and Kobayashi, 2013)

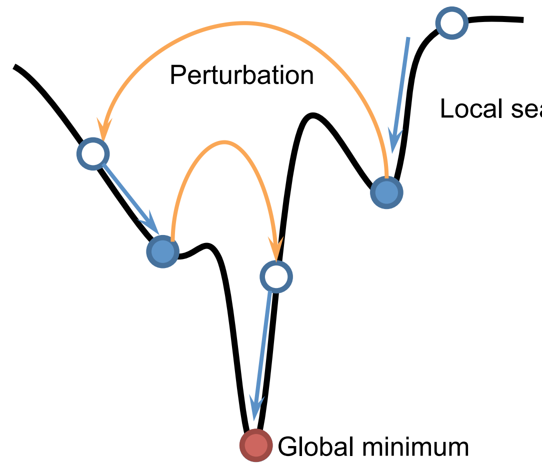
Sampling and constructing LONs

Data: I, TSP instance
Result: L, set of local optima,
E, set of escape edges
$L \leftarrow \{\}; E \leftarrow \{\}$
for $i \leftarrow 1$ **to** 1000 **do**
  $s_{start} \leftarrow \text{initialSolution}()$
  $s_{start} \leftarrow \text{LK}(s_{start})$
  $L \leftarrow L \cup \{s_{start}\}$
  while $j < 10000$ **do**
    $s_{end} \leftarrow \text{applyKick}(s_{start})$
    $s_{end} \leftarrow \text{LK}(s_{end})$
    $j \leftarrow j + 1$
    if $Objective(s_{end}) \leq Objective(s_{start})$ **then**
      $L \leftarrow L \cup \{s_{end}\}$
      $E \leftarrow E \cup \{(s_{start}, s_{end})\}$
      $s_{start} \leftarrow s_{end}$
      $j \leftarrow 0$
    end
  end
end

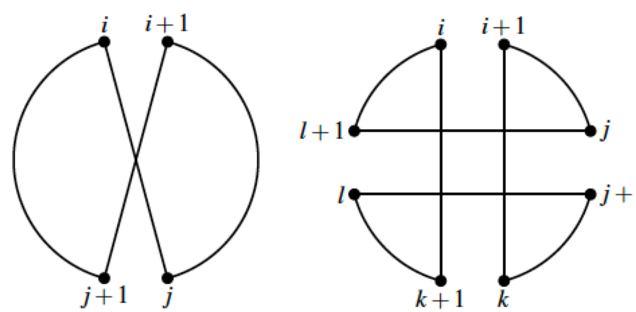
TSP heuristic, Chained Lin-Kernighan

(Martin, Otto, Felten, 1992)

- Form of Iterated Local Search
- Diversification & Intensification stages



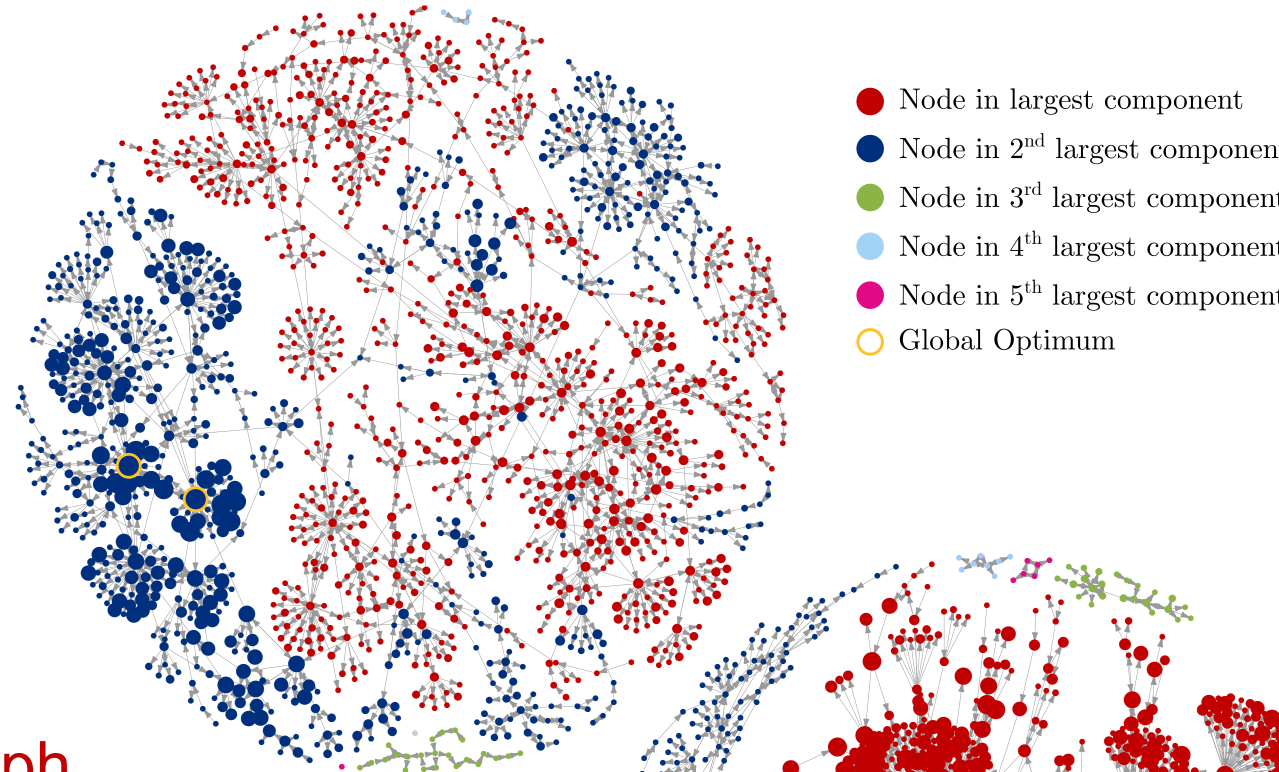
- Nodes. Lin-Kernighan
- Edges. Double-bridge



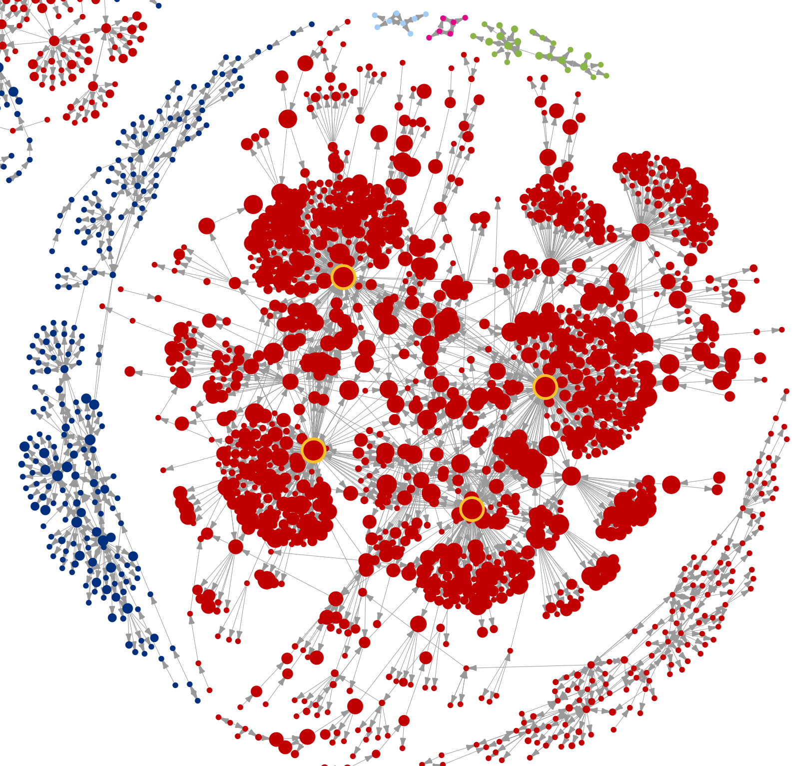
(a) 2-exchange
K-opt in general

(b) Double-bridge

att532



u574



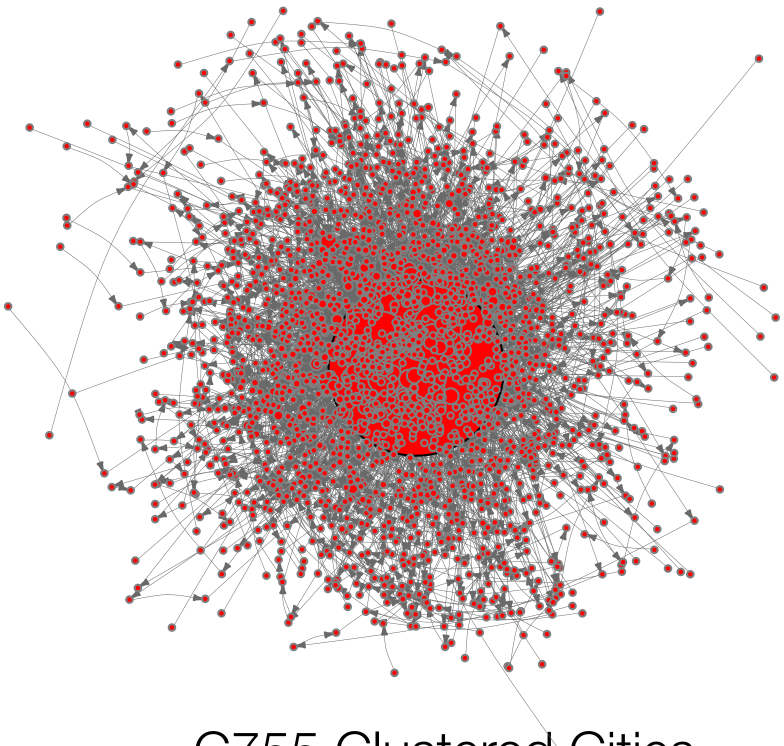
R, igraph

Fruchterman & Reingold Layout (force-directed method)

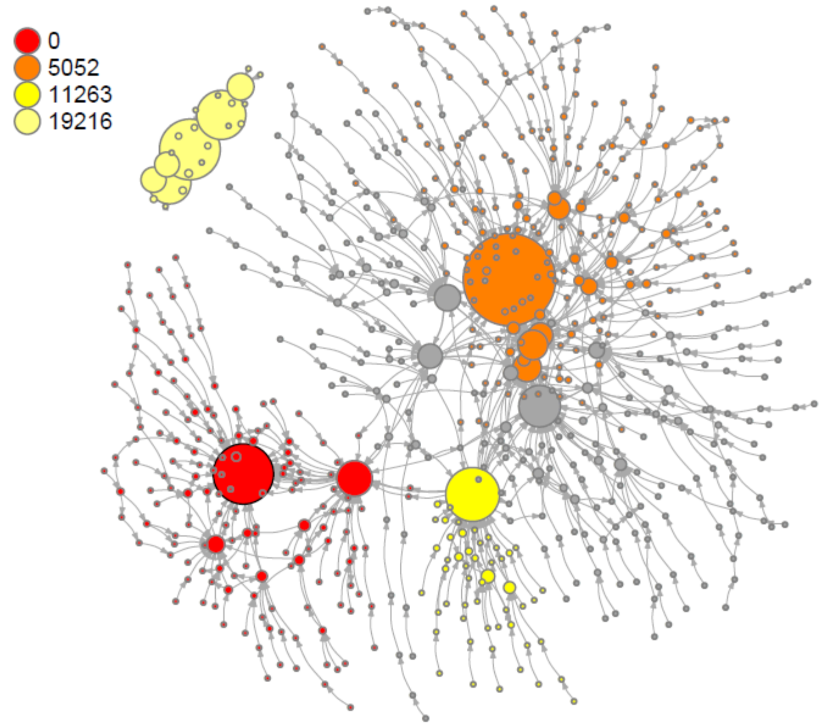
- Position nodes in 2D
- Edges of similar length
- Minimise crossings
- Exhibit symmetries

(Ochoa & Veerapen. EvoCOP 2016)

TSP Synthetic Instances
Funnels as monotonic sequences



C755 Clustered Cities
Funnels: 1, Success: 100%

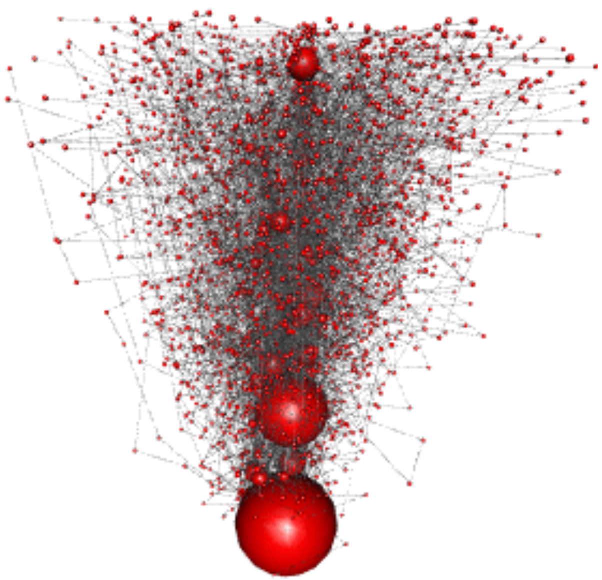


E755 Uniform Cities
Funnels: 4, Success: 13%

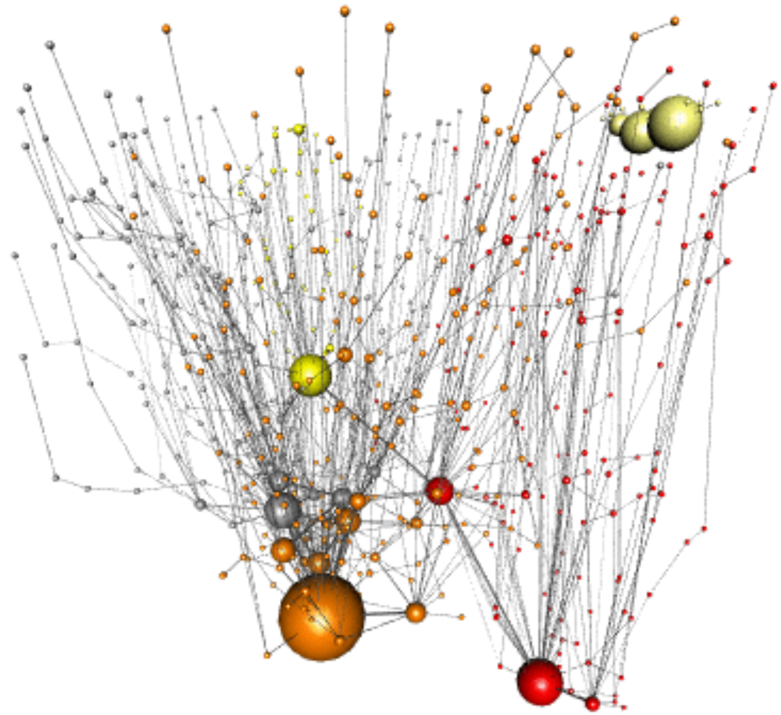
DIMACS random instances

(Ochoa & Veerapen, JoH 2017)

TSP Synthetic Instances



C755 Clustered Cities
Funnels: 1, Success: 100%

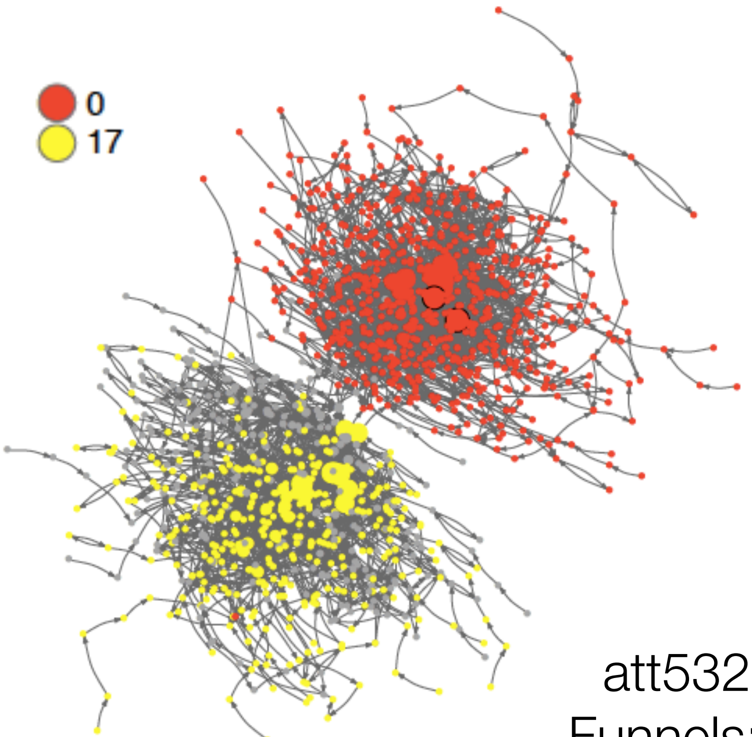


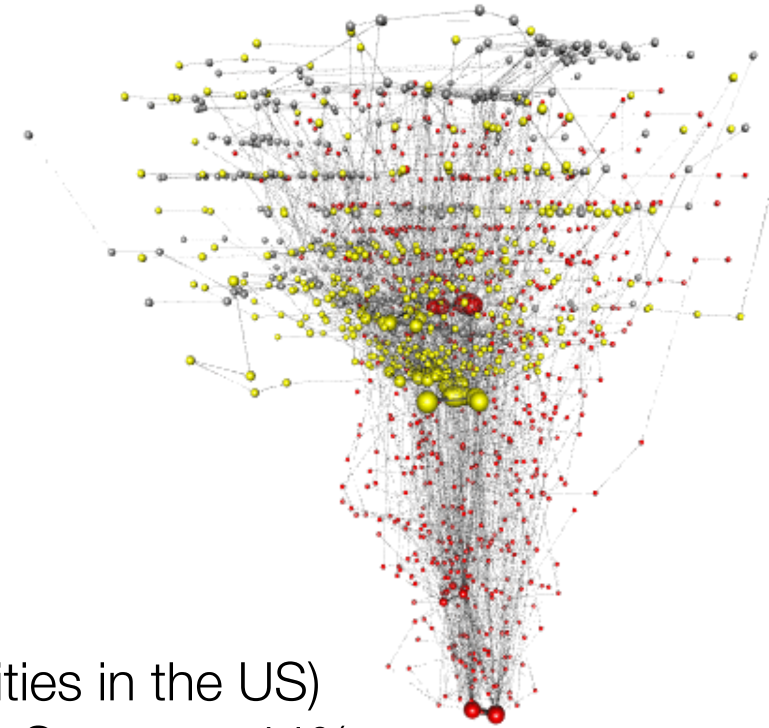
E755 Uniform Cities
Funnels: 4, Success: 13%

DIMACS random instances

Same layout, 3D projection where z coordinate is fitness

TSPLIB City Instance att532





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

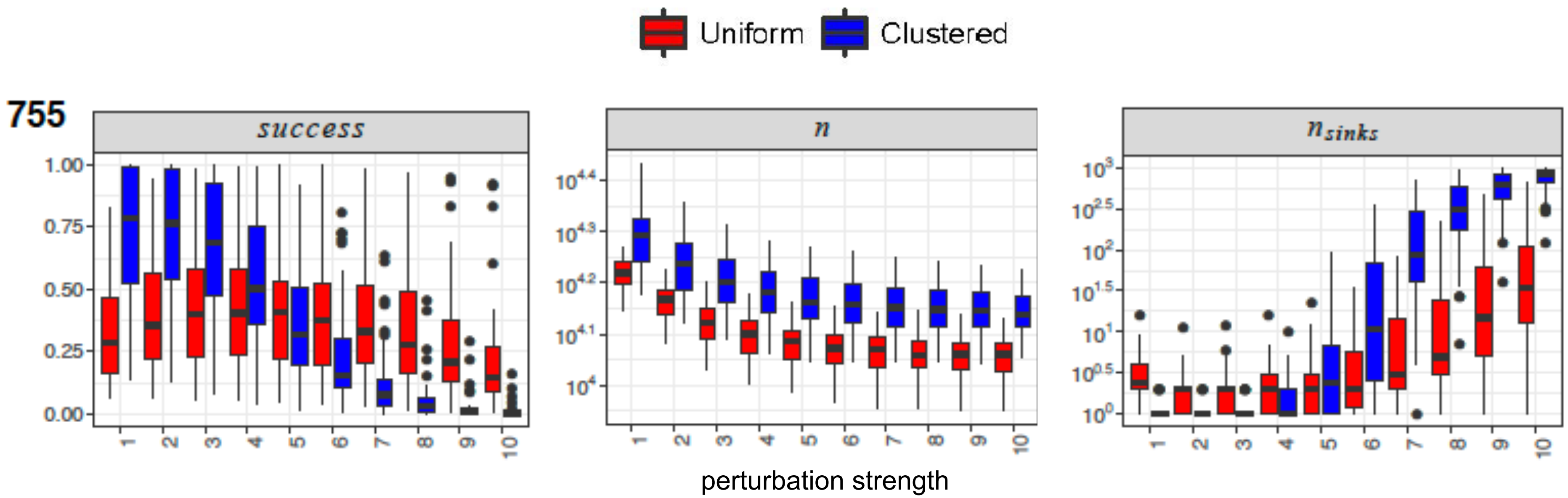
2D layout and 3D projection where z coordinate is fitness

Exploiting knowledge of the global structure

- Instances of several combinatorial optimisation problems have a multi-funnel structure
- Sub-optimal funnels act as traps to the search process
- Can we devise mechanisms for escaping sub-optimal funnels?
  - Restarts
  - Stronger perturbation in ILS implementations
  - Crossover

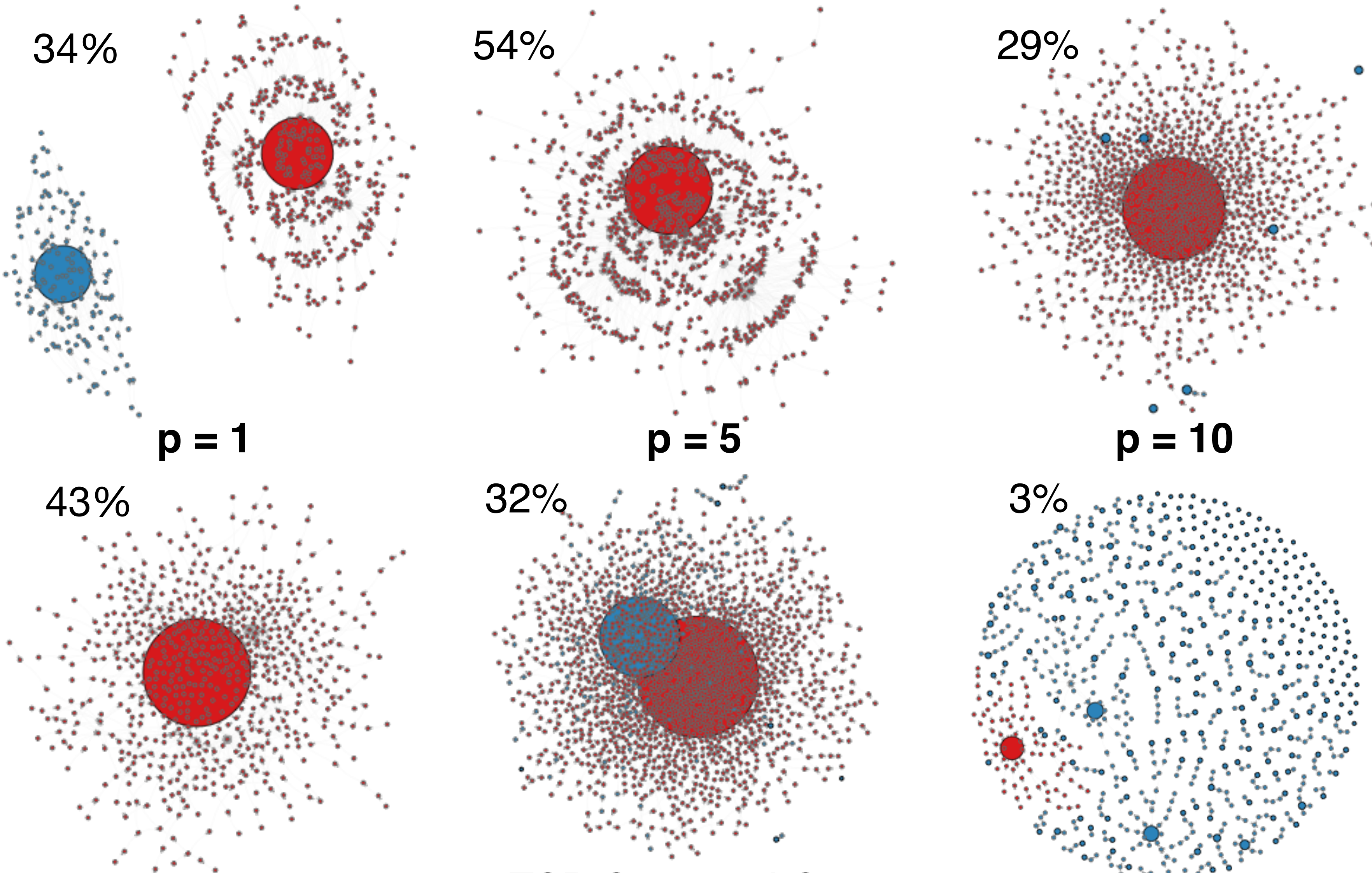
Increasing perturbation strength

- Chained-LK, Perturbation: 1 to10 double-bridge kicks
- TSP synthetic instances DIMACS: Uniform & Clustered
- Sizes 506, 755, 1010



(McMenemy, Veerapen & Ochoa. EvoCOP 2018)

TSP Uniform E755



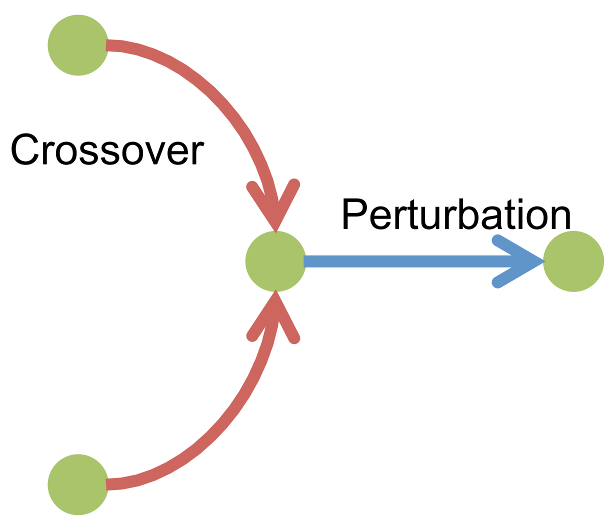
TSP Clustered C755

Other types of edges

- The LON model is not restricted to basin transition edges or escape edges.
- The model can also accommodate more than one type of edge.
- One example are LONs for Hybrid Evolutionary Algorithms.

LONs for Hybrid EAs

- Consider a Hydrid EA which incorporates a local search component to generate local optima.
- Two types of edges
  - Crossover (followed by local search)
  - Perturbation (followed by local search)



$P \leftarrow \text{popInit}()$
while *termination condition is not satisfied* **do**
  $Q(1) \leftarrow \text{bestSolution}(P)$
  for $i \leftarrow 2$ **to** $maxPop$ **do**
    $(p_1, p_2) \leftarrow \text{selection}(P)$
    $Q(i) \leftarrow \text{crossover}(p_1, p_2)$; $s \leftarrow \text{3opt}(Q(i))$
    $LO \leftarrow LO \cup \{s\}$; $E \leftarrow E \cup \{(p_1, s), (p_2, s)\}$
    if *crossover did not improve the solutions* **then**
      $best \leftarrow \text{chooseBest}(p_1, p_2)$
      $Q(i) \leftarrow \text{doubleBridgeMutation}(best)$; $s \leftarrow \text{3opt}(Q(i))$
      $LO \leftarrow LO \cup \{s\}$; $E \leftarrow E \cup \{(best, s)\}$
    end
  end
  if *best sol. did not improve in last 20 gen.* **then** $Q \leftarrow \text{immigration}(P)$
  $P \leftarrow Q$
end

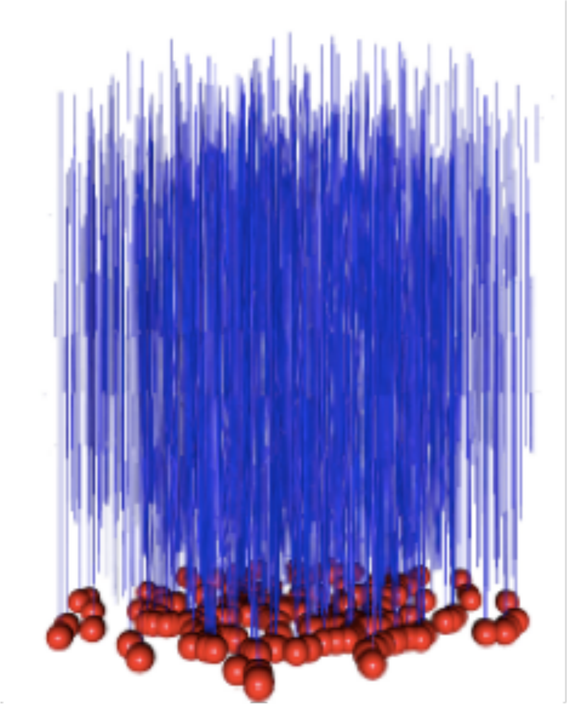
(Veerapen, Ochoa, Tinós, Whitley. PPSN 2016)

Contrasting LONs from two solving methods

- Hybrid GA vs ILS

Asymmetric TSP
Instance rbg323 LONs

Only edges and global optima are plotted.

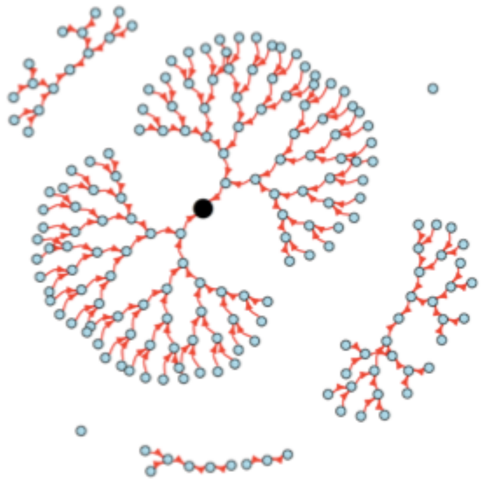


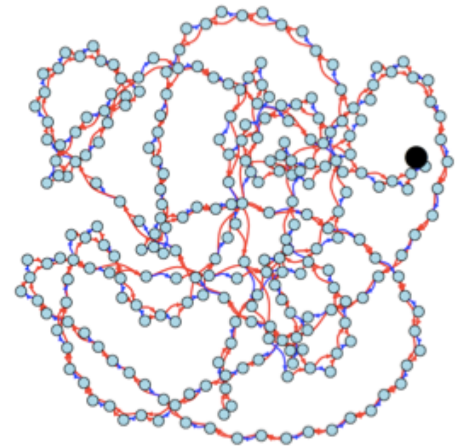
Hybrid GA
Partition Crossover (PX)
Success: 100%

Chained LK
Success: 0%

Contrasting LONs from two solving methods

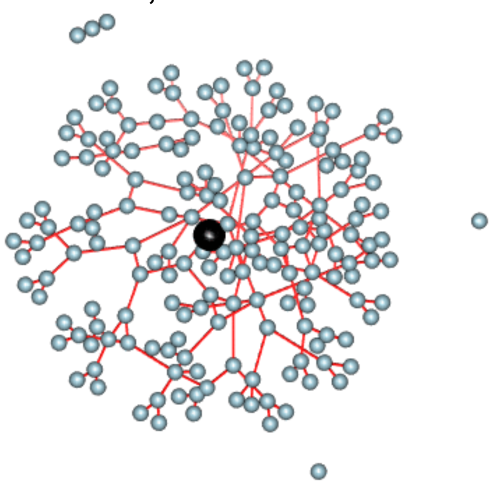
- Grey-box hybrid EA, 1 million variables NK

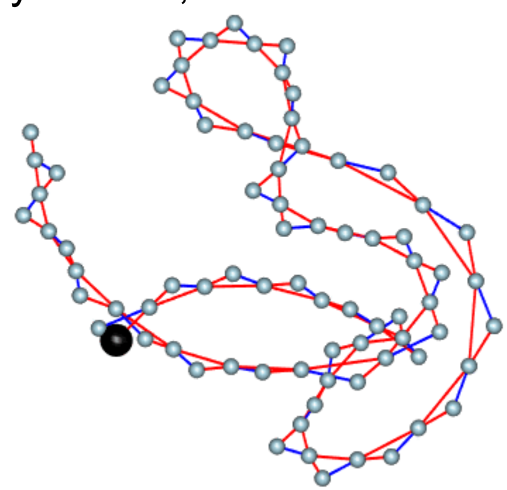




Hierarchical GA, Partition Crossover (PX)

Hybrid ILS, PX + Perturbation

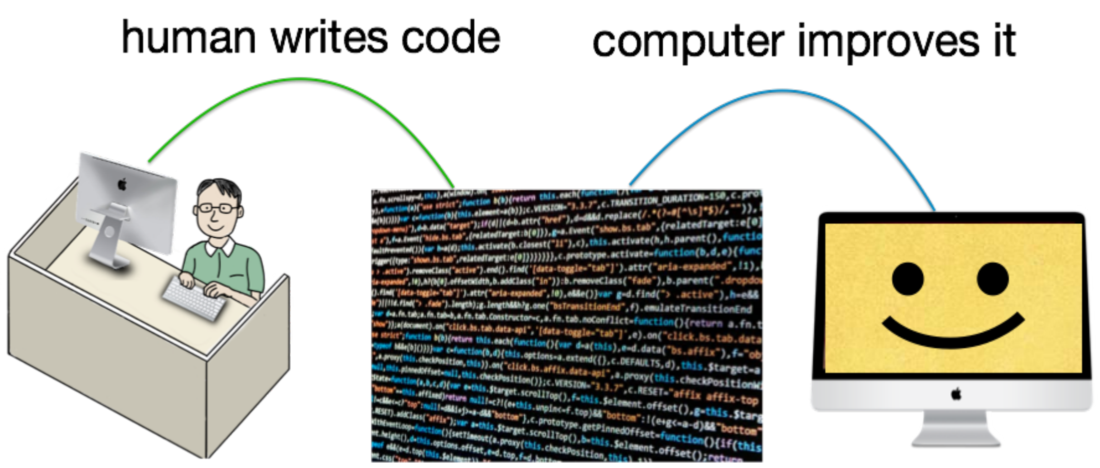




(Chicano, Whitley, Ochoa, Tinos. GECCO 2017)

Genetic Improvement of Software

- **Genetic improvement (GI)** uses automated search to find improved versions of existing software
- GI is different from Genetic Programming since it modifies existing code
- It is not necessary to use Genetic Programming
- Other methods such a Genetic Algorithms may be used
- Local Search is used in this case study



Program Search Test Bench

- Introduce random mutations to a bug free-program
- Try to recover a version passing all test cases (Competent programmer hypothesis, DeMillo et al., 1978)
- Mutations restricted to Comparison (<, <=, ==, !=, >=, >) and Boolean operators (&&, ||)
- Objective function: Minimise number of failed test cases

Input 1	Input 2	Input 3	Expected Output	Output	Failed
1	1	2	3	3	FALSE
1	2	1	3	4	TRUE
1	2	2	1	1	FALSE

Program Search Test Bench

- Mutations of comparison operators
  (<, <=, ==, !=, >=, >)
- Mutations of Boolean operators (&&, ||)
- Mutation operator: change one operator randomly
- Hill climber neighbourhood: change one operator
- Representation: vector of integers

2	2	0	4	6	7

```
if ( side1 == side2 ) {
      triang = triang + 1 ;
}
if ( side1 == side3 ) {
      triang = triang + 2 ;
}
```

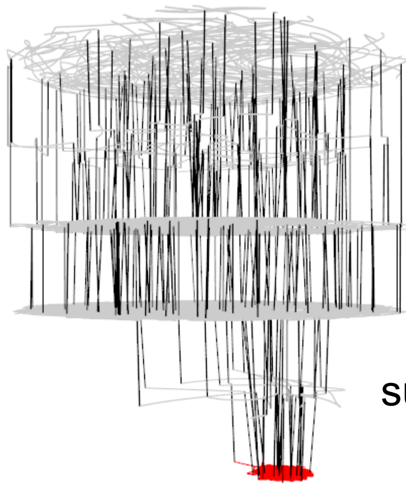
Program Search Test Bench

- Program and search space characteristics

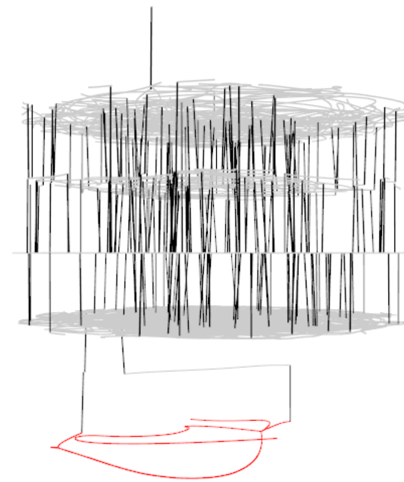
	triangle.c	tcas.c
Lines of code	40	135
Number of comparison operators	17	14
Number of Boolean operators	7	16
Number of input parameters	3	12
Number of output values	1	3
Number of test cases	14	1578
Size of search space with comparison operators only	1.69×10^{13}	7.84×10^{10}
Size of search space with comparison and Boolean operators	2.17×10^{15}	5.14×10^{15}

Comparison Operators Only | Comparison and Boolean Operators

triangle.c

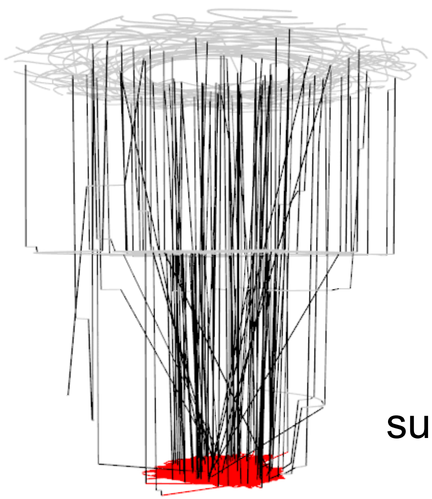


success: 87%

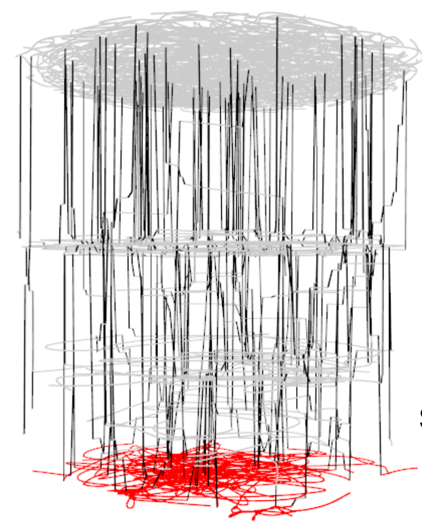


success: 31%

tcas.c



success: 94%



success: 98%

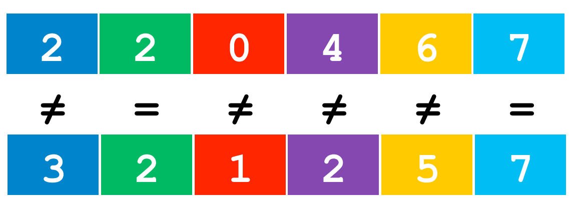
(Langdon, Veerapen, Ochoa. EuroGP 2017)

(Veerapen, Daolio, Ochoa. GECCO comp. 2017)

Preserving some info about solutions

- t-Distributed Stochastic Neighbor Embedding (t-SNE)
  - Non-linear dimensionality reduction
  - Similar objects are modelled by nearby points and dissimilar objects are modelled by distant points
  - Ability to reveal structure at the local and global levels

- Euclidean distance as default, here Hamming distance

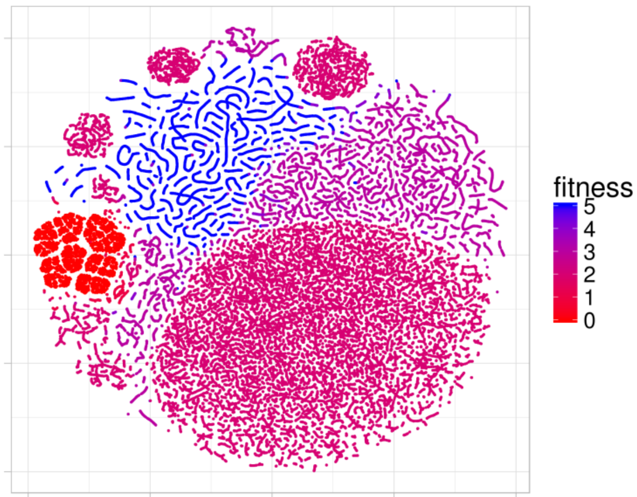


Hamming distance = 4

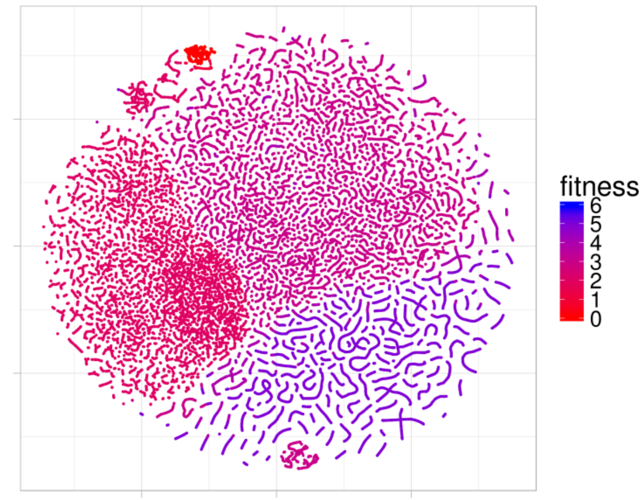
(Veerapen, Ochoa. GENP. 2018)

t-SNE layout

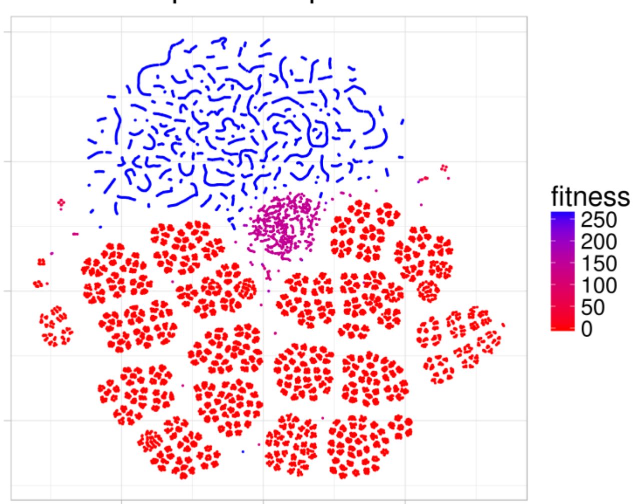
triangle - Comparison ops



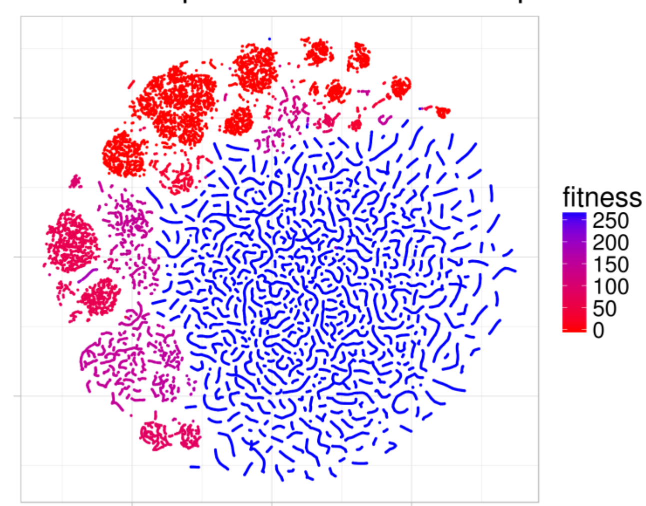
triangle - Comparison and Boolean ops



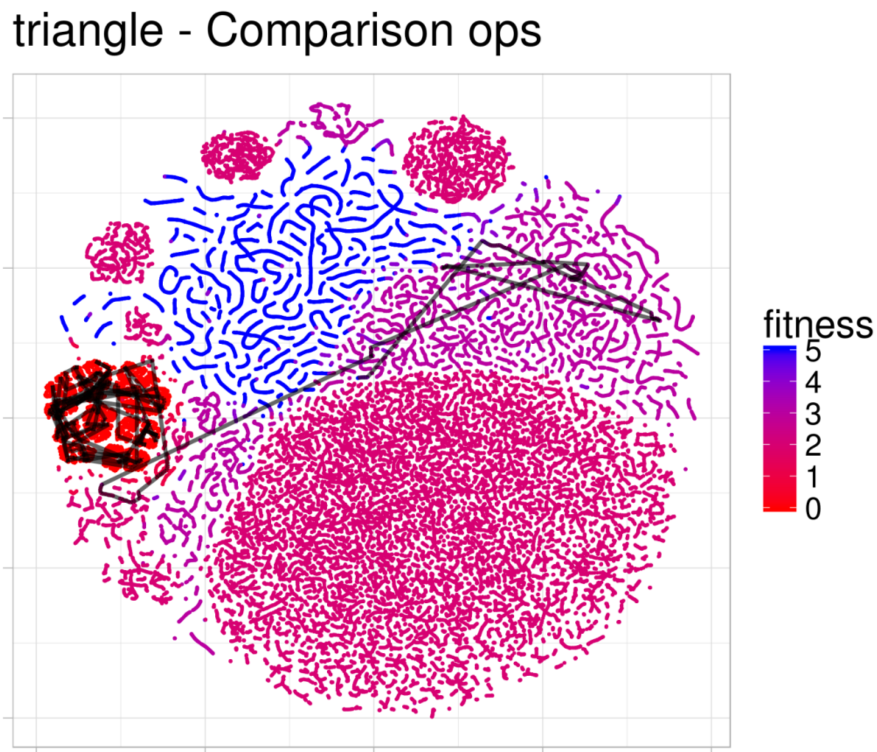
tcas - Comparison ops

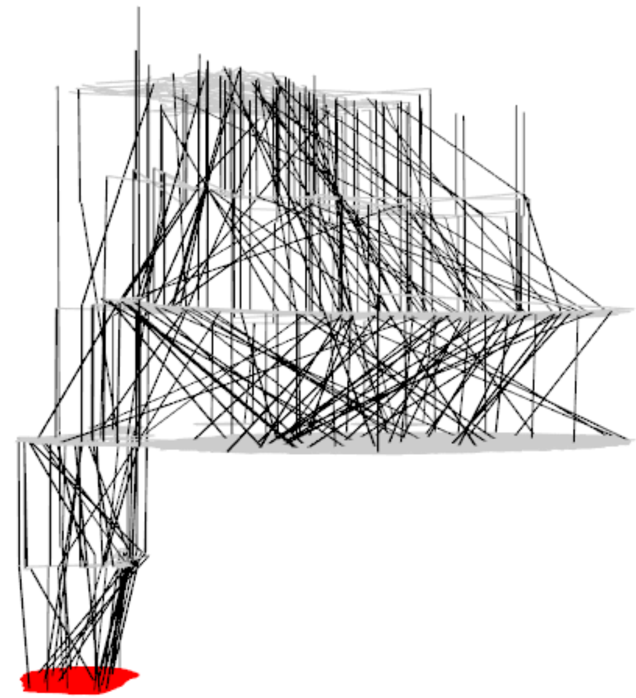


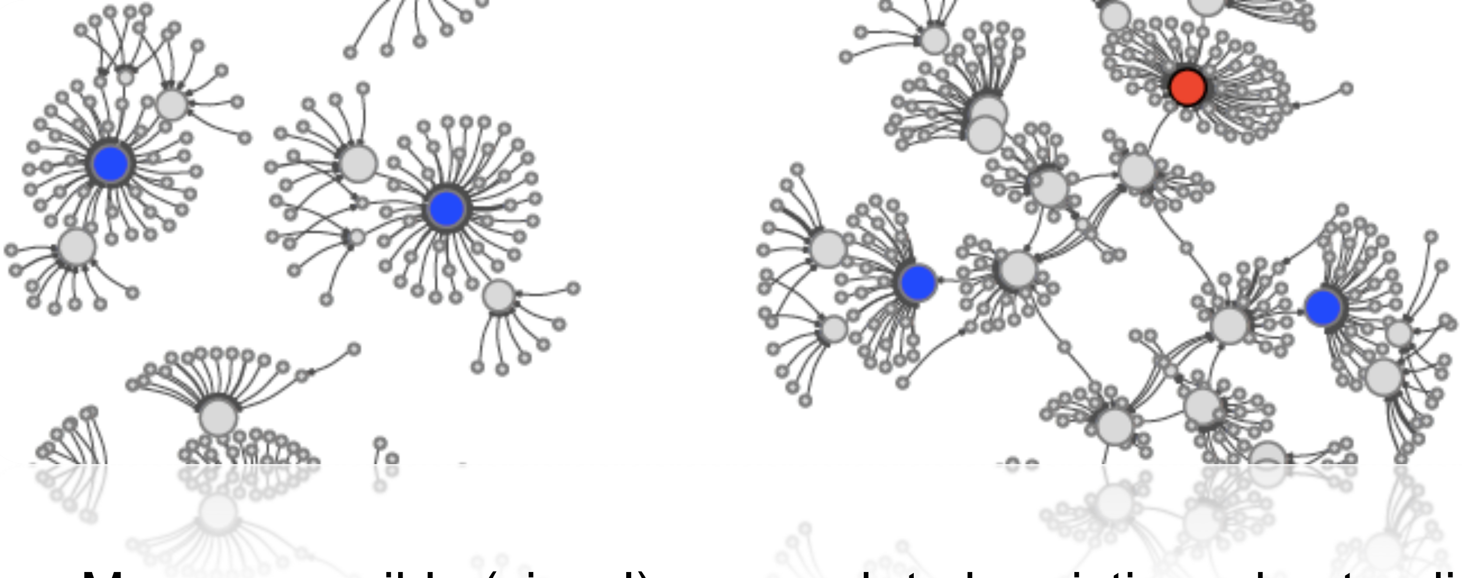
tcas - Comparison and Boolean ops



t-SNE layout







- More accessible (visual) approach to heuristic understanding
- Rigorous characterisation of funnels
- Global structure impacts search
- lonmaps.com - New website with resources available to assist researchers

CLOSING

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