Fitness Landscapes and Graphs: Multimodularity, Ruggedness and Neutrality

Sébastien Verel

I3S laboratory - Université Nice Sophia Antipolis / CNRS, France
DOLPHIN team - INRIA Lille-Nord Europe
http://www.i3s.unice.fr/∼verel

July, 6 2013

GECCO'13 Companion, July 6-10, 2013, Amsterdam, The Netherlands.
ACM 978-1-4503-1964-5/13/07.

Fitness landscapes : Motivations

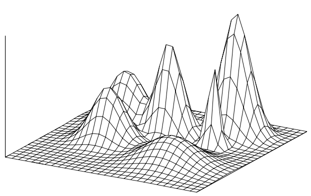
Basic idea

- Concept to study the search space
  from the point of view of local search
- Description of the search space "geometry"
- To design effective search algorithms

L. Barnett, U. Sussex, DPhil Diss. 2003

"the more we know of the ***statistical properties*** *of a class of fitness landscapes, the better equipped we will be for the* ***design*** *of effective search algorithms for such landscapes"*

Fitness landscapes in biology

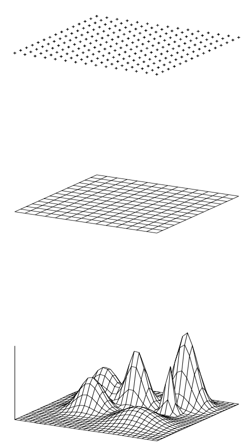


Origin in biological science :
Wright 1930 [45]

Biological evolution :

- Metaphorical uphill struggle across a "fitness landscape"
  - mountain **peaks** represent high "fitness" (ability to survive),
  - **valleys** represent low fitness.
- Evolution proceeds : population of organisms performs an "**adaptive walk**"

Fitness landscapes in biology and others sciences



In biology :

- Modelisation of species evolution

Extended to model dynamical systems :

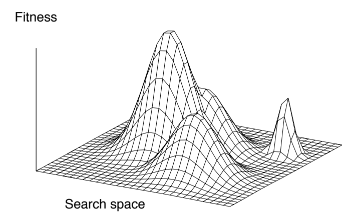
- statistical physic,
- molecular evolution,
- ecology, etc

Fitness landscapes in biology

2 sides of Fitness Landscapes

- **Metaphor** : most profound concept in evolutionary dynamics
  - give pictures of evolutionary process
  - be careful of misleading pictures :
    "smooth landscape without noise"
- **Quantitative** concept : predict the evolutionary paths
  - Quasispecies equation :
    mean field analysis with differential equations
  - Stochastic process :
    markov chain
  - Network analysis

In combinatorial optimization



Definition

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

- $\mathcal{S}$ is the **search space**
- $\mathcal{N} : \mathcal{S} \rightarrow 2^{\mathcal{S}}$ is a **neighborhood relation**
- $f : \mathcal{S} \rightarrow \mathbb{R}$ is a **objective function**

Fitness landscapes for black-box optimisation

Black box Scenario

We have only $\{(x_0, f(x_0)), (x_1, f(x_1)), ...\}$ given by an "oracle"
No information is either not available or needed on the definition of objective function

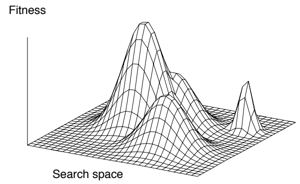
- Objective function given by a computation, or a simulation
- Objective function can be irregular, non differentiable, non continous, etc.
- (Very) large search space for discrete case (combinatorial optimization), *i.e.* NP-complete problems
- etc.

Fitness landscapes in evolutionary computation

2 sides of Fitness Landscapes

- **Metaphor** : most profound concept in EA
  - give pictures of the search dynamic :
    "if the fitness landscapes have big valleys,
    I can use this algorithm"
  - be careful of misleading pictures :
    "smooth landscape without noise"
- **Quantitative** concept : predict the evolutionary paths
  - Quasispecies equation :
    mean field analysis with differential equations
  - Stochastic process :
    markov chain
  - Network analysis

What is a neighborhood ?



Neighborhood function :

$$\mathcal{N} : \mathcal{S} \to 2^{\mathcal{S}}$$

Set of "**neighbor**" solutions associated to each solution

Important !

Neighborhood must be based on the operator(s) of the EA

Neighborhood $\Leftrightarrow$ Operator

$\mathcal{N}(x) = \{y \in \mathcal{S} \mid \mathbb{P}(y = op(x)) > 0\}$
or
$\mathcal{N}(x) = \{y \in \mathcal{S} \mid \mathbb{P}(y = op(x)) > \epsilon\}$
or
$\mathcal{N}(x) = \{y \in \mathcal{S} \mid \text{distance}(x, y) \leq 1\}$

Typical example : bit strings

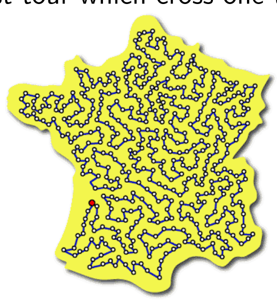
***Search space** : $\mathcal{S} = \{0, 1\}^N$*

$$\mathcal{N}(x) = \{y \in \mathcal{S} \mid d_{Hamming}(x, y) = 1\}$$

Example :
$\mathcal{N}(01101) = \{01100, 01111, 01001, 00101, 11101\}$

Typical example : permutations

Traveling Salesman Problem :
find the shortest tour which cross one time every town



***Search space** : $\mathcal{S} = \{\sigma \mid \sigma$ permutations $\}$*

$$\mathcal{N}(x) = \{y \in \mathcal{S} \mid \mathbb{P}(y = op_{2opt}(x)) > 0\}$$

More than 1 operator...

What can we do with 2 operators (ex : memetic algorithm) ?

$\mathcal{N}_1(x) = \{y \in \mathcal{S} \mid y = op_1(x)\}$ $\quad$ $\mathcal{N}_2(x) = \{y \in \mathcal{S} \mid y = op_2(x)\}$

Severals possibilities according to the goal :

- Study 2 landscapes : $(\mathcal{S}, \mathcal{N}_1, f)$ and $(\mathcal{S}, \mathcal{N}_2, f)$
- Study the landscape of "union" : $(\mathcal{S}, \mathcal{N}, f)$

$$\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2 = \{y \in \mathcal{S} \mid y = op_1(x) \text{ or } y = op_2(x)\}$$

- Study the landscape of "composition" : $(\mathcal{S}, \mathcal{N}, f)$

$$\mathcal{N} = \{y \in \mathcal{S} \mid y = op_1(x) \text{ or } y = op_2(x) \text{ or } y = op_1 \circ op_2(x) \text{ or } y = op_2 \circ op_1(x)\}$$

Goal of the fitness landscapes study

- Geometry (features) of fitness landscape
  $\Rightarrow$ dynamics of a local search algorithm
- Geometry is linked to the problem difficulty :
  - If there are a lot of local optima, the probability to find the global optimum is lower.
  - If the fitness landscape is flat, discovering better solutions is rare.
  - What is the best search direction in the landscape ?

Study of the fitness landscape **features**
allows to study
the **performance** of search algorithms

Goal of the fitness landscapes study

1. To compare the difficulty of two search spaces :
   - One problem with 2 (or more) possible codings :
     $(\mathcal{S}_1, \mathcal{N}_1, f_1)$ and $(\mathcal{S}_2, \mathcal{N}_2, f_2)$
     different coding, mutation operator, objective function, etc.

   Which one is easier to solve ?
2. To choose the algorithm :
   - analysis of global geometry of the landscape

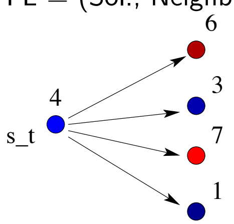
   Which algorithm can I use ?
3. To tune the parameters :
   - *off-line* analysis of structure of fitness landscape

   Which is the best mutation operator ? the size of the population ? number of restarts ? etc.
4. To control the parameters during the run :
   - *on-line* analysis of structure of fitness landscape

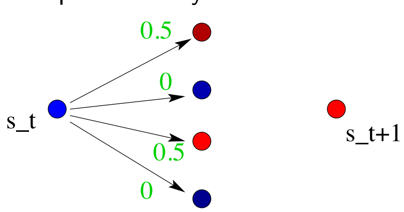
   Which is the optimal mutation operator according to the estimation of the structure ?

Point of view : Before putting a particular heuristic

FL = (Sol., Neighbors, Fitness)



Put prob. from your heuristic :



- Sample the neighborhood to have information on **local features** of the search space
- From local information : deduce some **global features** like general shape of search space, "difficulty", etc.

Goal of the fitness landscapes study

Study of the **geometry** of the landscape
allows to
study the **difficulty**, and **design** a good optimisation algorithm

Fitness landscape is a **graph** $(\mathcal{S}, \mathcal{N}, f)$:

- nodes are solutions which have a value (fitness),
- edges are defined by the neighborhood relation.

pictured as a real landscape

Two main geometries have been studied

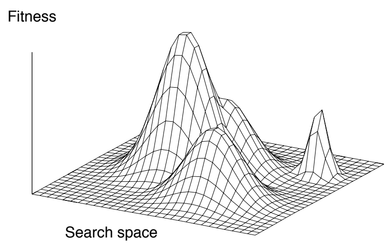
- multimodal and ruggedness
- neutral

Multimodal Fitness landscapes

Local optima s^*

no neighbor solution with higher fitness value

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



Multimodal Fitness landscapes

Adaptive walk

$(s_0, s_1, \ldots)$ where $s_{i+1} \in \mathcal{N}(s_i)$ and $f(s_i) < f(s_{i+1})$

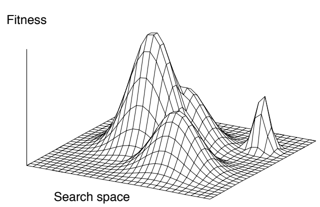
Hill-Climbing (HC) algorithm

Choose initial solution $s \in \mathcal{S}$
repeat
  choose $s' \in \mathcal{N}(s)$ such that $f(s') = max_{y \in \mathcal{N}(s)} f(y)$
  if $f(s) < f(s')$ **then**
    $s \leftarrow s'$
  end if
until s is a Local Optimum

Basin of attraction of s^*

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

Multimodal Fitness landscapes



Optimisation difficulty :
number and size of attractive basins (Garnier *et al* [10])

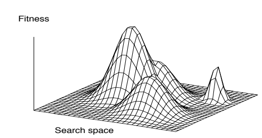
The idea :

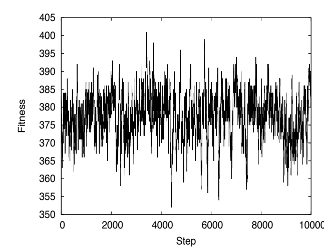
- if the size of attractive basin of global optimum is relatively "small"
- the "time" to find the global optimum is "long"

The measure :

- Length of adaptive walks (distribution, avg, etc.)

Walking on fitness landscapes



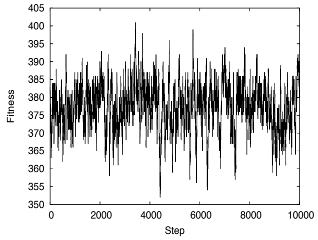


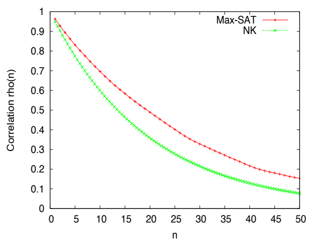
fitness vs. step of a random walk (example of max-SAT problem)

Random walk : $(s_1, s_2, \ldots)$ such that $s_{i+1} \in \mathcal{N}(s_i)$ and equiprobability on $\mathcal{N}(s_i)$

- Fitness seems to be very "chaotic"
- Analysis the fitness during the random walk as a signal

Rugged/smooth fitness landscapes





Autocorrelation of time series of fitnesses $(f(s_1), f(s_2), \ldots)$ along a random walk $(s_1, s_2, \ldots)$ [37] :

$$\rho(n) = \frac{E[(f(s_i) - \bar{f})(f(s_{i+n}) - \bar{f})]}{var(f(s_i))}$$

autocorrelation length $\tau = \frac{1}{\rho(1)}$

- small τ : rugged landscape
- long τ : smooth landscape

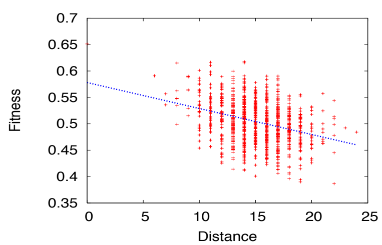
Results on rugged fitness landscapes (Stadler 96 [28])

Problem	parameter	$\rho(1)$
symmetric TSP	n number of towns	$1 - \frac{4}{n}$
anti-symmetric TSP	n number of towns	$1 - \frac{4}{n-1}$
Graph Coloring Problem	n number of nodes α number of colors	$1 - \frac{2\alpha}{(\alpha-1)n}$
NK landscapes	N number of proteins K number of epistasis links	$1 - \frac{K+1}{N}$

Ruggedness decreases with the size of thoses problems : small variation has less effect on the fitness values

Fitness Distance Correlation (FDC) (Jones 95 [15])

Correlation between distance to global optimum and fitness



Classification based on experimental studies :

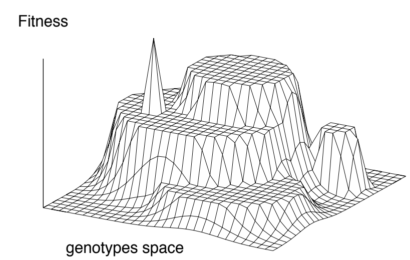
- $\rho < -0.15$, easy optimization
- $\rho > 0.15$, hard optimization
- $-0.15 < \rho < 0.15$, undecided zone

Neutral Fitness Landscapes

Neutral theory (Kimura ≈ 1960 [17])

Theory of mutation and random drift

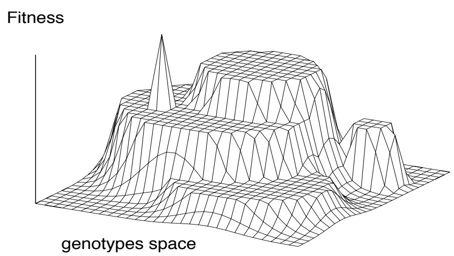
A considerable number of mutations have no effects on fitness values



- plateaus
- neutral degree
- neutral networks [Schuster 1994 [27], RNA folding]

Neutral Fitness Landscapes
Combinatorial optimization

- Redundant problem (symetries, ...) (Goldberg 87 [12])
- Problem "not well" defined or dynamic environment (Torres 04 [14])



Applicative problems :

- Robot controler
- Circuit design
- Genetic Programming
- Protein folding
- Learning problems

Neutrality and difficulty

- In our knowledge, there is no definitive answer about neutrality / problem hardness
- Certainly, it is dependent on the "nature" of neutrality

⇒ Sharp description of the geometry of neutral fitness landscapes is needed

Neutrality and difficulty

We know for certain that :

- **No information** is better than **Bad information** : Hard trap functions are more difficult than needle-in-a-haystack functions
- **Good information** is better than **No information**

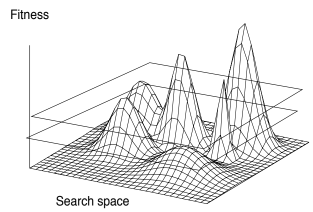
- When there is No information : you should have a good method to find it !

In the following

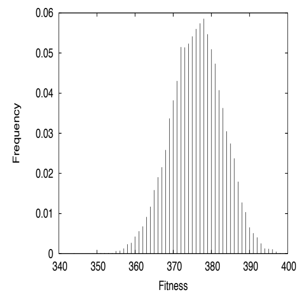
Description of neutral fitness landscapes :

- Neutral sets : set of solutions with the same fitness
- Neutral networks : add neighborhood information

Neutral sets : Density Of States



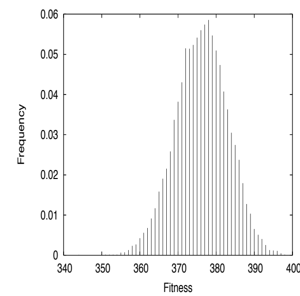
Set of solutions with fitness value



Density of states (D.O.S.)

- Introduce in physics (Rosé 1996 [26])
- Optimization (Belaidouni, Hao 00 [4])

Neutral sets : Density Of States

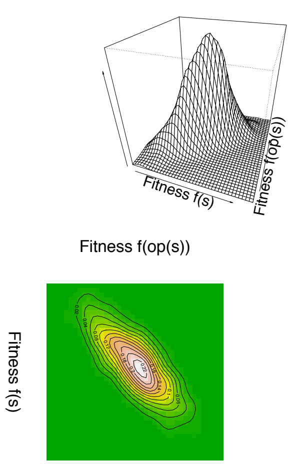


Density of states (D.O.S.)

Informations given :

- Performance of random search
- Tail of the distribution is an indicator of difficulty :
  - the faster the decay, the harder the problem
- But do not care about the neighborhood relation

Neutral sets : Fitness Cloud



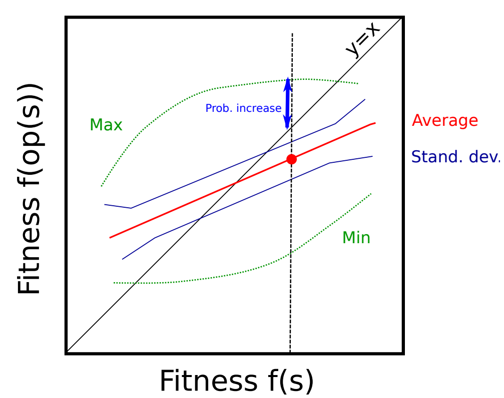
- $(\mathcal{S}, \mathcal{F}, \mathbb{P})$: probability space
- $op : \mathcal{S} \rightarrow \mathcal{S}$ stochastic operator of the local search

- $X(s) = f(s)$
- $Y(s) = f(op(s))$

Fitness Cloud of op

Conditional probability density function of Y given X

Fitness cloud : Measure of evolvability

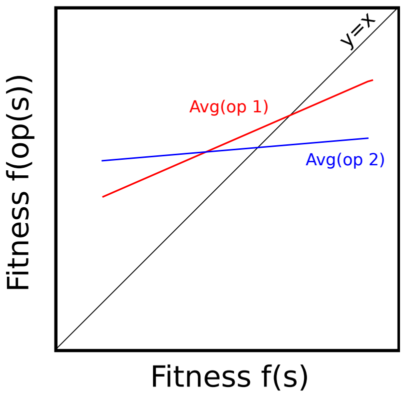


Evolvability

Ability to evolve : fitness in the neighborhood compared to the fitness of the solution

- Probability of finding better solutions
- Average fitness of better neighbor solutions
- Average and standard deviation of fitnesses

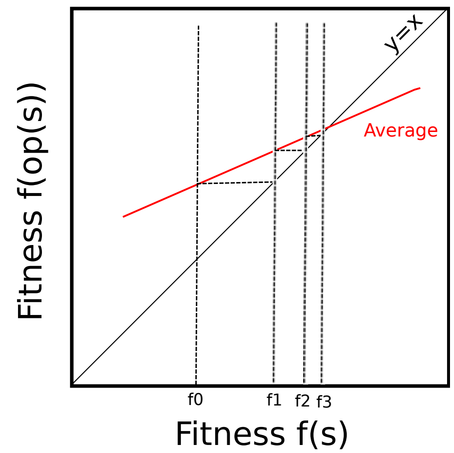
Fitness cloud : Comparaison of difficulty



- Operator 1 > Operator 2
- Because Average 1 more correlated to fitness
- Linked to autocorrelation
- Average is often a line :
  - See works on Elementary Landscapes (D. Wihtley and others)
  - See Negative Slope Coefficient (NSC)

Fitness cloud

Prediction of fitness (CEC 2003)

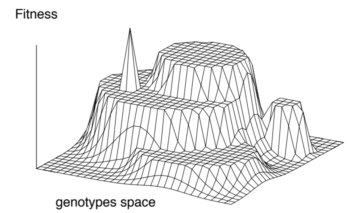


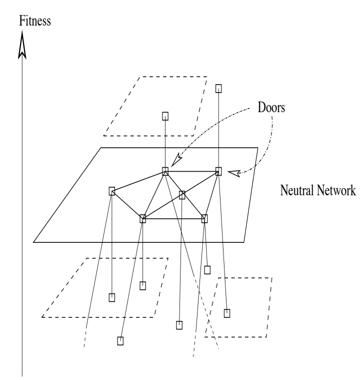
- Approximation (only approximation) of the fitness value after few steps of local operator
- Indication on the quality of the operator

Neutral fitness landscapes

- Neutral sets (done) :
  set of solutions with the same fitness
  $\Rightarrow$ No structure
- Fitness cloud (done) :
  Bivariate density $(f(s), f(op(s)))$
  $\Rightarrow$ Neighborhood relation **between** neutral sets
- Neutral networks (to be done) :
  $\Rightarrow$ Neighborhood structure **into** the neutral sets : Graph

Neutral networks (Schuster 1994 [27])





Definitions

Test of neutrality

$$isNeutral : S \times S \to \{true, false\}$$

For example, $isNeutral(s_1, s_2)$ is *true* if :

- $f(s_1) = f(s_2)$.
- $|f(s_1) - f(s_2)| \leq 1/M$ with M is the search population size.
- $|f(s_1) - f(s_2)|$ is under the evaluation error.

Neutral neighborhood

of s is the set of neighbors which have the same fitness $f(s)$

$$\mathcal{N}_{neut}(s) = \{s^{'} \in \mathcal{N}(s) \mid isNeutral(s, s^{'})\}$$

Neutral degree of s

Number of neutral neighbors : $nDeg(s) = \sharp(\mathcal{N}_{neut}(s) - \{s\})$.

Definitions

Neutral walk

$W_{neut} = (s_0, s_1, \ldots, s_m)$

- for all $i \in [0, m-1]$, $s_{i+1} \in \mathcal{N}(s_i)$
- for all $(i, j) \in [0, m]^2$, $isNeutral(s_i, s_j)$ is *true*.

Neutral Network

graph $G = (N, E)$

- $N \subset \mathcal{S}$: for all s and $s^{'}$ from V, there is a neutral walk belonging to V from s to $s^{'}$,
- $(s_1, s_2) \in E$ if they are neutral neighbors : $s_2 \in \mathcal{N}_{neut}(s_1)$

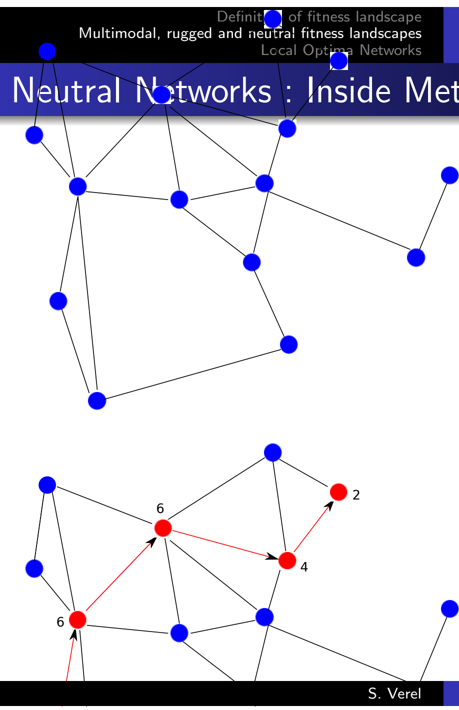
A fitness landscape is neutral
if there are many solutions with high neutral degree.

Neutral Networks (NN) : Inside Metrics

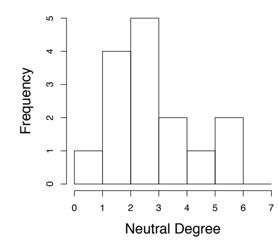
Classical graph metrics :

- **Size of NN** :
  number of nodes of NN,
- **Neutral degree distribution** :
  - measure of the quantity of "neutrality"
- **Autocorrelation of neutral degree** (Bastolla 03 [3]) :
  during neutral random walk
  - comparaison with random graph,
  - measure of the correlation structure of *NN*

Neutral Networks : Inside Metrics

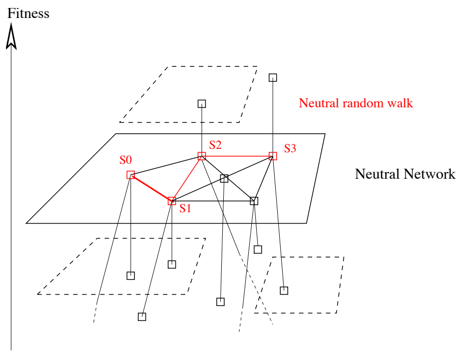


- Size : 15 solutions
  Distribution of size overall landscapes
- Neutral degree distribution



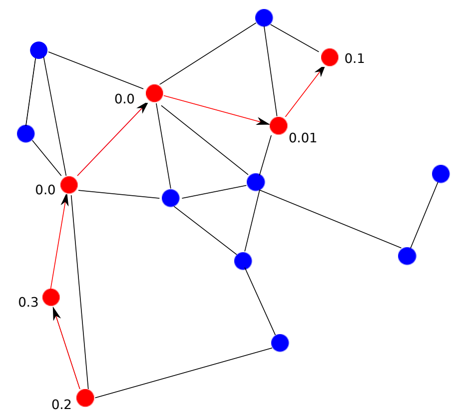
- Autocorrelation of

Neutral Networks : Outside Metrics



1. Rate of innovation (Huynen 96 [13]) : The number of new accessible structures (fitness) per mutation
2. Autocorrelation of evolvability [34] : autocorrelation of the sequence $(evol(s_0), evol(s_1), \ldots)$.

Neutral Networks : Outside Metrics

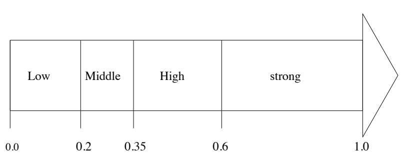


- Autocorrelation of evolvability :
  - Evolvability $evol$ = avg fitness in the neighborhood
  - Autocorrelation of $(evol(s_0), evol(s_1), \ldots)$.
- Informations :
  - if high correlation $\Rightarrow$ "easy" (you can use this information)
  - if low correlation $\Rightarrow$ "difficult"

Summary of metrics

- Neutral degrees distribution :

  "How neutral is the fitness landscape ?"
- Autocorrelation of neutral degrees : network "structure"



- Rate of innovation :

  low information for combinatorial optimization
- Autocorrelation of evolvability :

  information on the links between NN

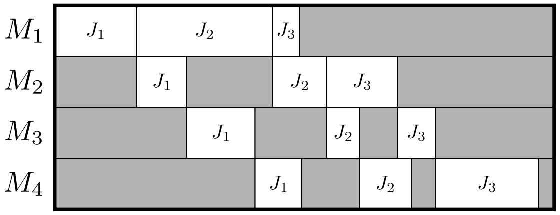
From fitness landscapes to design

Example of Flow Shop Scheduling problem

Join work with : Marie-Eleonore Marmion, Arnaud Liefooghe, Clarisse Dhaenens, Laetitia Jourdan,
DOLPHIN Team, INRIA Lille - Nord Europe, France

From fitness landscapes to design

Example of Flow Shop Scheduling problem



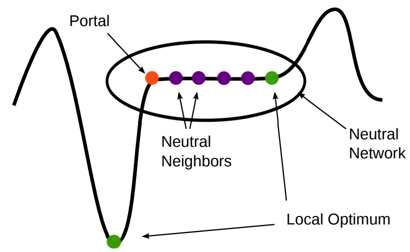
- N jobs, M machines
- Processing time can be different on each machine
- Solution representation = Permutation
- Minimization of the makespan

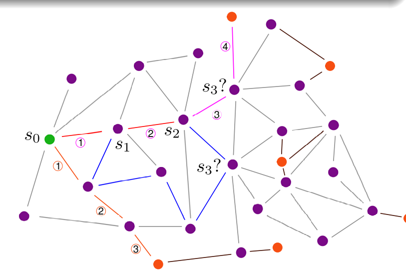
From fitness landscapes to design

[LION'11]

Analysis / Questions

- Is there some neutrality and plateaus ?
- Is it large plateaus ?
- Can we escape from plateaus ?





From fitness landscapes ...

Analysis / Questions

- Is there some neutrality and plateaus ?

Average neutral degree :

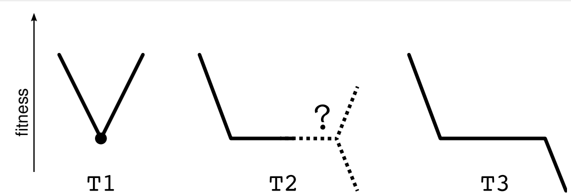
M / N	20	50	100	200
5	87 (24%)	720 (30%)	3038 (31%)	
10	32 (9%)	336 (14%)	1666 (17%)	7920 (20%)
20	14 (4%)	168 (7%)	882 (9%)	3960 (10%)

YES

From fitness landscapes ...

Analysis / Questions

- Is it large plateaus ?



- No T_1 for $N = 50, 100, 200$
- 0 - 20% T_1 T_2 for $N = 20$
- $>$ 97% of T_3

YES

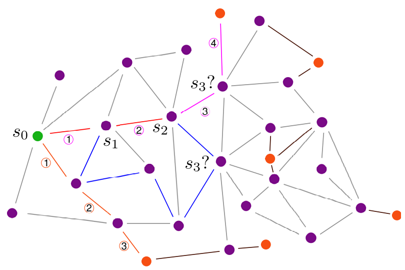
From fitness landscapes ...

Analysis / Questions

- Can we escape from plateaus ?

Average number of steps to find a portal :

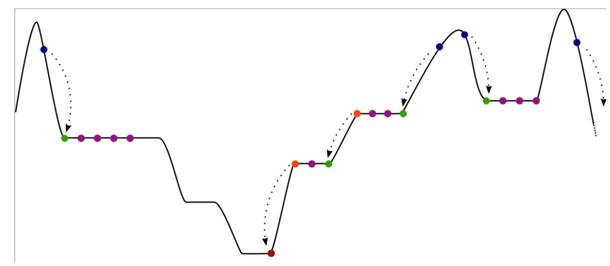
M / N	20	50	100	200
5	17	33	34	
10	10	14	17	30
20	6	6	6	6



YES

From fitness landscapes to design of LS

Neutrality based Iterated Local Search (NILS) [EVOCOP'11]



NILS principle

- Local Search :
  - First-improvement Hill-Climbing
- Perturbation :
  - Neutral moves until portal or maximum number of steps
  - Kick move when no improvement

From fitness landscapes to design of LS

Neutrality based Iterated Local Search (NILS)

- Efficient local search compare to previous ones
- Much simpler one, and performances are well understood
- One new best known solution on strutured a real-like instance
- The methodology can be applied to others combinatorial problems

Basic Methodology of fitness landscapes analysis

- Density of States : pure random search, initialization ?
- Length of adaptive walks : multimodality ?
- Autocorrelation of fitness : ruggedness ?
- Neutral Degree Distribution : neutrality ?
- Fitness Cloud : Quality of the operator, evolvability ?
- Fitness Distance Correlation from best known
- Neutral walks and evolvability : neutral information ?
- ... be creative from your algorithm and problem point of view
- ... be careful on the computed measures : one measure is not enough, and must be very well understand

Recent review : Katherine M. Malan, Information Sciences, (2013)

Sofware to perform fitness landscape analysis

Framework ParadisEO

http://paradiseo.gforge.inria.fr

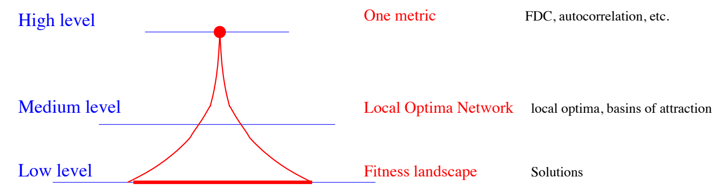
Software Framework for Metaheuristics (local search, EA, continous, discrete, parallel, island, fitness landscape, etc.)
See documentation, tutorials

```
moAutocorrelationSampling<Neighbor> sampling(randomInitialization,
                                             neighborhood,
                                             fitness,
                                             incrementalEvaluation,
                                             nbStep);

sampling();

sampling.fileExport(str_out);
```


Motivation and general idea : Levels of description



- **Fitness landscapes** : based on an huge number of solutions
- **One metric** : based on one real number, or curve to catch all the complexity
- **Local optima Network** : based on local optima

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.

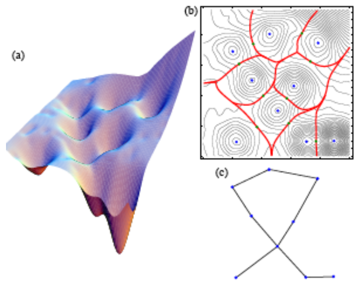
Small-world networks (Watts and Strogatz, 1998)

- 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

Energy surface and inherent networks (Doye, 2002)



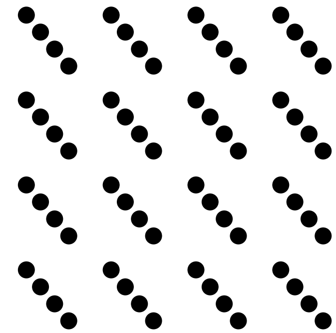
- a Model of 2D energy surface
- b Contour plot, partition of the configuration space into basins of attraction surrounding minima
- c landscape as a network

Inherent network :

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

Basins of attraction in combinatorial optimisation

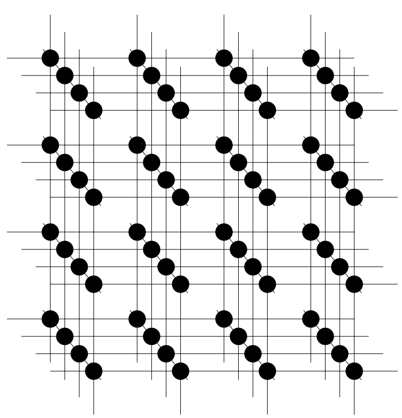
Example of small *NK* landscape with $N = 6$ and $K = 2$



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

Basins of attraction in combinatorial optimisation

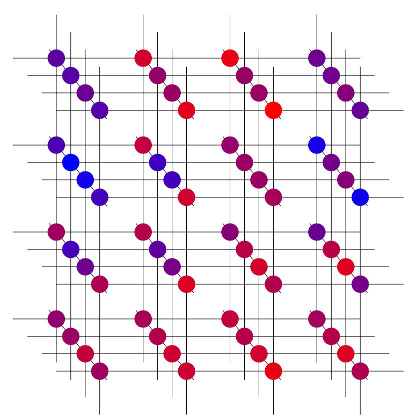
Example of small *NK* landscape with $N = 6$ and $K = 2$



- Bit strings of length $N = 6$
- Neighborhood size = 6
- Line between points = solutions are neighbors
- Hamming distances between solutions are preserved (except for at the border of the cube)

Basins of attraction in combinatorial optimisation

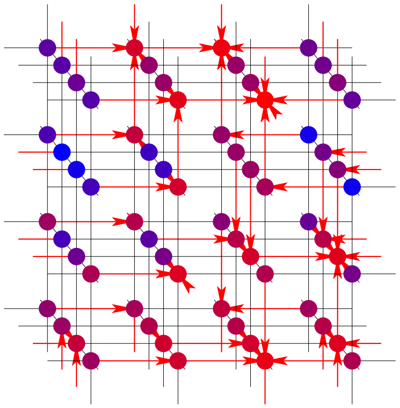
Example of small *NK* landscape with $N = 6$ and $K = 2$



Color represent fitness value
- high fitness
- low fitness

Basins of attraction in combinatorial optimisation

Example of small NK landscape with $N = 6$ and $K = 2$

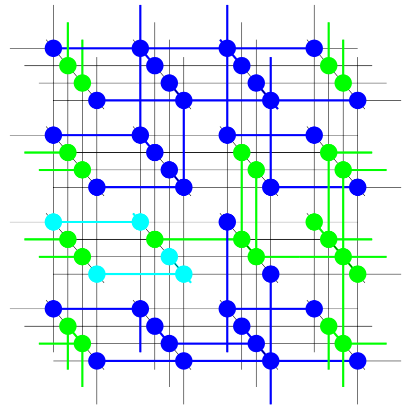


- Color represent fitness value
  - high fitness
  - low fitness
- → point towards the solution with highest fitness in the neighborhood

Exercise :
Why not make a Hill-Climbing walk on it ?

Basins of attraction in combinatorial optimisation

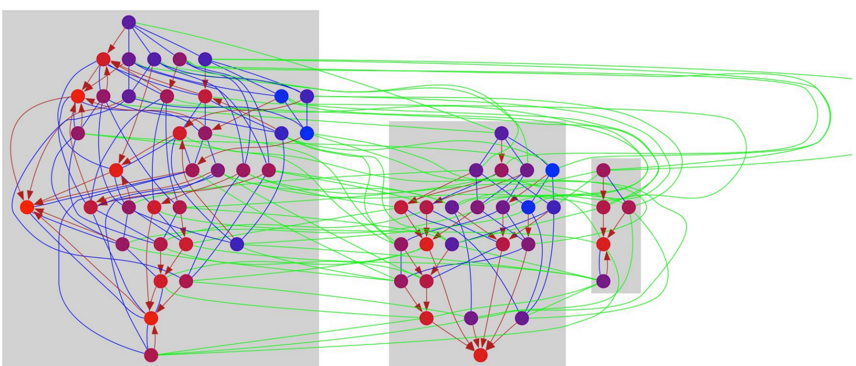
Example of small NK landscape with $N = 6$ and $K = 2$



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

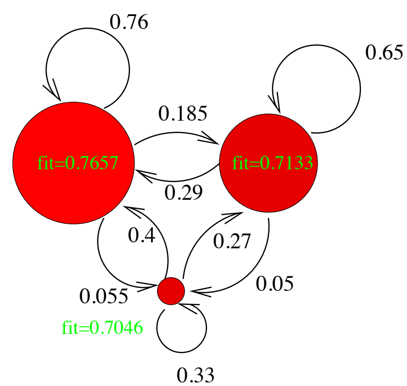
Basins of attraction in combinatorial optimisation

Example of small NK landscape with $N = 6$ and $K = 2$



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

Local optima network



- Nodes :
  local optima
- Edges :
  transition probabilities

Basin of attraction

Hill-Climbing (HC) algorithm

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

Basin of attraction of s^* :

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

local optima network

Local optima network

- Nodes : set of local optima $\mathcal{S}^*$
- Edges : notion of connectivity between basins of attraction

2 possible definitions of edges

- **Basin-transition edges** :
  transition between random solutions from basin b_i to basin b_j
  (GECCO 2008 [23])
  (ALIFE 2008 [35], Phys. Rev. E 2008 [32], CEC 2010)
- **Escape edges** :
  transition from Local Optimum i to basin b_j
  (EA 2011, GECCO 2012, PPSN 2012)

Basin-transition edges : random transition between basins

Edges

e_{ij} between LO_i and LO_j if $\exists\ s_i \in b_i$ and $s_j \in b_j : s_j \in \mathcal{N}(s_i)$

Prob. from solution s to solution s'

$$p(s \rightarrow s') = \mathbb{P}(s' = op(s))$$

For example, $\mathcal{S} = \{0,1\}^N$ and bit-flip operator

- if $s' \in \mathcal{N}(s)$, $p(s \rightarrow s') = \frac{1}{N}$
- if $s' \notin \mathcal{N}(s)$, $p(s \rightarrow s') = 0$

Prob. from solution s to basin b_j

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

Weights : Transition prob. from basin b_i to basin b_j

Escape edges : transition prob. from local optimum

Edges

e_{ij} between LO_i and LO_j if $\exists s : distance(LO_i, s) \leq D$ and $s \in b_j$.

Weights

$$w_{ij} = \sharp\{s \in S \mid d(LO_i, s) \leq D \text{ and } s \in b_j\}$$

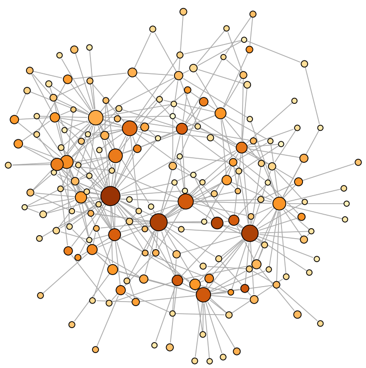
can be normalized by the number of solutions at distance D

$\Rightarrow$ local optima network : weighted oriented graph

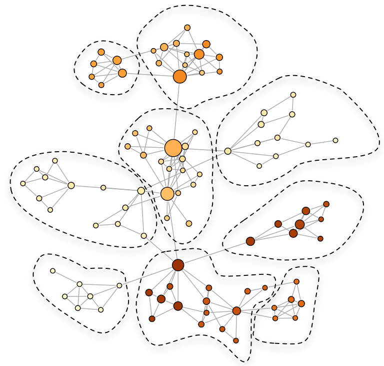
Structure of Local Optima Network

Quadratic Assignment Problem [CEC'10 - Phys A'11]

Random instance



Real-like instance



Structure of the Local Optima Network related to search difficulty

NK fitness landscapes : ruggedness and epistasis

NK-landscapes : Model of problems

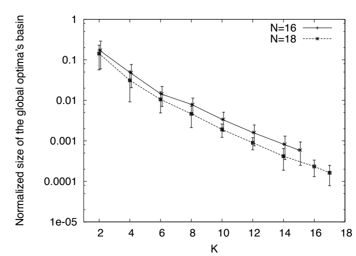
N size of the bit-strings
K from 0 to $N-1$, NK landscapes can be **tuned** from smooth to rugged (easy to difficult respectively) :

- $K=0$ 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)

Methods

- Extracted and analysed networks
  - $N \in \{14, 16, 18\}$,
  - $K \in \{2, 4, \ldots, N-2, N-1\}$
  - 30 random instances for each case
- Measures :
  - Statistics on **basins** sizes and fitness of optima
  - **Network features** : clustering coefficient, shortest path to the global optimum, weight distribution, disparity, boundary of basins

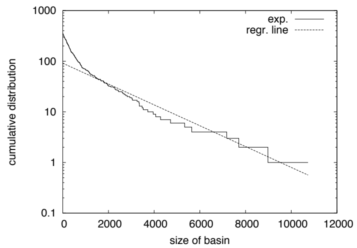
Global optimum basin size versus K



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

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

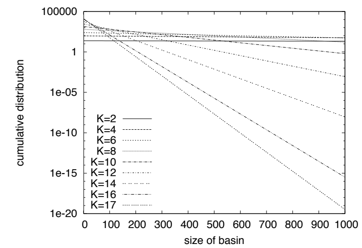
Analysis of basins : basin size



Cumulative distribution of basins sizes for $N = 18$ and $K = 4$

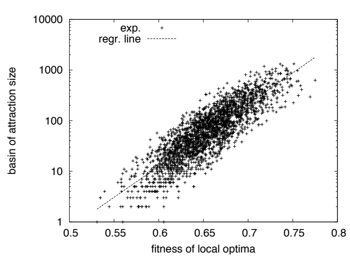
- Trend : small number of large basin, large number of small basin
- Log-normal cumulative distribution : not uniform !
- Slope of correlation increases with K
- When K large : basin sizes are nearly equals
  the distribution becomes more uniform

Analysis of basins : basin size



- Trend : small number of large basin, large number of small basin
- log-normal cumulative distribution
- slope of correlation increases with K
- when K large : basin sizes are nearly equals

Analysis of basins : fitness *vs.* basin size



Correlation fitness of local optima vs. their corresponding basins sizes

- Trend : clear positive correlation between the fitness values of maxima and their basins' sizes

The highest, the largest

- On average, the global optimum easier to find than one other local optimum
- But more difficult to find, as the number of local optima increases exponentially with increasing K

General network statistics

Weighted clustering coefficient

local density of the network

$$c^w(i) = \frac{1}{s_i(k_i - 1)} \sum_{j,h} \frac{w_{ij} + w_{ih}}{2} a_{ij} a_{jh} a_{hi}$$

where $s_i = \sum_{j \neq i} w_{ij}$, $a_{nm} = 1$ if $w_{nm} > 0$, $a_{nm} = 0$ if $w_{nm} = 0$ and $k_i = \sum_{j \neq i} a_{ij}$.

Disparity

dishomogeneity of nodes with a given degree

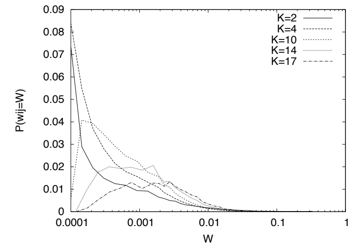
$$Y_2(i) = \sum_{j \neq i} \left(\frac{w_{ij}}{s_i} \right)^2$$

General network statistics $N = 16$

K	$\sharp$ nodes	$\sharp$ edges	$\bar{C}^w$	$\bar{Y}$	$\bar{d}$
2	33_{15}	516_{358}	$0.96_{0.0245}$	$0.326_{0.0579}$	56_{14}
4	178_{33}	9129_{2930}	$0.92_{0.0171}$	$0.137_{0.0111}$	126_{8}
6	460_{29}	41791_{4690}	$0.79_{0.0154}$	$0.084_{0.0028}$	170_{3}
8	890_{33}	93384_{4394}	$0.65_{0.0102}$	$0.062_{0.0011}$	194_{2}
10	$1,470_{34}$	162139_{4592}	$0.53_{0.0070}$	$0.050_{0.0006}$	206_{1}
12	$2,254_{32}$	227912_{2670}	$0.44_{0.0031}$	$0.043_{0.0003}$	207_{1}
14	$3,264_{29}$	290732_{2056}	$0.38_{0.0022}$	$0.040_{0.0003}$	203_{1}
15	$3,868_{33}$	321203_{2061}	$0.35_{0.0022}$	$0.039_{0.0004}$	200_{1}

- **Clustering Coefficient** : For high K, transition between a given pair of neighboring basins is less likely to occur
- **Disparity** : For high K the transitions to other basins tend to become equally likely, an indication of the randomness of the landscape

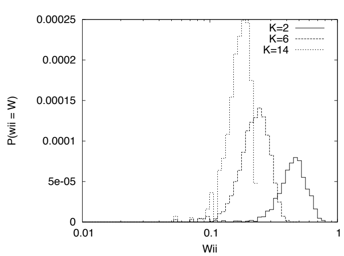
Weights distribution : transition probability between basins



distribution of the network weights w_{ij} for outgoing edges with $j \neq i$ in log-x scale, $N = 18$

- Weights are small
- For high K the decay is faster
- Low K has longer tails
- On average, the transition probabilities are higher for low K (less local optima)

Weight distribution remain in the same basin

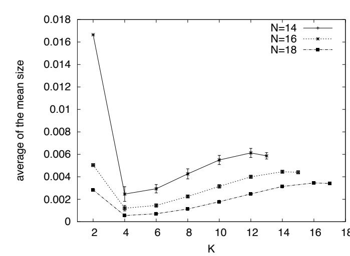


Average weight w_{ii} according to the parameter N and K

Question :
Is it easy to escape a basin ?

- Weights to remains in the same are large compare to w_{ij} with $i \neq j$
- w_{ii} are higher for low K
- Easier to leave the basin for high K : high "natural" exploration
- But : number of local optima increases fast with K

Interior and border size



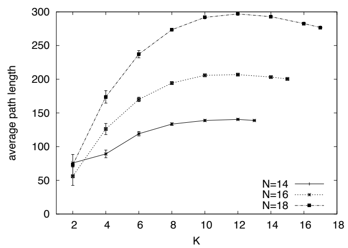
Average of the mean size of basins interiors

Question :
Do basins look like a "montain" with interior and border ?

solution is in the interior if all neighbors are in the same basin

Answer
- Interior is very small
- Nearly all solution are in the border

Shortest path length between local optima

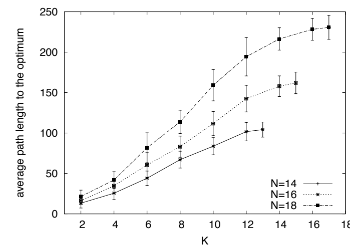


Average distance (shortest path) between nodes

Question :
Are the basins "far" from each other ?

- Increase with N (♯ of nodes increases exponentially)
- For a given N, increase with K up to $K = 10$, then stagnates

Shortest path length to global optima

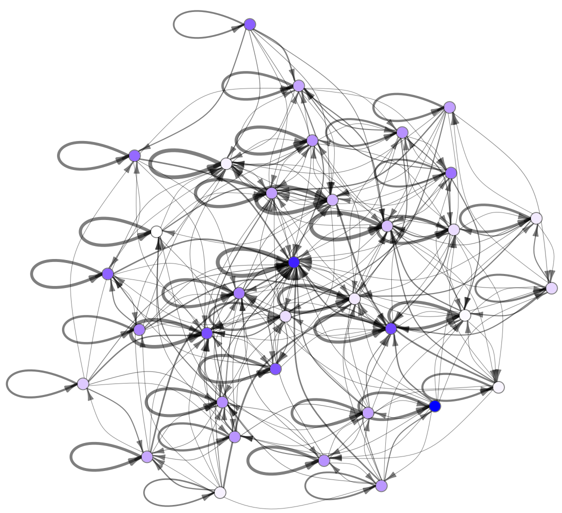


Average path length to the global optimum from all the other basins

Question :
Is the global optimum basin is far ?

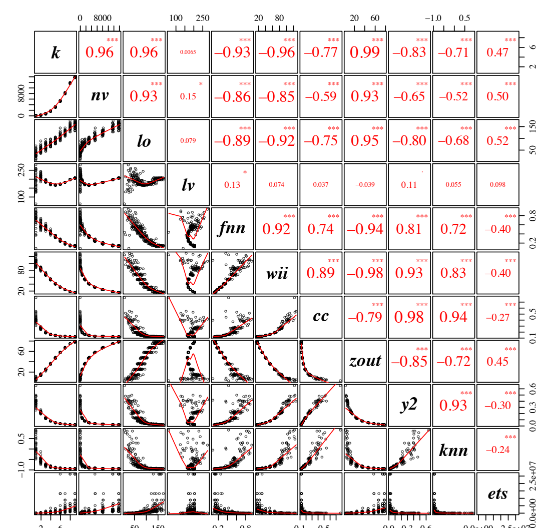
- More relevant for optimisation
- Increase steadily with increasing K

Network Metrics

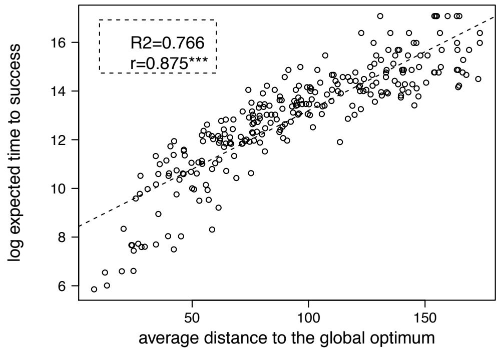


- *nv* : ♯vertices
- *lo* : path to best
- *lv* : avg path
- *fnn* : fitness corr.
- *wii* : self loops
- *cc* : clust. coef.
- *zout* : out degree
- *y2* : disparity
- *knn* : degree corr.

Correlation Matrix



ILS Performance vs LON Metrics
[GECCO'12]



Expected running times
vs.
Average shortest path to the global optimum.

ILS Performance vs LON Metrics
[GECCO'12]

1. Multiple linear regression on all possible predictors :

$$\log(ets) = \beta_0 + \beta_1 k + \beta_2 \log(nv) + \beta_2 lo + \cdots + \beta_{10} knn + \epsilon$$

2. Step-wise backward elimination of each predictor in turn.

Predictor	$\widehat{\beta_i}$	Std. Error	p-value
(Intercept)	10.3838	0.58512	$9.24 \cdot 10^{-47}$
lo	0.0439	0.00434	$1.67 \cdot 10^{-20}$
zout	-0.0306	0.00831	$2.81 \cdot 10^{-04}$
y2	-7.2831	1.63038	$1.18 \cdot 10^{-05}$
knn	-0.7457	0.40501	$6.67 \cdot 10^{-02}$

Multiple R-squared : 0.8494, Adjusted R-squared : 0.8471.

Tuning of parameters and Local Optima Network

- Relevant features using "complex system" technics
- Search difficulty is related to the features of LON :
  - Classification of instances
  - Understanding the search difficulty
  - Guideline of design
- Time complexity can be estimated :
  - Tuning with **Portefolio** technics

Future on local optima network

- Design a method for sampling large search space (under construction)
- Compare the properties of Loc. Opt. Network and the optimal tradeoff between exploration and exploitation
- Study the LON like a fitness landscape

Summary on fitness landscapes

Fitness landscape is a representation of

- search space
- notion of neighborhood
- fitness of solutions

Goal :

- **local description** : fitness between neighbor solutions
  Ruggedness, local optima, fitness cloud, neutral networks, local optima networks...
- and to deduce **global features** :
  - Difficulty !
  - To decide (and control) a good choice of the representation, operator and fitness function

Open questions

- How to control the parameters and/or operators of the algorithm with the local description of fitness landscape ?
- Can fitness landscape describe the dynamics of a population of solutions ?
- Links between neutrality and fitness difficulty ?
- Which intermediate description shows relevant properties of the optimization problem according to the local search heuristic ?
- What is the fitness landscapes for a *multiobjective problem* ?

Integration of the FL tools into the open framework *paradisEO*
`http://paradiseo.gforge.inria.fr`

L. Barnett.
Ruggedness and neutrality - the NKp family of fitness landscapes.
In C. Adami, R. K. Belew, H. Kitano, and C. Taylor, editors, *ALIFE VI, Proceedings of the Sixth International Conference on Artificial Life*, pages 18–27. ALIFE, The MIT Press, 1998.

Lionel Barnett.
Netcrawling - optimal evolutionary search with neutral networks.
In *Proceedings of the 2001 Congress on Evolutionary Computation CEC2001*, pages 30–37, COEX, World Trade Center, 159 Samseong-dong, Gangnam-gu, Seoul, Korea, 27-30 2001. IEEE Press.

U. Bastolla, M. Porto, H. E. Roman, and M. Vendruscolo.
Statiscal properties of neutral evolution.
Journal Molecular Evolution, 57(S) :103–119, August 2003.

Meriema Belaidouni and Jin-Kao Hao.
An analysis of the configuration space of the maximal constraint satisfaction problem.
In *PPSN VI : Proceedings of the 6th International Conference on Parallel Problem Solving from Nature*, pages 49–58, London, UK, 2000. Springer-Verlag.

P. Collard, M. Clergue, and M. Defoin Platel.
Synthetic neutrality for artificial evolution.
In *Artificial Evolution : Fourth European Conference AE'99*, pages 254–265. Springer-Verlag, 2000.
Selected papers in Lecture Notes in Computer Sciences 1829.

J. C. Culberson.
Mutation-crossover isomorphisms and the construction of discrimination function.
Evolutionary Computation, 2 :279–311, 1994.

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.

Ricardo Garcia-Pelayo and Peter F. Stadler.
Correlation length, isotropy, and meta-stable states.
Physica D, 107 :240–254, 1997.
Santa Fe Institute Preprint 96-05-034.

Josselin Garnier and Leila Kallel.
Efficiency of local search with multiple local optima.
SIAM Journal on Discrete Mathematics, 15(1) :122–141, 2002.

P. Gitchoff and G. Wagner.
Recombination induced hypergraphs : A new approach to mutation-recombination isomorphism, 1996.

David E. Goldberg and Philip Segrest.
Finite markov chain analysis of genetic algorithms.
In *ICGA*, pages 1–8, 1987.

M. Huynen.
Exploring phenotype space through neutral evolution.
Journal Molecular Evolution, 43 :165–169, 1996.

E. Izquierdo-Torres.
The role of nearly neutral mutations in the evolution of dynamical neural networks.
In J. Pollack and al, editors, *Ninth International Conference of the Simulation and Synthesis of Living Systems (Alife 9)*, pages 322–327. MIT Press, 2004.

T. Jones.
Evolutionary Algorithms, Fitness Landscapes and Search.
PhD thesis, University of New Mexico, Albuquerque, 1995.

S. A. Kauffman.
The Origins of Order.
Oxford University Press, New York, 1993.

M. Kimura.
The Neutral Theory of Molecular Evolution.
Cambridge University Press, Cambridge, UK, 1983.

J. Lobo, J. H. Miller, and W. Fontana.
Neutrality in technology landscape, 2004.

M. Newman and R. Engelhardt.
Effect of neutral selection on the evolution of molecular species.

In *Proc. R. Soc. London B.*, volume 256, pages 1333–1338, 1998.

Erik Van Nimwegen, James P. Crutchfield, and Martijn Huynen.
Metastable evolutionary dynamics : Crossing fitness barriers or escaping via neutral paths ?
Technical Report 99-07-041, SanteFe institute, 1999.

Marmion, M.-É., Dhaenens, C., Jourdan, L., Liefooghe, A., Verel, S., 2011. NILS : a neutrality-based iterated local search and its application to flowshop scheduling. In : Proceedings of the 12th European Conference of Evolutionary Computation in Combinatorial Optimization. Vol. 6622 of EvoCOP 2011. LNCS, Springer, pp. 191– 202.

Marmion, M.-É., Dhaenens, C., Jourdan, L., Liefooghe, A., Verel, S., 2011. On the neutrality of flowshop scheduling fitness landscapes. In : Proceedings of the 5th Learning and

Intelligent OptimizatioN Conference. Vol. 6683 of LION 2011. LNCS, Springer, pp. 238–252.

Gabriela Ochoa, Marco Tomassini, Sébastien Verel, and Christian Darabos.
A Study of NK Landscapes' Basins and Local Optima Networks.
In *Proceedings of the 10th annual conference on Genetic and evolutionary computation Genetic And Evolutionary Computation Conference*, pages 555–562, Atlanta États-Unis d'Amérique, 07 2008. ACM New York, NY, USA.
best paper nomination.

M. Defoin Platel.
Homologie en Programmation Génétique - Application à la résolution d'un problème inverse.
PhD thesis, Université Nice Sophia Antipolis, France, 2004.

Eduardo Rodriguez-Tello, Jin-Kao Hao, and Jose Torres-Jimenez.
A new evaluation function for the minla problem.
In *Proceedings of the MIC 2005*, pages 796–801, Vienna Austria, 2005.

Helge Rosé, Werner Ebeling, and Torsten Asselmeyer.
The density of states - a measure of the difficulty of optimisation problems.
In *Parallel Problem Solving from Nature*, pages 208–217, 1996.

P. Schuster, W. Fontana, P. F. Stadler, and I. L. Hofacker.
From sequences to shapes and back : a case study in RNA secondary structures.
In *Proc. R. Soc. London B.*, volume 255, pages 279–284, 1994.

Peter F. Stadler.
Landscapes and their correlation functions.

J. Math. Chem., 20 :1–45, 1996.

Peter F. Stadler and W. Schnabl.
The landscape of the traveling salesmen problem.
Phys. Letters, A(161) :337–344, 1992.

Peter F. Stadler and Gunter P. Wagner.
Algebraic theory of recombination spaces.
Evolutionary Computation, 5(3) :241–275, 1997.

Terry Stewart.
Extrema selection : Accelerated evolution on neutral networks.
In *Proceedings of the 2001 Congress on Evolutionary Computation CEC2001*, pages 25–29, COEX, World Trade Center, 159 Samseong-dong, Gangnam-gu, Seoul, Korea, 27-30 May 2001. IEEE Press.

Marco Tomassini, Sébastien Verel, and Gabriela Ochoa.

Complex-network analysis of combinatorial spaces : The NK landscape case.
Physical Review E : Statistical, Nonlinear, and Soft Matter Physics, 78(6) :066114, 12 2008.
89.75.Hc ; 89.75.Fb ; 75.10.Nr.

Vesselin K. Vassilev and Julian F. Miller.
The advantages of landscape neutrality in digital circuit evolution.
In *ICES*, pages 252–263, 2000.

Sebastien Verel, Philippe Collard, and Manuel Clergue.
Measuring the evolvability landscape to study neutrality.
In M. Keijzer and et al., editors, *Poster at Genetic and Evolutionary Computation – GECCO-2006*, pages 613–614, Seatle, 8-12 July 2006. ACM Press.

Sébastien Verel, Gabriela Ochoa, and Marco Tomassini.

The Connectivity of NK Landscapes' Basins : A Network Analysis.
In *Proceedings of the Eleventh International Conference on the Simulation and Synthesis of Living Systems Artificial Life XI*, pages 648–655, Winchester France, 08 2008. MIT Press, Cambridge, MA.
tea team.

F. Chicano, F. Daolio, G. Ochoa, S. Verel, M. Tomassini, and E. Alba.
Local optima networks, landscape autocorrelation and heuristic search performance.
In *Proceedings of Parallel Problem Solving from Nature - PPSN XII*, volume 7492 of *Lecture Notes in Computer Science*, pages 337–347. Springer, 2012.

E. D. Weinberger.

Correlated and uncorrelatated fitness landscapes and how to tell the difference.
In *Biological Cybernetics*, pages 63 :325–336, 1990.

F. Daolio, M. Tomassini, S. Verel, and G. Ochoa.
Communities of minima in local optima networks of combinatorial spaces.
Physica A : Statistical Mechanics and its Applications, 390(9) :1684–1694, 2011.

G. Ochoa, S. Verel, and M. Tomassini.
First-improvement vs. best-improvement local optima networks of nk landscapes.
In *Proceedings of Parallel Problem Solving from Nature - PPSN XI*, volume 6238 of *Lecture Notes in Computer Science*, pages 104–113. Springer, 2010.

L. Vanneschi, M. Tomassini, P. Collard, and S. Verel.

Negative slope coefficient. a measure to characterize genetic programming fitness landscapes.
In P. Collet et al., editor, *Proceedings of the 9th European Conference on Genetic Programming*, volume 3905 of *Lecture Notes in Computer Science*, pages 178–189. Springer, Berlin, Heidelberg, New York, 2006.

S. Verel, F. Daolio, G. Ochoa, and M. Tomassini.
Local optima networks with escape edges.
In *Proceedings of the International Conference on Artificial Evolution, EA-2011*, volume 7401 of *Lecture Notes in Computer Science*, pages 49–60. Springer, 2012.

S. Verel, G. Ochoa, and M. Tomassini.
Local optima networks of NK landscapes with neutrality.
IEEE Transactions on Evolutionary Computation, 15(6) :783–797, 2011.

Katherine M. Malan and Andries P. Engelbrecht.

A survey of techniques for characterising fitness landscapes and some possible ways forward.
Information Sciences, (0) :–, 2013.

Guanzhou Lu, Jinlong Li, and Xin Yao.
Fitness-probability cloud and a measure of problem hardness for evolutionary algorithms.
In *Proceedings of the 11th European conference on Evolutionary computation in combinatorial optimization*, EvoCOP'11, pages 108–117, Berlin, Heidelberg, 2011. Springer-Verlag.

S. Wright.
The roles of mutation, inbreeding, crossbreeding, and selection in evolution.
In *Proceedings of the Sixth International Congress of Genetics 1*, pages 356–366, 1932.