2. Two typical geometries of fitness landscapes

Fitness landscape analysis for understanding and designing local search heuristics

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Outline of this part

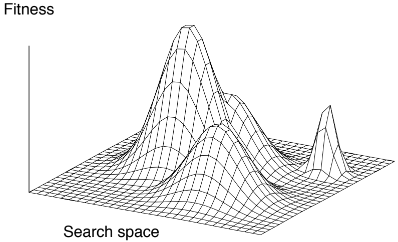
- Basis of fitness landscape :
  - introductory example *(Done)*
  - brief history and background of fitness landscape *(Done)*
  - fundamental definitions *(Done)*
- **Two typical geometries of fitness landscapes** :
  - multimodality
  - ruggedness
  - neutrality
  - neutral networks

Multimodal Fitness landscapes

Local optima s^*

no neighbor solution with strictly higher fitness value (maximization)

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



Typical example : bit strings

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

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

Example :
$x = 01101$ and $f_1(x) = f_2(x) = f_3(x) = 5$

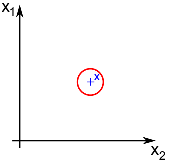
	11101	00101	01001	01111	01100
f_1	4	2	3	0	3
f_2	2	3	6	2	3
f_3	1	5	2	2	4

Question

Is x is a local maximum for f_1, f_2, and/or f_3 ?

Not so typical example : continuous optimization

Still an open question...



Search space : $X = [0,1]^d$

$$\mathcal{N}_\alpha(x) = \{y \in X \mid \|y - x\| \leqslant \alpha\}$$

with $\alpha > 0$

Classical definition of local optimum

x is local maximum iff

$$\exists \varepsilon > 0, \forall y \text{ such that } \|y - x\| \leqslant \varepsilon,\ f(y) \leqslant f(x)$$

Questions

Local search definition with $\mathcal{N}_\alpha \Rightarrow$ classical definition ?

Classical definition $\Rightarrow$ local search definition with $\mathcal{N}_\alpha$?

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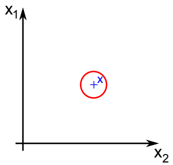

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Classical definition $\Rightarrow$ local search definition with $\mathcal{N}_\alpha$?

Still some works to do...

Sampling local optima

Basic estimator (Alyahya, K., & Rowe, J. E. 2016 [AR16])

Expected proportion of local optima :

Proportion of local optima in a sample of random solutions

- Complexity : $n \times |\mathcal{N}|$
- Pros :
  unbiased estimator
- Cons :
  poor estimation when expected proportion is lower than $1/n$

Sampling local optima by adaptive walks

Adaptive walk

$(x_1, x_2, \ldots, x_\ell)$ such that $x_{i+1} \in \mathcal{N}(x_i)$ and $f(x_i) < f(x_{i+1})$

Sampling local optima by adaptive walks

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Hill-Climbing algorithm (first-improvement)

Choose initial solution $x \in X$
repeat
    choose $x' \in \{y \in \mathcal{N}(x) \mid f(y) > f(x)\}$
    if $f(x) < f(x')$ **then**
        $x \leftarrow x'$
    end if
until x is a Local Optimum

Sampling local optima by adaptive walks

Adaptive walk

$$(x_1, x_2, \ldots, x_\ell) \text{ such that } x_{i+1} \in \mathcal{N}(x_i) \text{ and } f(x_i) < f(x_{i+1})$$

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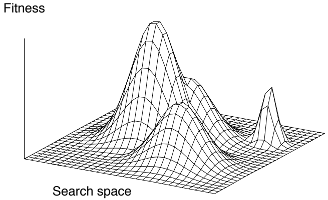
Basin of attraction of x^*

$$\{x \in X \mid HillClimbing(x) = x^*\}.$$

Multimodal Fitness landscapes and difficulty



The idea :

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

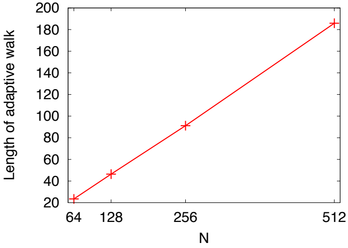
Optimisation difficulty :
Number and size of attractive basins (Garnier *et al.* [GK02])

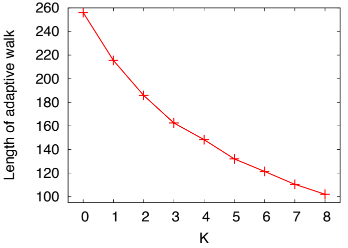
Feature to estimate basin size :

- **Length of adaptive walks**

complexity : sample size $\times \ell \times |\mathcal{N}|$

Multimodal Fitness landscapes and difficulty





ex. nk-landscapes with $n = 512$

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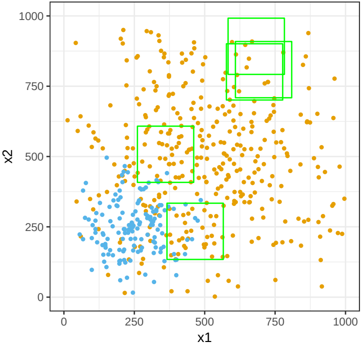
complexity : sample size $\times \ell \times |\mathcal{N}|$

Practice : the Squares Problem

a program design problem ?

Squares Problem (SP)

Find the position of 5 squares in order to maximize inside squares the number of brown points without blue points



Candidate solutions

$$X = ([0,1000] \times [0,1000])^5$$

	x_1	x_2
1	577	701
2	609	709
3	366	134
4	261	408
5	583	792

Fitness function

$f(x) =$ number of brown points $-$ number of blue points inside squares

Source code in R : ex01.R

Source code : `http://www-lisic.univ-littoral.fr/~verel/`

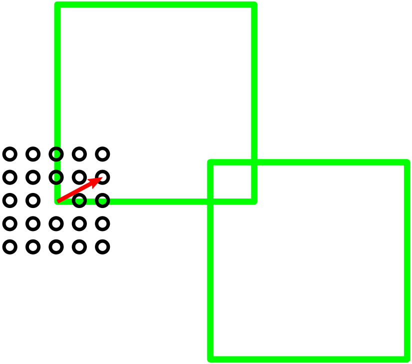
Different functions are already defined :

- `main` : example to execute the following functions
- `draw` and `draw_solution` :
  draw a problem and the squares of a solution
- `fitness_create` :
  create a fitness function from a data frame of points
- `pb1_create` and `pb2_create` :
  create two particular SP problems
- `init` :
  create a random solution with *n* squares
- `hc_ngh` :
  hill-climbing local search based on neighborhood

Neighborhood

Questions

- Execute line by line the `main` function
- Define the `neighborhood_create` which creates a neighborhood : a neighbor move one square



Adaptive walks to compare problem difficulty

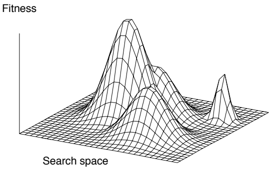
Pre-defined functions :

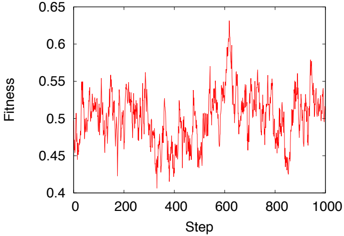
- `adaptive_length` :
  run the hill-climber and compute a data frame with the length of adaptive walks
- `main_adaptive_length_analysis` :
  Compute the adaptive length of two different SP problems

Questions

- Execute line by line the `main_adaptive_length_analysis` function to compute a sample of adaptive walk lengths.
- Compare the lengths of adaptive walks for the two SP problems.
- Which one is the more multi-modal ?

Random Walk to measure the ruggedness





Random walk :

- $(x_1, x_2, \ldots)$ where $x_{i+1} \in \mathcal{N}(x_i)$ and equiprobability on $\mathcal{N}(x_i)$

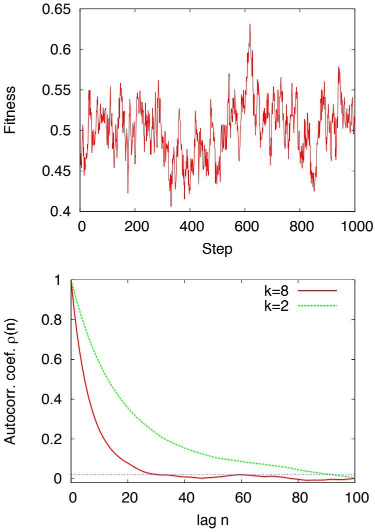
The idea :

- if the profile of fitness is irregular,
- then, the "information" between neighbors is low.

Feature :

- Study the fitness profile like a signal

Rugged/smooth fitness landscapes



Autocorrelation function of time series of fitnesses along a random walk (Weinberger 90 [Wei90]) :

$$\rho(n) = \frac{\mathrm{E}[(f(x_i) - \bar{f})(f(x_{i+n}) - \bar{f})]}{\mathrm{var}(f(x_i))}$$

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

"How many random steps such that correlation becomes insignificant"

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

complexity : sample size $\approx 10^3$

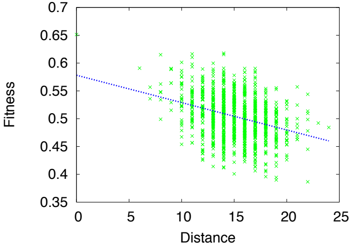
Results on rugged fitness landscapes (Stadler 96 [Sta96])

Ruggedness decreases with the size of thoses problems

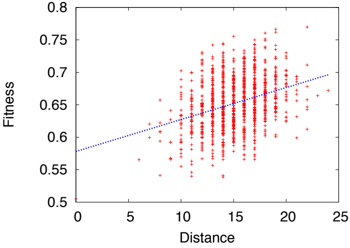
Problem	parameter	$\rho(1)$
symmetric TSP	n number of towns	$1 - \frac{4}{n}$
anti-symmetric TSP	n number of towns	$1 - \frac{4}{n-1}$
Graph Coloring Problem	n number of nodes α number of colors	$1 - \frac{2\alpha}{(\alpha-1)n}$
NK landscapes	N number of proteins K number of epistasis links	$1 - \frac{K+1}{N}$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

Fitness Distance Correlation (FDC) (Jones 95 [Jon95])

Correlation between fitness and distance to global optimum



easy



hard

Classification based on experimental studies :

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

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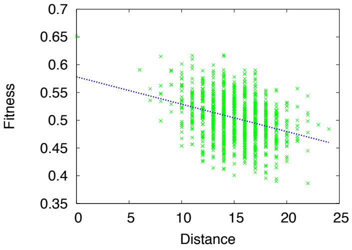

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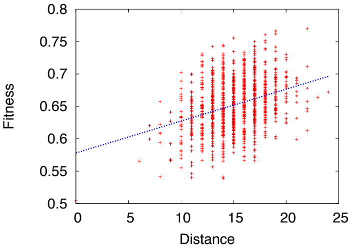


hard

- Important concept to understand
- Not useful in "practice" (difficult to estimate)

Practice : computation the autocorrelation function

Source code `exo02.R` :

- `mutation_create` :
  Create a mutation operator,
  modify each square according to rate p,
  a new random value from $[(x-r, y-r), (x+r, y+r)]$.
- `main` :
  Code to obtain autocorrelation function

Questions

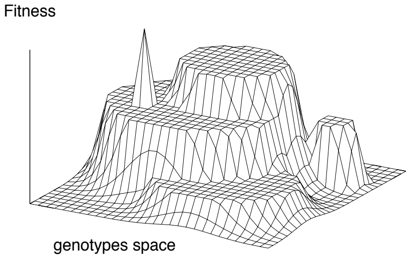
- Define the function `random_walk` to compute the fitness values during a random walk.
- Execute line by line the `main` function to compute a sample of fitness value collected during a random walk.
- Compare the first autocorrelation coefficient of the SP problems 1 and 2.

Neutral Fitness Landscapes

Neutral theory (Kimura ≈ 1960 [Kim83])

Theory of mutation and random drift

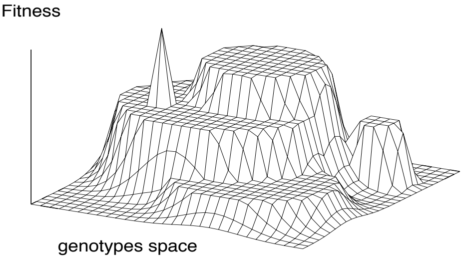
A considerable number of mutations have no effects on fitness values



- plateaus
- neutral degree
- neutral networks [Schuster 1994 [SFSH94], RNA folding]

Neutral Fitness Landscapes

- Redundant problem (symmetries, etc.) [GS87]
- Problem “not well” defined or dynamic environment [IT04]
- Unused variables, discrete values, etc.



Real-world problems :

- Robot controler
- Circuit design
- Genetic Programming
- Protein folding
- Learning problems
- Scheduling problems
- Graph problems...

Neutrality and difficulty

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

Solving optimization problem and neutrality

3 ways to deals with neutrality :

- Decrease the neutrality : reduce the entropy barrier
- Increase the neutrality : reduce the fitness barrier
- Unchange the neutrality : use a specific algorithm

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** :
  From a non-optimal solution, hard trap functions are more difficult than needle-in-a-haystack functions
- **Good information** is better than **No information** :
  Onemax problem is much easier than needle-in-a-haystack functions

Neutrality and difficulty

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

Objects of neutral fitness landscapes

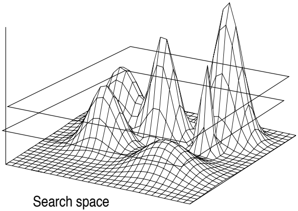
Description of multimodal fitness landscapes is based on :

- Local optima
- Basins of attraction

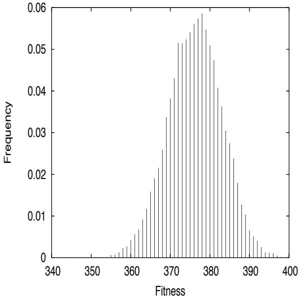
Description of neutral fitness landscapes is based on :

- **Neutral sets** :
  set of solutions with the same fitness
- **Neutral networks** :
  neutral sets with neighborhood relation

Neutral sets : Density Of States



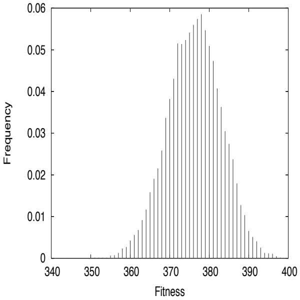
Set of solutions with fitness value



Density of states (D.O.S.)

- Introduce in physics (Rosé 1996 [REA96])
- Optimization (Belaidouni, Hao 00 [BH00])

Neutral sets : Density Of States



Informations given :

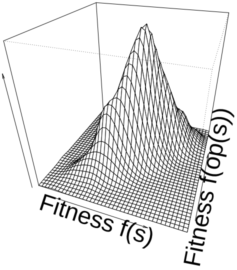
- Performance of random search
- Tail of the distribution is an indicator of difficulty :
  - the faster the decay, the harder the problem
- But do not care about the neighborhood relation

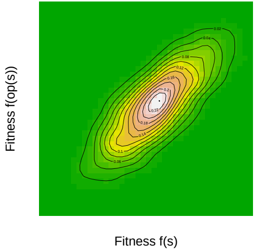
Features :

- **Average**, **sd**, **kurtosis**, etc.

complexity : sample size

Neutral sets : Fitness Cloud [Verel et al. 2003]





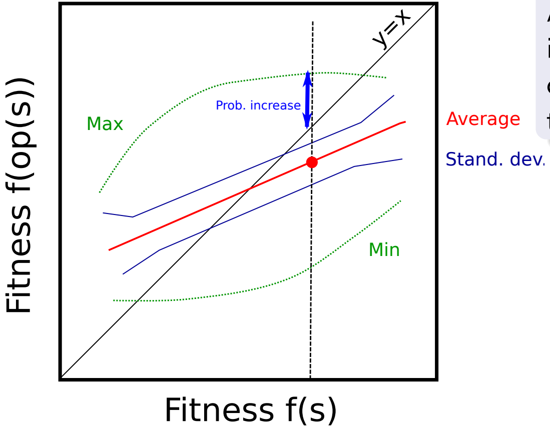
- $(X, \mathcal{F}, \Pr)$: probability space
- $op : X \to X$ stochastic operator of the local search

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

Fitness Cloud of *op*

Conditional probability density function of Y given X

Fitness cloud : Measure of evolvability



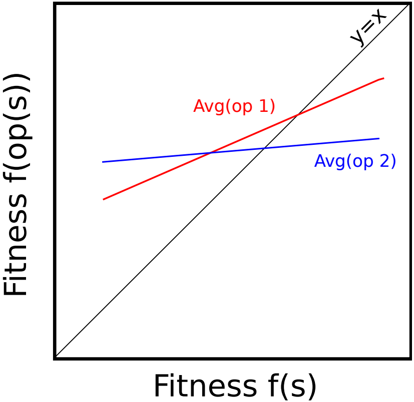
Evolvability

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 : Comparison of difficulty

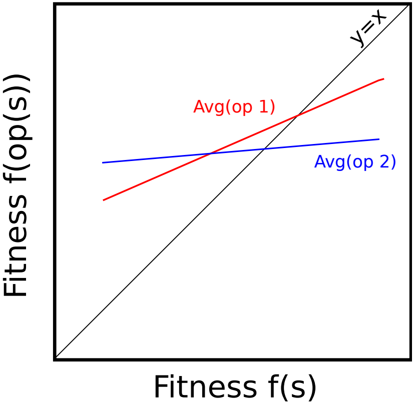
Average of evolvability



- Operator 1 ? ? Operator 2

Fitness cloud : Comparison of difficulty

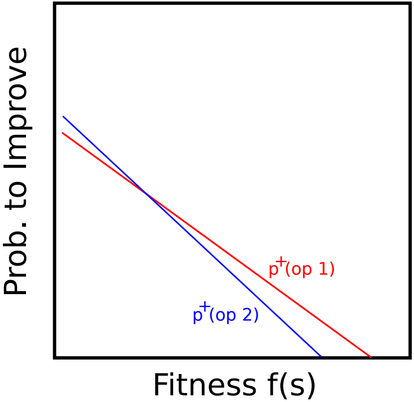
Average of evolvability



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

Fitness cloud : Comparison of difficulty

Probability to improve



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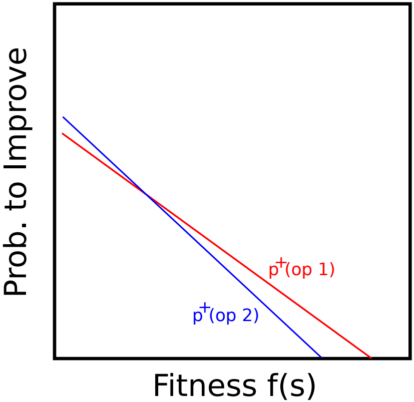
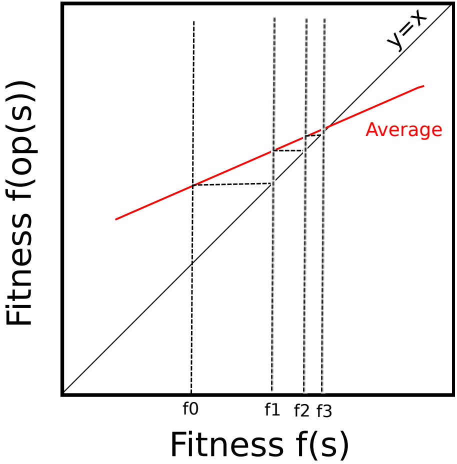
Fitness cloud : Comparison of difficulty

Probability to improve



- Operator 1 > Operator 2
- Prob. to improve of 1 is often higher than Prob. to improve of 2
- Probability to improve is often a line
- See also works on fitness-probability cloud (G. Lu, J. Li, X. Yao [LLY11])
- See theory of EA and fitness level technics.

Fitness cloud : estimation of convergence point

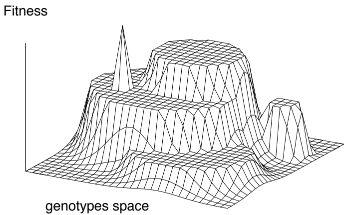


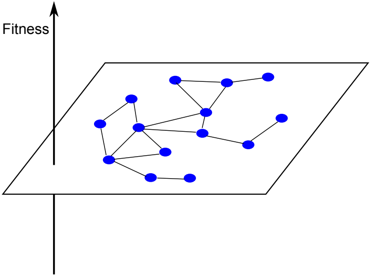
- Approximation (only approximation) of the fitness value after few steps of local operator
- Indication on the quality of the operator
- See fitness level technic

Outline

- 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) :
  $\Rightarrow$ neutral sets with neighborhood relation : graph

Neutral networks (Schuster 1994 [SFSH94])





Basic definition of Neutral Network

Node = solution with same fitness value

Edge = neighborhood relation

Definitions

Test of neutrality

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

For example, $isNeutral(x_1, x_2)$ is *true* if :

- $f(x_1) = f(x_2)$.
- $|f(x_1) - f(x_2)| \leqslant 1/M$ with M is the search population size.
- $|f(x_1) - f(x_2)|$ 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

$W_{neut} = (x_0, x_1, \ldots, x_m)$

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

Neutral Network

graph $G = (N, E)$

- $N \subset X$: for all s and $s^{'}$ from N, there is a neutral walk belonging to N from s to $s^{'}$,
- $(x_1, x_2) \in E$ if they are neutral neighbors : $x_2 \in \mathcal{N}_{neut}(x_1)$

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

Practice : computation of the neutral rate

The neutral rate is the proportion of neutral neighbors.
It can be estimated by a random walk :

$$\frac{\sharp\{(x_t, x_{t+1}) \ : \ f(x_t) = f(x_{t+1}), t \in \{1, \ell - 1\}\}}{\ell - 1}$$

Source code `exo03.R` :

- `main` :
  Code to compute the neutral rates

Questions

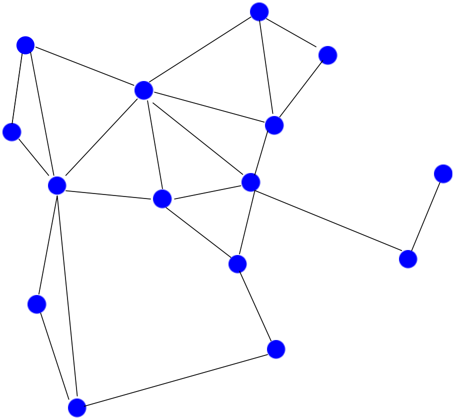
- Define the function `neutral_rate` to compute the neutral rate estimated with a random walk.
- Execute the `main` function to compute the neutral rate.
- Compare the neutrality of the SP problems 1 and 2.

Features inside neutral network

Classical graph metrics :

1. **Size of NN** :
   - number of nodes of NN,
2. **Neutral degree distribution** :
   - measure of the quantity of "neutrality"
3. **Autocorrelation of neutral degree** (Bastolla 03 [BPRV03]) during neutral random walk :
   - comparaison with random graph,
   - measure of the correlation structure of *NN*

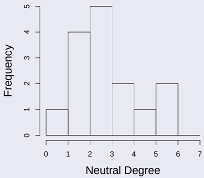
Features inside neutral network



1. **Size**

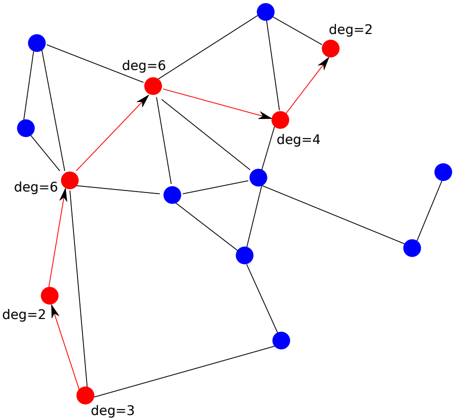
   avg,distribution,etc.

2. **Neutral degree distribution**



3. **Autocorrelation of neutral degree**
   - random walk on NN
   - autocorr. of degrees

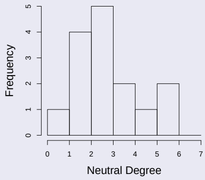
Features inside neutral network



1. **Size**

   avg,distribution,etc.

2. **Neutral degree distribution**



3. **Autocorrelation of neutral degree**
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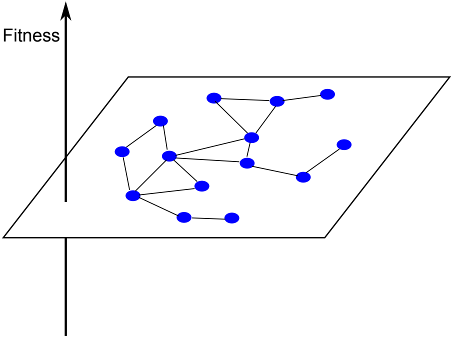
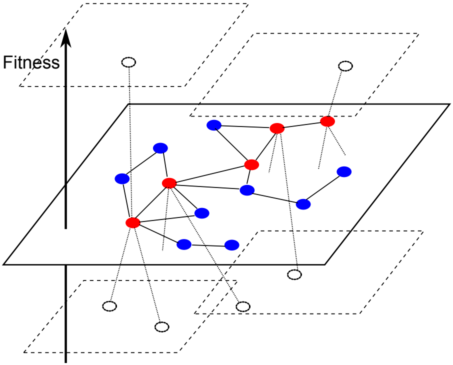
   - autocorr. of degrees

Features between neutral networks



1. **Rate of innovation** (Huynen 96 [Huy96]) : the number of new accessible structures (fitness) per mutation
2. **Autocorrelation of evolvability** [VCC06] : autocorrelation of the sequence $(evol(x_0), evol(x_1), \ldots)$.

Features between neutral networks



1. **Rate of innovation** (Huynen 96 [Huy96]) : the number of new accessible structures (fitness) per mutation
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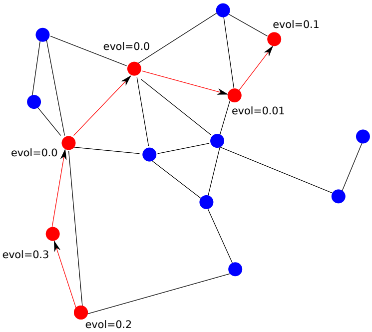
Features between neutral networks



- Autocorrelation of evolvability :
  - Autocorrelation of $(evol(x_0), evol(x_1), \ldots)$.
  - Evolvability *evol* :
    - average fitness in the neigh.
    - prob. to improve, etc.
- Informations :
  - if high correlation $\Rightarrow$ "easy" (you can use this information)
  - if low correlation $\Rightarrow$ "difficult"

Summary of neutral fitness landscapes features

- Density of States :
  Size of neutral sets
- Fitness cloud and related statistics :
  Evolvability of solutions
- Neutral degrees distribution :
  "How neutral is the fitness landscape ?"
- Autocorrelation of neutral degrees :
  Network "structure"
- Autocorrelation of evolvability :
  Evolution of evolvability on NN

Practice : Performance *vs.* fitness landscape features

Explain the performance of ILS with fitness landscape features ?

- 20 random SP problems have been generated : `pb_xx.csv`
- The performance of Iterated Local Search have been computed in `perf_ils_xx.csv` (30 runs)
- Goal : regression of ILS performance with fitness landscape features

Practice : Performance *vs.* fitness landscape features

Source code `exo04.R` :

- `fitness_landscape_features` :
  Compute the basic fitness landscape features
- `random_walk_samplings` :
  Random walk sampling on each problem (save into file)
- `fitness_landscape_analysis` :
  Compute the features for each problems
- `ils_performance` :
  Add the performance of ILS into the data frame
- `main` :
  Execute the previous functions.

Practice : Performance *vs.* fitness landscape features

Questions

- What are the features computed by the function `fitness_landscape_features`?
- Execute the `random_walk_samplings` function to compute the random walks samplings.
- Compute the correlation plots between features and ILS performance (use ggpairs).
- Compute the linear regression of performance with fitness landscape features.

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