

Generalised Local Search Machines and Fitness Landscape Characterisation

FIT4012 Advanced topics in computational science

This material is based on the book 'Stochastic Local Search: Foundations and Applications' by Holger H. Hoos and Thomas Stützle (Morgan Kaufmann, 2004)
- see www.sls-book.net for further information.

August 26, 2014

The Basic GLSM Model

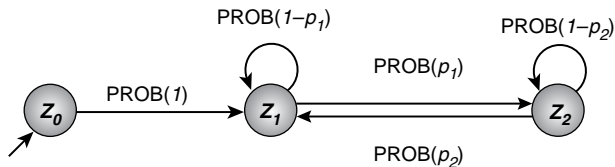
Many high-performance SLS methods are based on combinations of *simple (pure) search strategies* (e.g., ILS, MA).

These hybrid SLS methods operate on two levels:

- ▶ **lower level:** execution of underlying simple search strategies
- ▶ **higher level:** activation of and transition between lower-level search strategies.

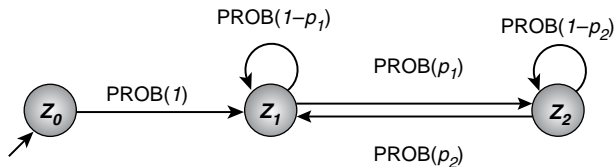
Key idea: Explicitly represent higher-level search control mechanism in the form of a *finite state machine*.

Example: Simple 3-state GLSM



- ▶ States z_0, z_1, z_2 represent simple search strategies, such as Random Picking (for initialisation), Iterative Best Improvement and Uninformed Random Walk.
- ▶ $\text{PROB}(p)$ refers to a probabilistic state transition with probability p after each search step.

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Generalised Local Search Machines (GLSMs)

- ▶ States \cong simple search strategies.
- ▶ State transitions \cong search control.
- ▶ GLSM \mathcal{M} starts in initial state.
- ▶ In each iteration:
 - ▶ \mathcal{M} executes one search step associated with its current state z ;
 - ▶ \mathcal{M} selects a new state (which may be the same as z) in a nondeterministic manner.
- ▶ \mathcal{M} terminates when a given termination criterion is satisfied.

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Formal definition of a GLSM

A *Generalised Local Search Machine* is defined as a tuple

$\mathcal{M} := (\mathbf{Z}, \mathbf{z}_0, M, m_0, \Delta, \sigma_Z, \sigma_\Delta, \tau_Z, \tau_\Delta)$ where:

- ▶ \mathbf{Z} is a set of states;
- ▶ $\mathbf{z}_0 \in \mathbf{Z}$ is the *initial state*;
- ▶ M is a set of *memory states* (as in SLS definition)
- ▶ m_0 is the *initial memory state* (as in SLS definition);
- ▶ $\Delta \subseteq \mathbf{Z} \times \mathbf{Z}$ is the *transition relation*;
- ▶ σ_Z and σ_Δ are sets of *state types* and *transition types*;
- ▶ $\tau_Z : \mathbf{Z} \mapsto \sigma_Z$ and $\tau_\Delta : \Delta \mapsto \sigma_\Delta$ associate every state z and transition (z, z') with a state type $\sigma_Z(z)$ and transition type $\tau_\Delta((z, z'))$, respectively.

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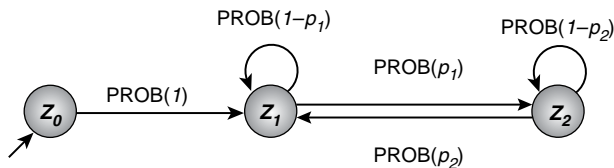
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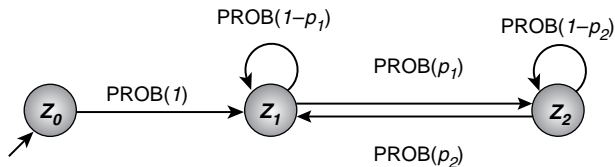
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Example: Simple 3-state GLSM (formal definition)



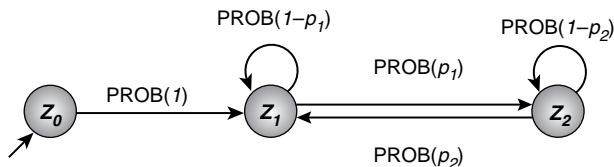
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- ▶ $\Delta := \{(z_0, z_1), (z_1, z_2), (z_1, z_1), (z_2, z_1), (z_2, z_2)\}$
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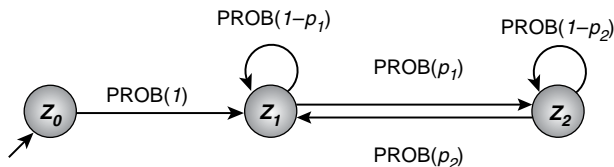
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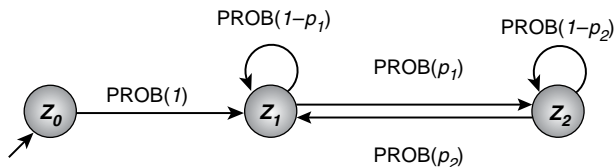
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- ▶ *Transition types* formally represent mechanisms used for switching between GLSM states.
- ▶ σ_Z, σ_Δ should include only state and transition types that are actually used in given GLSM ('no junk').
- ▶ Not all states in Z may actually be reachable when running a given GLSM.
- ▶ *Termination condition* is not explicitly captured in GLSM model, but considered part of the execution environment.

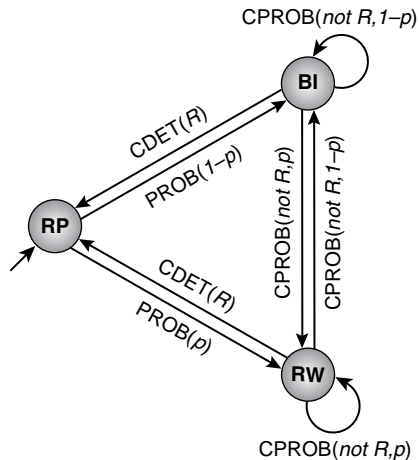
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Example: Randomised Iterative Best Improvement with Random Restart



GLSM Semantics

Behaviour of a GLSM is specified by *machine definition* + *run-time environment* comprising specifications of

- ▶ state types,
- ▶ transition types;
- ▶ problem instance to be solved,
- ▶ search space,
- ▶ solution set,
- ▶ neighbourhood relations for subsidiary SLS algorithms;
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Run GLSM \mathcal{M} :

set *current machine state* to z_0 ; set *current memory state* to m_0 ;

While *termination criterion* is not satisfied:

perform *search step* according to type of current machine state;
this results in a new *search position*

select *new machine state* according to *types of transitions*
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GLSMs are factored representations of SLS strategies

- ▶ GLSM represents the way in which *initialisation* and *step function* of a hybrid SLS method are composed from respective functions of *subsidiary component SLS methods*.
- ▶ When modelling hybrid SLS methods using GLSMs, *subsidiary SLS methods* should be as simple and pure as possible, leaving *search control* to be represented explicitly at the GLSM level.
- ▶ *Initialisation* is modelled using *GLSM states* (advantage: simplicity and uniformity of model).
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State, Transition and Machine Types

In order to completely specify the search method represented by a given GLSM, we need to define:

- ▶ the GLSM model (states, transitions, ...);
- ▶ the search method associated with each *state type*, i.e., step functions for the respective subsidiary SLS methods;
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State types

- ▶ State type semantics are often most conveniently specified procedurally.
- ▶ *initialising state type* = state type τ for which search position after one τ step is independent of search position before step.
initialising state = state of initialising type.
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Transitions types

- ▶ *Unconditional deterministic transitions* – type *DET*:
 - ▶ executed always and independently of memory state or search position;
 - ▶ every GLSM state can have at most one outgoing DET transition;
 - ▶ frequently used for leaving initialising states.
- ▶ *Conditional probabilistic transitions* – type *PROB(p)*:
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- ▶ DET transitions are a special case of PROB transitions.
- ▶ For a GLSM \mathcal{M} any state that can be reached from initial state z_0 by following a chain of $\text{PROB}(p)$ transitions with $p > 0$ will eventually be reached with arbitrarily high probability in any sufficiently long run of \mathcal{M} .
- ▶ In any state z with a $\text{PROB}(p)$ self-transition (z, z) with $p > 0$, the number of GLSM steps before leaving z is distributed geometrically with mean and variance $1/p$.

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 - ▶ executed with probability proportional to p iff *condition predicate* C is satisfied;
 - ▶ all CPROB transitions from the current GLSM state whose condition predicates are not satisfied are *blocked*, i.e., cannot be executed.
- ▶ Special cases of $CPROB(C, p)$ transitions:
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Commonly used simple condition predicates

\top	always true
$\text{count}(k)$	total number of GLSM steps $\geq k$
$\text{countm}(k)$	total number of GLSM steps modulo $k = 0$
$\text{scount}(k)$	number of GLSM steps in current state $\geq k$
$\text{scountm}(k)$	number of GLSM steps in current state modulo $k = 0$
lmin	current candidate solution is a local minimum w.r.t. the given neighbourhood relation
$\text{evalf}(y)$	current evaluation function value $\leq y$
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All based on local information; can also be used in negated form.

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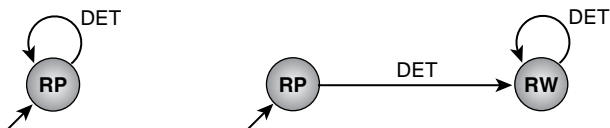
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Transition actions

- ▶ Associated with individual transitions; provide mechanism for modifying current memory states.
- ▶ Performed whenever GLSM executes respective transition.
- ▶ Modify memory state only, *cannot* modify GLSM state or search position.
- ▶ Have read-only access to search position and can hence be used to memorise current candidate solution.
- ▶ Can be added to any of the previously defined transition types.

Modelling SLS Methods Using GLSMs

Uninformed Picking and Uninformed Random Walk



procedure *step-RP*(π, s)

input: *problem instance* $\pi \in \Pi$,
candidate solution $s \in S(\pi)$

output: *candidate solution* $s \in S(\pi)$

$s' := \text{selectRandom}(S)$;

return s'

end *step-RP*

procedure *step-RW*(π, s)

input: *problem instance* $\pi \in \Pi$,
candidate solution $s \in S(\pi)$

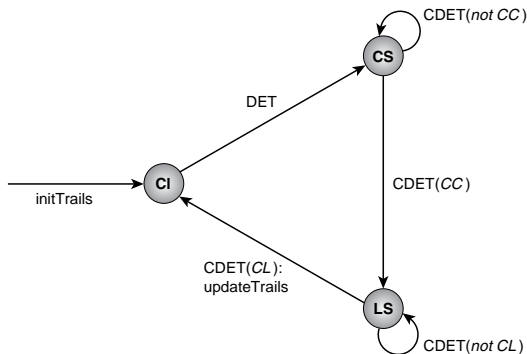
output: *candidate solution* $s \in S(\pi)$

$s' := \text{selectRandom}(N(s))$;

return s'

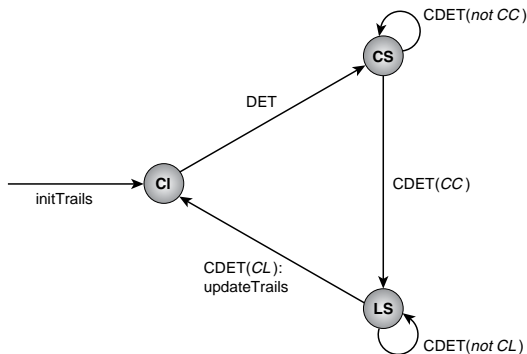
end *step-RW*

Ant Colony Optimisation



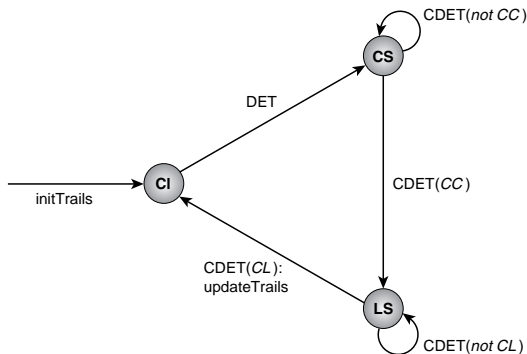
- ▶ The condition predicate *CC* determines the end of the construction phase.
- ▶ The condition predicate *CL* determines the end of the local search phase; in many algorithms, $CL := l_{min}$.

Ant Colony Optimisation



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- ▶ The condition predicate **CL** determines the end of the local search phase; in many algorithms, $CL := lmin$.

Ant Colony Optimisation



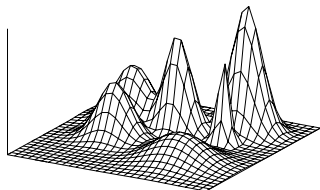
- ▶ The condition predicate *CC* determines the end of the construction phase.
- ▶ The condition predicate *CL* determines the end of the local search phase; in many algorithms, $CL := lmin$.

Fitness Landscape Characterisation

- ▶ study the search space
- ▶ description of the search space 'geometry'
- ▶ to understand what makes problems difficult
- ▶ to design effective search algorithms

Fitness landscapes in biology

Origin in biological science: Wright 1932 [45]

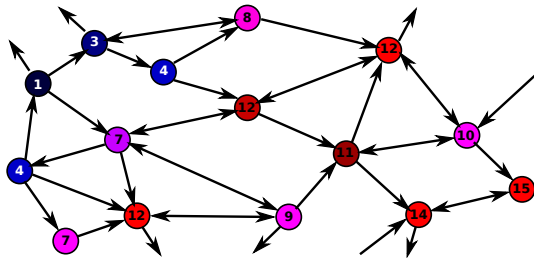


Fitness landscape is a graph (S, N, f)

- ▶ S is the search space
- ▶ $N : S \rightarrow 2^S$ is a neighbourhood relation
- ▶ $f : S \rightarrow R$ is a objective function

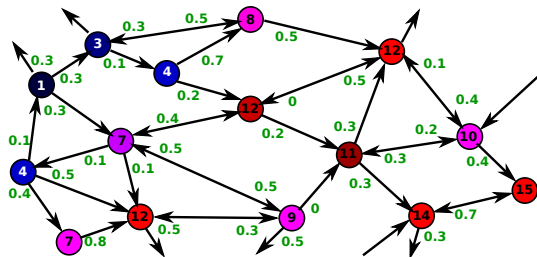
Fitness landscapes are graphs

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



Fitness landscapes are graphs

Specific local search puts probability transitions on edges according to f and history of the search

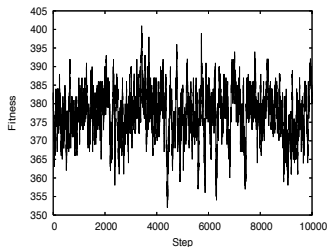
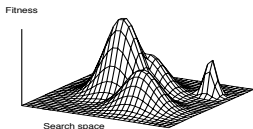


How does fitness landscape characterisation work?

- ▶ sample the neighbourhood 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.
- ▶ study of the geometry of the landscape allows to study the difficulty, and design a good optimisation algorithm

What makes a problem difficult to optimise?

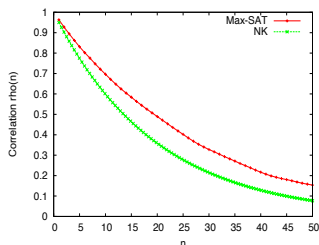
Number and size of attractive basins (Garnier et al [10])



Ruggedness

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

$$\rho(n) = \frac{E[(f(s_i) - \bar{f})(f(s_{i+n}) - \bar{f})]}{\text{var}(f(s_i))} \quad (1)$$



Results

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	$1 - \frac{K+1}{N}$

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

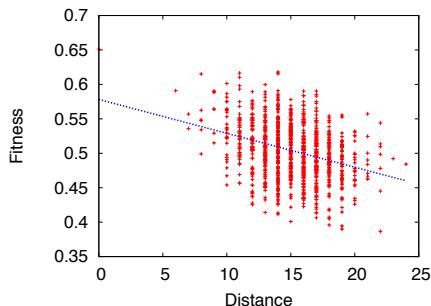
Correlation between distance to global optimum and fitness

- ▶ given a set $F = f_1, f_2, \dots, f_n$ of solution fitnesses
- ▶ with corresponding $D = d_1, d_2, \dots, d_n$ Hamming distances to the nearest global optimum

$$\text{fdc} = \frac{(f_i - \bar{f})(d_i - \bar{d})}{n} \sum_{i=1}^n \quad (2)$$

$$r = \frac{\text{fdc}}{\sigma_F \sigma_D} \quad (3)$$

where σ_F and σ_D are the standard deviations of F and D .



Classification based on experimental studies:

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

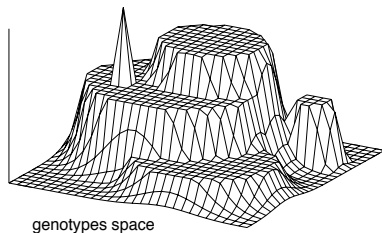
Neutral Fitness Landscapes

Neutral sets: set of solutions with the same fitness

Neutral networks: includes neighbourhood information

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

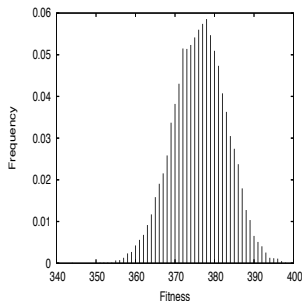
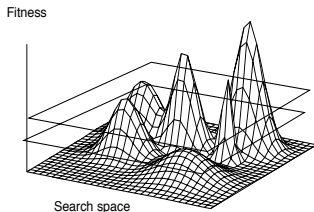
Fitness



Neutrality and difficulty

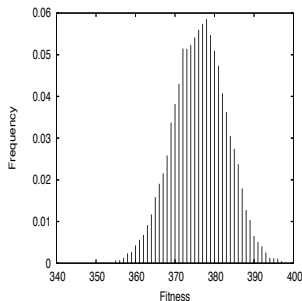
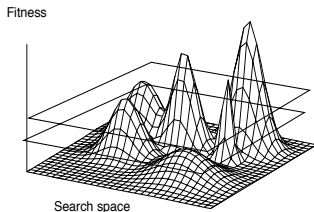
- ▶ there is no definitive answer about neutrality / problem hardness
- ▶ certainly, it is dependent on the 'nature' of neutrality
- ▶ no information is better than bad information : Hard trap functions are more difficult than needle-in-a-haystack functions

Measuring neutrality: Density Of States



Tail of the distribution is an indicator of difficulty: the faster the decay, the harder the problem

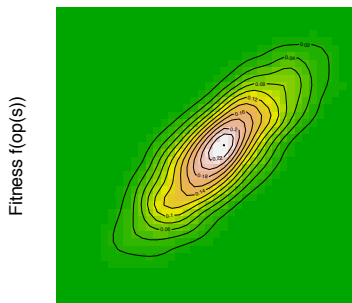
Measuring neutrality: Density Of States



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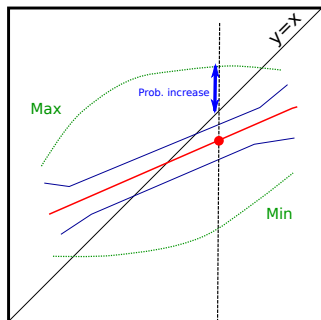
Measuring evolvability: Fitness Cloud [Verel et al. 2003]

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



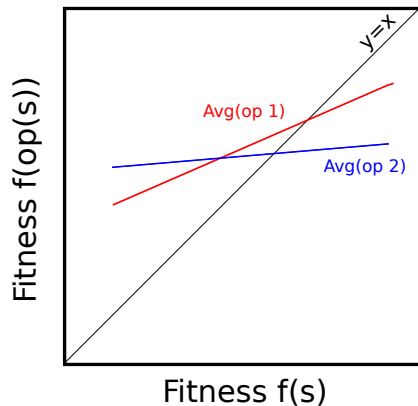
Fitness $f(s)$

Fitness $f(op(s))$



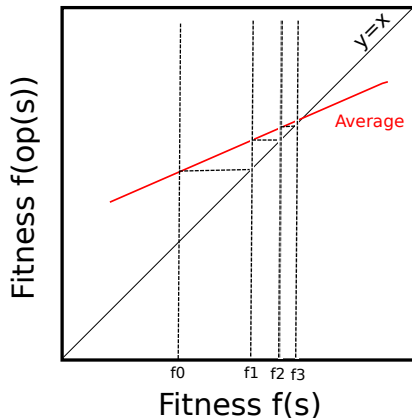
Fitness $f(s)$

Evolvability as an indication of problem difficulty

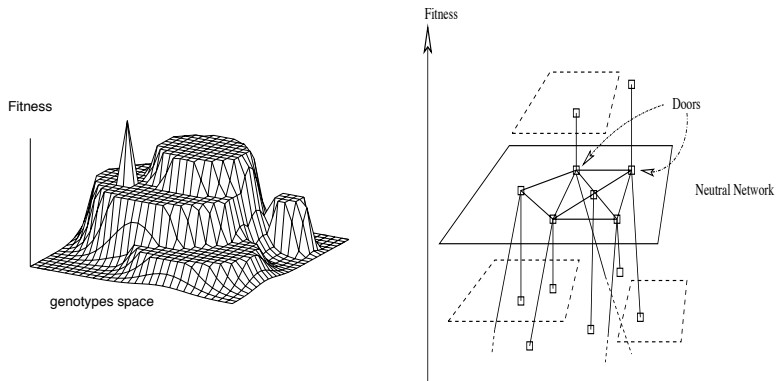


Predicting fitness using fitness clouds

- ▶ Approximation of the fitness value after few steps of local operator
- ▶ Indication on the quality of the operator

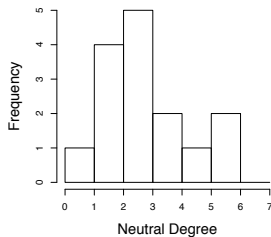


Neutral networks (Schuster 1994 [27])

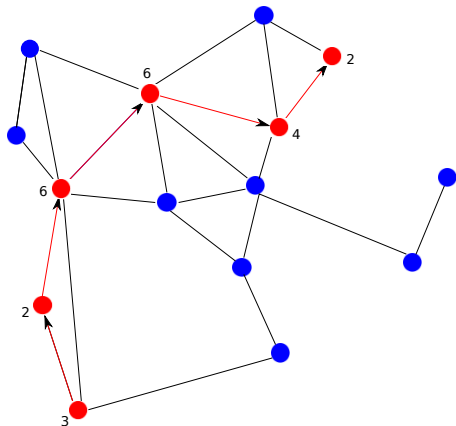


Metrics of neutral networks

- ▶ Size of NN: number of nodes of NN,
- ▶ Neutral degree distribution



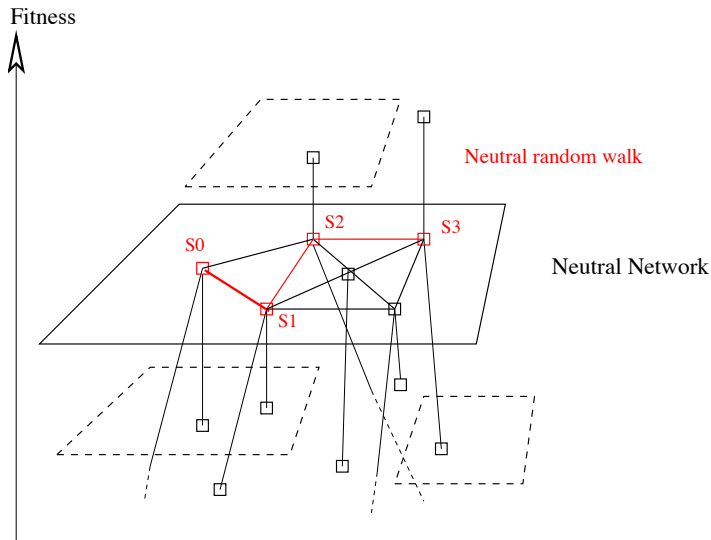
Autocorrelation of neutral degree (Bastolla 03 [3])



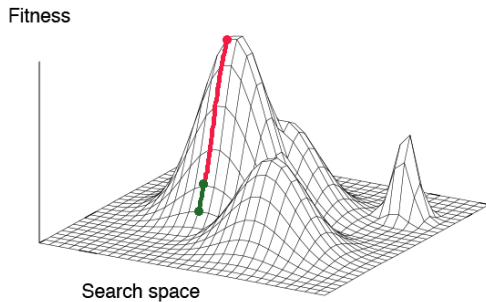
- ▶ random walk on NN
- ▶ autocorrelation of degrees

Rate of innovation (Huynen 96 [13])

The number of new accessible structures (fitness) per mutation



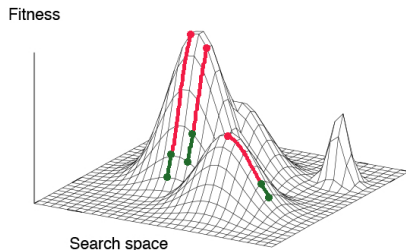
Predictors



Predictor definition:

- ▶ $p'_i = \frac{f(s'_i) - f(s_i)}{f(s'_i)}$
- ▶ $p''_i = \frac{f(s''_i) - f(s_i)}{f(s'_i) - f(s_i)}$

Predictive Local Search



Learning phase

- Predictor pool

$$\{(p'_1, p''_1), (p'_2, p''_2), \dots, (p'_n, p''_n)\}$$

- Similarity measure

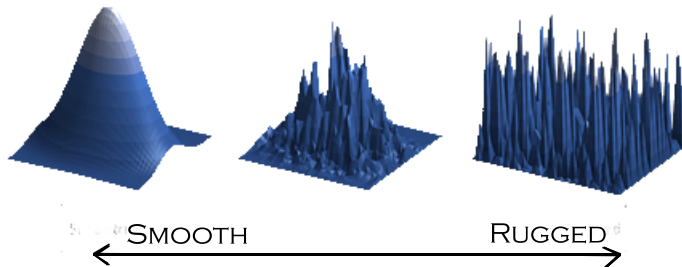
$$C = \frac{|p'_i - p'_j|}{|p'_i| + |p'_j|} + \frac{|p''_i - p''_j|}{|p''_i| + |p''_j|}$$

Predictive Local Search (continued)

Testing phase

1. Create a random solution
2. Calculate its fitness
3. Perform a local search (hill climbing) for a certain number of function evaluations
4. Calculate the fitness of the improved solution
5. Select the predictor that best matches the improvement in the first step
6. Perform a local search to the local optimum
7. Calculate the fitness of the local optimum
8. Calculate the error in prediction

How hard is an optimisation problem?



So what?

- ▶ The nature of the search-space is the key factor determining the performance of the optimisation algorithm,
- ▶ Define/characterize the search-space,
- ▶ Analyse what makes problems difficult,
- ▶ Guide the optimisation process
 - ▶ Select the right search strategy

