DM811

Heuristics for Combinatorial Optimization

Lecture 11

Neighborhoods and Landscapes

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

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Computational Complexity of LS

For a local search algorithm to be effective, search initialization and individual search steps should be efficiently computable.

Complexity class $\mathcal{PLS}$: class of problems for which a local search algorithm exists with polynomial time complexity for:

- search initialization
- any single search step, including computation of evaluation function value

For any problem in $\mathcal{PLS}$ ...

- local optimality can be verified in polynomial time
- improving search steps can be computed in polynomial time
- **but:** finding local optima may require super-polynomial time

Computational Complexity of LS

$\mathcal{PLS}$-complete: Among the most difficult problems in $\mathcal{PLS}$;
if for any of these problems local optima can be found
in polynomial time, the same would hold for all problems in $\mathcal{PLS}$.

Some complexity results:

- TSP with k-exchange neighborhood with $k > 3$ is $\mathcal{PLS}$-complete.
- TSP with 2- or 3-exchange neighborhood is in $\mathcal{PLS}$, but $\mathcal{PLS}$-completeness is unknown.

Outline

Learning goals of this section

- Review basic formal and theoretical concepts
- Learn about techniques and goals of experimental search space analysis
- Develop intuition on features of local search that may guide the design of LS algorithms

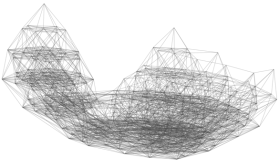
Definitions

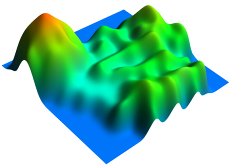
- Problem instance π
- Search space S_π
- Neighborhood function $\mathcal{N} : S \subseteq 2^S$
- Evaluation function $f_\pi : S \to \mathbf{R}$

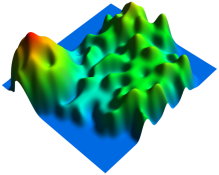
Definition:

The **search landscape** L is the vertex-labeled neighborhood graph given by the triplet $\mathcal{L} = \langle S_\pi, N_\pi, f_\pi \rangle$.

Search Landscape







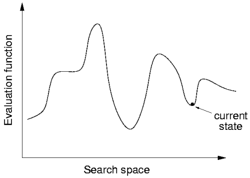
Transition Graph of Iterative Improvement

Given $\mathcal{L} = \langle S_\pi, N_\pi, f_\pi \rangle$, the transition graph of iterative improvement is a directed acyclic subgraph obtained from $\mathcal{L}$ by deleting all arcs (i, j) for which it holds that the cost of solution j is worse than or equal to the cost of solution i.

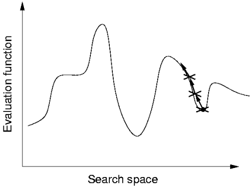
It can be defined for other algorithms as well and it plays a central role in the theoretical analysis of proofs of convergence.

Ideal visualization of landscapes principles

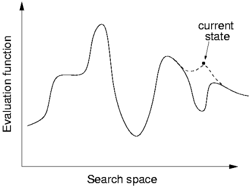
- Simplified landscape representation



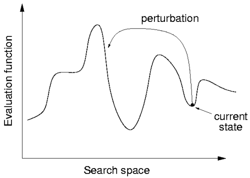
- Tabu Search



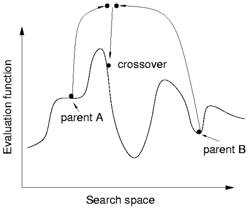
- Guided Local Search



- Iterated Local Search



- Evolutionary Alg.



Fundamental Properties

The behavior and performance of an LS algorithm on a given problem instance crucially depends on properties of the respective search landscape.

Simple properties:

- search space size $|S|$
- reachability: solution j is reachable from solution i if neighborhood graph has a path from i to j.
  - strongly connected neighborhood graph
  - weakly optimally connected neighborhood graph
- distance between solutions
- neighborhood size (ie, degree of vertices in neigh. graph)
- cost of fully examining the neighborhood
- relation between different neighborhood functions (if $N_1(s) \subseteq N_2(s)$ forall $s \in S$ then $\mathcal{N}_2$ dominates $\mathcal{N}_1$)

Neighborhood Operator

Goal: providing a formal description of neighborhood functions for the three main solution representations:

- Permutation
  - linear permutation: Single Machine Total Weighted Tardiness Problem
  - circular permutation: Traveling Salesman Problem
- Assignment: Graph Coloring Problem, SAT, CSP
- Set, Partition: Max Independent Set

A neighborhood function $\mathcal{N} : S \to 2^S$ is also defined through an operator. An operator Δ is a collection of operator functions $\delta : S \to S$ such that

$$s' \in N(s) \iff \exists \delta \in \Delta \mid \delta(s) = s'$$

Permutations

$\Pi(n)$ indicates the set all permutations of the numbers $\{1, 2, \ldots, n\}$

$(1, 2 \ldots, n)$ is the identity permutation ι.

If $\pi \in \Pi(n)$ and $1 \leq i \leq n$ then:

- π_i is the element at position i
- $pos_\pi(i)$ is the position of element i

Alternatively, a permutation is a bijective function $\pi(i) = \pi_i$

The permutation product $\pi \cdot \pi'$ is the composition $(\pi \cdot \pi')_i = \pi'(\pi(i))$

For each π there exists a permutation such that $\pi^{-1} \cdot \pi = \iota$
$\pi^{-1}(i) = pos_\pi(i)$

$$\Delta_N \subset \Pi$$

Linear Permutations

Swap operator

$$\Delta_S = \{\delta_S^i | 1 \leq i \leq n\}$$

$$\delta_S^i(\pi_1 \dots \pi_i \pi_{i+1} \dots \pi_n) = (\pi_1 \dots \pi_{i+1} \pi_i \dots \pi_n)$$

Interchange operator

$$\Delta_X = \{\delta_X^{ij} | 1 \leq i < j \leq n\}$$

$$\delta_X^{ij}(\pi) = (\pi_1 \dots \pi_{i-1} \pi_j \pi_{i+1} \dots \pi_{j-1} \pi_i \pi_{j+1} \dots \pi_n)$$

($\equiv$ set of all transpositions)

Insert operator

$$\Delta_I = \{\delta_I^{ij} | 1 \leq i \leq n, 1 \leq j \leq n, j \neq i\}$$

$$\delta_I^{ij}(\pi) = \begin{cases} (\pi_1 \dots \pi_{i-1} \pi_{i+1} \dots \pi_j \pi_i \pi_{j+1} \dots \pi_n) & i < j \\ (\pi_1 \dots \pi_j \pi_i \pi_{j+1} \dots \pi_{i-1} \pi_{i+1} \dots \pi_n) & i > j \end{cases}$$

Circular Permutations

Reversal (2-edge-exchange)

$$\Delta_R = \{\delta_R^{ij} | 1 \leq i < j \leq n\}$$

$$\delta_R^{ij}(\pi) = (\pi_1 \ldots \pi_{i-1}\pi_j \ldots \pi_i \pi_{j+1} \ldots \pi_n)$$

Block moves (3-edge-exchange)

$$\Delta_B = \{\delta_B^{ijk} | 1 \leq i < j < k \leq n\}$$

$$\delta_B^{ij}(\pi) = (\pi_1 \ldots \pi_{i-1}\pi_j \ldots \pi_k \pi_i \ldots \pi_{j-1}\pi_{k+1} \ldots \pi_n)$$

Short block move (Or-edge-exchange)

$$\Delta_{SB} = \{\delta_{SB}^{ij} | 1 \leq i < j \leq n\}$$

$$\delta_{SB}^{ij}(\pi) = (\pi_1 \ldots \pi_{i-1}\pi_j \pi_{j+1}\pi_{j+2}\pi_i \ldots \pi_{j-1}\pi_{j+3} \ldots \pi_n)$$

Assignments

An assignment can be represented as a mapping $\sigma : \{X_1 \dots X_n\} \to \{v : v \in D, |D| = k\}$:

$$\sigma = \{X_i = v_i, X_j = v_j, \dots\}$$

One-exchange operator

$$\Delta_{1E} = \{\delta_{1E}^{il} | 1 \leq i \leq n, 1 \leq l \leq k\}$$

$$\delta_{1E}^{il}(\sigma) = \left\{\sigma' : \sigma'(X_i) = v_l \text{ and } \sigma'(X_j) = \sigma(X_j) \ \forall j \neq i\right\}$$

Two-exchange operator

$$\Delta_{2E} = \{\delta_{2E}^{ij} | 1 \leq i < j \leq n\}$$

$$\delta_{2E}^{ij}(\sigma) = \left\{\sigma' : \sigma'(X_i) = \sigma(X_j), \sigma'(X_j) = \sigma(X_i) \text{ and } \sigma'(X_l) = \sigma(X_l) \forall l \neq i, j\right\}$$

Partitioning

An assignment can be represented as a partition of objects selected and not selected $s : \{X\} \to \{C, \overline{C}\}$
(it can also be represented by a bit string)

One-addition operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in \overline{C}\}$$

$$\delta_{1E}^{v}(s) = \{s : C' = C \cup v \text{ and } \overline{C}' = \overline{C} \setminus v\}$$

One-deletion operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in C\}$$

$$\delta_{1E}^{v}(s) = \{s : C' = C \setminus v \text{ and } \overline{C}' = \overline{C} \cup v\}$$

Swap operator

$$\Delta_{1E} = \{\delta_{1E}^{v} \mid v \in C, u \in \overline{C}\}$$

$$\delta_{1E}^{v}(s) = \{s : C' = C \cup u \setminus v \text{ and } \overline{C}' = \overline{C} \cup v \setminus u\}$$

Distances

Set of paths in $\mathcal{L}$ with $s, s' \in S$:

$$\Phi(s, s') = \{(s_1, \ldots, s_h) \mid s_1 = s, s_h = s' \, \forall i : 1 \leq i \leq h - 1, \langle s_i, s_{i+1} \rangle \in E_{\mathcal{L}}\}$$

If $\phi = (s_1, \ldots, s_h) \in \Phi(s, s')$ let $|\phi| = h$ be the length of the path; then the distance between any two solutions s, s' is the length of shortest path between s and s' in $\mathcal{L}$:

$$d_{\mathcal{N}}(s, s') = \min_{\phi \in \Phi(s,s')} |\Phi|$$

$\mathtt{diam}(\mathcal{L}) = \max\{d_{\mathcal{N}}(s, s') \mid s, s' \in S\}$ (= maximal distance between any two candidate solutions)
(= worst-case lower bound for number of search steps required for reaching (optimal) solutions)

Note: with permutations it is easy to see that:

$$d_{\mathcal{N}}(\pi, \pi') = d_{\mathcal{N}}(\pi^{-1} \cdot \pi', \iota)$$

Distances for Linear Permutation Representations

- Swap neighborhood operator
  computable in $O(n^2)$ by the precedence based distance metric:
  $d_S(\pi, \pi') = \#\{\langle i, j\rangle | 1 \leq i < j \leq n, pos_{\pi'}(\pi_j) < pos_{\pi'}(\pi_i)\}$.
  $\mathtt{diam}(G_{\mathcal{N}}) = n(n-1)/2$

- Interchange neighborhood operator
  Computable in $O(n) + O(n)$ since
  $d_X(\pi, \pi') = d_X(\pi^{-1} \cdot \pi', \iota) = n - c(\pi^{-1} \cdot \pi')$
  $c(\pi)$ is the number of disjoint cycles that decompose a permutation.
  $\mathtt{diam}(G_{\mathcal{N}_X}) = n - 1$

- Insert neighborhood operator
  Computable in $O(n) + O(n\, log(n))$ since
  $d_I(\pi, \pi') = d_I(\pi^{-1} \cdot \pi', \iota) = n - |lis(\pi^{-1} \cdot \pi')|$ where $lis(\pi)$ denotes the length of the longest increasing subsequence.
  $\mathtt{diam}(G_{\mathcal{N}_I}) = n - 1$

Distances for Circular Permutation Representations

- Reversal neighborhood operator
  sorting by reversal is known to be NP-hard
  surrogate in TSP: bond distance

- Block moves neighborhood operator
  unknown whether it is NP-hard but there does not exist a proved polynomial-time algorithm

Distances for Assignment Representations

- Hamming Distance

- An assignment can be seen as a partition of n in k mutually exclusive non-empty subsets

  One-exchange neighborhood operator
  The *partition-distance* $d_{1E}(\mathcal{P}, \mathcal{P}')$ between two partitions $\mathcal{P}$ and $\mathcal{P}'$ is the minimum number of elements that must be moved between subsets in $\mathcal{P}$ so that the resulting partition equals $\mathcal{P}'$.

  The partition-distance can be computed in polynomial time by solving an assignment problem. Given the assignment matrix M where in each cell (i, j) it is $|S_i \cap S'_j|$ with $S_i \in \mathcal{P}$ and $S'_j \in \mathcal{P}'$ and defined $A(\mathcal{P}, \mathcal{P}')$ the assignment of maximal sum then it is $d_{1E}(\mathcal{P}, \mathcal{P}') = n - A(\mathcal{P}, \mathcal{P}')$

Example: Search space size and diameter for the TSP

- Search space size = $(n-1)!/2$

- Insert neighborhood
  size = $(n-3)n$
  diameter = $n-2$

- 2-exchange neighborhood
  size = $\binom{n}{2} = n \cdot (n-1)/2$
  diameter in $[n/2, n-2]$

- 3-exchange neighborhood
  size = $\binom{n}{3} = n \cdot (n-1) \cdot (n-2)/6$
  diameter in $[n/3, n-1]$

Example: Search space size and diameter for SAT

SAT instance with n variables, 1-flip neighborhood:
$G_{\mathcal{N}} = n$-dimensional hypercube; diameter of $G_{\mathcal{N}} = n$.

Let $\mathcal{N}_1$ and $\mathcal{N}_2$ be two different neighborhood functions for the same instance (S, f, π) of a combinatorial optimization problem.

If for all solutions $s \in S$ we have $N_1(s) \subseteq N_2(s)$ then we say that $\mathcal{N}_2$ dominates $\mathcal{N}_1$

Example:

In TSP, 1-insert is dominated by 3-exchange.
(1-insert corresponds to 3-exchange and there are 3-exchanges that are not 1-insert)

Other Search Space Properties

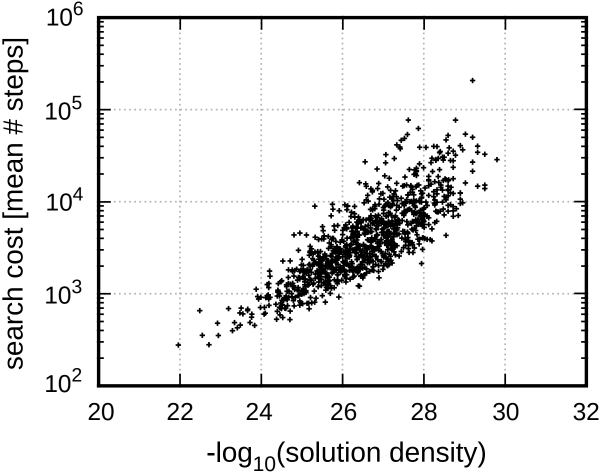
- number of (optimal) solutions $|S'|$, solution density $|S'|/|S|$
- distribution of solutions within the neighborhood graph

Solution densities and distributions can generally be determined by:

- exhaustive enumeration;
- sampling methods;
- counting algorithms (often variants of complete algorithms).

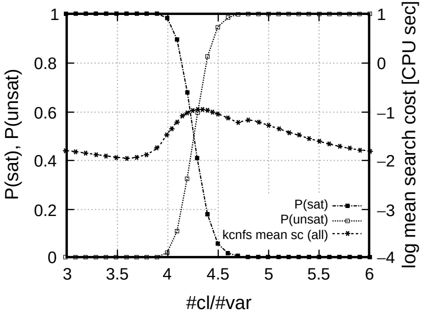
Example: Correlation between solution density and search cost for GWSAT over set of hard Random-3-SAT instances:

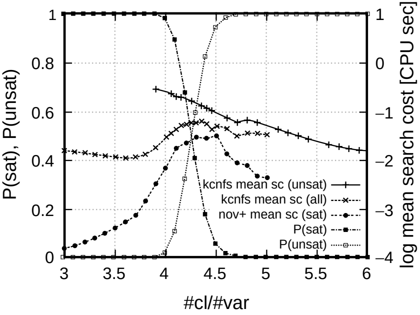
The less solutions, the harder to find them



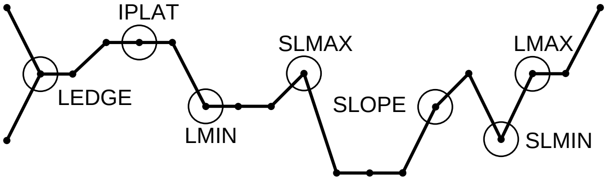
Phase Transition for 3-SAT

Random instances $\rightsquigarrow$ m clauses of n uniformly chosen variables





Classification of search positions



position type	$>$	$=$	$<$
SLMIN (strict local min)	+	−	−
LMIN (local min)	+	+	−
IPLAT (interior plateau)	−	+	−
SLOPE	+	−	+
LEDGE	+	+	+
LMAX (local max)	−	+	+
SLMAX (strict local max)	−	−	+

"+" = present, "–" absent; table entries refer to neighbors with larger ("$>$") , equal ("$=$"), and smaller ("$<$") evaluation function values

Example: Complete distribution of position types for hard Random-3-SAT instances

instance	*avg sc*	SLMIN	LMIN	IPLAT
uf20-91/easy	13.05	0%	0.11%	0%
uf20-91/medium	83.25	$< 0.01\%$	0.13%	0%
uf20-91/hard	563.94	$< 0.01\%$	0.16%	0%

instance	SLOPE	LEDGE	LMAX	SLMAX
uf20-91/easy	0.59%	99.27%	0.04%	$< 0.01\%$
uf20-91/medium	0.31%	99.40%	0.06%	$< 0.01\%$
uf20-91/hard	0.56%	99.23%	0.05%	$< 0.01\%$

(based on exhaustive enumeration of search space;
sc refers to search cost for GWSAT)

Example: Sampled distribution of position types for hard Random-3-SAT instances

instance	*avg sc*	SLMIN	LMIN	IPLAT
uf50-218/medium	615.25	0%	47.29%	0%
uf100-430/medium	3 410.45	0%	43.89%	0%
uf150-645/medium	10 231.89	0%	41.95%	0%

instance	SLOPE	LEDGE	LMAX	SLMAX
uf50-218/medium	$< 0.01\%$	52.71%	0%	0%
uf100-430/medium	0%	56.11%	0%	0%
uf150-645/medium	0%	58.05%	0%	0%

(based on sampling along GWSAT trajectories;
sc refers to search cost for GWSAT)

Local Minima

Note: Local minima prevent local search progress.

Simple properties of local minima:

- *number of local minima:* $|lmin|$, *local minima density* $|lmin|/|S|$
- *localization of local minima:* distribution of local minima within the neighborhood graph

Problem: Determining these measures typically requires exhaustive enumeration of search space.

$\leadsto$ Approximation based on sampling or estimation from other measures (such as autocorrelation measures, see below).

Example: Distribution of local minima for the TSP

Goal: Empirical analysis of distribution of local minima for Euclidean TSP instances.

Experimental approach:

- Sample sets of local optima of three TSPLIB instances using multiple independent runs of two TSP algorithms (3-opt, ILS).
- Measure pairwise distances between local minima (using *bond distance* = number of edges in which two given tours differ).
- Sample set of purportedly globally optimal tours using multiple independent runs of high-performance TSP algorithm.
- Measure minimal pairwise distances between local minima and respective closest optimal tour (using bond distance).

Empirical results:

Instance	avg sq [%]	avg d_{lmin}	avg d_{opt}
	Results for 3-opt		
`rat783`	3.45	197.8	185.9
`pr1002`	3.58	242.0	208.6
`pcb1173`	4.81	274.6	246.0
	Results for ILS algorithm		
`rat783`	0.92	142.2	123.1
`pr1002`	0.85	177.2	143.2
`pcb1173`	1.05	177.4	151.8

(based on local minima collected from 1 000/200 runs of 3-opt/ILS)
avg sq [%]: average solution quality expressed in percentage deviation from optimal solution

Interpretation:

- Average distance between local minima is small compared to maximal possible bond distance, n.

  $\rightsquigarrow$ *Local minima are concentrated in a relatively small region of the search space.*

- Average distance between local minima is slightly larger than distance to closest global optimum.

  $\rightsquigarrow$ *Optimal solutions are located centrally in region of high local minima density.*

- Higher-quality local minima found by ILS tend to be closer to each other and the closest global optima compared to those determined by 3-opt.

  $\rightsquigarrow$ *Higher-quality local minima tend to be concentrated in smaller regions of the search space.*

Note: These results are fairly typical for many types of TSP instances and instances of other combinatorial problems.
In many cases, local optima tend to be clustered; this is reflected in multi-modal distributions of pairwise distances between local minima.

Fitness-Distance Correlation (FDC)

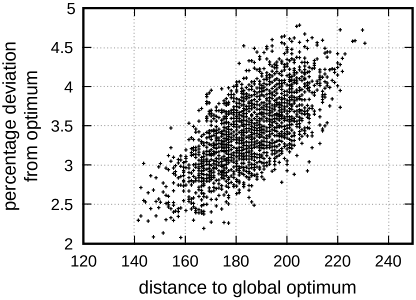
Idea: Analyze correlation between solution quality (fitness) g of candidate solutions and distance d to (closest) optimal solution.

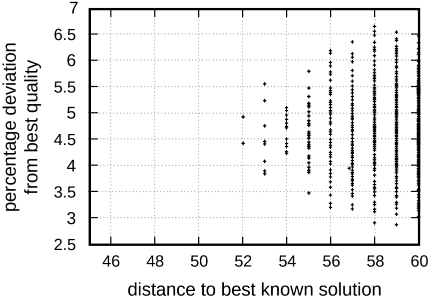
Measure for FDC: *empirical correlation coefficient* r_{fdc}.

Fitness-distance plots, *i.e.*, scatter plots of the (g_i, d_i) pairs underlying an estimate of r_{fdc}, are often useful to graphically illustrate fitness distance correlations.

- The FDC coefficient, r_{fdc} depends on the given neighborhood relation.
- r_{fdc} is calculated based on a sample of m candidate solutions (typically: set of local optima found over multiple runs of an iterative improvement algorithm).

Example: FDC plot for TSPLIB instance `rat783`, based on 2500 local optima obtained from a 3-opt algorithm





High FDC (r_{fdc} close to one):

- 'Big valley' structure of landscape provides guidance for local search;
- search initialization: high-quality candidate solutions provide good starting points;
- search diversification: (weak) perturbation is better than restart;
- typical, *e.g.*, for TSP.

Low FDC (r_{fdc} close to zero):

- global structure of landscape does not provide guidance for local search;
- typical for very hard combinatorial problems, such as certain types of QAP (Quadratic Assignment Problem) instances.

Applications of fitness-distance analysis:

- algorithm design: use of strong intensification (including initialization) and relatively weak diversification mechanisms;
- comparison of effectiveness of neighborhood relations;
- analysis of problem and problem instance difficulty.

Limitations and short-comings:

- *a posteriori* method, requires set of (optimal) solutions,
  but: results often generalize to larger instance classes;
- optimal solutions are often not known, using best known solutions can lead to erroneous results;
- can give misleading results when used as the sole basis for assessing problem or instance difficulty.

Ruggedness

Idea: Rugged search landscapes, *i.e.*, landscapes with high variability in evaluation function value between neighboring search positions, are hard to search.

Example: Smooth *vs* rugged search landscape

Note: Landscape ruggedness is closely related to local minima density: rugged landscapes tend to have many local minima.

The ruggedness of a landscape L can be measured by means of the empirical autocorrelation function $r(i)$:

$$r(i) := \frac{1/(m-i) \cdot \sum_{k=1}^{m-i}(g_k - \bar{g}) \cdot (g_{k+i} - \bar{g})}{1/m \cdot \sum_{k=1}^{m}(g_k - \bar{g})^2}$$

where $g_1, \dots g_m$ are evaluation function values sampled along an uninformed random walk in L.

Note: $r(i)$ depends on the given neighborhood relation.

- Empirical autocorrelation analysis is computationally cheap compared to, *e.g.*, fitness-distance analysis.
- (Bounds on) AC can be theoretically derived in many cases, *e.g.*, the TSP with the 2-exchange neighborhood.
- There are other measures of ruggedness, such as *empirical autocorrelation coefficient* and *(empirical) correlation length*.

High AC (close to one):

- "smooth" landscape;
- evaluation function values for neighboring candidate solutions are close on average;
- low local minima density;
- problem typically relatively easy for local search.

Low AC (close to zero):

- very rugged landscape;
- evaluation function values for neighboring candidate solutions are almost uncorrelated;
- high local minima density;
- problem typically relatively hard for local search.

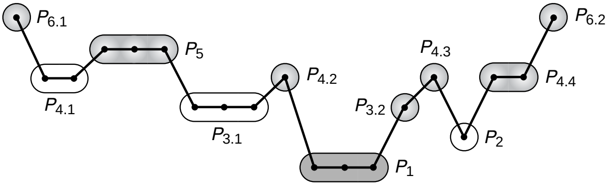
Note:

- Measures of ruggedness, such as AC, are often insufficient for distinguishing between the hardness of individual problem instances;
- but they can be useful for
  - analyzing differences between neighborhood relations for a given problem,
  - studying the impact of parameter settings of a given SLS algorithm on its behavior,
  - classifying the difficulty of combinatorial problems.

Plateaux

Plateaux, *i.e.*, ‘flat’ regions in the search landscape

Intuition: Plateaux can impede search progress due to lack of guidance by the evaluation function.



Definitions

- **Region:** connected set of search positions.
- **Border of region R:** set of search positions with at least one direct neighbor outside of R (**border positions**).
- **Plateau region:** region in which all positions have the same level, *i.e.*, evaluation function value, l.
- **Plateau:** maximally extended plateau region, *i.e.*, plateau region in which no border position has any direct neighbors at the plateau level l.
- **Solution plateau:** Plateau that consists entirely of solutions of the given problem instance.
- **Exit of plateau region R:** direct neighbor s of a border position of R with lower level than plateau level l.
- **Open / closed plateau:** plateau with / without exits.

Measures of plateau structure:

- *plateau diameter* = diameter of corresponding subgraph of $G_{\mathcal{N}}$
- *plateau width* = maximal distance of any plateau position to the respective closest border position
- *number of exits*, *exit density*
- *distribution of exits within a plateau*, *exit distance distribution* (in particular: avg./max. distance to closest exit)

Some plateau structure results for SAT:

- Plateaux typically don't have an interior, *i.e.*, almost every position is on the border.
- The diameter of plateaux, particularly at higher levels, is comparable to the diameter of search space. (In particular: plateaux tend to span large parts of the search space, but are quite well connected internally.)
- For open plateaux, exits tend to be clustered, but the average exit distance is typically relatively small.

Barriers and Basins

Observation:

The *difficulty of escaping* from closed plateaux or strict local minima is related to the *height of the barrier*, *i.e.*, the difference in evaluation function, that needs to be overcome in order to reach better search positions:

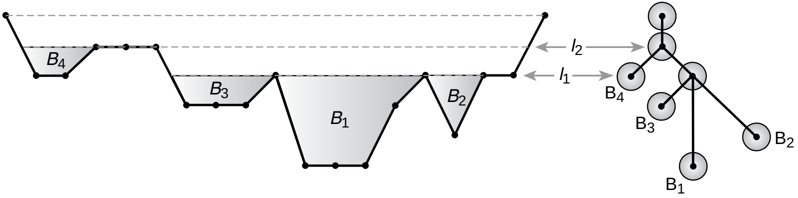
Higher barriers are typically more difficult to overcome (this holds, *e.g.*, for Probabilistic Iterative Improvement or Simulated Annealing).

Definitions:

- Positions s, s' are *mutually accessible at level* l iff there is a path connecting s' and s in the neighborhood graph that visits only positions t with $g(t) \leq l$.
- The *barrier level between positions* s, s', $bl(s, s')$ is the lowest level l at which s' and s' are mutually accessible;

  the difference between the level of s and $bl(s, s')$ is called the *barrier height between* s *and* s'.
- **Basins**, *i.e.*, maximal (connected) regions of search positions below a given level, form an important basis for characterizing search space structure.

Example: Basins in a simple search landscape and corresponding basin tree



Note: The basin tree only represents basins just below the critical levels at which neighboring basins are joined (by a *saddle*).