Fitness Landscapes and Graphs: Multimodularity, Ruggedness and Neutrality

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Outline of this tutorial

1. Introduction :
   contexte, goals, related theoretical works, definition
2. Fitness landscapes of multimodal, and neutral problems, a case study
3. Local optima network
4. Fitness landscapes for continous and multobjective problems

Optimization framework

Inputs

- Search space : Set of all feasible solutions,

$$\mathcal{S}$$

- Objective function : Quality criterium

$$f : \mathcal{S} \rightarrow \mathbb{R}$$

Goal

Find the best solution according to the criterium

$$s^\star = \text{argmax } f$$

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But, sometime, the set of all best solutions, good approximation of the best solution, good 'robust' solution...

Contexte

Black box Scenario

We have only $\{(s_0, f(s_0)), (s_1, f(s_1)), ...\}$ 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.

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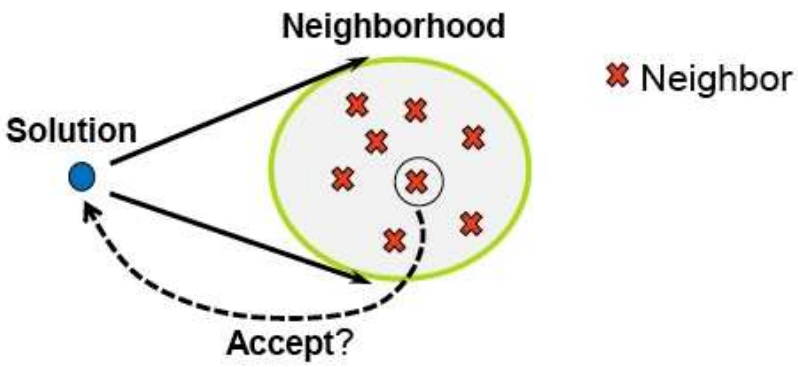
- Objective function given by a computation, or a simulation
- Objective function can be irregular, non differentiable, non continous, etc.
- (Very) large search space for discrete case (combinatorial optimization), *i.e.* NP-complete problems

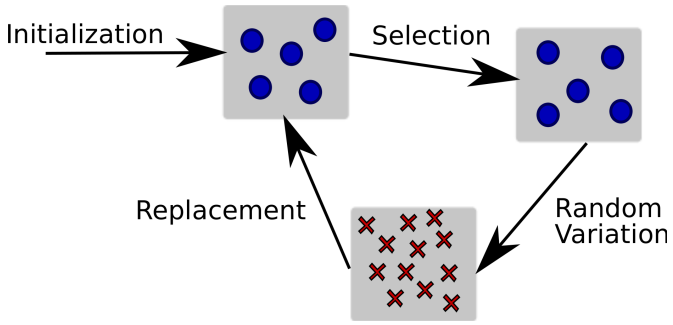
Search algorithms

Principle

Enumeration of the search space

- A lot of ways to enumerate the search space
- Using random sampling : Monte Carlo technics
- Local search technics :





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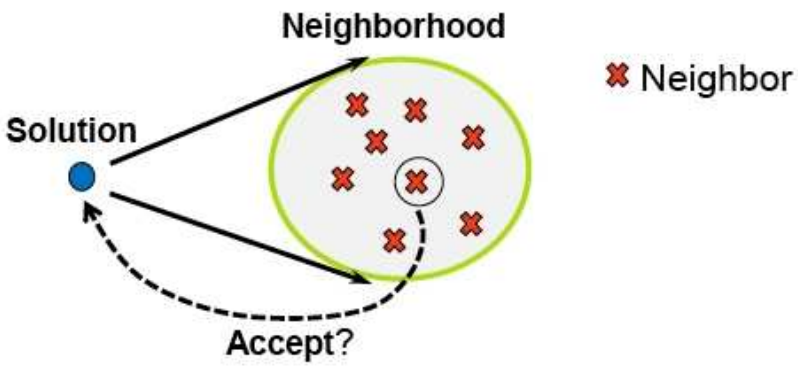
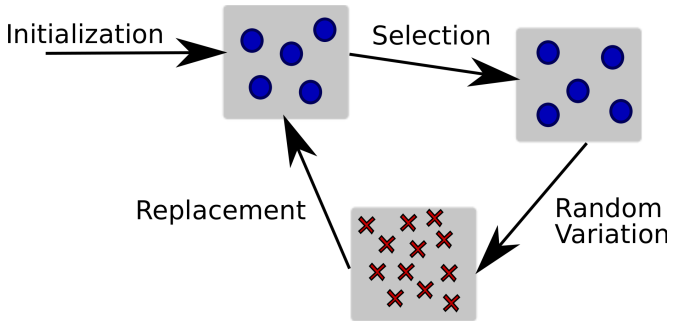




- If objective function f has no propertie : random search
- If not...

Fitness landscapes : Motivations

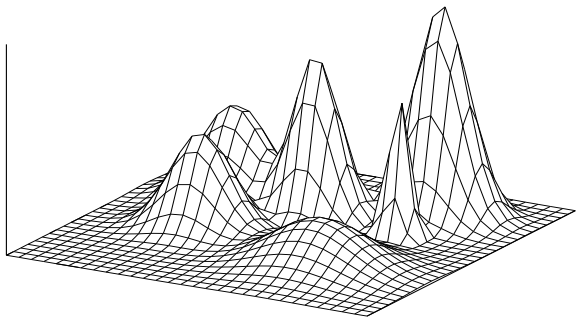
Why using fitness landscapes ?

- To analyse the structure of the search space
- To study problem (search) difficulty in combinatorial optimisation :
  information on runtime for a given problem and a class of LS
- 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

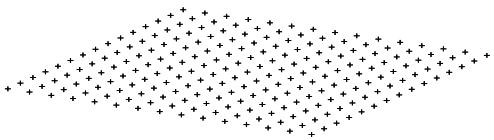


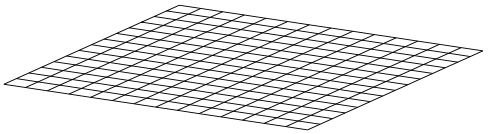
Biological science :
Wright 1930 [36]

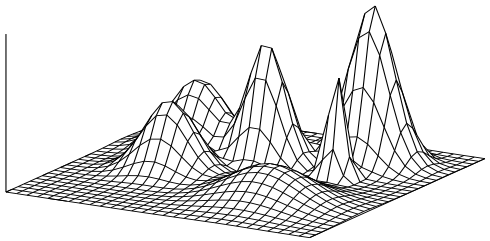
Biological evolution :

- 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 :

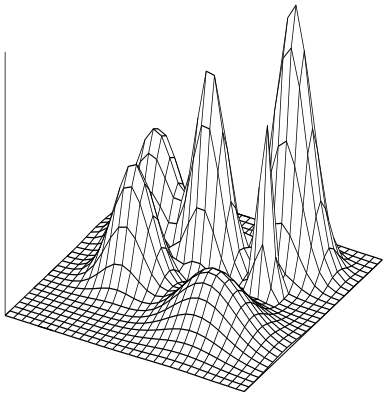
- statistical physic,
- molecular evolution,
- ecology, etc

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 $(\mathcal{S}, \mathcal{N}, f)$:

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

$2^{\mathcal{S}}$ is the set of sets : $\mathcal{N}(s) \subset \mathcal{S}$

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
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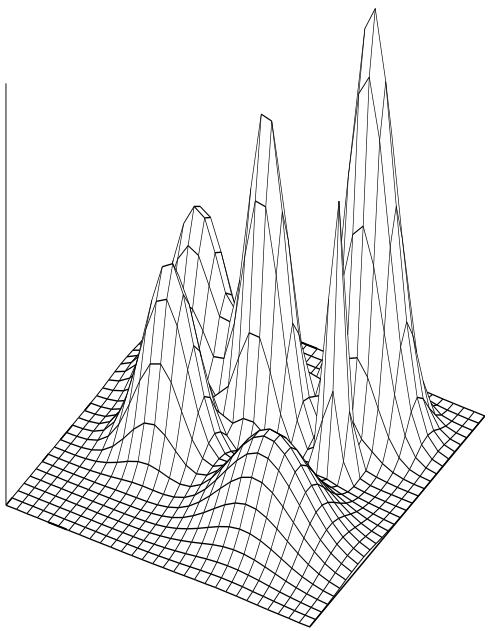
What is a neighborhood ?



Neighborhood function :

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

Set of "neighbor" solutions associated to each solution

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

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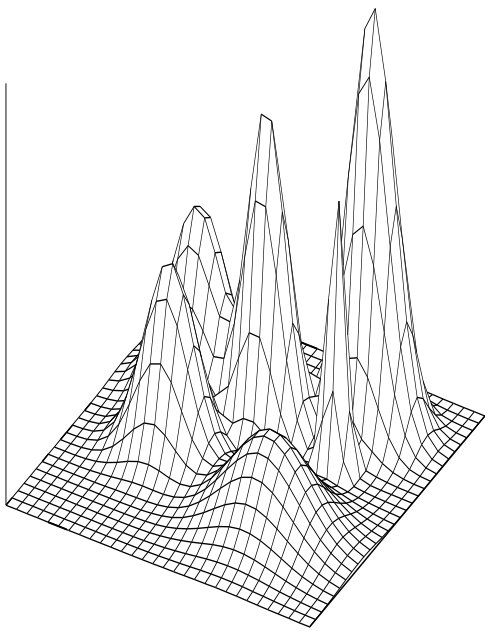

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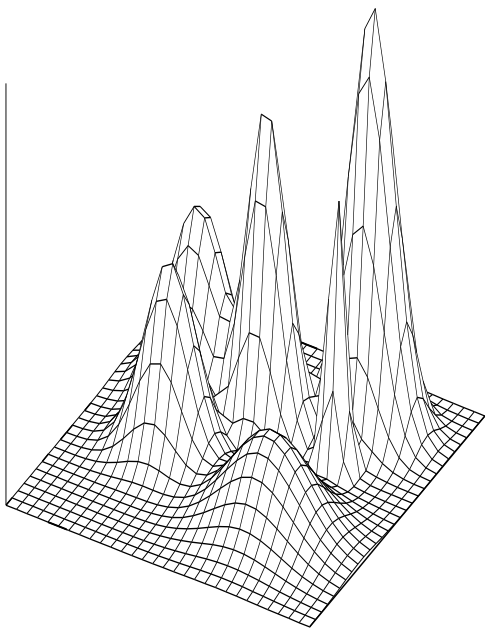

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or

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

Example of neighborhood : bit strings

Search space : $\mathcal{S} = \{0,1\}^N$
Algorithm : simple GA, hill-climbing, or simulated annealing, etc.

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

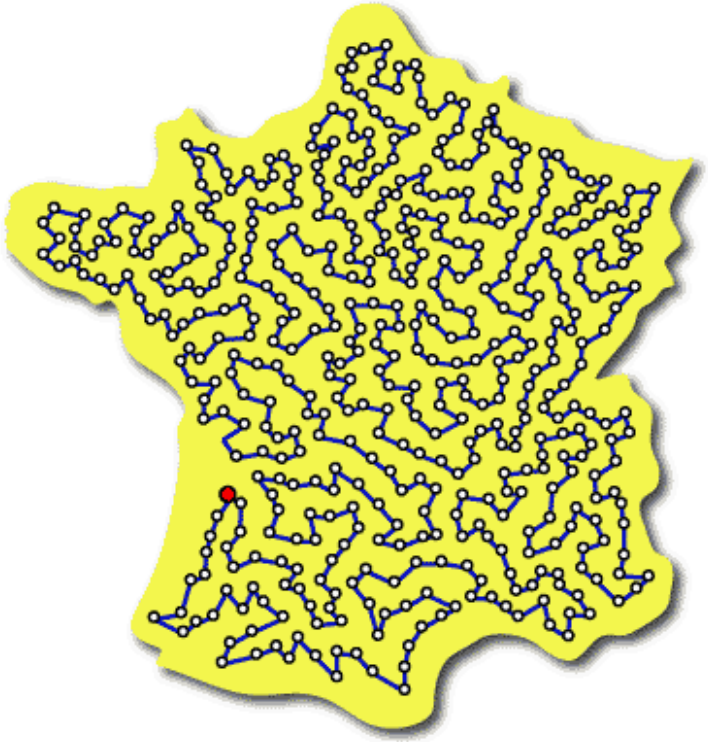
Important !

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

Neighborhood $\Leftrightarrow$ Operator

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

Example of neighborhood : permutations

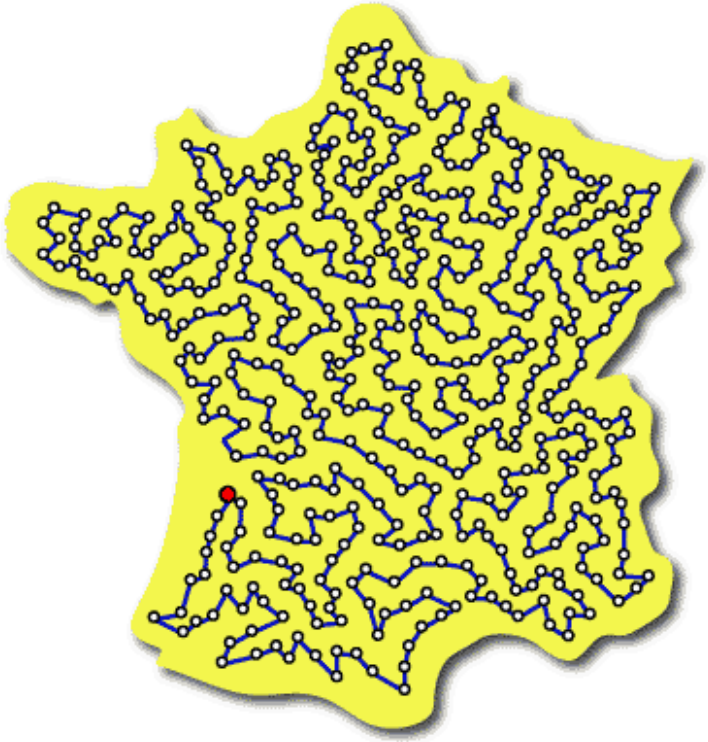


Traveling Salesman Problem : find the shortest tour which cross one time every town

- *Search space* : $\mathcal{S} = \{\sigma \mid \sigma \text{ permutations } \}$
- *Algorithm* : simple EA
  operator : 2-opt

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

Example of neighborhood



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

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  operators : 2-opt and 3-opt

$$\mathcal{N}(x) = \{y \in \mathcal{S} \mid \mathbb{P}(y = op_{2opt}(x)) > 0 \textbf{ or } \mathbb{P}(y = op_{3opt}(x)) > 0\}$$

Example of neighborhood : memetic algorithms

- *Algorithm* : memetic algorithm, EA + operator hill-climbing

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

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- *Algorithm* : memetic algorithm, EA + operator hill-climbing and bit-flip mutation

2 possibilities :

- Study 2 landscapes :
  one for *HC* operator, one for bit-flip mutation
- Study 1 landscape :
  $\mathcal{N}(x) = \{y \in \mathcal{S} \mid y = op_{HC}(x)$ **or** $\mathbb{P}(y = op_{bit-flip}(x)) > \epsilon\}$

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It depends on what you want to know

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 : $(S_1, \mathcal{N}_1, f_1)$ and $(S_2, \mathcal{N}_2, f_2)$
     different coding, mutation operator, fitness function, etc.

Which one is easier to solve ?

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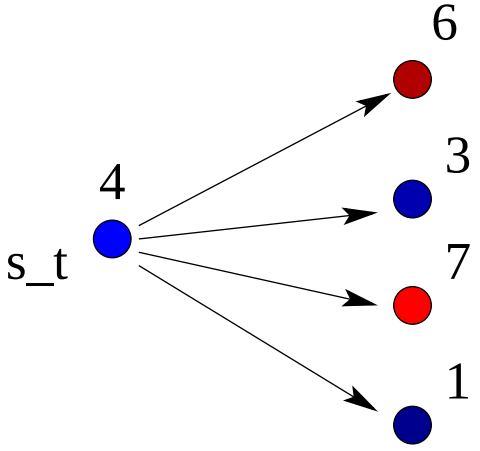
     Which is the best mutation operator ? the size of the population ? etc.
4. To control the parameters during the run :
   - *on-line* analysis of structure of fitness landscape

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

Fitness landscapes point of view

FL = (Sol., Neighbors, Fitness)



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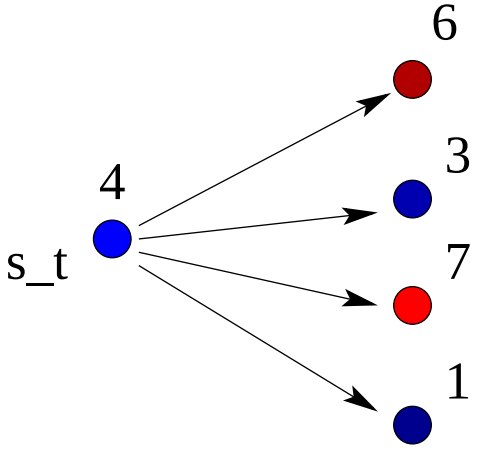
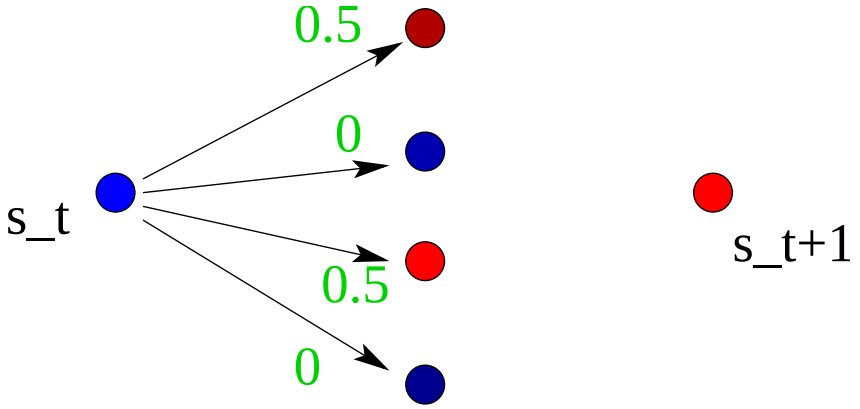


Put prob. from your heuristic :



No particular heuristic, heuristics based on the same neighborhood relation

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

Two main geometries have been studied :

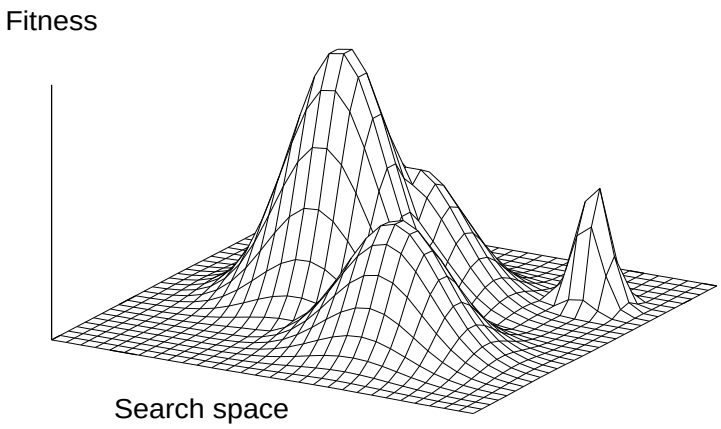
- multimodal and ruggedness
- neutral

Multimodal Fitness landscapes

Local optima s^* (maximization) :

no neighbor solution with higher fitness value

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



Multimodal Fitness landscapes

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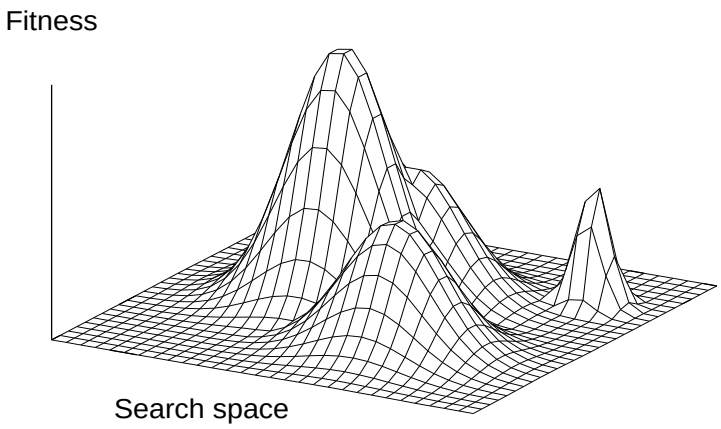
$$\forall s \in \mathcal{N}(s^*), f(s) \leq f(s^*)$$



Multimodal Fitness landscapes

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

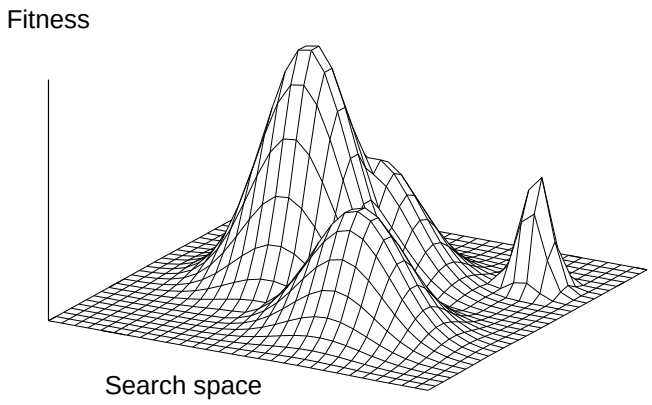
Hill-Climbing (HC) algorithm

Choose initial solution $s \in S$
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^* :

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

Multimodal Fitness landscapes



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

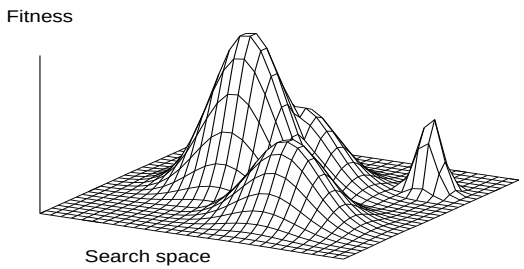
The idea :

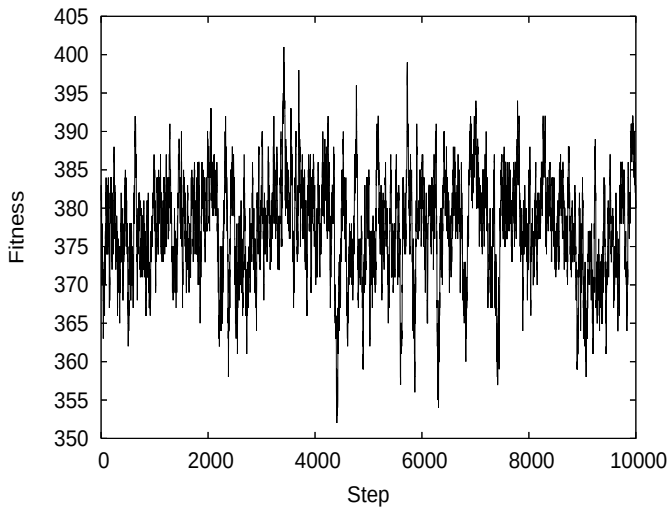
- if the size of attractive basin of global optima is relatively "small"
- the problem is difficult to optimize

The measure :

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

Walking on fitness landscapes



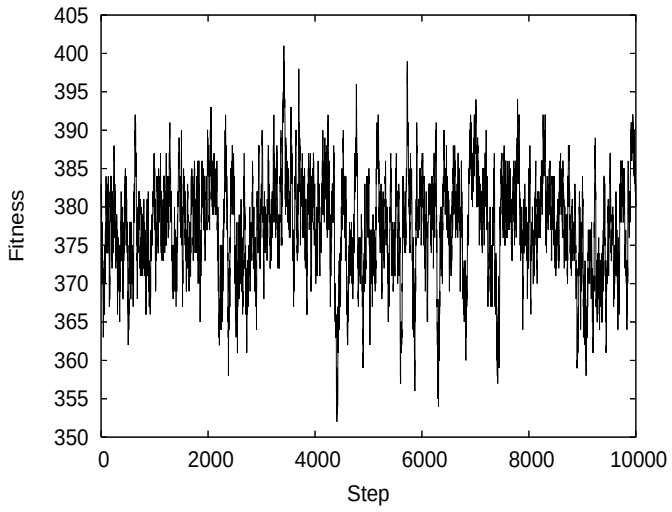


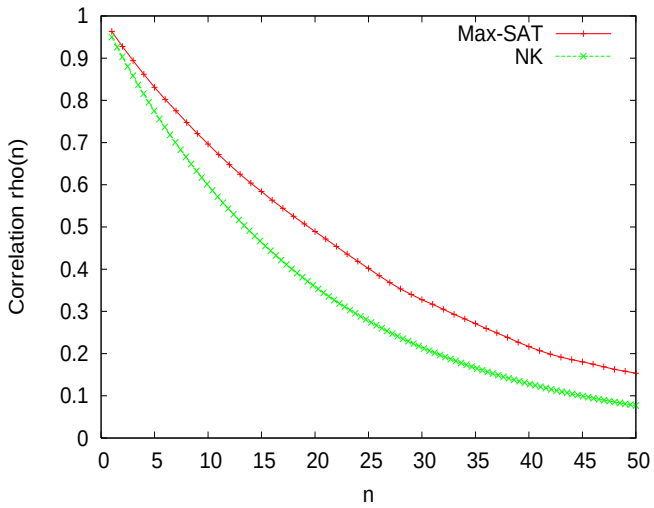
fitness vs. step of a random walk (example of max-SAT problem)

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 $(s_1, s_2, \ldots)$ [35] :

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

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

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

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

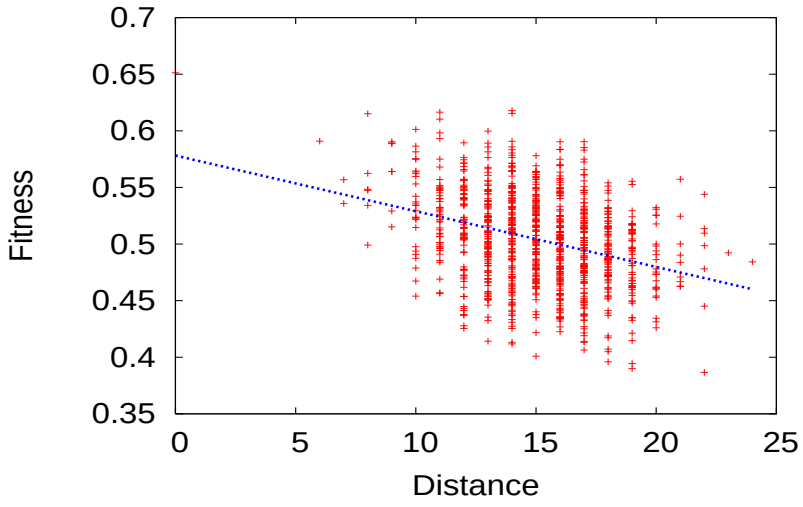
Problem	parameter	$\rho(1)$
symmetric TSP	n number of towns	$1 - \frac{4}{n}$
anti-symmetric TSP	n number of towns	$1 - \frac{4}{n-1}$
Graph Coloring Problem	n number of nodes α number of colors	$1 - \frac{2\alpha}{(\alpha-1)n}$
NK landscapes	N number of proteins K number of epistasis links	$1 - \frac{K+1}{N}$

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

Weinberger, Stadler, Whitley, Sutton : elementary landscapes

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

Correlation between distance to global optimum and fitness



Classification based on experimental studies :

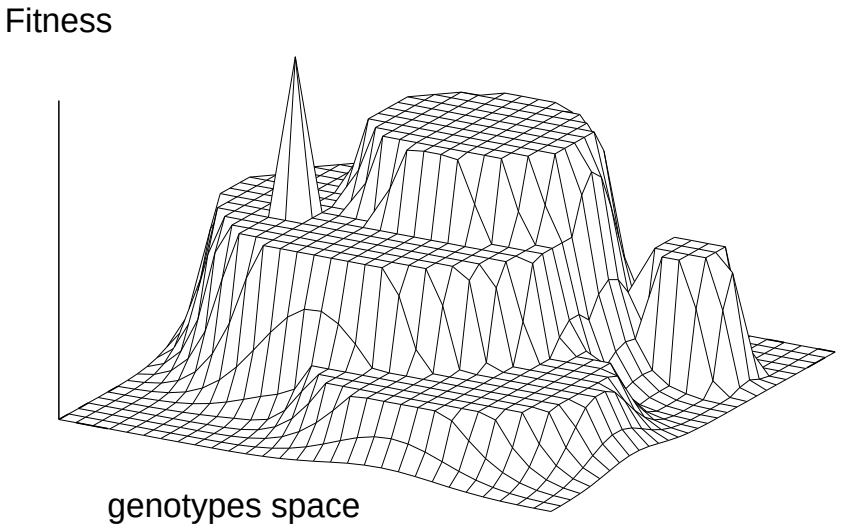
- $\rho < -0.15$, easy optimization
- $\rho > 0.15$, hard optimization
- $-0.15 < \rho < 0.15$, undecided zone

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

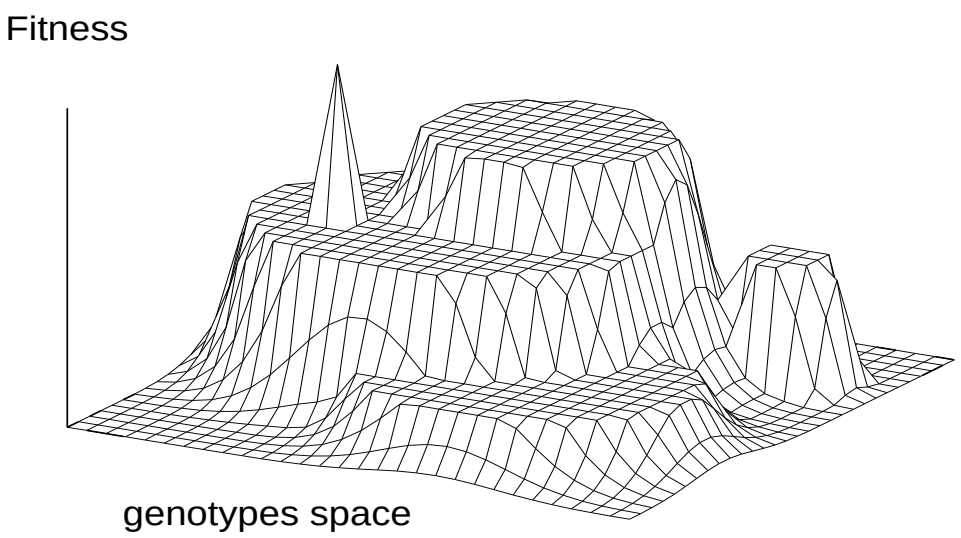


- plateaus
- neutral degree
- neutral networks [Schuster 1994 [25], RNA folding]

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 of the fitness landscape

⇒ 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

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

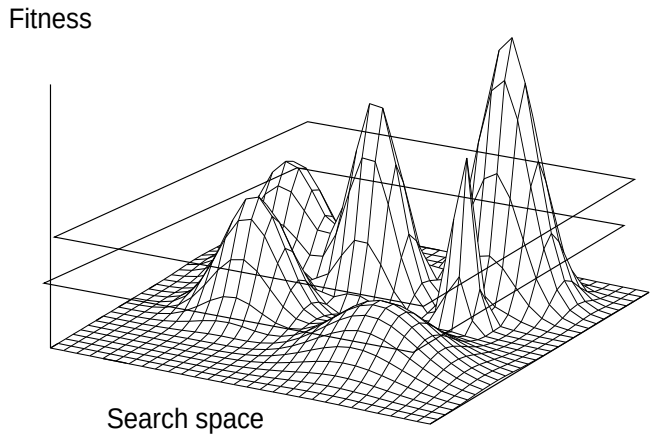
- When there is No information :
  you should have a good method to find it !

In the following

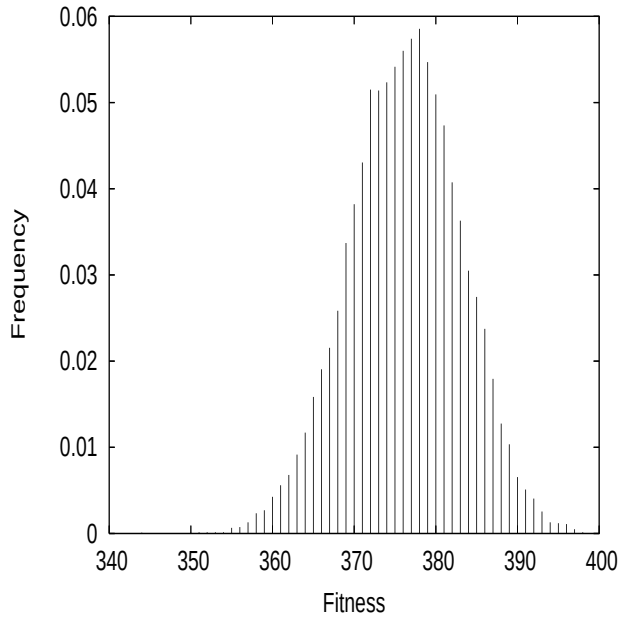
Description of neutral fitness landscapes :

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

Neutral sets : Density Of States



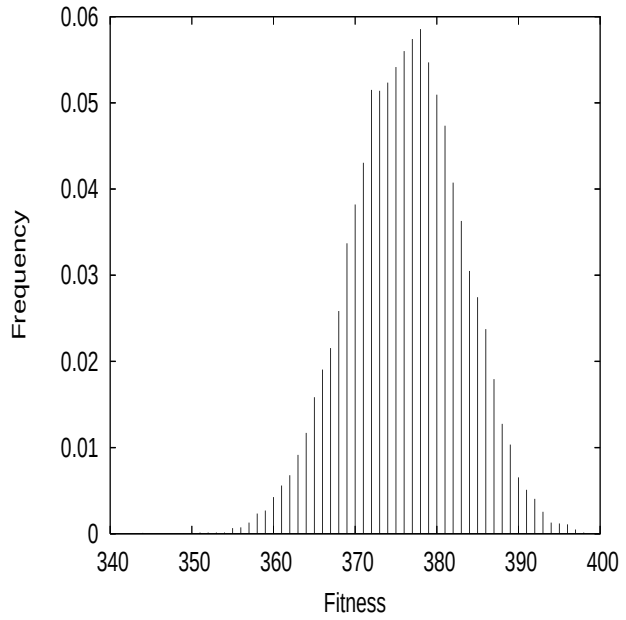
Set of solutions with fitness value



Density of states (D.O.S.)

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

Neutral sets : Density Of States

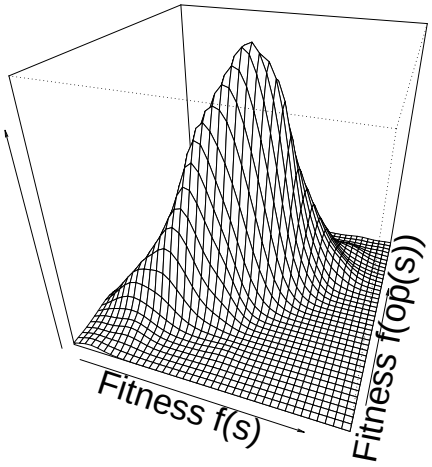


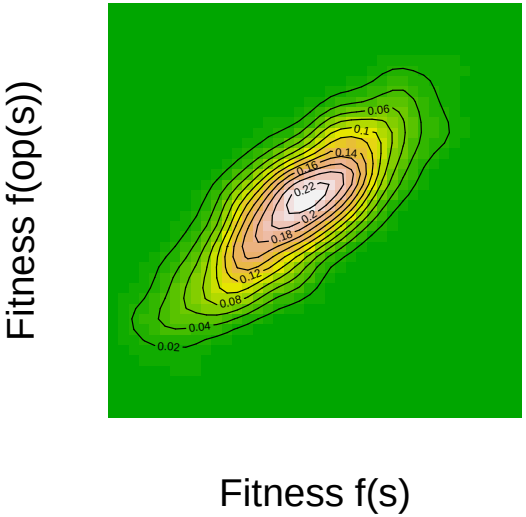
Density of states (D.O.S.)

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





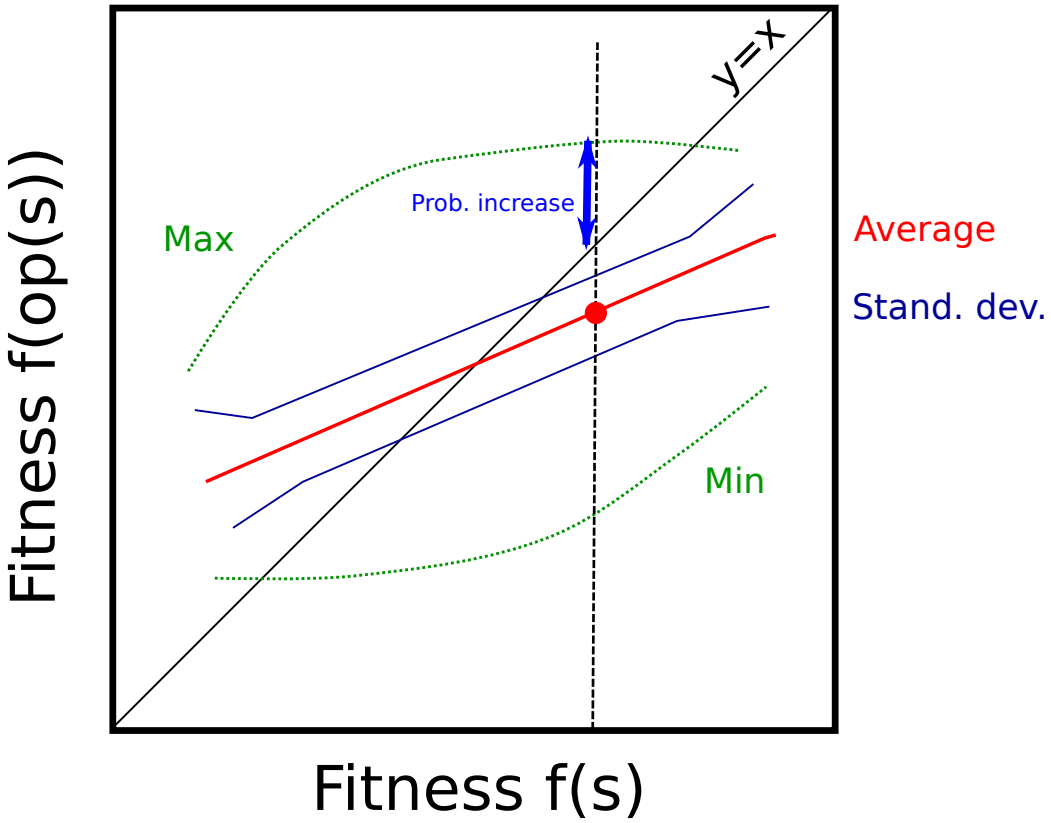
- $(\mathcal{S}, \mathcal{F}, \mathbb{P})$: probability space
- $op : \mathcal{S} \rightarrow \mathcal{S}$ stochastic operator of the local search

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

Fitness Cloud of *op*

Conditional probability density function of Y given X

Fitness cloud : Measure of evolvability

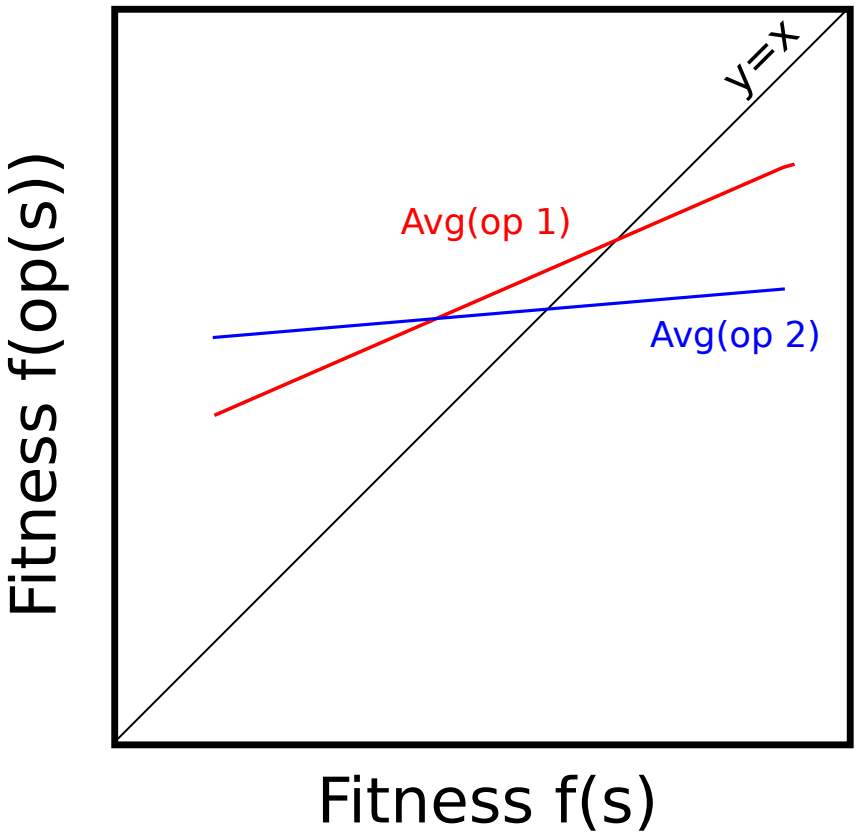


Evolvability

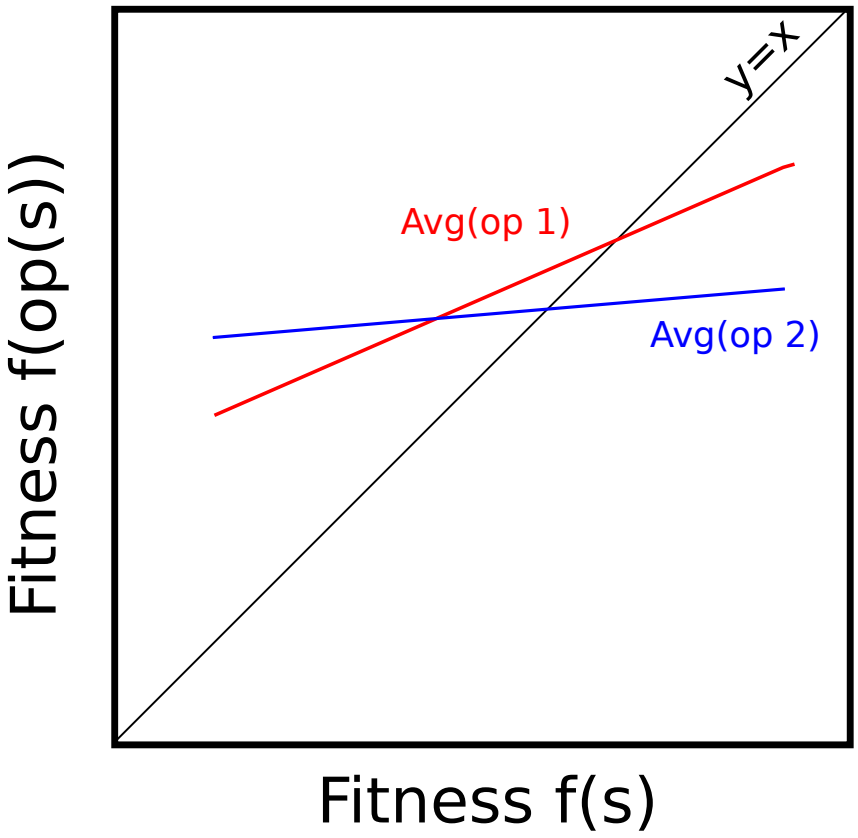
Ability to evolve : fitness in the neighborhood compared to the fitness of the solution

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

Fitness cloud : Comparaison of difficulty



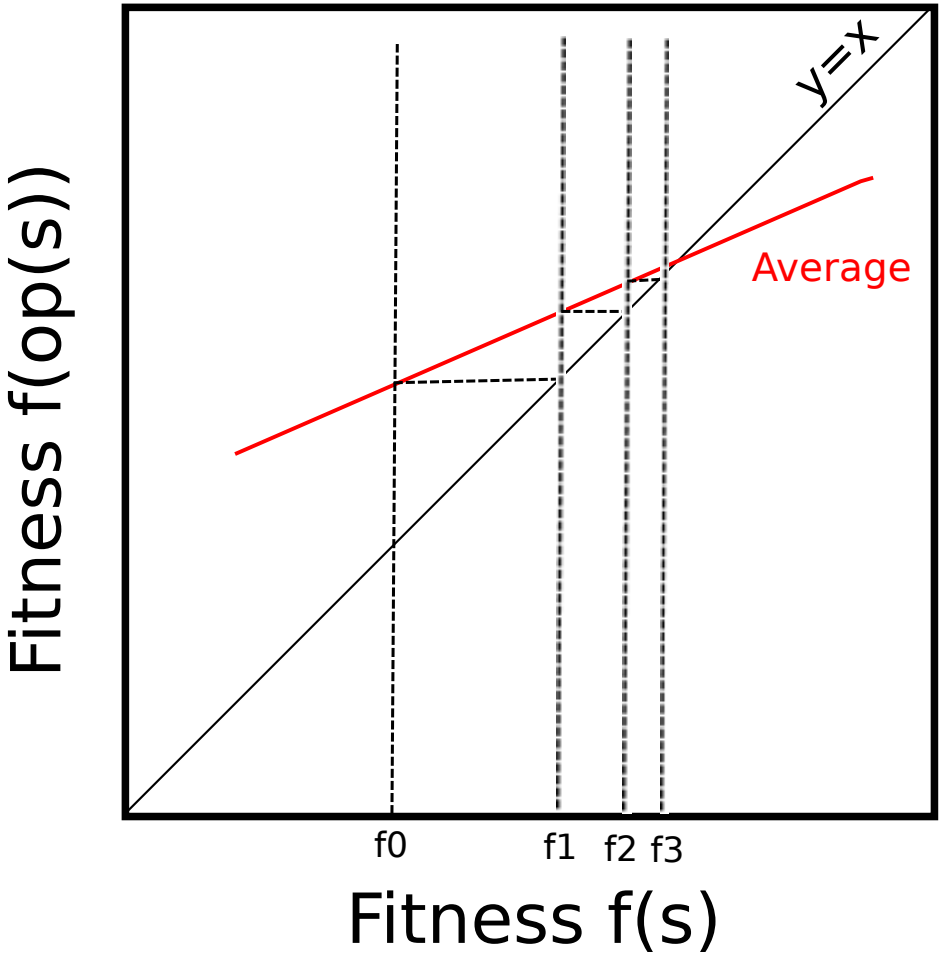
Fitness cloud : Comparaison of difficulty



- 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)

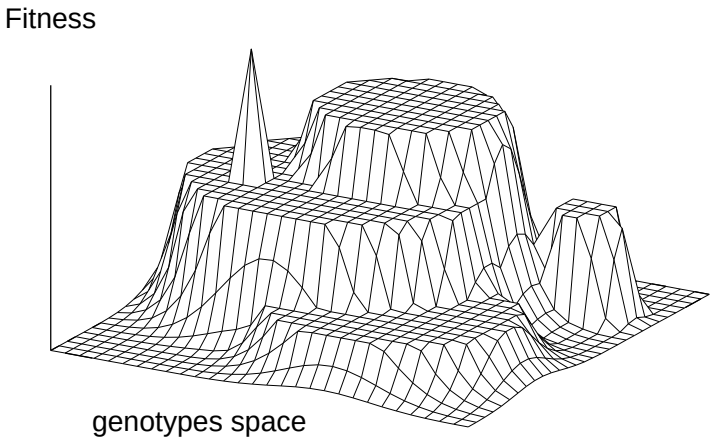


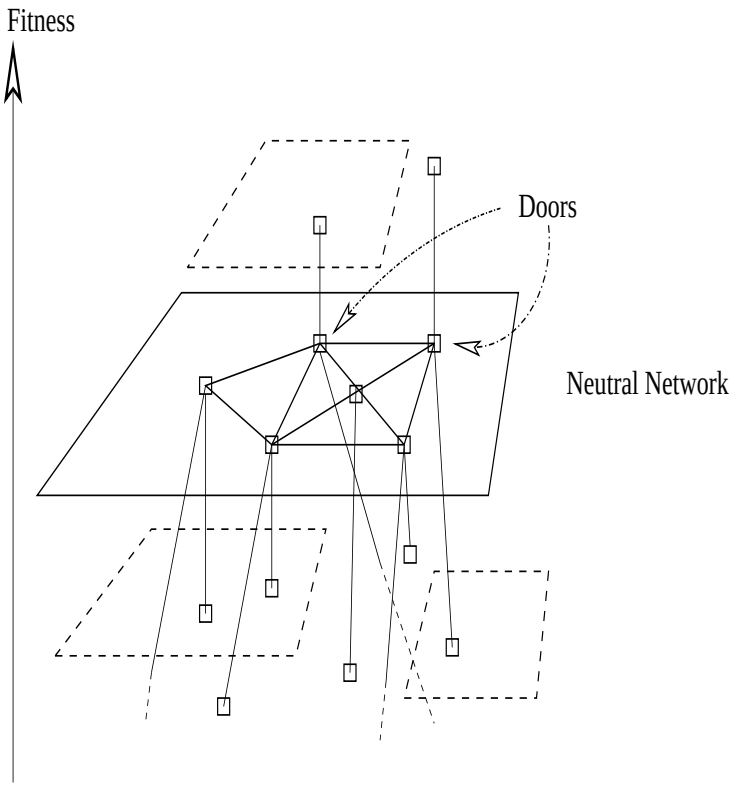
- Approximation (only approximation) of the fitness value after few steps of local operator
- Indication on the quality of the operator

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 [25])





Definitions (simple version)

Neutral neighborhood

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

$$\mathcal{N}_{neut}(s) = \{s' \in \mathcal{N}(s) \mid f(s) = f(s')\}$$

Neutral degree of s

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

Definitions

Test of neutrality

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

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.

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 : $s_2 \in \mathcal{N}_{neut}(s_1)$

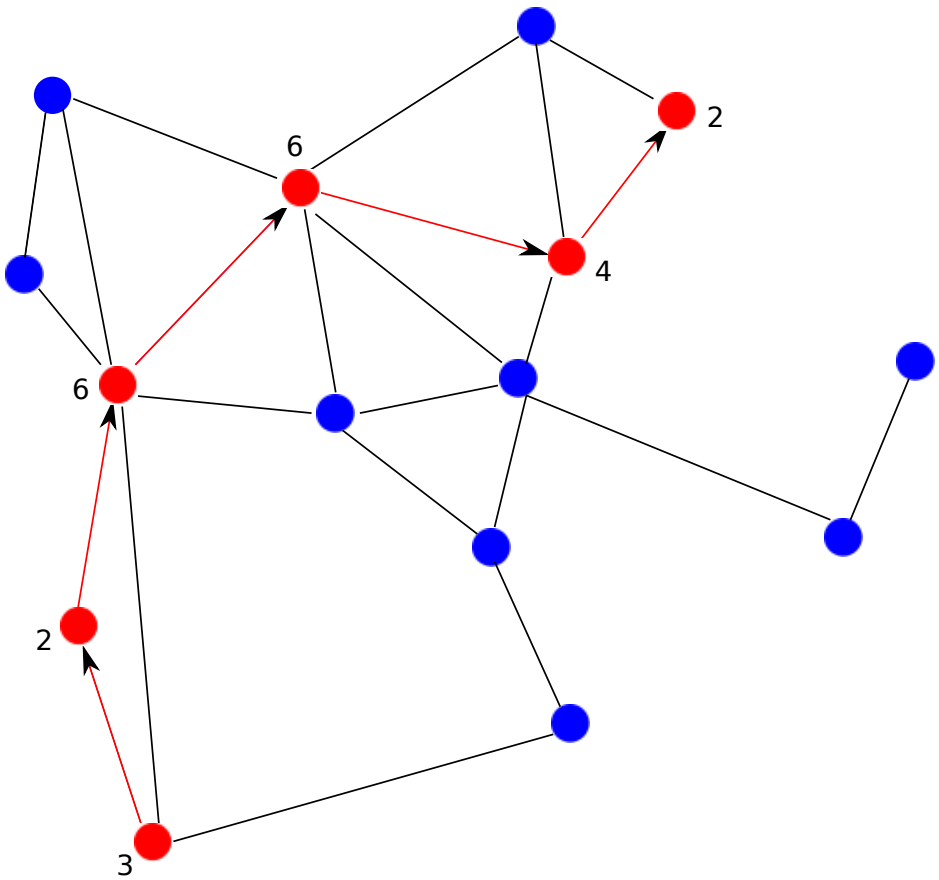
A fitness landscape is neutral
if there are many solutions with high neutral degree.

Neutral Networks (NN) : Inside Metrics

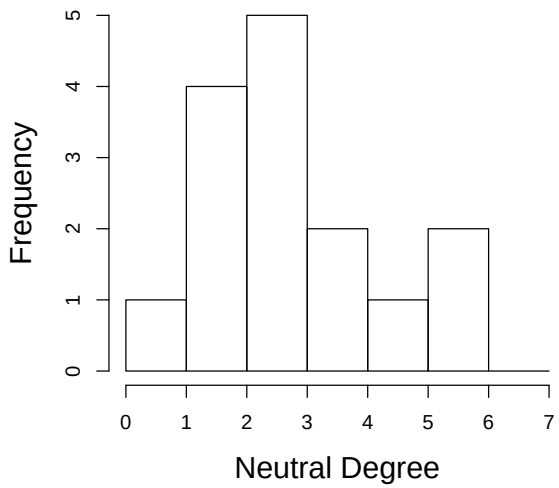
Classical graph metrics :

- 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*

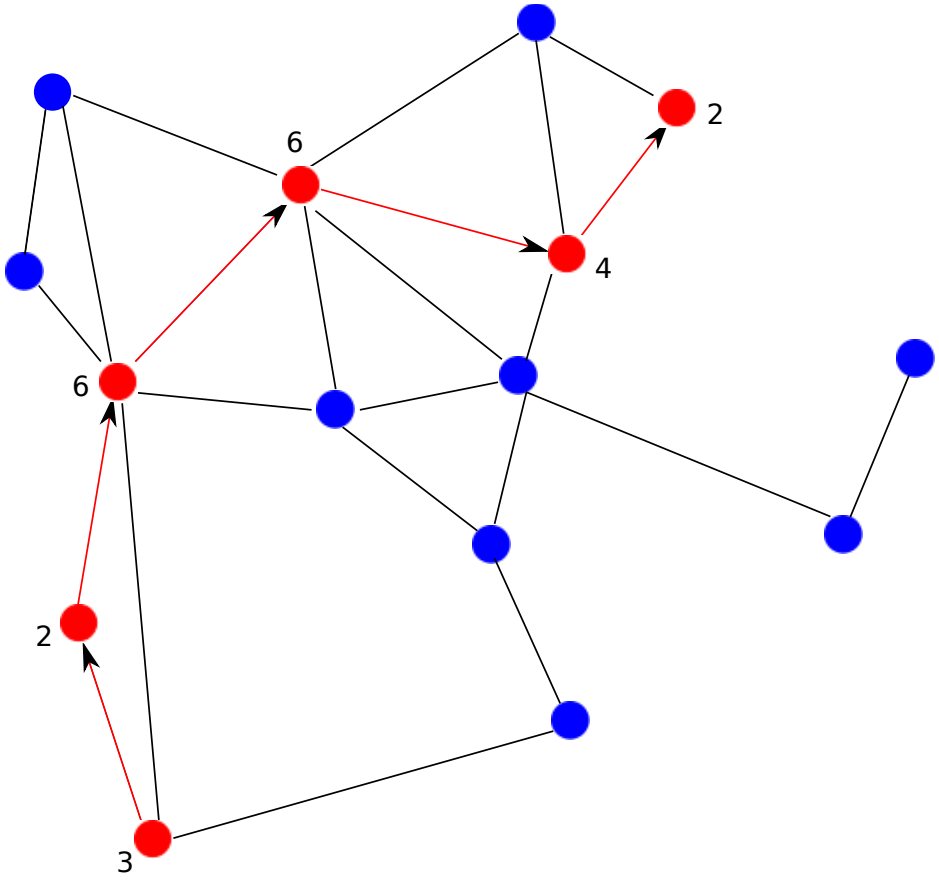
Neutral Networks : Inside Metrics



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

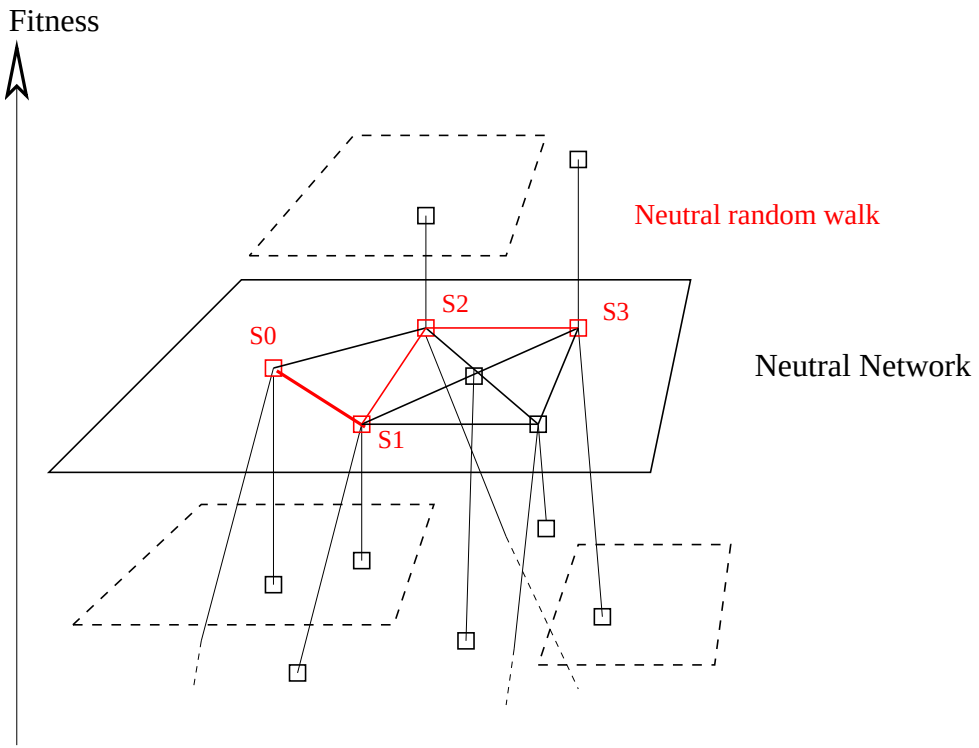


Neutral Networks : Inside Metrics



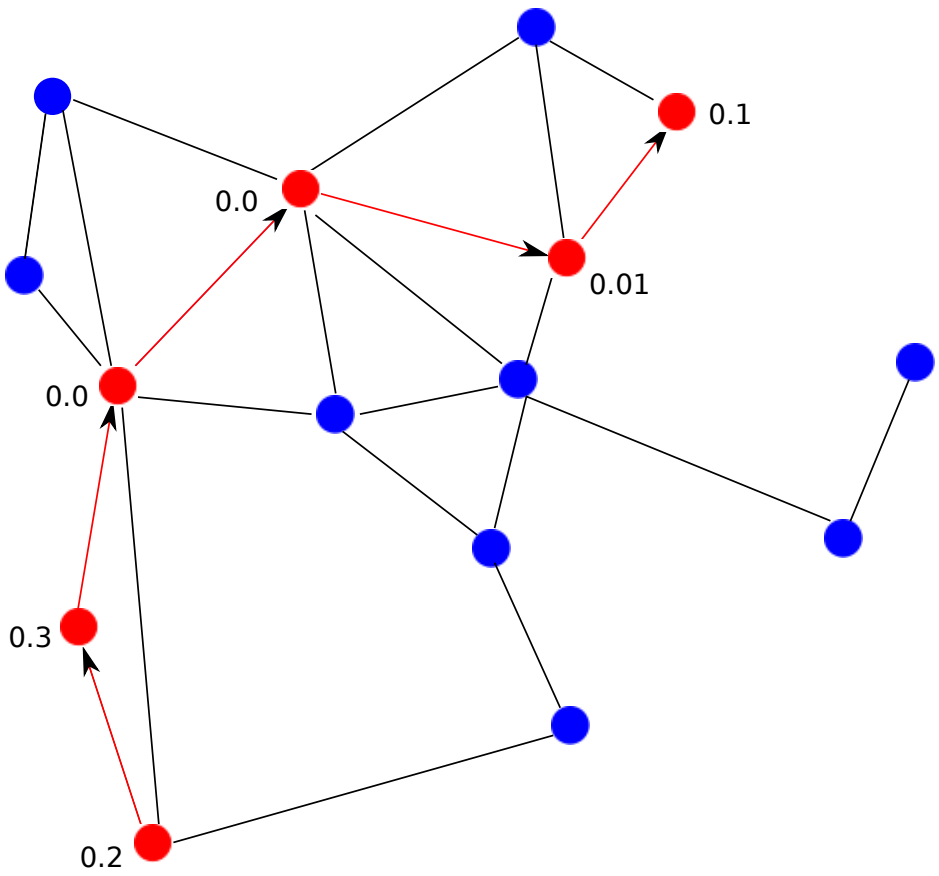
- Size : 15 solutions
  Distribution of size overall landscapes
- Neutral degree distribution
- Autocorrelation of neutral degree :
  - random walk on NN
  - autocorrelation of degrees

Neutral Networks : Outside Metrics



- Number of portals (exits toward better solutions), spreading of portals
- Autocorrelation of evolvability [33] : autocorrelation of the sequence $(evol(s_0), evol(s_1), \ldots)$.

Neutral Networks : Outside Metrics



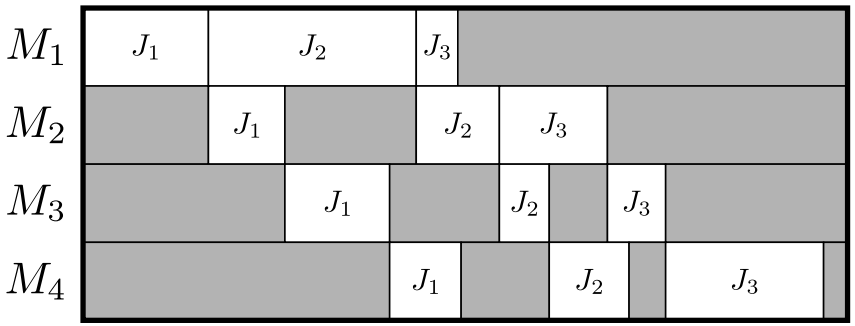
- Autocorrelation of evolvability :
  - Evolvability $evol$ = avg fitness in the neighborhood
  - Autocorrelation of $(evol(s_0), evol(s_1), \ldots)$.
- Informations :
  - if high correlation $\Rightarrow$ "easy" (you can use this information)
  - if low correlation $\Rightarrow$ "difficult"

From analysis to design : a case study

PhD work of Marie-Eléonore Marmion (December 2011)

An example :
From fitness landscapes analysis to design of efficient local search

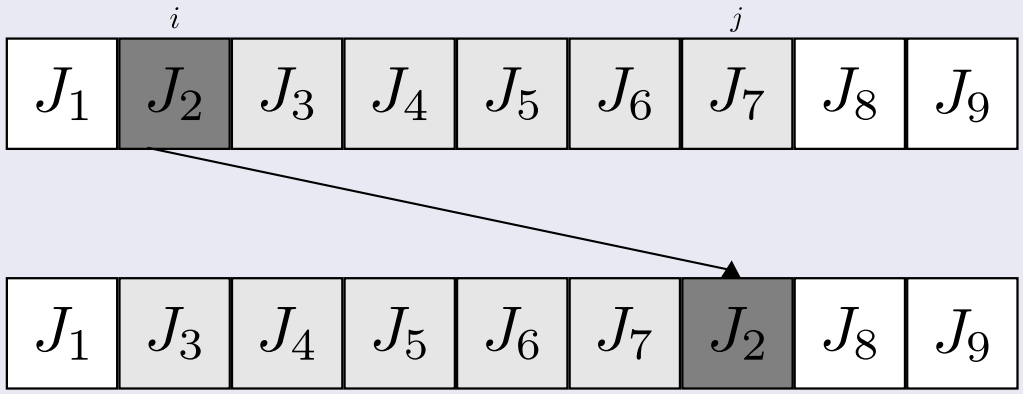
A case study : The Permutation Flowshop Scheduling Problem (FSP)



- N jobs, M machines
- Processing time of each job can be different on each machine
- Each job can be processed on at most one machine
- Each machine can process at most one job at a time
- Job order is the same on every machine :
  Representation = Permutation
- $\Rightarrow$ Makespan minimization

Neighborhood relation

Insertion operator



Neighborhood size : $(N-1)^2$

Something strange in the state-of-art local search (Iterated Greedy)
So a fitness analysis...

Neutrality

Question 1

Is there some neutrality in the problem ?

Neutral degree (ratio) of local optima

- Sample : set of local optima

N	20		50		100		200	
5	65	(18%)	792	(33%)	3920	(40%)		
10	7	(2%)	96	(4%)	784	(8%)	6732	(17%)
20	4	(1%)	24	(1%)	98	(1%)	396	(1%)

Neutrality

Question 1

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20	4	(1%)	24	(1%)	98	(1%)	396	(1%)

Yes ! There is some neutrality.

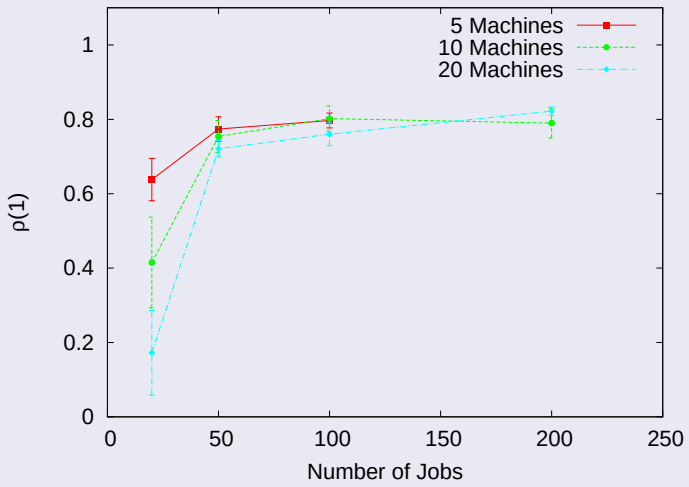
Continue the analysis to find information...

Neutral Networks

Question 2

The neutral networks have some structure ?

Autocorrelation of neutral degrees



Neutral Networks

Question 2

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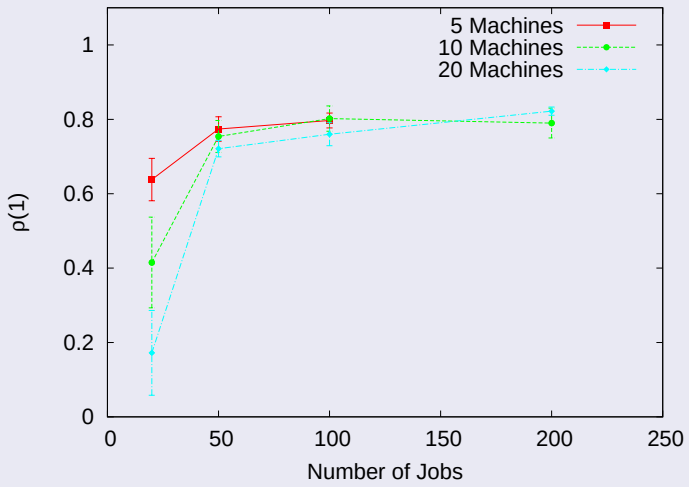
Autocorrelation of neutral degrees



Yes ! Neutral Networks are not random graphs.

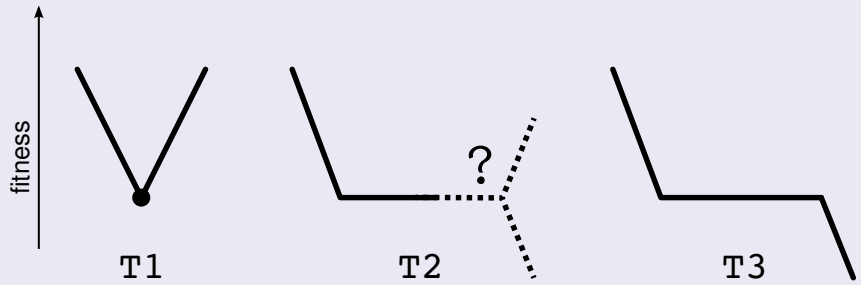
Continue the analysis to find information...

Portals, exits

Question 3

Can we reach a portal ?

Typology of neutral networks



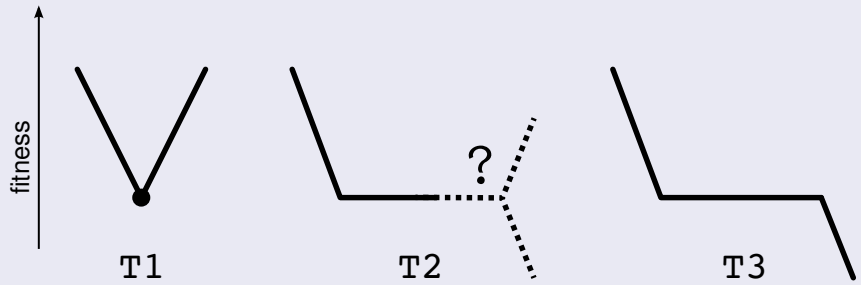
- No T1 for $N = 50, 100, 200$
- $< 20\%$ T1 and T2 for $N = 20$, $< 3\%$ T2 for $N = 50, 100, 200$
- $> 97\%$ T3

Portals, exits

Question 3

Can we reach a portal ?

Typology of neutral networks



- No T1 for $N = 50, 100, 200$
- $< 20\%$ T1 and T2 for $N = 20$, $< 3\%$ T2 for $N = 50, 100, 200$
- $> 97\%$ T3

Yes ! There is some portals.

Neutrality

Question 4

Is it easy to find a portal ?

Average number of steps before a portal

- During random neutral walks

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

Neutrality

Question 4

Is it easy to find a portal ?

Average number of steps before a portal

- During random neutral walks

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

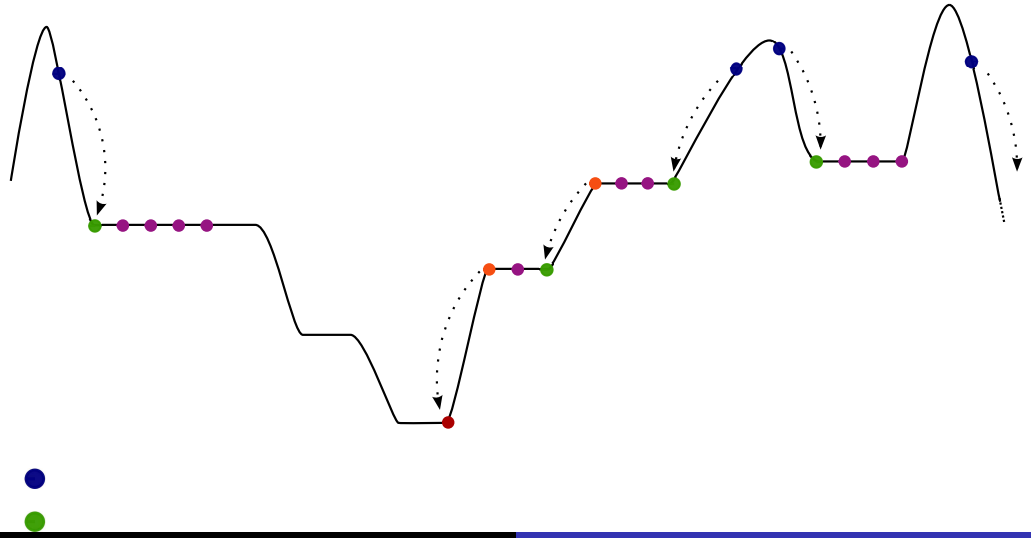
Yes ! The portals are closed to local optima.

Design efficient Local search

NILS : Neutral Iterated Local Search

- Local Search : First-improvement Hill-Climbing (until local optimum)
- Perturbation : to escape from plateau
  - Neutral moves (until maximum number of steps)
  - Kick move (from the IG local search)

⇒ Very competitive *vs.* the state-of-art IG, and we understand why.

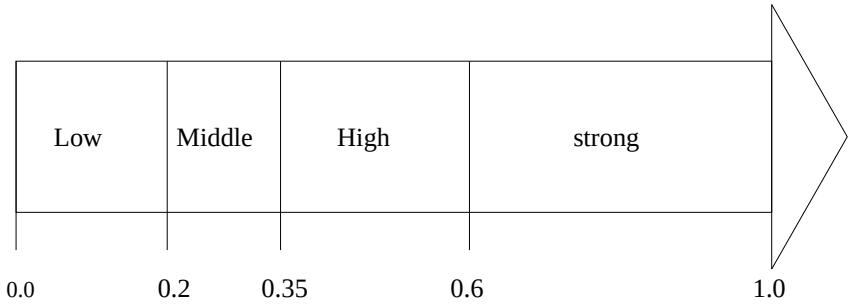


Summary of metrics

- Neutral degrees distribution :

  "How neutral is the fitness landscape ?"

- Autocorrelation of neutral degrees : network “structure”



- Portals, exits :

  Escaping of plateau to find better solutions

- Autocorrelation of evolvability :

  information on the links between NN

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 ?

Basic Methodology of fitness landscapes analysis

- Density of States : pure random search, initialization ?
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- 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

Sofware to perform fitness landscape analysis

Framework **ParadisEO 1.3**

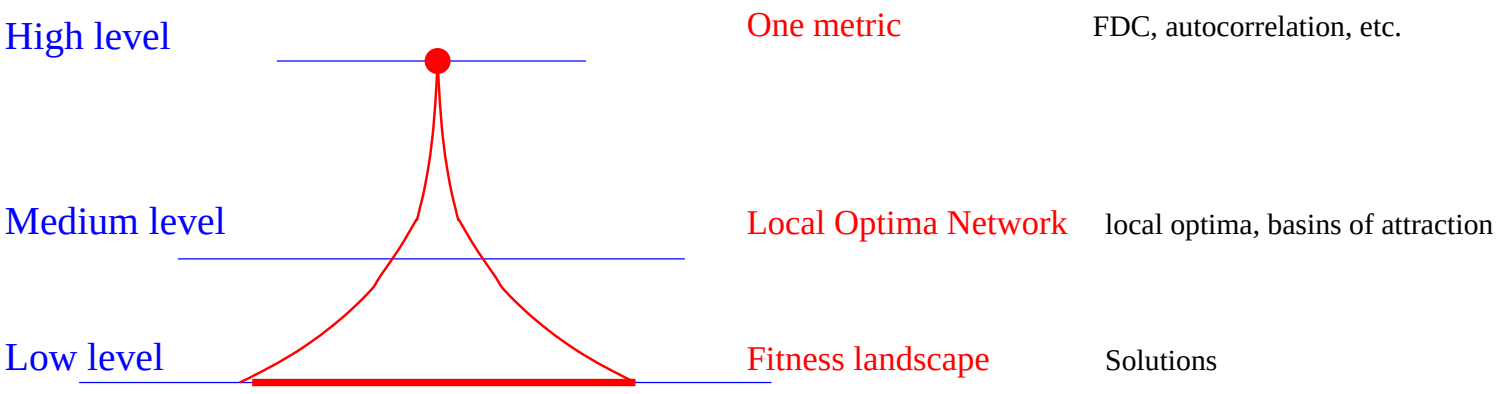
http://paradiseo.gforge.inria.fr/newWebsite/index.php?n=Doc.Tuto
and tutorials :
http://paradiseo.gforge.inria.fr/newWebsite/index.php?n=Doc.Tuto

```
moAutocorrelationSampling<Neighbor> sampling(randomInit,
                                             neighborhood,
                                             fullEval,
                                             incrementalEval,
                                             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.

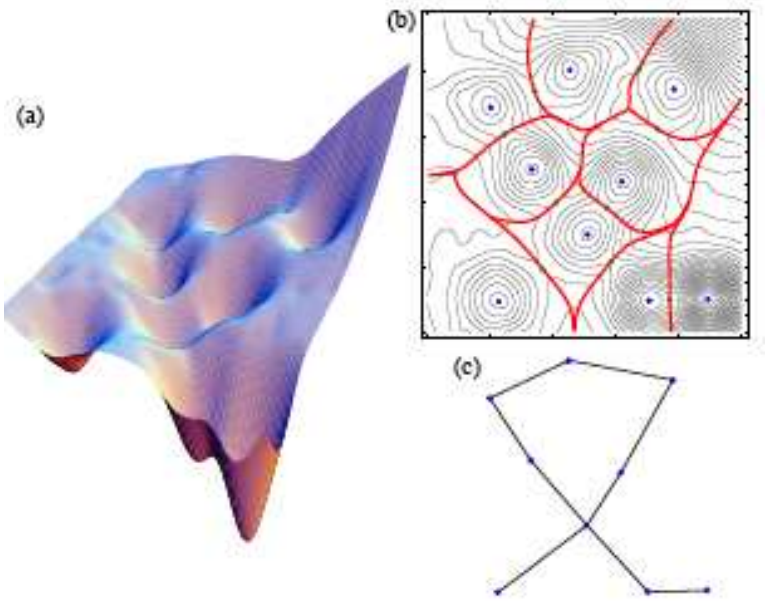
Small – world networks (Watts and Strogatz, 1998)

- 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

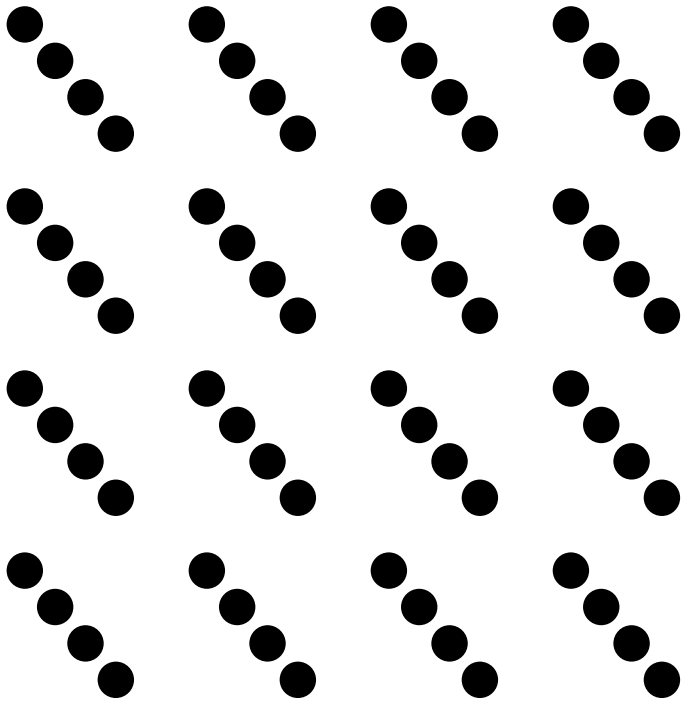
c landscape as a network

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

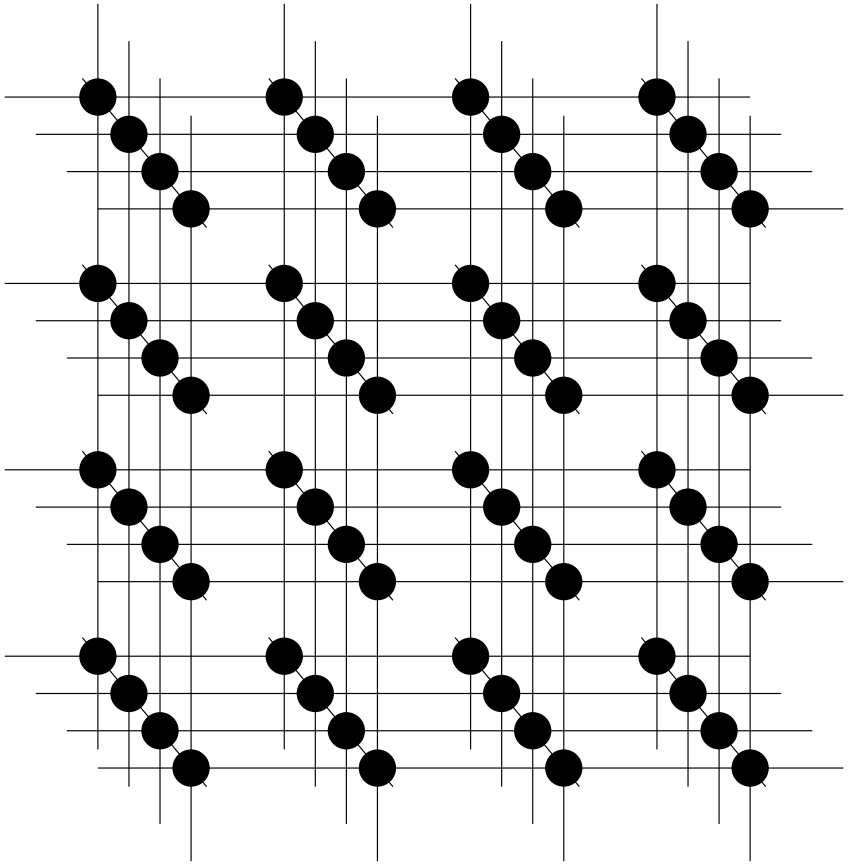
Example of small NK landscape with $N = 6$ and $K = 2$



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

Basins of attraction in combinatorial optimisation

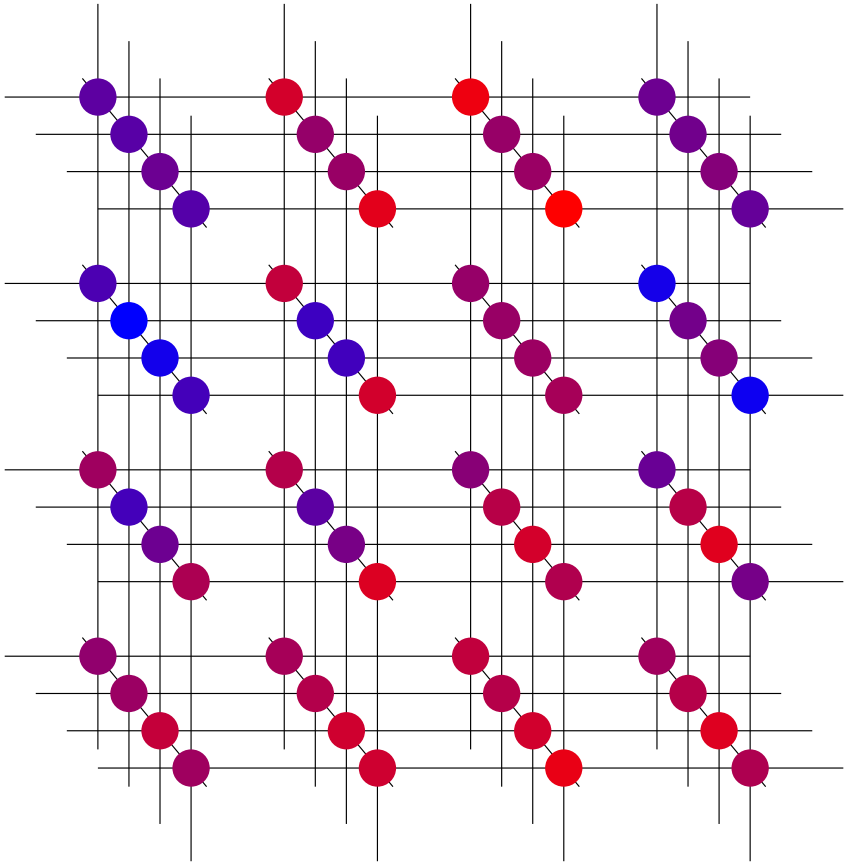
Example of small NK landscape with $N = 6$ and $K = 2$



- 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 $K = 2$

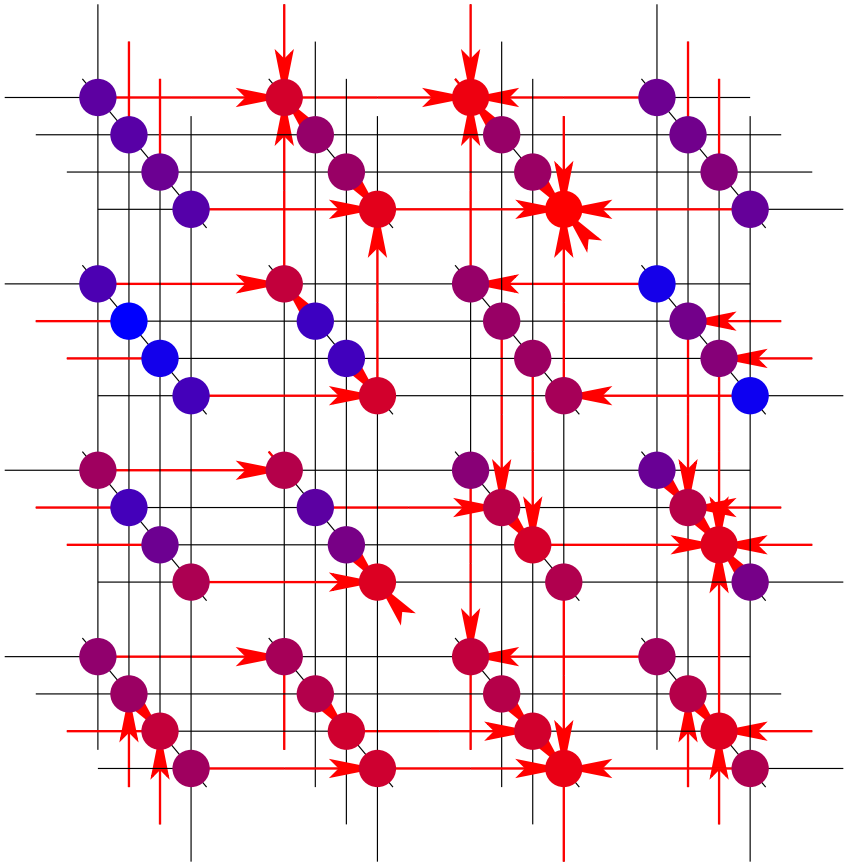


Color represent fitness value

- high fitness
- low fitness

Basins of attraction in combinatorial optimisation

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



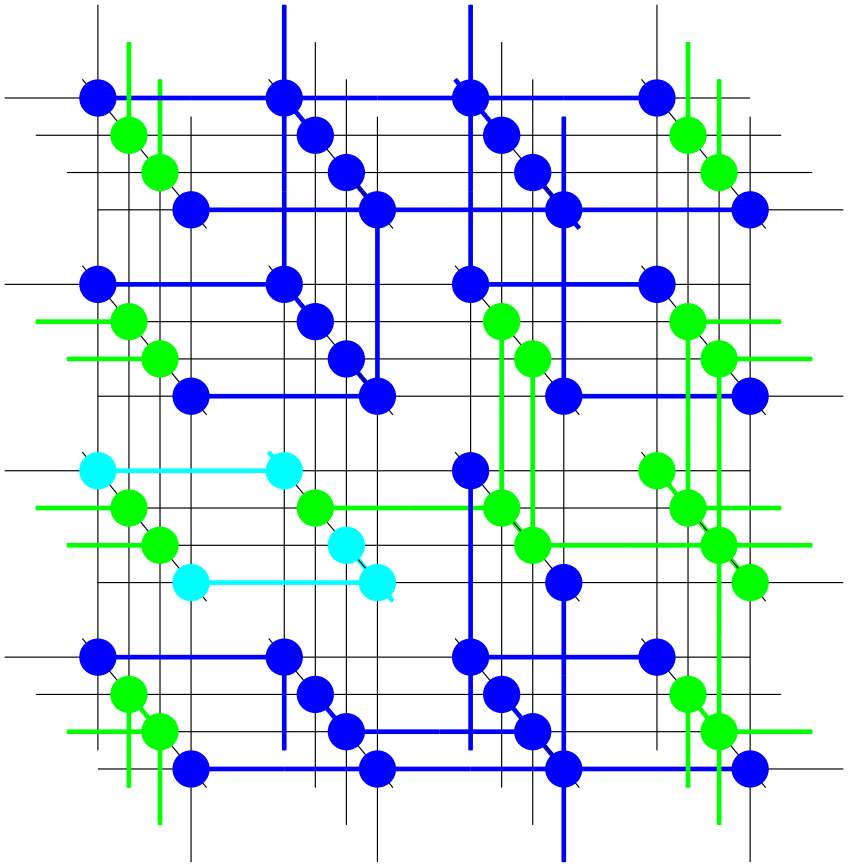
- Color represent fitness value
  - high fitness
  - low fitness
- $\longrightarrow$ point towards the solution with highest fitness in the neighborhood

Exercise :

Why not make a Hill-Climbing walk on it ?

Basins of attraction in combinatorial optimisation

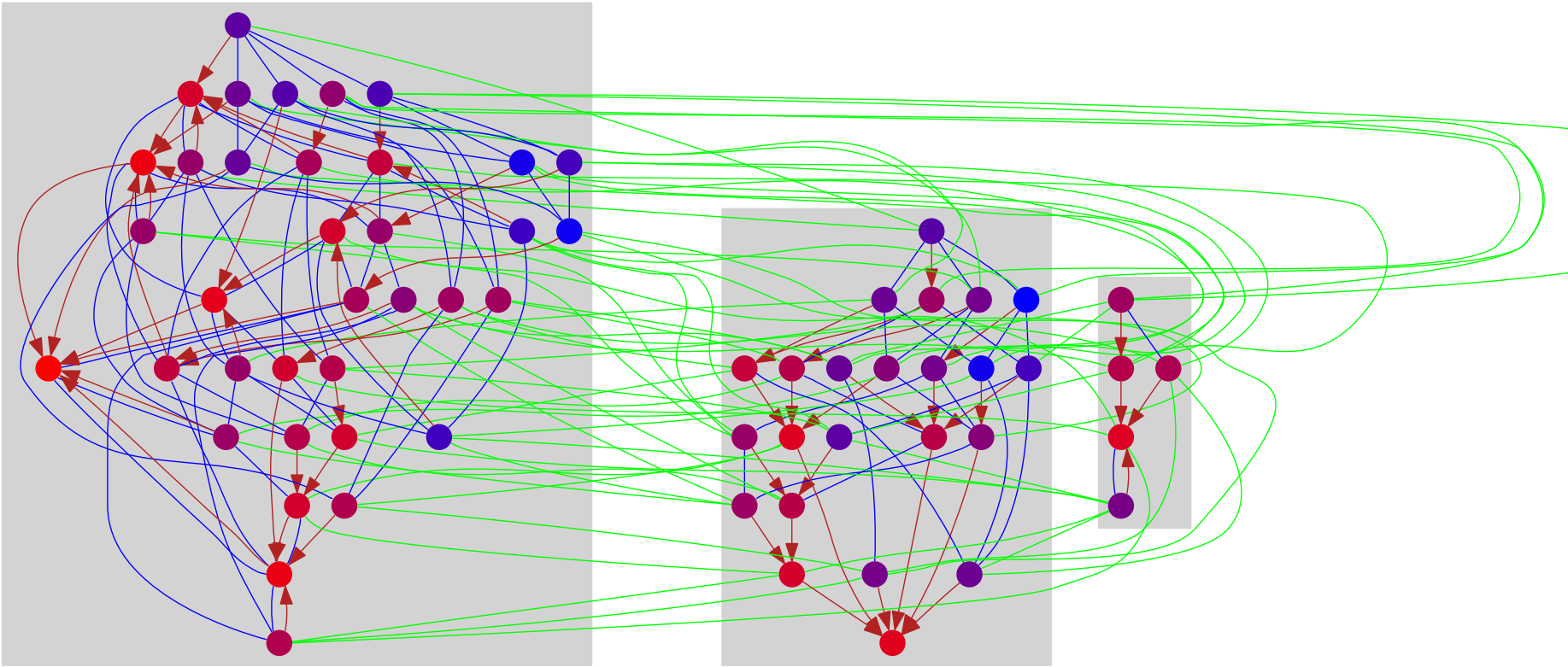
Example of small NK landscape with $N = 6$ and $K = 2$



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

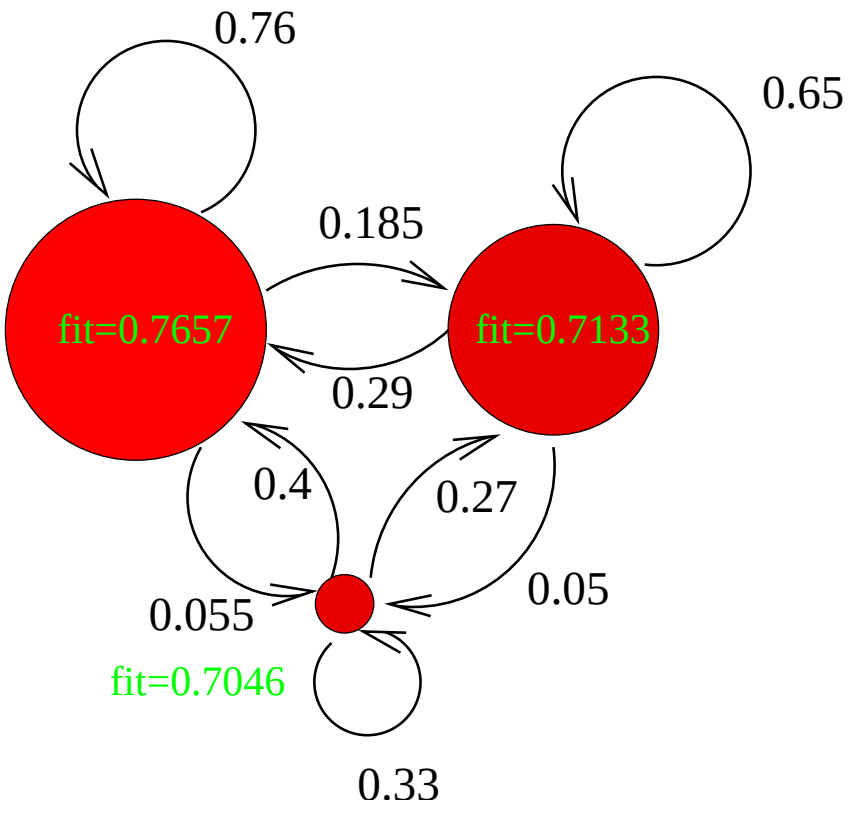
Basins of attraction in combinatorial optimisation

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^* :

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

local optima network

Local optima network

- Nodes : set of local optima $\mathcal{S}^*$
- Edges : notion of connectivity between basins of attraction
  - e_{ij} between i and j if there is at least a pair of neighbours s_i and $s_j \in \mathcal{N}(s_i)$ 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 [34], Phys. Rev. E 2008 [30], CEC 2010)
  - Escape edges : e_{ij} between i and j if
    Basins j which can be reached from the local optima i (Artificial Evolution 2011 [31])

Basin edges : Weights of edges

- From each s and $s^{'}$, $p(s \rightarrow s^{'}) = \mathbb{P}(s^{'} = op(s))$

  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 $s^{'} \notin \mathcal{N}(s)$, $p(s \rightarrow s^{'}) = 0$

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

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

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

- 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 $s^{'} \in b_j$:

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

Escape edges

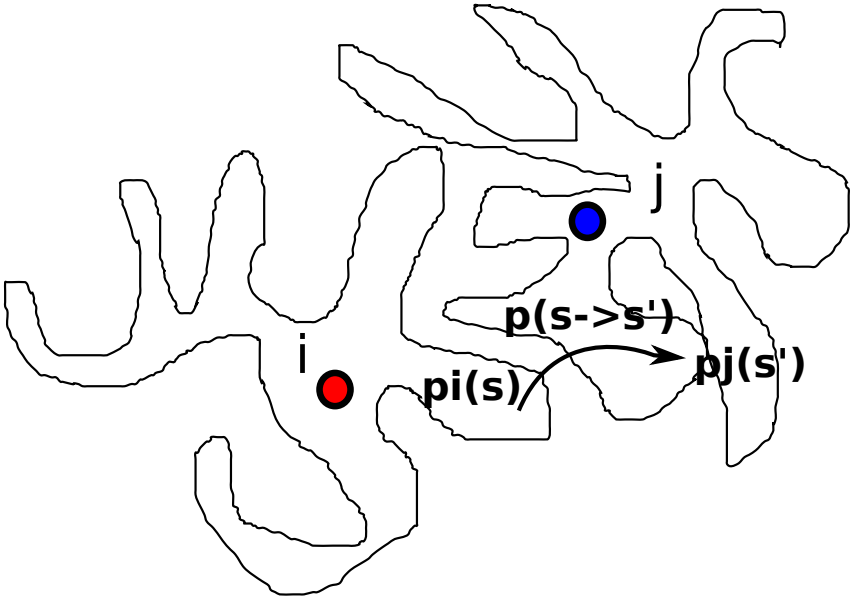
Escape edges

Given distance function d, and positive integer $D > 0$.

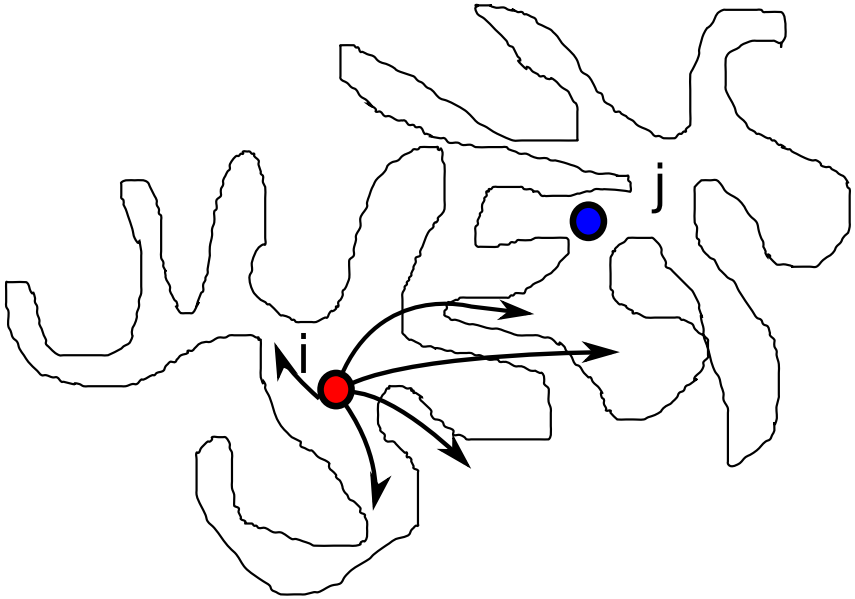
- e_{ij} between LO_i and LO_j :
  if it exists a solution s such that : $d(s, LO_i) \leq D$ and $h(s) = LO_j$.
- Weight w_{ij} of e_{ij} :
  $\sharp\{s \in S \mid d(s, LO_i) \leq D \text{ and } h(s) = LO_j\}$
  normalized by $\sharp\{s \in S \mid d(s, LO_i) \leq D\}$.

$\Rightarrow$ local optima network : weighted oriented graph

Basin edges *vs.* Escape edges



Basin edges



Escape edges

NK fitness landscapes : ruggedness and epistasis

NK-landscapes : Model of problems

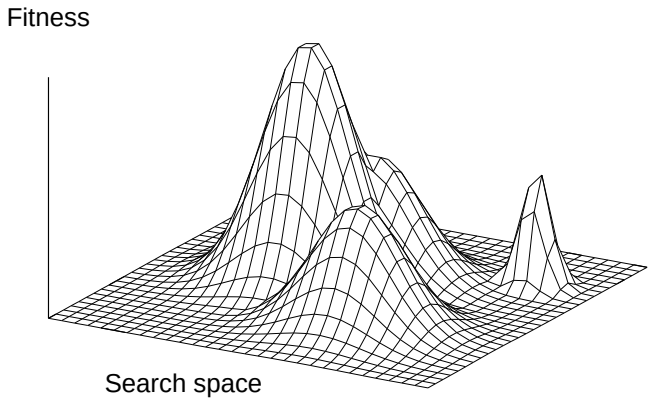
N size of the bit-strings
K from 0 to $N-1$, NK landscapes can be tuned from smooth to rugged (easy to difficult respectively) :

- $K = 0$ 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

Remember : Multimodal Fitness landscapes

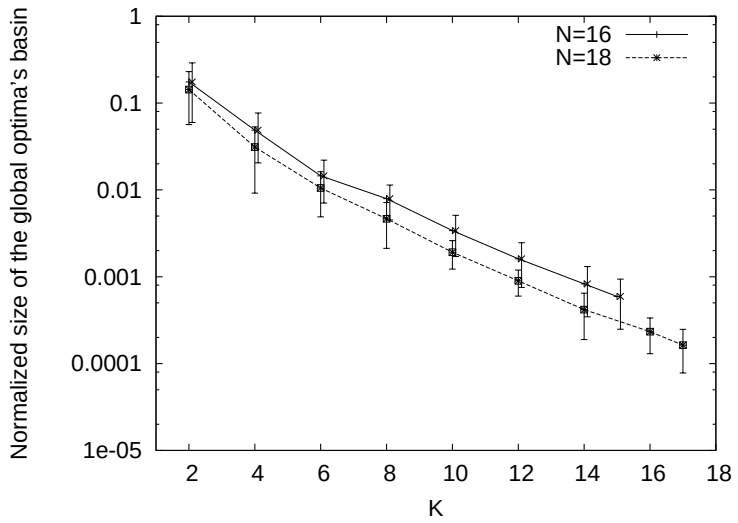


Optimisation difficulty :
number and size of attractive basins (Garnier *et al* [10])

The idea :

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

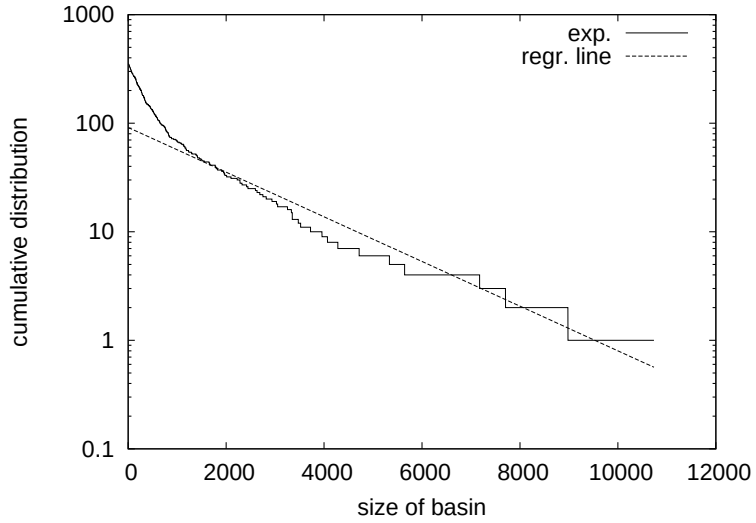
Global optimum basin size versus K



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

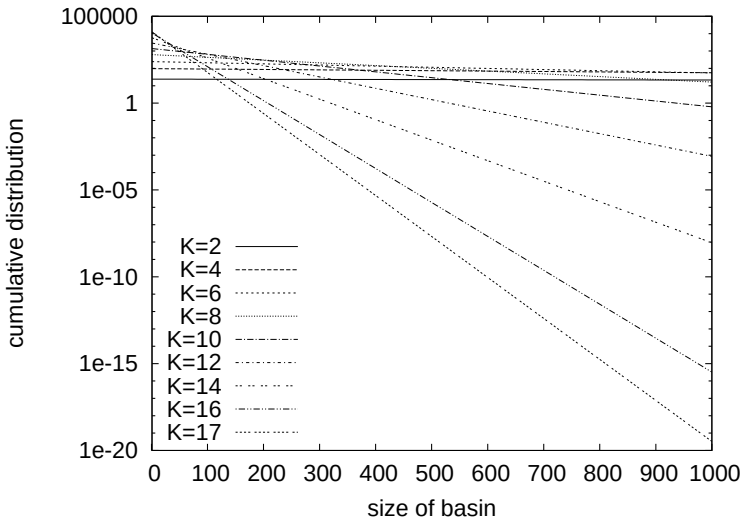
Analysis of basins : basin size



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

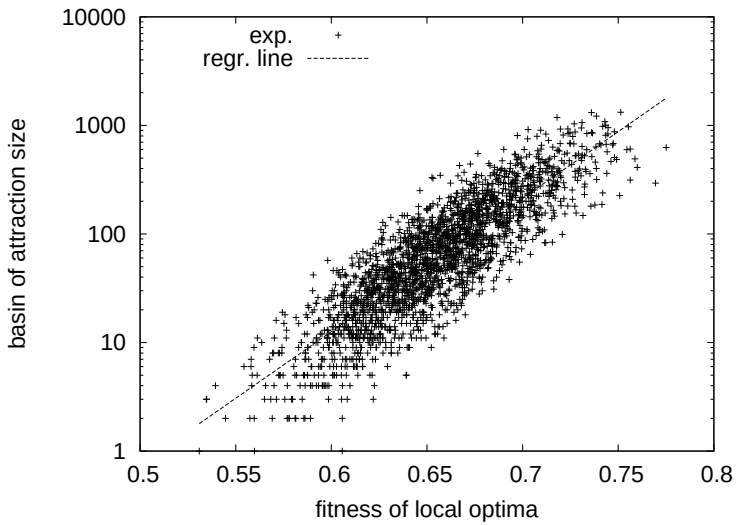
- Trend : small number of large basin, large number of small basin
- Log-normal cumulative distribution : not uniform !
- Slope of correlation increases with K
- When K large : basin sizes are nearly equals the distribution becomes more uniform

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

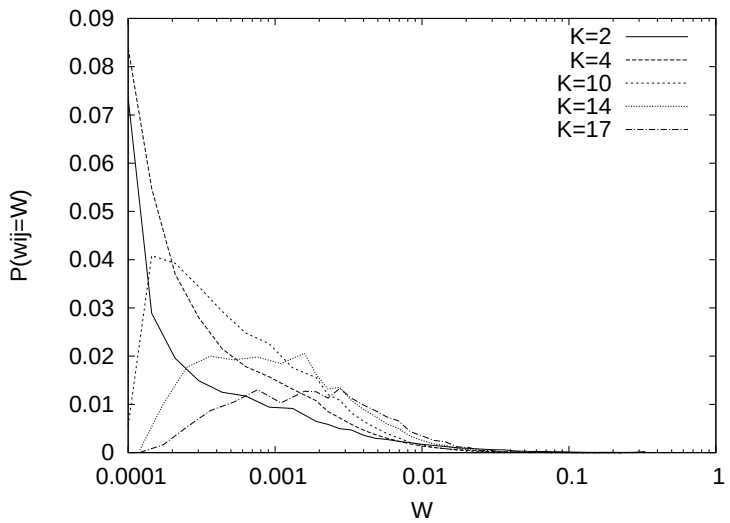
$$Y_2(i) = \sum_{j \neq i} \left(\frac{w_{ij}}{s_i} \right)^2$$

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

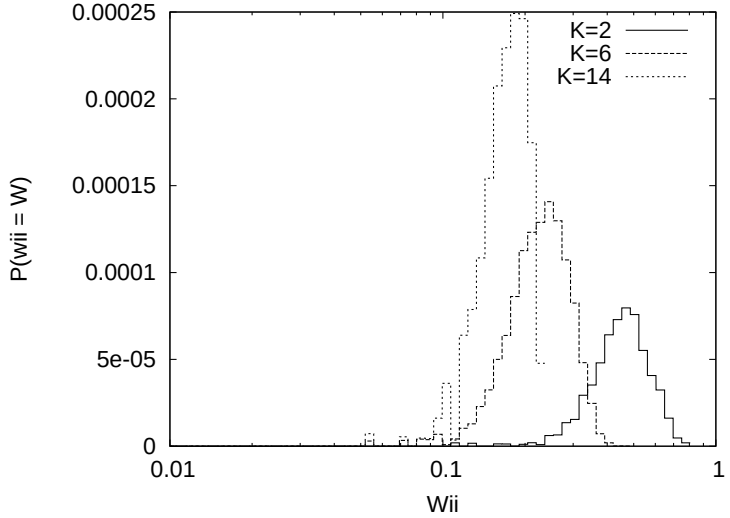
Weights distribution : transition probability between basins



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



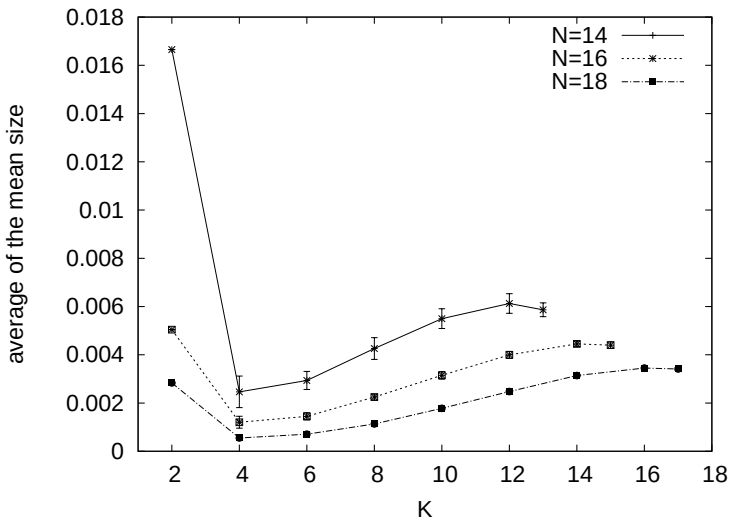
Average weight w_{ii} according to the parameter N and K

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



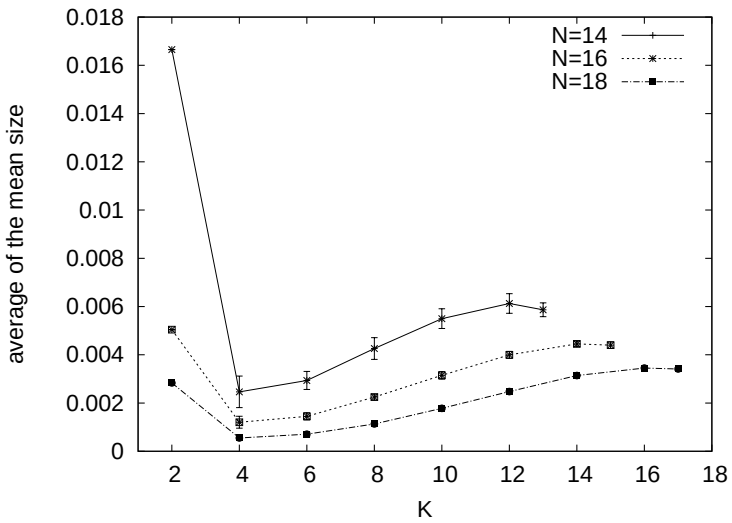
Average of the mean size of basins interiors

Question :

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

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

Interior and border size



Average of the mean size of basins interiors

Question :

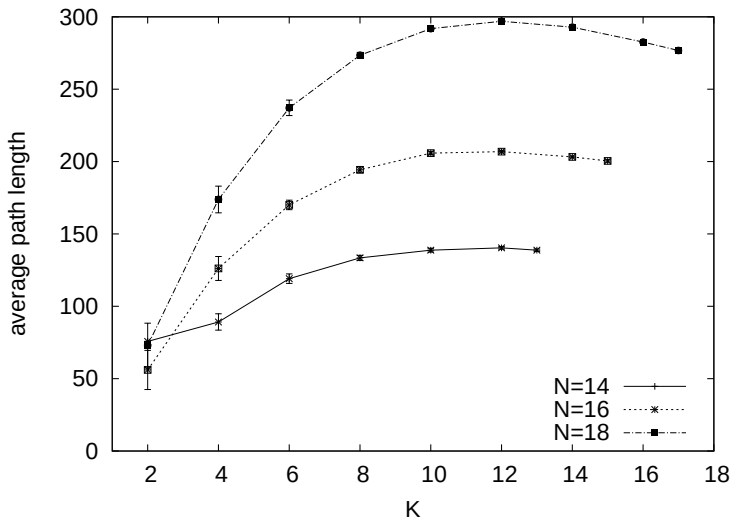
Do basins look like a "montain" with interior and border ?

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



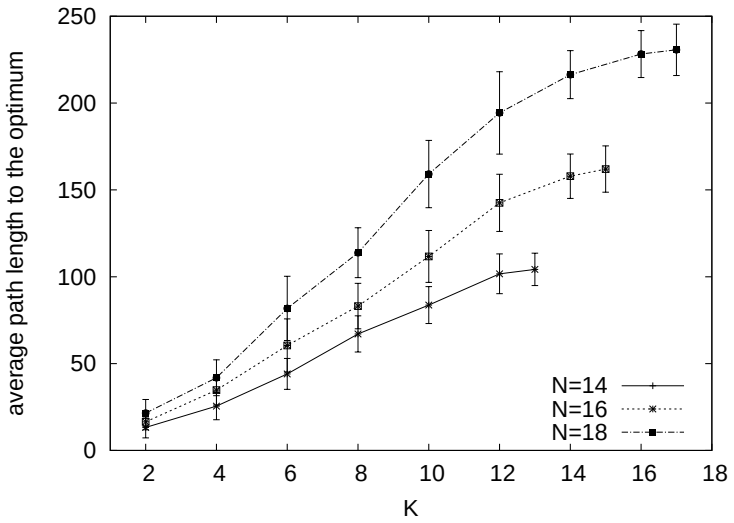
Average distance (shortest path) between nodes

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 ?

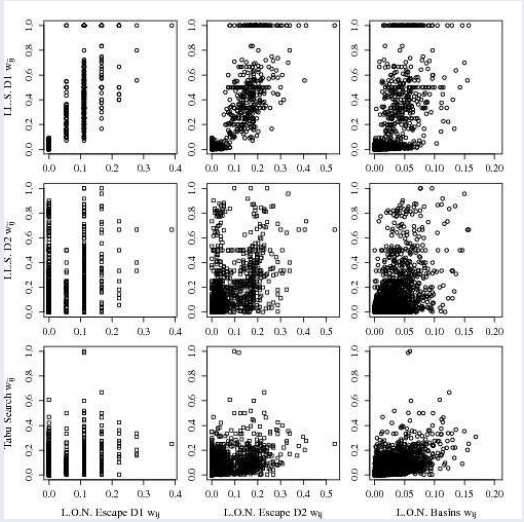
- More relevant for optimisation
- Increase steadily with increasing K

Summary on local optima network

- Medium level of description : proposed characterization of combinatorial landscapes as networks
- a new model for landscape analysis
- New findings about basin's structure : sizes, fitness *vs.* size, etc.
- Related some *network features* to *search difficulty*

Summary on local optima network

- Related some *network features* to *search difficulty*



- Weights edges of NK-landscapes LON
- Effective frequencies of TS and ILS from one basin to another

Wednesday, July 11th, 14 :32 "Local Optima Networks and the Performances of ILS", F. Daolio *et al.*

Continuous problems

Fitness landscape – FiL $(\mathcal{X}, \mathcal{N}, f)$

- $\mathcal{X} = \mathbb{R}^n$
- $\mathcal{N}$ defined by gaussian mutation
- $f : \mathbb{R}^n \rightarrow \mathbb{R}$

P. Caamano, A. Prieto, J.A. Becerra, F. Bellas and R.J. Duro, Real Valued Multimodal Fitness Landscape Characterization for Evolution, Lecture Notes in Computer Sciences, vol. 6443, pp. 567-574, Springer-Verlag, 2010

Function	m	Attr. Basin Size		Distance	
		Largest	Optimum	lar.-opt.	Maxima
f_1 Cosine	$\approx 5^n$	$2.60E{-2}$	$2.60E{-2}$	$0.00E{+0}$	$2.15E{-1}$
f_2 Rastrigin	$\approx 11^n$	$8.00E{-3}$	$8.00E{-3}$	$0.00E{+0}$	$4.86E{-1}$
f_3 Schwefel	$\approx 8^n$	$2.36E{-1}$	$2.96E{-5}$	$9.20E{-1}$	$9.20E{-1}$
f_4 Ackleys	$\approx 65^n$	$1.00E{-3}$	$1.00E{-3}$	$0.00E{+0}$	$5.00E{-1}$
f_5 Griewank	$\approx 4^n$	$1.00E{-3}$	$2.00E{-4}$	$3.97E{-1}$	$4.55E{-1}$
f_6 Levy	$\approx 5^n$	$5.77E{-1}$	$5.77E{-1}$	$0.00E{+0}$	$2.61E{-1}$
f_7 Penalized1	$\approx 5^n$	$1.28E{-1}$	$1.28E{-1}$	$0.00E{+0}$	$1.13E{-1}$
f_8 Penalized2	$\approx 5^n$	$1.74E{-1}$	$1.74E{-1}$	$0.00E{+0}$	$5.00E{-2}$

Function	Dim.	CMA		DE	
		SR	SP	SR	SP
f_1 Cosine	5	1.00	2636.60	**1.00**	**2232.84**
f_2 Rastrigin	5	0.08	621949.00	**1.00**	**5142.76**
f_3 Schwefel	5	0.08	608619.00	**1.00**	**7483.64**
f_4 Ackleys	5	**1.00**	**1864.60**	1.00	5171.72
f_5 Griewank	5	0.04	1232999.00	**1.00**	**19992.92**
f_6 Levy	5	**1.00**	**815.00**	1.00	2210.80
f_7 Penalized1	5	**1.00**	**1484.20**	1.00	2759.96
f_8 Penalized2	5	**1.00**	**2074.60**	1.00	2869.88

Continuous fitness landscapes

Main difficulty

- Which step size to define the neighborhood ? 10^{-3} ?
  - Different step size, different landscape ?
  - Use the standard definition of LO ?
    $\exists \epsilon > 0,\ \forall x,\ |x - x^\star| \leq \epsilon \Rightarrow f(x) \leq f(x^\star)$
- Toward measure like $||f(x) - f(y)||/||x - y||$?
- But is it better than derivate function ?

Continuous fitness landscapes

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- Which step size to define the neighborhood ? 10^{-3} ?
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    $\exists \epsilon > 0,\ \forall x,\ |x - x^\star| \leq \epsilon \Rightarrow f(x) \leq f(x^\star)$
- Toward measure like $||f(x) - f(y)||/||x - y||$?
- But is it better than derivate function ?

Personal fealing

Main different between combinatorial and continuous FiL

- No search "direction" in combinatorial problem
- Probability to improve the current solution
- Shape of the attraction basins

Multiobjective optimization

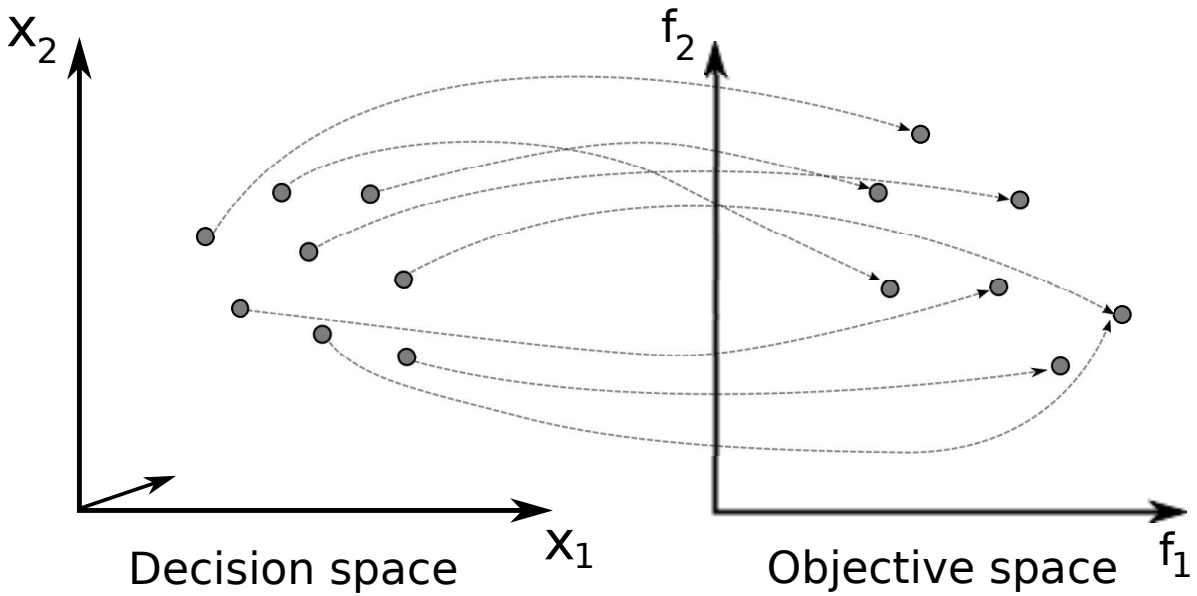
What is the structure of a mutiobjective search space ?

Have you seen the multiobjective tutorial by Dimo Brockhoff ?

Multiobjective optimization

Multiobjective optimization problem

- $\mathcal{X}$: set of feasible solutions in the decision space
- $M \geqslant 2$ objective functions $f = (f_1, f_2, \ldots, f_M)$ (to maximize)
- $\mathcal{Z} = f(\mathcal{X}) \subseteq \mathbb{R}^M$: set of feasible outcome vectors in the objective space

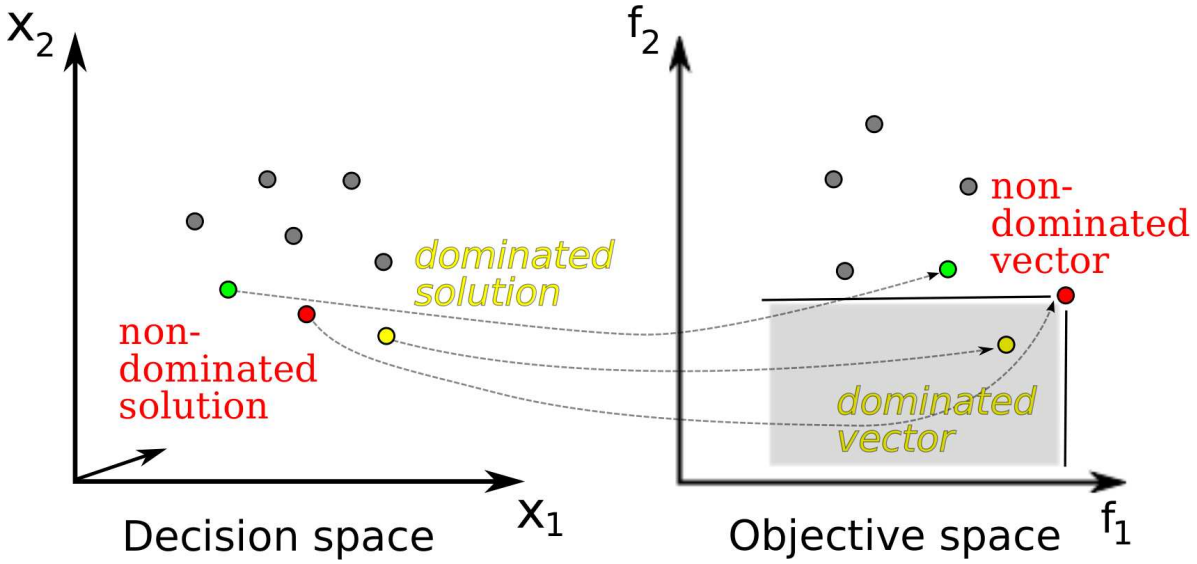


Definition

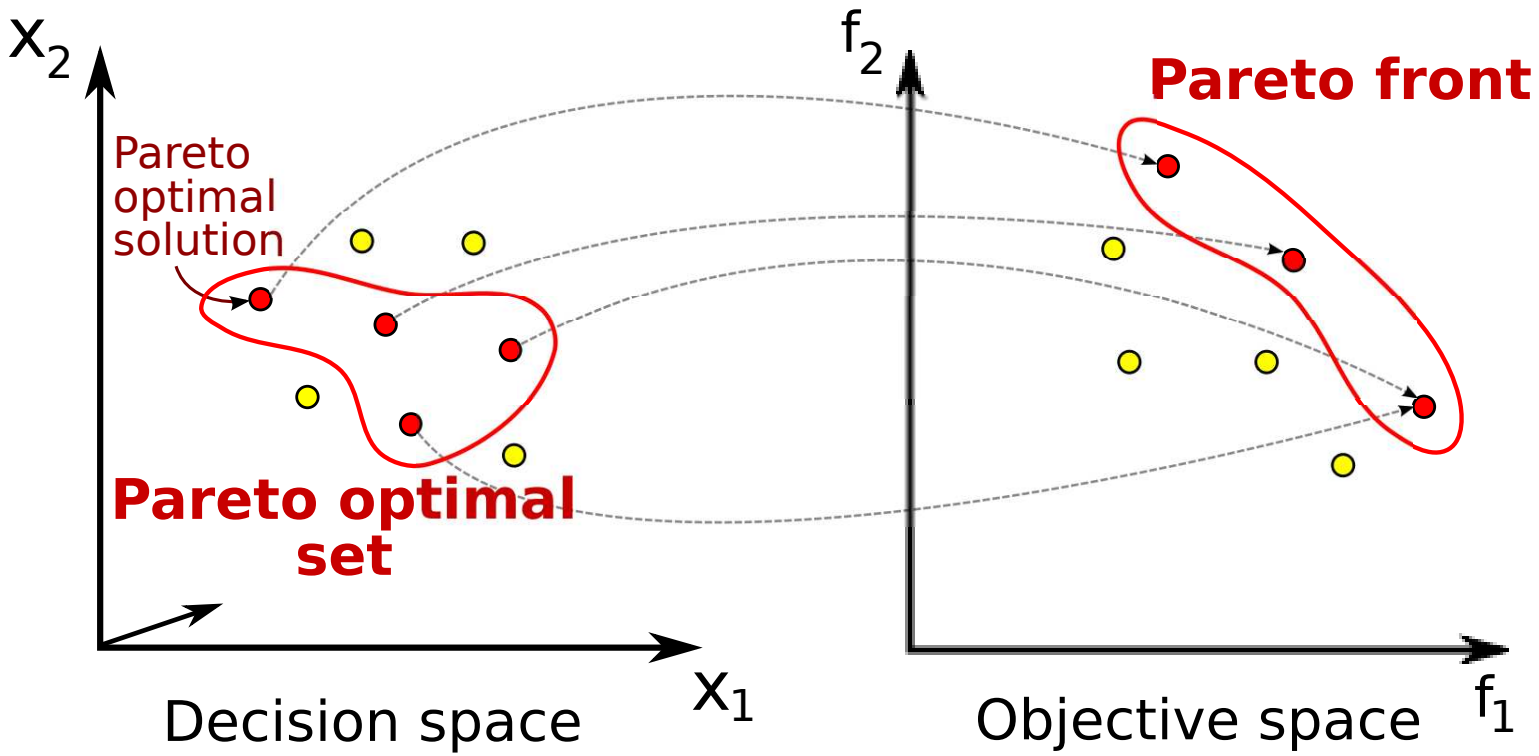
Pareto dominance relation

A solution $x \in \mathcal{X}$ dominates a solution $x' \in \mathcal{X}$ ($x' \prec x$) iff

- $\forall i \in \{1, 2, \ldots, M\}$, $f_i(x) \geqslant f_i(x')$
- $\exists j \in \{1, 2, \ldots, M\}$ such that $f_j(x) > f_j(x')$



Pareto set, Pareto front



Set-based multiobjective fitness landscape

Definition

A set-based multiobjective fitness landscape is defined as a triplet $(\Sigma, \mathtt{N}, \mathtt{I})$ such that :

- $\Sigma \subset 2^{\mathcal{X}}$ is a set of feasible solution-sets (where $\mathcal{X}$ is the set of feasible solutions)
- $\mathtt{N} : \Sigma \rightarrow 2^{\Sigma}$ is a neighborhood relation between solution-sets
- $\mathtt{I} : \Sigma \rightarrow \mathbb{R}$ is a unary quality indicator, *i.e.* a fitness function measuring the quality of solution-sets

State-of-the-art tools from single-objective FiL can be reused

Set-based search space

Illustrative examples

- Population-based approaches
  $\Sigma = \{\sigma \in 2^{\mathcal{X}} \ : \ |\sigma| = \mu\}$, where μ is the population size
- Bounded archive-based approaches
  $\Sigma = \{\sigma \in 2^{\mathcal{X}} \ : \ |\sigma| \leqslant \mu\}$, where μ is the max archive size
- Dominance-based approaches (with mutually *n-d* solutions)
  $\Sigma = \{\sigma \in 2^{\mathcal{X}} \ : \ \forall s, s' \in \sigma, s \not\prec s'\}$
- Bounded archive- + Dominance-based approaches
  $\Sigma = \{\sigma \in 2^{\mathcal{X}} \ : \ |\sigma| \leqslant \mu \text{ and } \forall s, s' \in \sigma, s \not\prec s'\}$
- No restriction
  $\Sigma = 2^{\mathcal{X}}$
- ...

Set-based neighborhood relation

Illustrative examples

- Set-level replacement neighborhood
  $\sigma' = \sigma \cup \{s'\} \setminus \{s\}$ such that $s \in \sigma$, $s' \in \mathcal{N}(s)$
  $\rightarrow |\mathbb{N}(\sigma)| \leqslant |\sigma| \cdot \sum_{s \in \sigma} |\mathcal{N}(s)|$
- Set-level insertion neighborhood
  $\sigma' = \sigma \cup \{s'\}$ such that $s \in \sigma$, $s' \in \mathcal{N}(s)$
  $\rightarrow |\mathbb{N}(\sigma)| \leqslant \sum_{s \in \sigma} |\mathcal{N}(s)|$
- Set-level deletion neighborhood
  $\sigma' = \sigma \setminus \{s\}$ such that $s \in \sigma$
  $\rightarrow |\mathbb{N}(\sigma)| = |\sigma|$
- ... (recombination)

Set-based fitness function

Illustrative example : **hypervolume** ($\mathtt{I}_H$)

- Compliant with the (weak) Pareto dominance relation
  $\rightarrow A \prec B \Rightarrow \mathtt{I}_H(A) \leqslant \mathtt{I}_H(B)$
- A single parameter : the reference point
- Minimal solution-set maximizing $\mathtt{I}_H$
  $\rightarrow$ subset of the Pareto optimal set

$$\arg\max_{\sigma \in \Sigma} \ \mathtt{I}_H(\sigma)$$

Main Fitness Landscape measures can be used

Ruggedness, autocorrelation

→ Based on random walk sampling

- Is the fitness of neighboring solutions random ?

Autocorrelation length $\tau = \frac{1}{\rho}$, with ρ correlation $(f(s), f(s'))$, $s' \in \mathcal{N}(s)$

small τ : rugged landscape | large τ : smooth landscape

Local optima

→ Based on adaptive walk sampling

- What is the number of local optima, and the size of basins ?

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

small $\mathcal{L}$: high multi-modality	large $\mathcal{L}$: low multi-modality
(many local optima, small basin size)	(few local optima, large basin size)

What is the structure of the search space ?

Facts

- Very large search space
- Very large neighborhood
- High computational cost to compute the fitness

What is the structure of the search space ?

Facts

- Very large search space
- Very large neighborhood
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Open questions

(combinatorial) multiobjective problems :

- Escaping from local loptima ?
- Exploring the neighborhood is an optimization problem ?

Summary on fitness landscapes

Fitness landscape is a representation of

- search space
- notion of neighborhood
- fitness of solutions

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 (design, tune or 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 ?

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

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