

GECCO'09 Tutorial

Fitness Landscapes and Graphs: Multimodularity, Ruggedness and Neutrality

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(Please, thank the great speakers for me)

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Goals of this tutorial

- Defining the concept of fitness landscape :
Define your own fitness landscape according to your problem
- Giving all standard tools to study fitness landscape
- Giving an overview of fitness landscapes with mountains
- Giving an overview of fitness landscapes with plateaus :
Practical example of analysis of such FL
- Define the local optima network of FL :
Example of such networks on NK —landscapes

Study of Fitness landscapes : Motivations

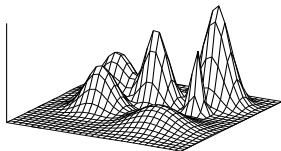
Use the fitness landscapes :

- To analyse the structure of the search space
- To study problem (search) difficulty in combinatorial optimisation
- 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



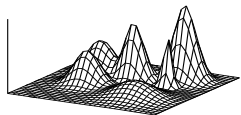
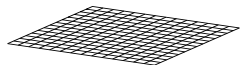
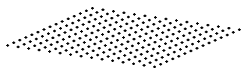
Biological science :

Wright 1930 [35]

Evolution :

- a metaphorical uphill struggle across a "fitness landscape"
- mountain peaks represent high "fitness", or ability to survive,
- valleys represent low fitness.
- evolution proceeds :
population of organisms performs an "adaptive walk"

Fitness landscapes in biology



In biology :

- Modelisation of species evolution

Used to model dynamical systems :

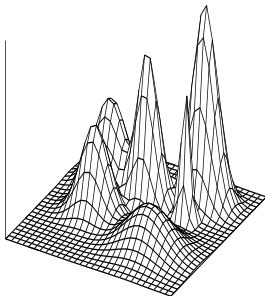
- statistical physic,
- molecular evolution,
- ecology, etc

Fitness landscapes in biology

2 sides for **Fitness Landscapes** :

- Powerful **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

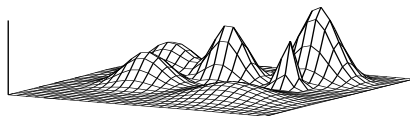
In combinatorial optimization



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.

Fitness landscapes in evolutionary computation



FL : Tools for **black-box optimisation**

Search space analysis where "no" information is either not available or needed on the definition of fitness function.

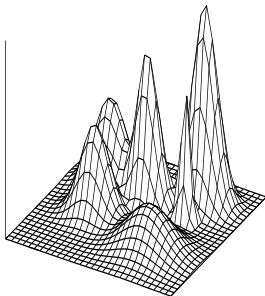
We have only $\{(x, f(x)), \dots\}$

Fitness landscapes in evolutionary computation

2 sides for **Fitness Landscapes** :

- Powerful **metaphor** : most profound concept
 - give pictures of the search dynamic :
"if the fitness landscapes have big valleys, I can use this algorithm"
 - be careful of misleading pictures : set of smooth mountains
- **Quantitative** concept : predict the evolutionary dynamic
 - Quasispecies equation : mean field analysis with differential equations
 - Stochastic process : markov chain
 - Network analysis

Definition of the neighborhood



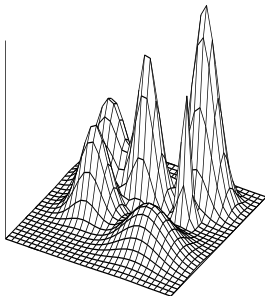
$\mathcal{V} : \mathcal{S} \rightarrow 2^{\mathcal{S}}$: neighborhood function

$\forall x \in \mathcal{S},$

$\mathcal{V}(x) = \{y \in \mathcal{S} \mid P(y = op(x)) > 0\}$

or

Definition of the neighborhood



$\mathcal{V} : \mathcal{S} \rightarrow 2^{\mathcal{S}}$: neighborhood function

$\forall x \in \mathcal{S},$

$\mathcal{V}(x) = \{y \in \mathcal{S} \mid P(y = op(x)) > 0\}$

or

$\mathcal{V}(x) = \{y \in \mathcal{S} \mid d(y, x) \leq 1\}$

Example of neighborhood

Search space : $\{0, 1\}^N$

Algorithm : simple GA,
 hill-climbing, or simulated
 annealing, etc.

$$x = 01101$$

$$\mathcal{V}(x) = \{01101$$

01100

01111

01001

00101

11101

}

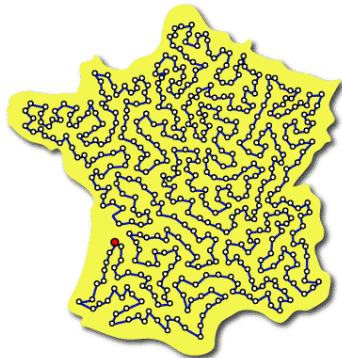
Important

Definition of neighborhood must be based on the local search operator used in the algorithm

$$\mathcal{S} = \{0, 1\}^N$$

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid d_{\text{hamming}}(y, x) \leq 1\}$$

Example of neighborhood

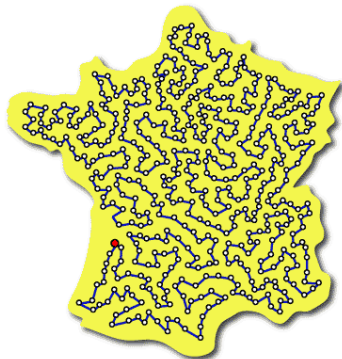


- *Search space* : set of permutations
- *Algorithm* : simple EA with 2-opt mutation operator op_{2-opt}

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

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

Example of neighborhood



- *Search space* : set of permutations
- *Algorithm* : simple EA with 2-opt and 3-opt mutation operators op_{2-opt} and op_{3-opt}

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid P(y = op_{2-opt}(x)) > 0 \text{ or } P(y = op_{3-opt}(x)) > 0\}$$

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

Example of neighborhood

- *Algorithm* : memetic algorithm, EA with hill-climbing mutation operator op_{HC}

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x)\}$$

Example of neighborhood

- *Algorithm* : memetic algorithm, EA with hill-climbing mutation operator op_{HC}

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x)\}$$

- *Algorithm* : memetic algorithm, EA with hill-climbing mutation operator op_{HC} and bit-flip mutation

2 possibilities :

- Study 2 landscapes :
one for HC operator, one for bit-flip mutation

- Study 1 landscape :
 $\mathcal{V}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x) \text{ or } P(y = op_{bit-flip}(x)) > 0\}$

Example of neighborhood

- *Algorithm* : memetic algorithm, EA with hill-climbing mutation operator op_{HC}

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x)\}$$

- *Algorithm* : memetic algorithm, EA with hill-climbing mutation operator op_{HC} and bit-flip mutation

2 possibilities :

- Study 2 landscapes :
one for HC operator, one for bit-flip mutation
- Study 1 landscape :

$$\mathcal{V}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x) \text{ or } P(y = op_{bit-flip}(x)) > 0\}$$

What is your question ?

Goal of the fitness landscapes study

- "geometry" of fitness landscape
⇒ dynamic of a local search algorithm
- geometry is linked to the problem hardness :
 - probability or time to have a fitness level for a given local search heuristic

Study of the geometry of the landscape allows to study the difficulty

Goal of the fitness landscapes study

- Compare the difficulty of two search spaces :
 - One problem with 2 (or more) possible codings : $(S_1, \mathcal{V}_1, f_1)$ and $(S_2, \mathcal{V}_2, f_2)$
different coding, mutation operator, fitness function, etc.

Which one is easier to solve?

Goal of the fitness landscapes study

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Which one is easier to solve?
- Choose the algorithm :
 - analysis of global geometry of the landscape
Which algorithm can I use?

Goal of the fitness landscapes study

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Which one is easier to solve?
- Choose the algorithm :
 - analysis of global geometry of the landscape
Which algorithm can I use?
- Tune the parameters :
 - *off-line* analysis of structure of fitness landscape
Which is the mutation rate? the size of the population ? etc.

Goal of the fitness landscapes study

- Compare the difficulty of two search spaces :
 - One problem with 2 (or more) possible codings : $(S_1, \mathcal{V}_1, f_1)$ and $(S_2, \mathcal{V}_2, f_2)$
different coding, mutation operator, fitness function, etc.
Which one is easier to solve?
- Choose the algorithm :
 - analysis of global geometry of the landscape
Which algorithm can I use?
- Tune the parameters :
 - *off-line* analysis of structure of fitness landscape
Which is the mutation rate? the size of the population ? etc.
- Tune the parameters during the run :
 - *on-line* analysis of structure of fitness landscape
Which is the optimal mutation rate according to the estimation of structure?

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 $(\mathcal{S}, \mathcal{V}, f)$ where the nodes have a value (fitness) : can be "pictured" as a "real" landscape

Two main geometries have been studied :

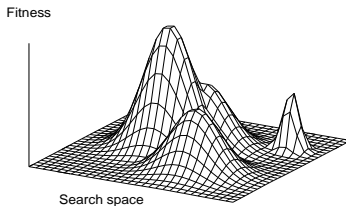
- multimodal and ruggedness
- neutral

Multimodal Fitness landscapes

Local optima s^* :

no neighbor solution with higher fitness value

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



Multimodal Fitness landscapes

Adaptive walk : (s_0, s_1, \dots) where $s_{i+1} \in \mathcal{V}(s_i)$ and $f(s_i) < f(s_{i+1})$

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**

$s \leftarrow s'$

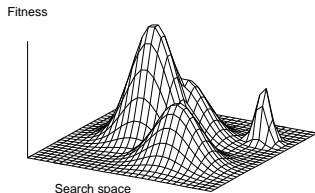
end if

until s is a Local optimum

Basin of attraction of s^* :

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

Multimodal Fitness landscapes

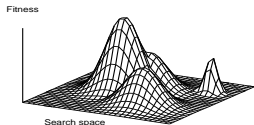


Optimisation difficulty :
number and size of attractive
basins (Garnier *et al* [10])

The idea :

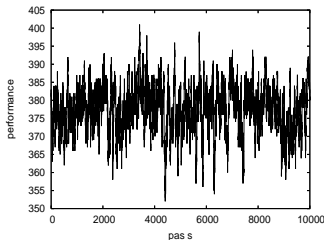
- if the size of attractive basin of global optima is relatively "small"
- the problem is difficult to optimize

Walking on fitness landscapes



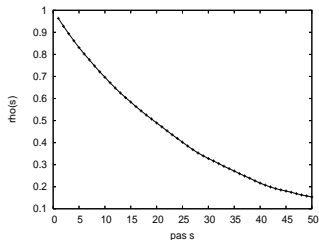
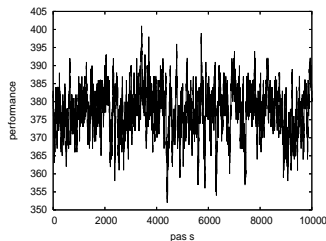
Random walk : (s_1, s_2, \dots) such that $s_{i+1} \in \mathcal{V}(s_i)$ and equiprobability on $\mathcal{V}(s_i)$

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



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

Rugged/smooth fitness landscapes



Autocorrelation of fitness
 $(f(s_1), f(s_2), \dots)$ along a random
walk (s_1, s_2, \dots) (Weinberger
1990 [34]) :

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

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

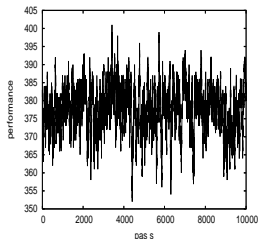
- small τ : rugged landscape
- long τ : smooth landscape

Results on rugged fitness landscapes (Stadler 96 [26])

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 those problems :
 small variation has less effect on the fitness values

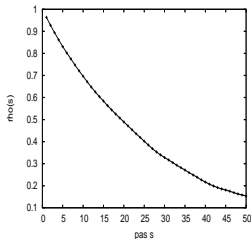
Links multimodality, ruggedness, epistasis ?



- Links between multimodality and ruggedness :

Conjecture (Stadler 92 [27], Garcia 97 [9])

on average, 1 local optimum per sphere of radius τ



- Links between epistasis and ruggedness : NK fitness landscapes (Kauffman [16])

NK fitness landscapes

$$f(x) = \frac{1}{N} \sum_{i=1}^N f_i(x_i, x_{i_1}, \dots, x_{i_K})$$

- N : length of the bit string (protein length)
- $K \leq N - 1$ number of interactions
- $x_i \in \{0, 1\}$
- $\{i_1, \dots, i_K\} \subset \{1, \dots, i-1, i+1, \dots, N\}$
- $f_i : \{0, 1\}^{K+1} \rightarrow [0, 1]$ chosen at random

Example $N = 4$ $K = 2$

$$x = 0110$$

$x_1 x_2 x_4$	f_1
000	0.9
001	0.6
010	0.1
011	0.2
...	...

$x_1 x_2 x_3$	f_2
000	0.4
001	0.8
010	0.3
011	0.2
...	...

$x_2 x_3 x_4$	f_3
000	0.2
...	...
101	0.9
110	0.1
111	0.5

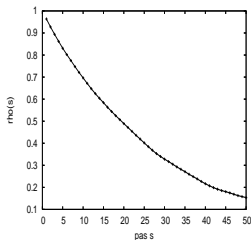
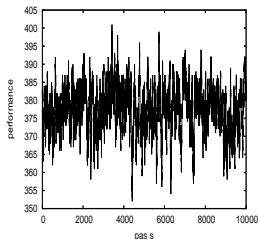
$x_1 x_2 x_4$	f_4
000	0.1
001	0.2
010	0.8
011	0.0
...	...

$$\begin{aligned}
 f(x) &= \frac{1}{4} (f_1(010) + f_2(011) + f_3(110) + f_4(010)) \\
 &= \frac{1}{4} (0.1 + 0.2 + 0.1 + 0.8) \\
 &= 0.3
 \end{aligned}$$

NK fitness landscapes : ruggedness and epistasis

- 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)

Links multimodality, ruggedness, epistasis ?

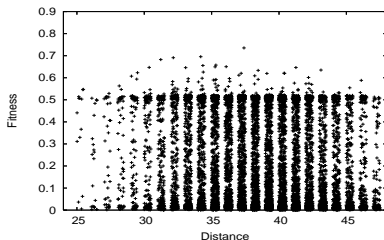


- multimodality/ruggedness :
conjecture (Stadler 92 [27], Garcia 97 [9]) :
on average, 1 local optimum per
sphere of radius τ
- epistasis/ruggedness :
NK fitness landscapes (Kauffman [16])
$$\tau = \frac{-1}{\ln(1 - \frac{K+1}{N})} \text{ et } d = \frac{N \log_2(K+1)}{2(K+1)}$$
- But some counterexamples...
$$\sum_{i=1}^N \exp(i)x_i \text{ et } \prod_{i=1}^N x_i$$

... open question ?

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

Fitness landscape and crossover ?

- Crossover of complementary strings (Culberson 94 [6]) : comparison with mutation-landscape
- Generalisation of graph theory :
 - Hypergraph of Gitchoff [11]
 - P-structure of Stadler [28]
- crossover with a random solution
- Space of pair of solutions (Jones, Defoin [22] : study of linear GP crossover)

Maybe the schemata theorem or the study of distances between pairs give better results?...

Synthesis

- Metaphor from the biology
- Study of multimodal fitness landscapes :
→ optimization algorithms (SA, Tabu Search, Island Model...)

Goal of study of fitness landscapes :

- Links with problem hardness :
choice of coding, fitness function, operators
- design of algorithms
- Auto-adaptation of parameters

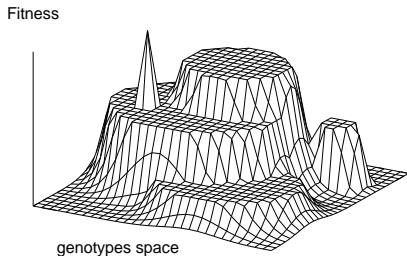
Limits :

- 1 operator = 1 landscape ?
- Crossover ? and links with population ?
- Edges : useful information ?

Neutral Fitness Landscapes

Neutral theory (Kimura \approx 1960 [17])
Theory of mutation and random drift

A considerable number of mutations have no effects on fitness values



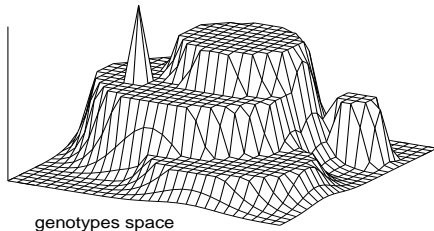
- plateaus
- neutral degree
- neutral networks
[Schuster 1994 [25],
RNA folding]

Neutral fitness landscapes

Combinatorial optimization

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

Fitness



Applicative problems :

- Robot controller
- Circuit design
- genetic programming
- Protein Folding
- learning problems

What optimizers do with neutrality?

Three possibilities :

- Decrease the neutrality
- Use a specific metaheuristic
- Increase the neutrality with redundant genotype/phenotype mapping

Decreasing the neutrality (minLA : E. Rodriguez, PPSN05 [23])

Redundant encoding is a drawback, lack of information

graph $G = (V, E)$: labeled each nodes

$$LA(G, \varphi) = \sum_{(u,v) \in E} |\varphi(u) - \varphi(v)| \in \mathbb{N}$$

“LA represents a potential drawback because different linear arrangements can result in the same total edge length. This incomplete information can prevent the search process from finding better solution.”

$$\phi(G, \varphi) = LA(G, \varphi) + I_{norm}(G, \varphi)$$

with $I_{norm}(G, \varphi) \in [0, 1]$

- I_{norm} is higher when the differents could be optimized
- I_{norm} makes different between equivalent labelling

Use a specific metaheuristic

Neutrality of the problem can not be changed

Netcrawler (L. Barnett [2])

```
step  $\leftarrow$  0  
Choose initial solution  $s \in \mathcal{S}$   
repeat  
  choose  $s' \in \mathcal{V}(s)$  randomly  
  if  $f(s) \leq f(s')$  then  
     $s \leftarrow s'$   
  end if  
  step  $\leftarrow$  step + 1  
until stepMax  $\leq$  step
```

Good results on ϵ -correlated landscapes, problems where :

- low probability to find a better solution
- high probability to find a solution with same fitness

Use a specific metaheuristic

Neutrality of the problem can not be changed

- Extrema selection (Stewart 2001 [29]) :

"It is sufficient to recognise that the neutrality of a fitness function may be a significant issue when evolving solutions. With this in mind, the remainder of this paper describes a novel modification to the standard GA which is **specifically designed to take in advantage of Neutral Networks**." When the solutions are in the same plateau (at 90% from best solution)
→ selection according to the distance from the centroid of the population

Increase the neutrality of the landscape with a redundant coding

Escape from local optima

- crossing a Barrier (Nimwegen et Crutchfield 99 [20]) :
 - fitness barrier : decreases the fitness by crossing a valley
 - Entropy barrier : lack of information on a plateau
- in Cartesian GP (Vassilev *et al* 00 [31]) :

“(...) the role of landscape neutrality for adaptive evolution is to provide a path for crossing landscape regions with poor fitness.”
- Duality (Collard, Clergue 00 [5]) : add one bit and use a specific operator
$$f(x0) = f(x), f(x1) = f(\bar{x}) \text{ et } op(x1) = \bar{x}0$$

What do we do ?

- In our knowledge, there is no definitive answer about neutrality / problem hardness
 - Certainly, it is dependent on the nature of neutrality of the fitness landscape
- ⇒ Sharp description of the geometry of neutral fitness landscapes is needed

What do we do ?

- **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**

What do we do ?

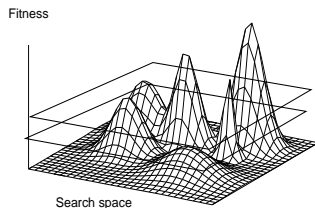
- **No information** is better than **Bad information** :
Hard trap functions are more difficult than
needle-in-a-haystack functions
- **Good information** is better than **No information**
- When there is No information : you should have a good
method to find it !

In the following

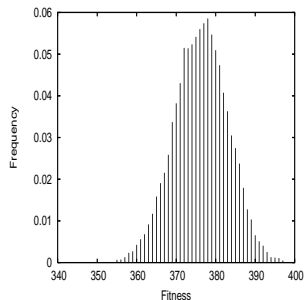
Description of neutral fitness landscapes :

- Neutral sets :
set of solutions with the same fitness
- Neutral networks :
add neighborhood information
- Application on an optimisation problem

Neutral sets



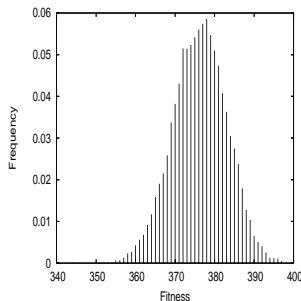
Set of solution with fitness value



Density of state (D.O.S.)

- Introduce in physics (Rosé 1996 [24])
- Optimization (Belaidouni, Hao 00 [4])

Neutral sets

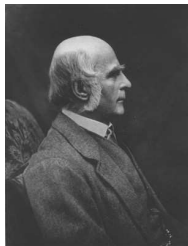


Density of state (D.O.S.)

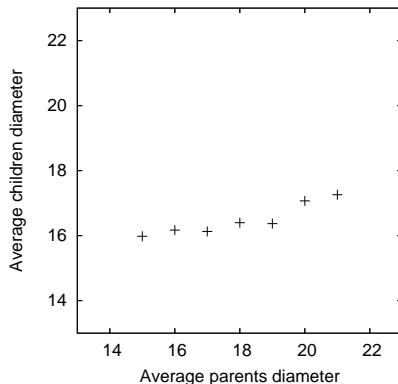
Informations given :

- Performance of random search
- the 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

Make a roundabout with Sir F. Galton

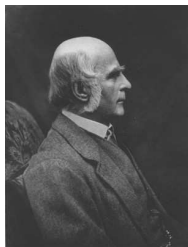


(1822 - 1911)

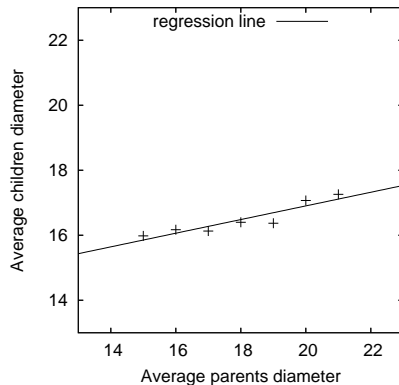


Original data of sweet peas sizes (1877)

Make a roundabout with Sir F. Galton

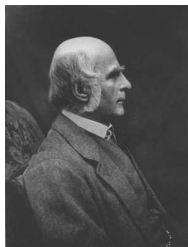


(1822 - 1911)

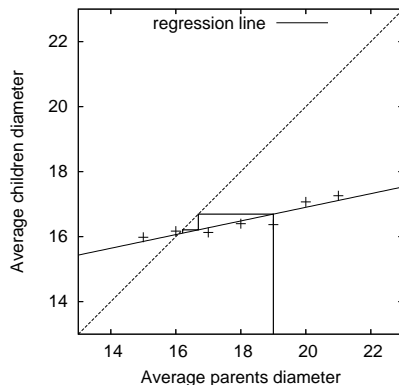


Original data of sweet peas sizes (1877)

Make a roundabout with Sir F. Galton



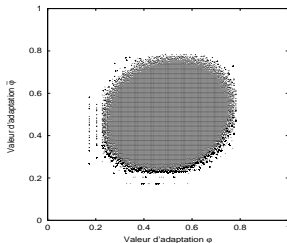
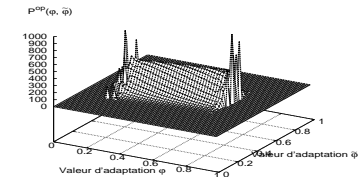
(1822 - 1911)



Original data of sweet peas sizes (1877)

Fitness Cloud

Combinatorial optimization

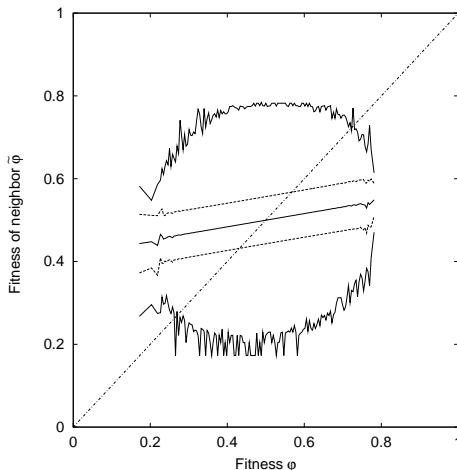


- $(\mathcal{S}, \mathcal{F}, P)$: probability space
- $op : \mathcal{S} \rightarrow \mathcal{S}$ stochastic operator of the local search
- $X(s) = f(s)$
- $Y(s) = f(op(s))$

Fitness Cloud of op

conditional probability density function of Y given X

Fitness cloud : Measure of evolvability



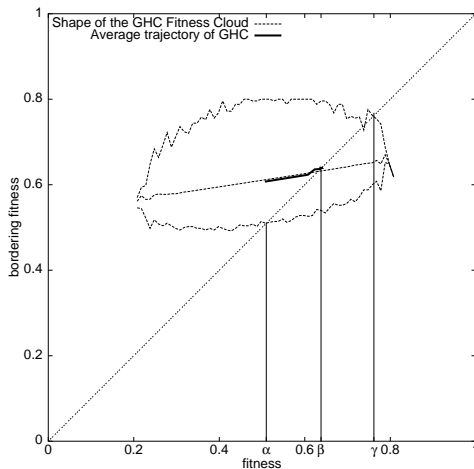
Evolvability

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

Prediction of evolution (CEC 2003)

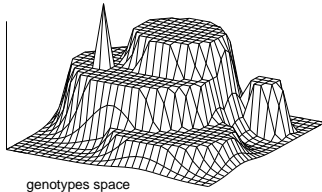


Neutral fitness landscapes

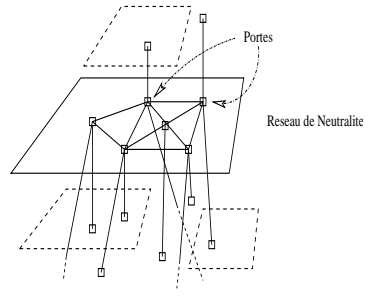
- Neutral sets : set of solutions with same fitness
→ no structure
- **Fitness cloud** : neighborhood relation between neutral sets
- Introduction of neighborhood structure in the neutral sets
→ Neutral Networks

Neutral networks (Schuster 1994 [25])

Fitness



Fitness



Definitions

- A *test of neutrality* is a predicate

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

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.
- The *neutral neighborhood* of s is the set of neighbors which have the same fitness $f(s)$

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

- The *neutral degree* of a solution is the number of its neutral neighbors

$$nDeg(s) = \#(\mathcal{V}_{neut}(s) - \{s\}).$$

Definitions

- A *neutral walk* : $W_{neut} = (s_0, s_1, \dots, s_m)$
for all $i \in [0, m-1]$, $s_{i+1} \in \mathcal{V}(s_i)$
for all $(i, j) \in [0, m]^2$, $isNeutral(s_i, s_j)$ is true.
- A *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' ,
Two vertices are connected by an edge of E if they are neutral
neighbors.

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

Measures on neutral fitness landscapes

To introduce measure of neutrality,
we will use two possible families of neutral fitness landscapes :

- based on NK fitness landscapes :
 \mathcal{S} : bit strings of length N ,
$$f(x) = \frac{1}{N} \sum_{i=1}^N f_i(x_i, x_{j_1}, \dots, x_{j_K})$$
- corresponding to two possible ways to introduce redundancy in additive fitness functions
- two parameters :
one for non-linearity (epistasis K), one for neutrality
- the measures could be analysed with the parameters and supposed difficulty

Neutral NK fitness landscapes

NK (Kauffman 1993)

$$f(s) = \frac{1}{N} \quad (\quad 0.02 \quad + \quad 0.31 \quad + \quad 0.91 \quad + \dots + \quad 0.20 \quad)$$

NK_q (Newmann *et al* 1998 [19]) : q values for the terms

$$f(s) = \frac{1}{N(q-1)} \quad (\quad 1 \quad + \quad 3 \quad + \quad 3 \quad + \dots + \quad 0 \quad)$$

NK_p (Barnett 1998 [1]) : prob. p to have 0

$$f(s) = \frac{1}{N} \quad (\quad 0.0 \quad + \quad 0.31 \quad + \quad 0.0 \quad + \dots + \quad 0.20 \quad)$$

Intra network Measures

Classical measures of graph to describe NN :

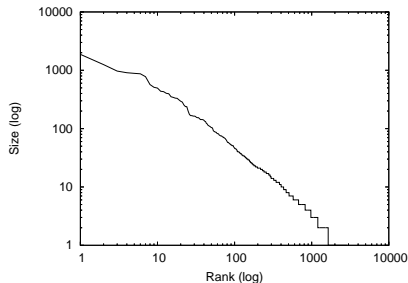
- 1 the **size** : number of nodes of NN,
- 2 **neutral degree distribution** :
measure of the quantity of "neutrality"
- 3 **Autocorrelation of neutral degree** during neutral random walk
(Bastolla 03 [3]) :
comparaison with random graph,
measure of the correlation structure of *NN*

Intra network Measures

Size

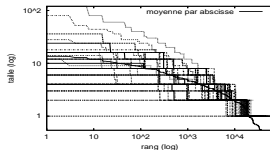
Classical measures of graph to describe NN :

- 1 The *size* : number of nodes of NN,
rank-size of *NN* in log-log :

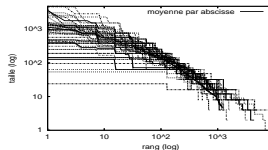


Frequency of apparition of a word in a text (Ziff law 1960)

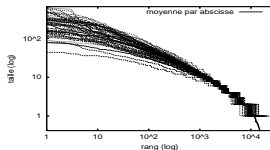
Size of neutral networks



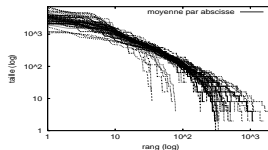
$$K = 1 \quad q = 10$$



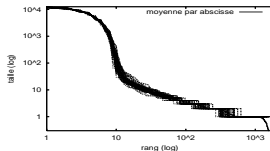
$$K = 1 \quad p = 0.8$$



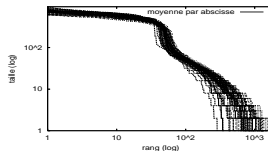
$$K = 2 \quad q = 4$$



$$K = 2 \quad p = 0.9$$



$$K = 5 \quad q = 2$$



$$K = 5 \quad p = 0.95$$

Size of neutral networks

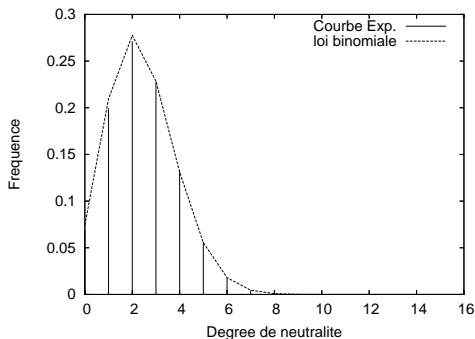
- Existence of few and large neutral networks :
maybe, could be proved with percolation theory...
→ important information to design search algorithms
- The power-law is approached only when epistasis and neutrality are low
- When epistasis and neutrality increase,
the random variation of distribution of size decreases

Intra network Measures

Classical measures of graph to describe NN :

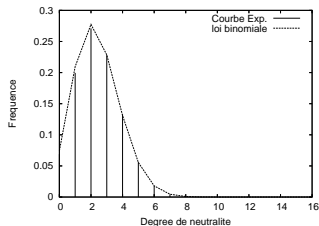
- 1 the *size* : number of nodes of NN,
- 2 *neutral degree distribution* :
measure of the quantity of "neutrality"
- 3 Autocorrelation of neutral degree during random neutral walk
(Bastolla 03 [3]) :
comparaison with random graph,
measure of the correlation structure of *NN*

Distribution of neutral degrees ($N = 16$, $K = 2$, $q = 4$)

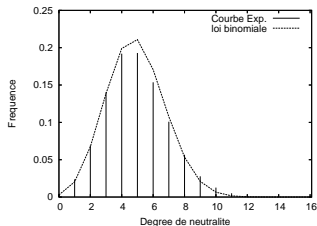


Experimental distribution (impulse), binomial distribution (line).

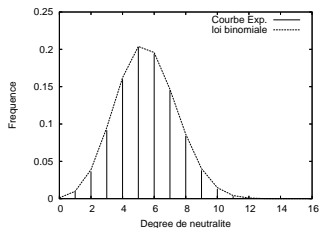
Distribution of neutral degrees ($N = 16, K = 2$)



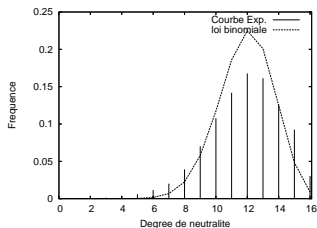
$q = 4$



$p = 0.8$



$q = 2$



$p = 0.95$

Distribution of neutral degrees

- Barnett (98) gives the probability of neutral mutation for NK_p -landscapes

$$p_{neutr} = p^2 \left(1 - \frac{K}{N-1} (1 - p^2)^{N-1}\right) \approx p^2 e^{-K(1-p^2)}$$

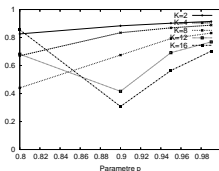
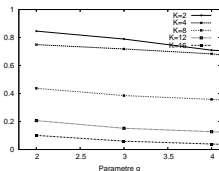
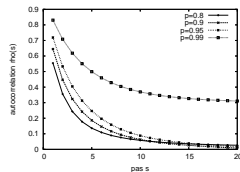
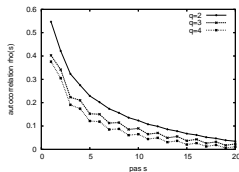
- For NK_q landscapes the distribution is nearly a binomial distribution

Intra network Measures

Classical measures of graph to describe NN :

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

Autocorrelation of neutral degrees



NK_q land.

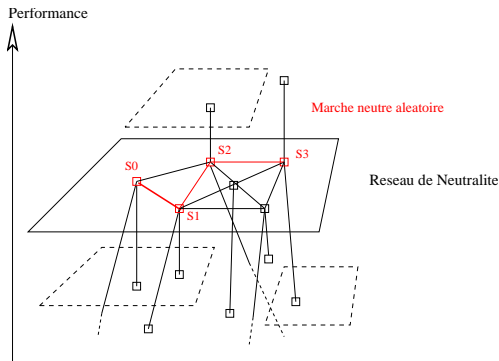
NK_p land.

Autocorrelation coefficient of order 1

Autocorrelation of neutral degrees

- Neutral networks should be not random graph
- epistasis parameter (K) has more influence on the structure of neutral networks than neutrality parameter
- \longrightarrow important to design search algorithm

Inter networks measures



- 1 rate of innovation (Huynen 96 [13]) :
The number of new accessible structures (fitness) per mutation
- 2 Autocorrelation of evolvability [32] :
autocorrelation of the sequence $(evol(s_0), evol(s_1), \dots)$.

Rate of innovation on neutral NK landscapes

The number of new accessible structures (fitness) per mutation

- No information on neutral NK fitness landscapes :
 - No link with the parameters
 - difficult to estimate for the whole fitness landscape

Autocorrelation of maximal evolvability (Verel 06 [32])

Evolvability : ability to evolve (fitness distribution in the neighborhood)

Definition

Autocorrelation of evolvability is the autocorrelation function of the serie $(evol(s_0), evol(s_1), evol(s_2), \dots)$ where (s_0, s_1, s_2, \dots) is neutral random walk on a neutral network and $evol$ is a measure of evolvability of a solution.

Measure of evolvability :

- Probability to have fitter solution in the neighborhood
- maximum evolvability : the fitness of best solution in the neighborhood

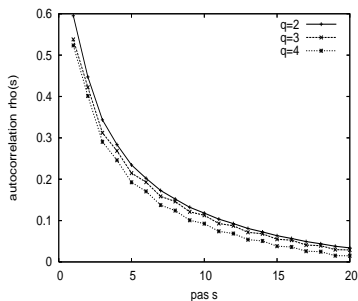
Autocorrelation of maximal evolvability (Gecco 06 [32])

- if correlation is high, then the neutral networks are not randomly distributed over the fitness landscapes.
The problem is easier to optimize than...
- if the correlation is low, the neutral networks are randomly distributed over the fitness landscapes

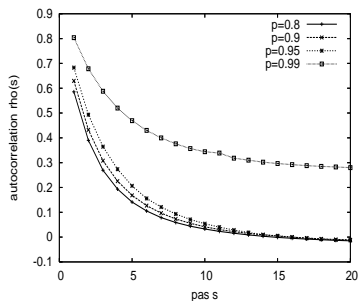
→ and this information could be introduced into a search algorithm

Autocorrelation of maximal evolvability (Verel 06 [32])

maximal evolvability autocorrelation function for $N = 16$, $K = 2$

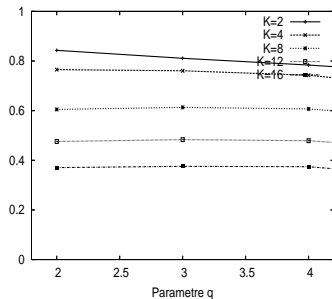


NK_q

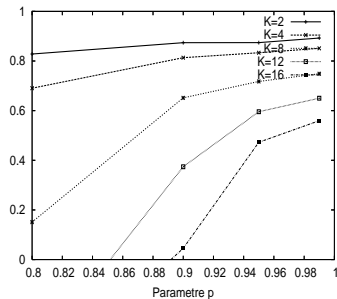


NK_p

Autocorrelation of maximal evolvability



NK_q



NK_p

Autocorrelation coefficient of order 1 for $N = 64$

Autocorrelation of maximal evolvability

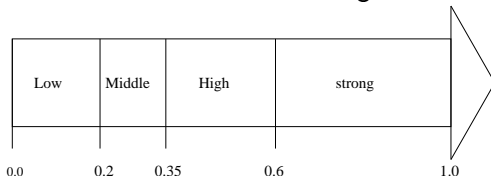
- Neutral networks are not randomly distributed
- Epistasis parameter (K) has more impact than the parameter of neutrality

→ Take care of neutrality to design efficient search algorithm !

Synthesis

Measures

- neutral degrees distribution :
“How neutral is the fitness landscape ?”
- Autocorrelation of neutral degrees : network “structure”

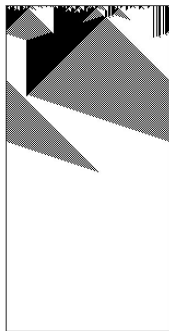


- rank-size of NN in log-log :
well adapted representation (complex systems, percolation)
- rate of innovation :
low information for combinatorial optimization
- Autocorrelation of maximal evolvability :
information on the links between NN

Presentation

majority or *density* task : two-state cellular automata (CA)

Goal : Find the set of rules which classified the initial configuration according density of 1s



$$\rho_0 < 0.5$$



$$\rho_0 > 0.5$$

- Difficult problem : coordination among the automata
- Paradigm of the phenomenon of *emergence* in complex systems.

Definition

Cellular Automata :

- two states : 0 and 1
- radius : $r = 3$

$\Rightarrow 2^{2^{3 \times 2 + 1}} = 2^{128}$ sets of rules

ρ_0 be the fraction of 1s in the *Initial Configuration* (IC) ($N = 149$).

- If $\rho_0 > 1/2$ then the CA must relax to $(1)^N$
- If $\rho_0 < 1/2$ then the CA must relax to $(0)^N$

after $M = 2N$ time steps

Definition

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after $M = 2N$ time steps

Standard performance (fitness function) :

fraction of correct classifications over $n = 10^4$ randomly chosen ICs.

Best Rules Known

- No CA can perform the task perfectly [Land 95]
- Finding a good CA is a hard Problem

Best Rules Known

- No CA can perform the task perfectly [Land 95]
- Finding a good CA is a hard Problem

Best rules knowed (till 2005) :

GKL (1978), By hand, 0.815 005F005F005F005FFF5F005FFF5F	Das (1996), By hand, 0.823 009F038F001F002FFB5F001FFF1F
Davis (1996), By hand, 0.818 070007FF0F000FFF0F0007FF0F310FFF	ABK (1996), Gen. Prog, 0.824 050055050500550555FF55FF55FF55FF
Coe1 (1998), coevol GA, 0.851 011430D7110F395705B4FF17F13DF957	Coe2 (1998), coevol GA, 0.860 1451305C0050CE5F1711FF5F0F53CF5F

Best Rules Known

- No CA can perform the task perfectly [Land 95]
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Best rules known (till 2005) :

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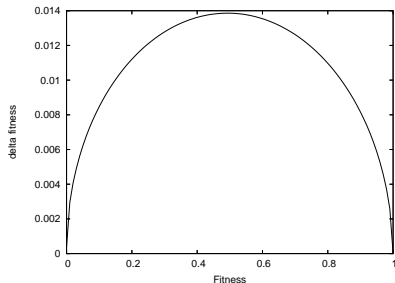
- No investigations of the difficulty of this fitness landscape
- ⇒ **One goal** : To statistically quantify the degree of difficulty

Neutrality in Majority Problem

Standard performance : error of evaluation due to random variation of samples of ICs.

ICs are chosen independently,

fitness value f follows a normal law $\mathcal{N}(f, \sqrt{\frac{f(1-f)}{n}})$



isNeutral(s, s') is true
if t-test accepts the hypothesis of
equality of $f(s)$ and $f(s')$ with
95% of confidence.

Definition of Olympus Landscape

Two symmetries that do not change performance :

0/1 symmetry and *right/left* symmetry.

Symmetries of *blok* which maximize the number of joint bits

$$\begin{aligned} \text{GKL}' &= \text{GKL}, & \text{Das}' &= \text{Das}, & \text{Davis}' &= S_{01}(\text{Davis}), \\ \text{ABK}' &= S_{01}(\text{ABK}), & \text{Coe1}' &= \text{Coe1} & \text{Coe2}' &= S_{rl}(\text{Coe2}). \end{aligned}$$

Olympus Landscape, subspace of dimension 77 :

```
000*0*0* 0****1** 0***00** **0**1** 000***** 0*0**1** ***** 0*0**1*1
0*0***** *****1** 111111** **0**111 ***** 0**1*1*1 11111**1 0*01*111
```

Whole landscape or Olympus Landscape ?

Comparison of hardness

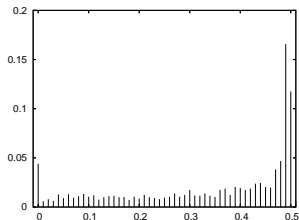
Is it easier to search in the Whole landscape or in the Olympus landscape ?

No direct mathematical definition of the fitness function : black-box optimisation

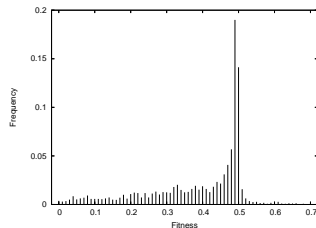
⇒ Analysis of the 2 fitness landscapes to compare their difficulty

Density Of States

% of null fitness value	Sampling method	
	Random	Metropolis-Hasting
Whole landscape	99.9%	4.4%
Olympus landscape	28.6%	0.3%



Whole landscape

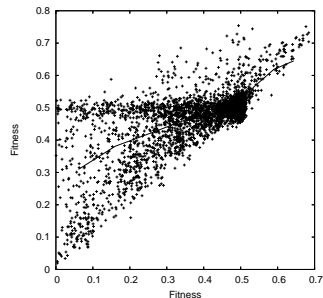
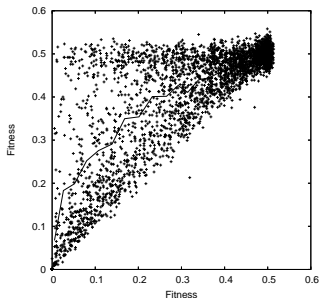


Olympus landscape

- From DOS : Olympus landscape is easier

Fitness cloud

Sampled with Metropolis-Hasting



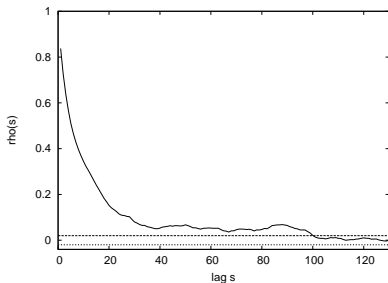
Whole landscape

Olympus landscape

- Expected fitness value is higher for Olympus landscape
- From fitness cloud : Olympus landscape is easier

Auto-correlation analysis

Impossible for whole landscape (only null fitness value)



$$\rho(1) = 0.838$$

- High auto-correlation :
similar to NK landscape with $N = 100$ and $K = 7$
- relative "smooth" landscape

Fitness distance correlation

FDC from best local optima
known

	Whole	Olympus
GLK	-0.1072	-0.19399
Davis	-0.0809	-0.15103
Das	-0.0112	-0.18476
ABK	-0.1448	-0.23128
Coe1	-0.1076	0.077606
Coe2	-0.1105	-0.17320
nearest		-0.20798
Centroid		-0.33612

- For Olympus landscape : correlation over 0.15
- From FDC : Olympus landscape is easier
- For Olympus landscape : fitness leads to the centroid

Neutral Degree : Sampling Method

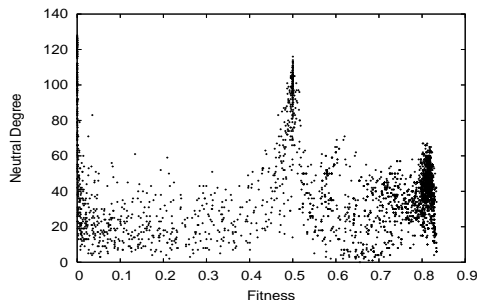
Sampling method :

- Solutions < 0.5 : randomly chosen in Olympus.
- Solutions > 0.5 : from 2 runs of a GA during 10^3 generations.

AG used :

- Based on GA defined by M. Mitchell
- Operators : restricted to Olympus subspace
- Selection : tournament selection taking into account the neutrality.

Neutral Degree



- Two large neutral networks at fitnesses 0 and 0.5 :
neutral degree > 70 .
- Over fitness 0.5 :
average of neutral degree is 37.6.

Study of Neutral Networks

Study of two important large neutral networks (NN) :

- $NN_{0.5}$: fitness around 0.5
Automata that solve the problem on only half of ICs,
5 neutral walks.
- $NN_{0.76}$: fitness around 0.765
Solutions near a CA found by M. Mitchell (GA),
19 neutral walks.

Neutral walks :

- Same starting point on each NN
- Strictly increasing the Hamming distance from the starting solution,
- Stops when there is no neutral step that increases distance.

Diameter

Average length of neutral walks (max 128) :

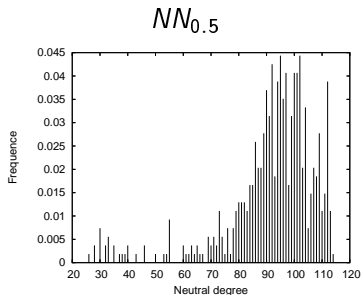
$NN_{0.5}$	108.2
$NN_{0.76}$	33.1

Result on diameter :

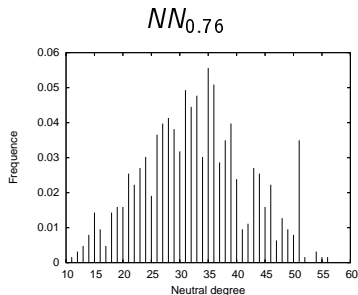
Diameter of $NN_{0.5} >$ Diameter of $NN_{0.76}$.

Neutral Degree Distribution

Distribution of neutral degree collected along all neutral walks.



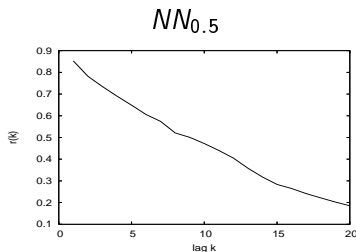
$$Avg_{stddev} = 91.6_{16.6}$$



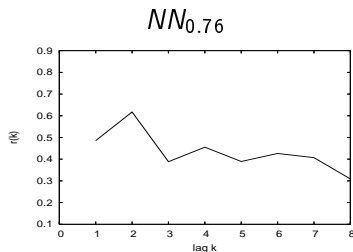
$$Avg_{stddev} = 32.7_{9.2}$$

- $NN_{0.76}$: close to normal,
- $NN_{0.5}$: skewed and approximately bimodal

Autocorrelation of Neutral Degree



$$\rho(1) = 0.85$$



$$\rho(1) = 0.49$$

- Correlation is not null
- Correlation for $NN_{0.5} >$ Correlation for $NN_{0.76}$
- Graphs of Neutral Networks are not random graphs
- Variation of neutral degree is smooth on NN

⇒ important consequence on metaheuristic design

Comparison of landscapes

- From DOS : Olympus $>$ Whole
- From Fitness cloud : Olympus $>$ Whole
- From FDC : Olympus $>$ Whole
- autocorrelation structure is relative favorable for Olympus landscape
- Important neutrality, and in particular in 0 and 0.5
- Neutral networks studies are not random graphs
- Fitness landscape of Majority Problem is hard

Result of the analysis

Choose Olympus landscape !

Result with simple GA

10^3 generations and 50 independent runs

GA	Average	Std Deviation	Best
simple GA in Olympus	0.8315	0.01928	0.8450
Simple GA in Olympus with neutrality	0.8323	0.00556	0.8472

- "With neutrality" :
Tournament selection taking into account the neutrality in evaluation

Motivation and general idea

- Fitness landscapes analysis :
 - study links between neighborhood and fitness
- Large search space :
 - estimation of statistical measures are difficult unless some hypothesis on fitness landscapes (isotropic)
 - sampling the solutions exploring by the meta-heuristic

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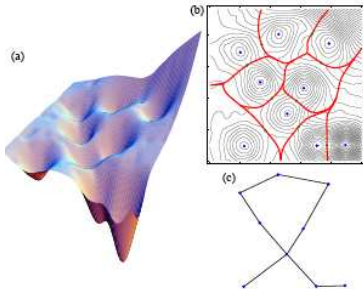
One possibility

Use an intermediate level of description of FL : **local optima network**

How ?

- Mapping fitness landscape to a network :
Smaller network with "good" properties
- conduct network analysis
- Relate (and exploit ?) network features to search operators

Energie surface and inherent networks (Doye [7] [8])



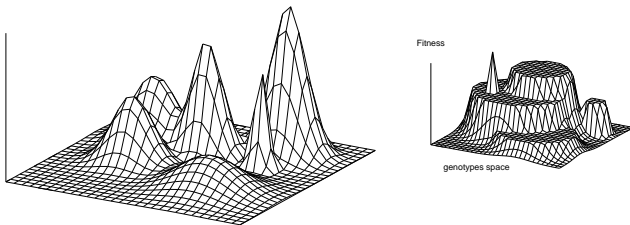
- a Model of 2D energy surface
- b Contour plot, partition of the configuration space into basins of attraction surrounding minima
- c landscape as a network

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

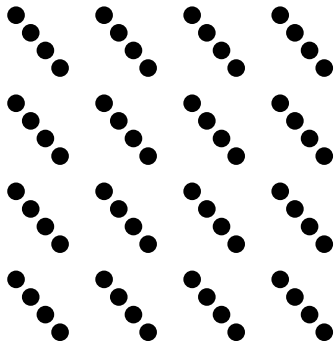
Classical representations :



- Very smooth representation as in real optimisation
- Neutral landscapes : not true (see previous description)
- Rugged landscapes : not true (see the following...)

Basins of attraction in combinatorial optimisation

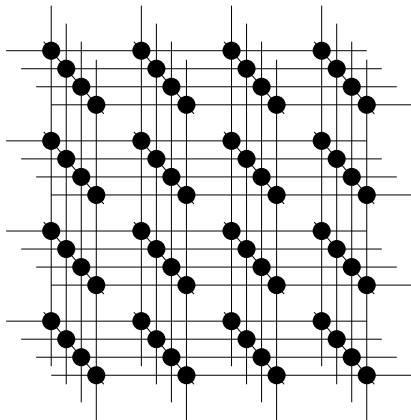
Example of small NK landscape with $N = 6$ and $K = 2$



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

Basins of attraction in combinatorial optimisation

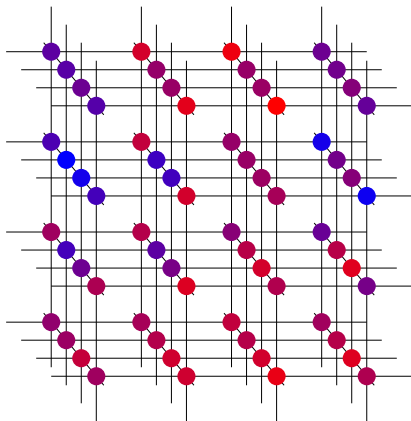
Example of small NK landscape with $N = 6$ and $K = 2$



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

Basins of attraction in combinatorial optimisation

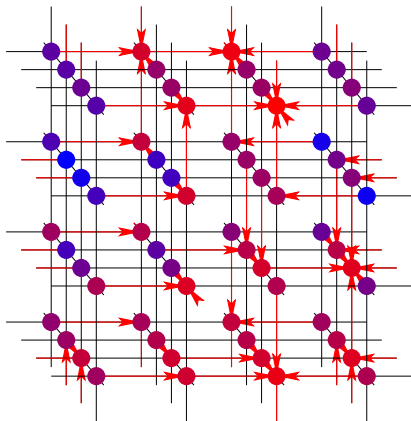
Example of small NK landscape with $N = 6$ and $K = 2$



- Color represent fitness value
- red = the fitness is high
- blue = the fitness is low

Basins of attraction in combinatorial optimisation

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

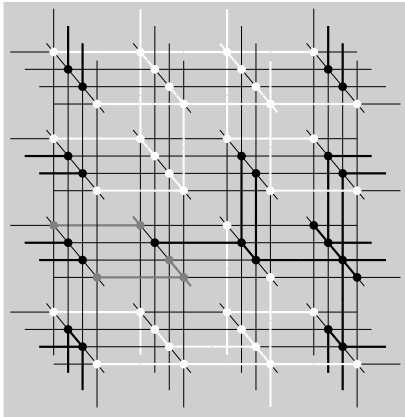


- Color represent fitness value
- Red arrow = toward the solution with the highest fitness in the neighborhood (if better)
remember that the size of the neighborhood is 6

Why not make a Hill-Climbing walk on it?

Basins of attraction in combinatorial optimisation

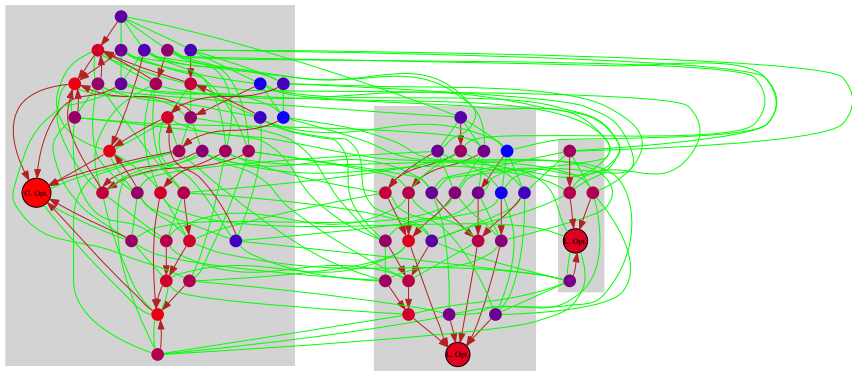
Example of small NK landscape with $N = 6$ and $K = 2$



- Each color correspond to one basin of attraction
- Basins of attraction are very imbricate
- Basins have no "interior"

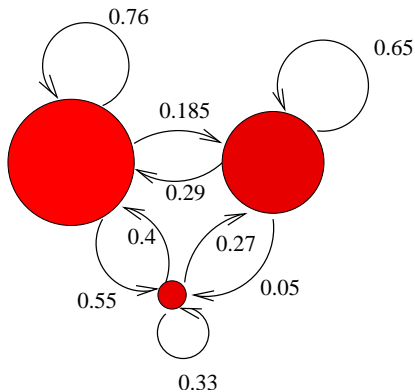
Basins of attraction in combinatorial optimisation

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



- Basins of attraction are very imbricate
- A lot of neighbor's solution outside the basin

Local optima network



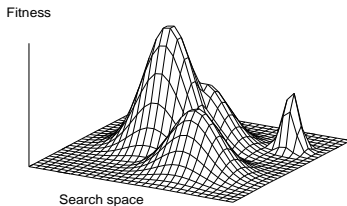
- Nodes : local optima
- Weighted edges : probability to pass from random solution of one basin to another

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

Local optima network

- Nodes : set of local optima \mathcal{S}^*
- Edges : notion of connectivity between basins of attraction
 - 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 [21])
 - weights w_{ij} is attached to the edges, account for transition probabilities between basins (ALIFE 2008 [33], Phys. Rev. E 2008 [30])

Weights of edges

- From each s and s' , $p(s \rightarrow s') = P(s' = op(s))$ the probability to pass from s to s'

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

- 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

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

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

- 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 $s' \in b_j$:

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

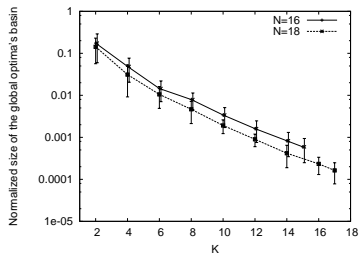
NK fitness landscapes : ruggedness and epistasis

- 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 for $N = 14, 16$ and 18 , $K = 2, 4, \dots, N - 2, N - 1$ (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

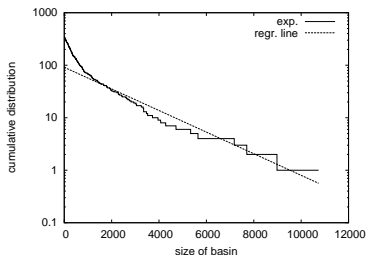
Global optimum basin size versus K



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

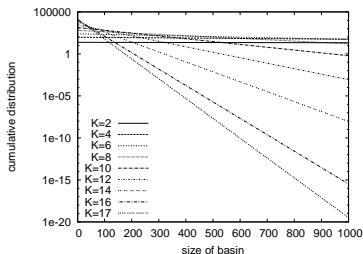
Analysis of basins : basin size



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

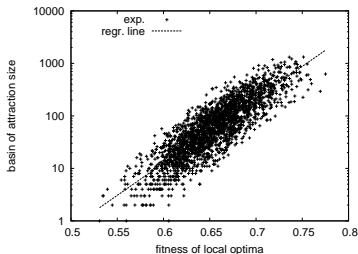
- Trend : small number of large basin, large number of small basin
- log-normal cumulative distribution
- slope of correlation increases with K
- when K large : basin sizes are nearly equals

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
- 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

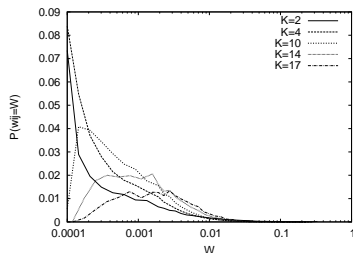
$$Y_2(i) = \sum_{j \neq i} \left(\frac{w_{ij}}{s_i} \right)^2$$

General network statistics $N = 16$

K	# nodes	# edges	\bar{C}^w	\bar{Y}	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

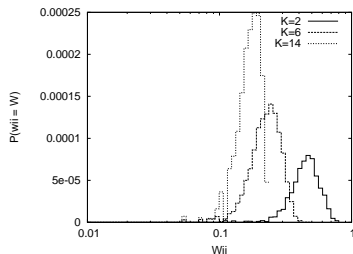
Weights distribution



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

- Weights (transition prob. between neighbouring basins) are small
- For high K the decay is faster
- Low K has longer tails
- On average, the transition probabilities are higher for low K

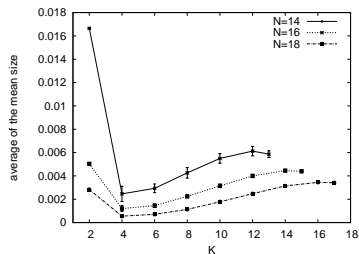
Weight distribution remain in the same basin



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

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

Interior and border size

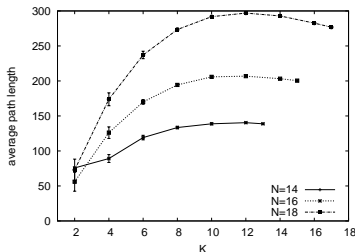


Average of the mean size of
basins interiors

Do basins look like a "mountain"
with interior and border ?

- solution is in the interior if all neighbors are in the same basin
- Interior is very small
- Nearly all solution are in the border

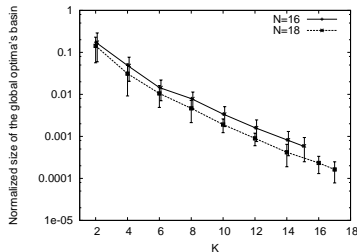
Shortest path length between local optima



Average distance (shortest path) between nodes

- 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

- More relevant for optimisation
- Increase steadily with increasing K

Summary on local optima network

- Proposed characterization of combinatorial landscapes as networks
- New findings about basin's structure
- Related some network features to search difficulty

Future on local optima network

- Define basin for neutral fitness landscapes
- Define sampling methodology
- Test on realistic combinatorial fitness landscapes
- Generalised the concept of basin

Summary on fitness landscapes

Fitness landscape is a representation of

- notion of neighborhood
- fitness of solutions

Summary on fitness landscapes

Fitness landscape is a representation of

- 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 results :
Difficulty!
to decide a good choice of the representation, operator and fitness function

Open questions

- How to dynamically change the parameters and/or operators of the algorithm with the local description of fitness landscape ?
- Can fitness landscape describe the dynamic of a population of solutions ?
- Links between neutrality and fitness difficulty ?
- Links between neutralities and fitness difficulty ?
- Which intermediate description shows relevant properties of the optimization problem according to the local search heuristic ?
-



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