

Local Optima Networks of NK Landscapes with and without Neutrality

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Overview and Motivation

- Bring the tools of *complex networks* analysis to the study the structure of combinatorial fitness landscapes
- **Goals** : Understand problem difficulty, design effective heuristic search algorithms
- **Methodology** : Extract a network that represents the landscape (Inspiration from energy landscapes (Doye, 2002)¹)
 - **Vertices** : local optima
 - **Edges** : a notion of adjacency between basins
- Conduct a network analysis
- Relate (exploit ?) network features to search algorithm design

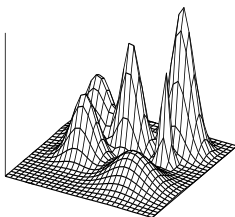
1. J. P. K. Doye, The network topology of a potential energy landscape : a static scale-free network., *Phys. Rev. Lett.*, 88 :238701, 2002.

Small – world networks (Watts and Strogatz, 1998)

- Neither ordered nor completely random
- Nodes highly clustered yet path length is small
- Network topological measures :
 - C : clustering coefficient, measure of local density
 - l : shortest path length global measure of separation

Scale – free networks (Barabasi and Albert, 1999)

- The distribution of the number of neighbours (the degree distribution) is *right – skewed* with a heavy tail
- Most of the nodes have less-than-average degree, whilst a small fraction of hubs have a large number of connections
- Described mathematically by a power-law



- Visual metaphor
- Tool for black-box optimisation analysis

Fitness landscape $(\mathcal{S}, \mathcal{V}, f)$:

- \mathcal{S} : set of admissible solutions,
- $\mathcal{V} : \mathcal{S} \rightarrow 2^{\mathcal{S}}$: neighborhood function,
- $f : \mathcal{S} \rightarrow \mathbb{R}$: fitness function.

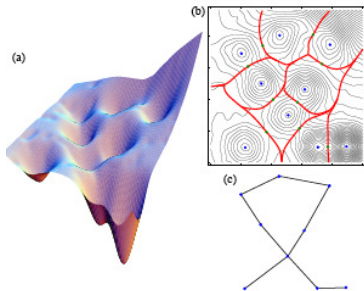
Our study :

- $\mathcal{S} : \{0, 1\}^N$
- $\mathcal{V}(x) = \{y \in \mathcal{S} \mid d_{hamming}(y, x) \leq 1\}$
- $f(x) = NK$ fitness function

NK fitness landscapes (Kauffman, 1993)

- Binary strings of length N
- K from 0 to $N - 1$, NK landscapes can be **tuned** from smooth to rugged (easy to difficult respectively)
- $K = 0$ no correlations, f is an additive function, and there is a **single maximum**
- $K = N - 1$ landscape **completely random**, the expected number of local optima is $\frac{2^N}{N+1}$
- Intermediate values of K interpolate between these two extreme cases and have a variable degree of **epistasis** (i.e. gene interaction) \rightarrow **ruggedness**

Energy surface and inherent networks (Doye, 2002)



- a Model of 2D energy surface
- b Contour plot, partition of the configuration space into basins of attraction surrounding minima
- c landscape as a network

Inherent network :

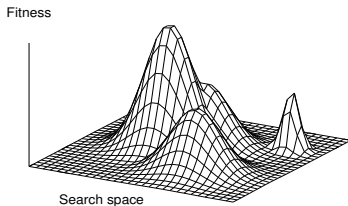
- **Nodes** : energy minima
- **Edges** : two nodes are connected if the energy barrier separating them is sufficiently low (transition state)

Local optima

Local optima s^* :

no neighbor solution with higher fitness value

$$\forall s \in \mathcal{V}(s^*), f(s) < f(s^*)$$



Basin of attraction

Hill-Climbing (HC) algorithm

Choose initial solution $s \in S$

repeat

 choose $s' \in \mathcal{V}(s)$ such that $f(s') = \max_{x \in \mathcal{V}(s)} f(x)$

if $f(s) < f(s')$ **then**

$s \leftarrow s'$

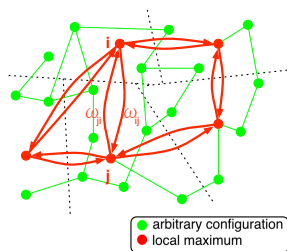
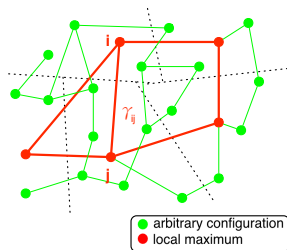
end if

until s is a Local optimum

Basin of attraction of s^* :

$$\{s \in S \mid \text{HillClimbing}(s) = s^*\}.$$

Local optima network



Nodes : set of local optima \mathcal{S}^*

Edges : notion of connectivity between basins

- e_{ij} between i and j if there is at least a pair of neighbours s_i and $s_j \in \mathcal{V}(s_i)$ such that $s_i \in b_i$ and $s_j \in b_j$ (GECCO 2008)
- weights w_{ij} attached to edges \rightarrow transition probabilities between basins (ALIFE 2008, Phys. Rev. E 2008)

Weight of edges

- For each pair of solutions s and s' , $p(s \rightarrow s') = P(s' = op(s))$
probability to pass from s to s'
 - if $s' \in \mathcal{V}(s)$, $p(s \rightarrow s') = \frac{1}{N}$
 - if $s' \notin \mathcal{V}(s)$, $p(s \rightarrow s') = 0$

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- Probability that a configuration $s \in S$ has a neighbor in a basin b_j

$$p(s \rightarrow b_j) = \sum_{s' \in b_j} p(s \rightarrow s')$$

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- w_{ij} : Total probability of going from basin b_i to basin b_j is the average over all $s \in b_i$ of the transition prob. to $s' \in b_j$:

$$p(b_i \rightarrow b_j) = \frac{1}{\#b_i} \sum_{s \in b_i} p(s \rightarrow b_j)$$

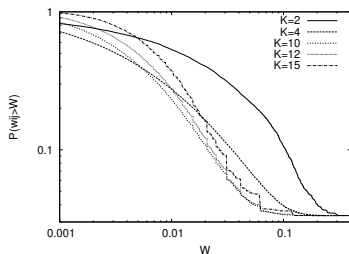
Experimental setup

- Extracted and analysed networks for $N = 14, 16$ and 18 , $K = 2, 4, \dots, N - 2, N - 1$ (30 random instances for each case)
- Network topological measurements
 - Number of nodes and edges
 - Clustering coefficient
 - Shortest path length and shortest path to the global optimum
 - Weight distribution
- Basin measurements
 - Basins sizes and fitness of optima
 - Visualisation

K	# nodes	# edges	Clustering	Path length
2	33	516	0.96	56
6	460	41,791	0.79	170
8	890	93,384	0.65	194
10	1,470	162,139	0.53	206
14	3,264	290,732	0.38	203
15	3,868	321,203	0.35	200

- # nodes and # edges : increase exponentially with K
- Clustering : decreases with K , transition between a given pair of neighboring basins is less likely to occur with high K
- Path length : increases steadily with K , distance between a given pair of nodes is longer with high K

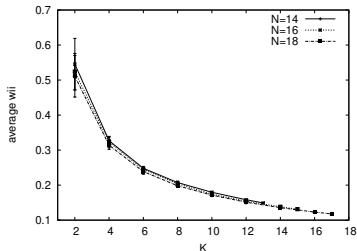
Outgoing weight distribution



Cumulative distribution of the network weights w_{ij} for outgoing edges with $j \neq i$ in log-log scale, $N = 16$

- Weights (transition prob. to neighbouring basins) are small
- The distributions are not uniform or Poissonian, nor power laws
- For high K the decay is faster
- Low K has longer tails (on average the transition probabilities are higher for low K)

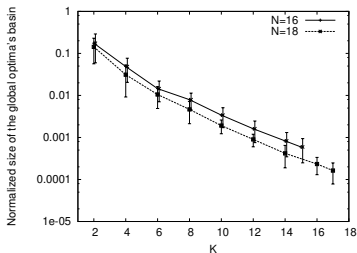
Average weights to remain in the same basin



Average weight w_{ii} according to the parameter N and K

- Weights to remain in the same basin w_{ii} , are large compare to w_{ij} with $i \neq j$
- w_{ii} are higher for low K (50% for $K = 2$, above 12% for high K),
- It seems easier to leave the basin for high K (high exploration), however, number the of local optima increases fast with K

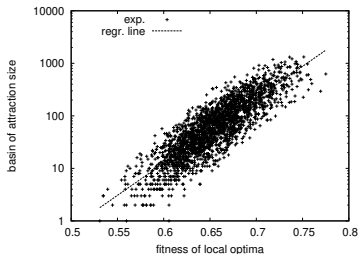
Global optimum basin size



Size of the basin corresponding to the global maximum for each K

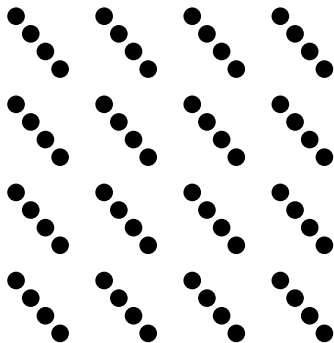
- **Trend** : the basin shrinks very quickly with increasing K.
- For higher K, it is more difficult for a search algorithm to locate the basin of attraction of the global optimum

Fitness vs. basin size

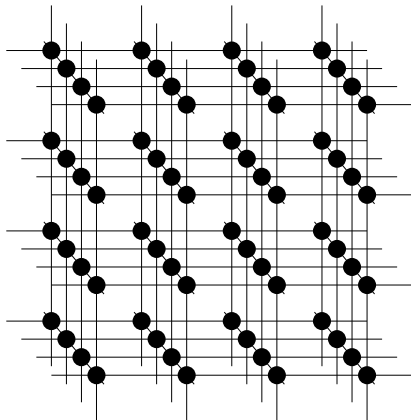


Fitness of local optima vs. their corresponding basins sizes

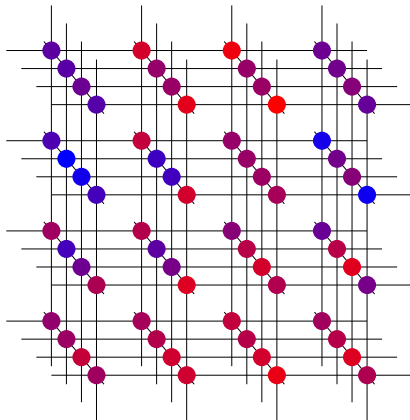
- **Trend** : clear positive correlation between the fitness values of maxima and their basins' sizes
- On average, the global optimum seems easier to find than another local optimum, however, the number of local optima increases exponentially with increasing K



- Bit strings of length $N = 6$
- $2^6 = 64$ solutions
- one point = one solution



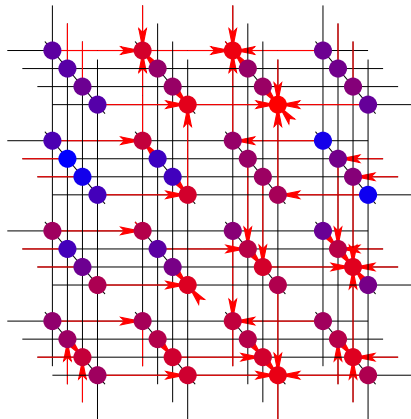
- Bit strings of length $N = 6$
- Neighborhood size = 6
- Line between points = solutions are neighbors




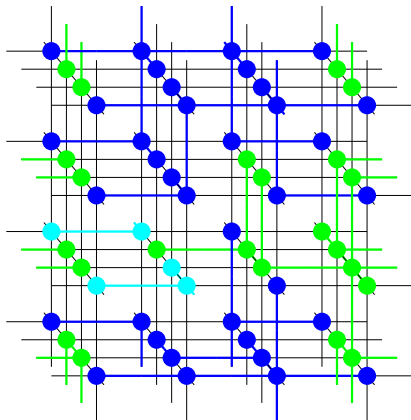
Color represent fitness value

● high fitness

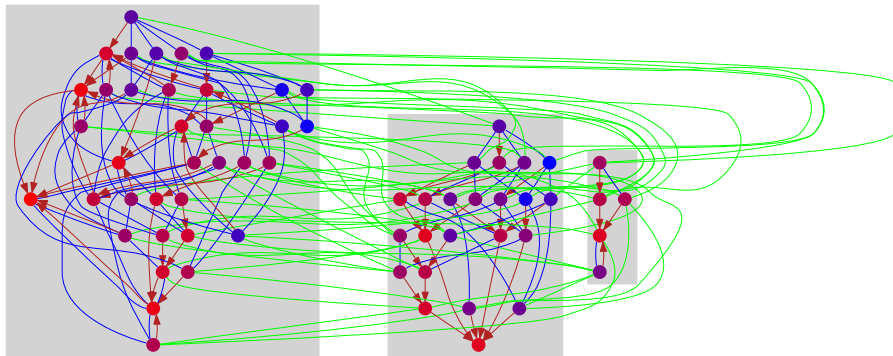
● low fitness



- Color represent fitness value
 - high fitness
 - low fitness
-  point towards the solution with highest fitness in the neighborhood

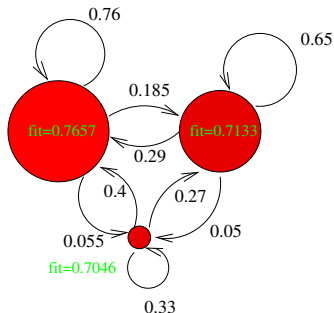


- Each color correspond to one basin of attraction
- Basins of attraction are interlinked and overlapped
- Basins have no "interior"



- Basins of attraction are interlinked and overlapped !
- Most neighbours of a given solution are outside its basin

Local optima networks



Nodes : local optima

Edges : transition probabilities





- G. Ochoa, M. Tomassini, S. Verel, C. Darabos (2008) [A Study of NK Landscapes' Basins and Local Optima](#) *GECCO 2008*, pages 555-562 (best paper nomination)
- S. Verel, G. Ochoa, M. Tomassini (2008) [The Connectivity of NK Landscapes' Basins : A Network Analysis](#), *Artificial Life XI*, MIT Press, Cambridge, MA.
- M. Tomassini, S. Verel, G. Ochoa (2008) [Complex Network analysis of Combinatorial Spaces : the NK Landscape Case](#), *Physical Review E*, Vol.78, No.6.
- S. Verel, G. Ochoa, M. Tomassini (under review) [Local Optima Networks of NK landscapes with Neutrality](#)

Summary and conclusions

- *Local optima networks* : a new model for landscape analysis
- New findings about basin's structure of NK landscapes
- Network features are related to previously observed search difficulty (with increasing K)

Future work

- Adapt the notion of optima network to landscapes with neutrality (done, under review)
- Design sampling methodologies to extract representative networks (test on realistic combinatorial problems)
- **Ultimate research question** : Given an optima network with certain properties, what is the best algorithm to search for nodes with high-fitness in this network ?

-  J. P. K. Doye, The network topology of a potential energy landscape : a static scale-free network., *Phys. Rev. Lett.*, 88 :238701, 2002.
-  J. P. K. Doye and C. P. Massen. Characterizing the network topology of the energy landscapes of atomic clusters. *J. Chem. Phys.*, 122 :084105, 2005.
-  S. A. Kauffman. *The Origins of Order*. Oxford University Press, New York, 1993.
-  Gabriela Ochoa, Marco Tomassini, Sébastien Verel, and Christian Darabos. A Study of NK Landscapes' Basins and Local Optima Networks. *Proceedings of the 10th annual conference on Genetic and evolutionary computation Genetic And Evolutionary Computation Conference*, pages 555–562, ACM New York, NY, USA.

best paper nomination.



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pages 648–655, 2008. MIT Press,