STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Search Space Structure and SLS Performance

Holger H. Hoos & Thomas Stützle

Outline

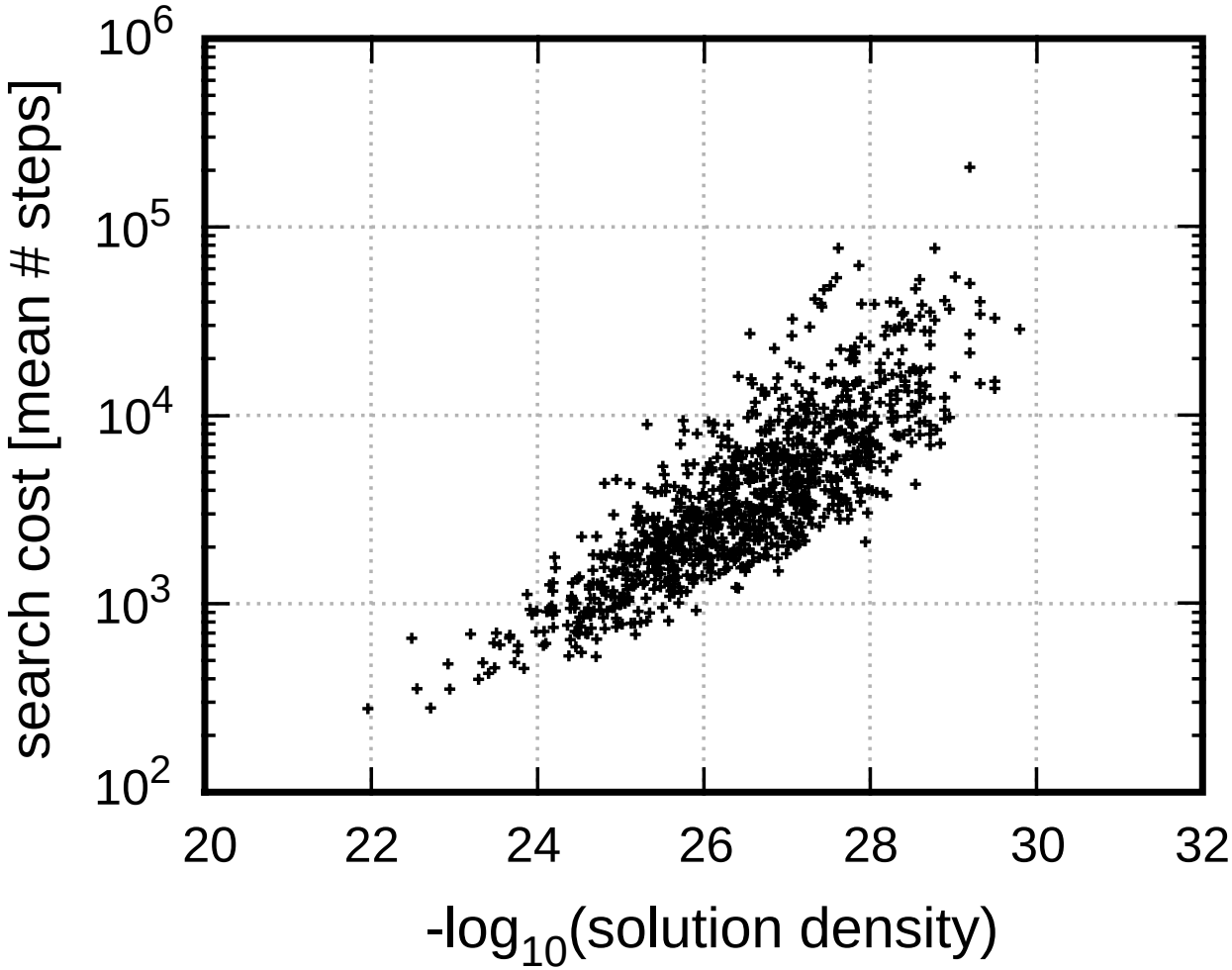
1. Fundamental Search Space Properties
2. Search Landscapes and Local Minima
3. Fitness-Distance Correlation
4. Ruggedness
5. Barriers and Basins

Fundamental Search Space Properties

Simple properties of search space S:

- search space size $\#S$
- number of (optimal) solutions $\#S'$, *solution density* $\#S'/\#S$
- search space diameter $diam(G_N)$
  (= maximal distance between any two candidate solutions)
- distribution of solutions within the neighbourhood graph

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



Search Landscapes

Given an SLS algorithm A and a problem instance π with associated search space $S(\pi)$, neighbourhood relation $N(\pi)$ and evaluation function $g(\pi) : S \mapsto \mathbb{R}$, the *search landscape of* π, $L(\pi)$, is defined as $L(\pi) := (S(\pi), N(\pi), g(\pi))$.

A landscape $L := (S, N, g)$ is ...

- *non-degenerate* (or *invertible*), iff
  $\forall s, s' \in S : [g(s) = g(s') \Longrightarrow s = s']$;
- *locally invertible*, iff
  $\forall r \in S : \forall s, s' \in N(r) \cup \{r\} : [g(s) = g(s') \Longrightarrow s = s']$;
- *non-neutral*, iff
  $\forall s \in S : \forall s' \in N(s) : [g(s) = g(s') \Longrightarrow s = s']$.

Classification of search positions (according to evaluation function values of direct neighbours):

position type	$>$	$=$	$<$
SLMIN (strict local min)	$+$	*0*	*0*
LMIN (local min)	$+$	$+$	*0*
IPLAT (interior plateau)	*0*	$+$	*0*
SLOPE	$+$	*0*	$+$
LEDGE	$+$	$+$	$+$
LMAX (local max)	*0*	$+$	$+$
SLMAX (strict local max)	*0*	*0*	$+$

"+" = present, "0" absent; table entries refer to neighbours with larger ("$>$") , equal ("$=$"), and smaller ("$<$") evaluation function values

Example: 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 enumaration of search space;
sc refers to search cost for GWSAT)

Example: 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 impede local search progress.

Simple measures related to local minima:

- number of local minima $\#lmin$, *local minima density* $\#lmin/\#S$
- distribution of local minima within the neighbourhood graph

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

Solutions: Approximations based on sampling or estimation from other measures (such as autocorrelation measures, see below)

Fitness-Distance Correlation (FDC)

Idea: Analyse (linear) correlation between solution quality (fitness) and distance to (closest) optimal solution.

Measure for FDC: *empirical correlation coefficient*

$$r_{fdc} := \frac{\widehat{Cov}(g,d)}{\widehat{\sigma}(g) \cdot \widehat{\sigma}(d)},$$

where

$$\widehat{Cov}(g,d) := \frac{1}{m-1} \sum_{i=1}^{m} (g_i - \bar{g})(d_i - \bar{d}),$$

$$\widehat{\sigma}(g) := \sqrt{\frac{1}{m-1} \sum_{i=1}^{m} (g_i - \bar{g})^2}, \quad \widehat{\sigma}(d) := \sqrt{\frac{1}{m-1} \sum_{i=1}^{m} (d_i - \bar{d})^2}$$

Note: r_{fdc} depends on the given neighbourhood relation.

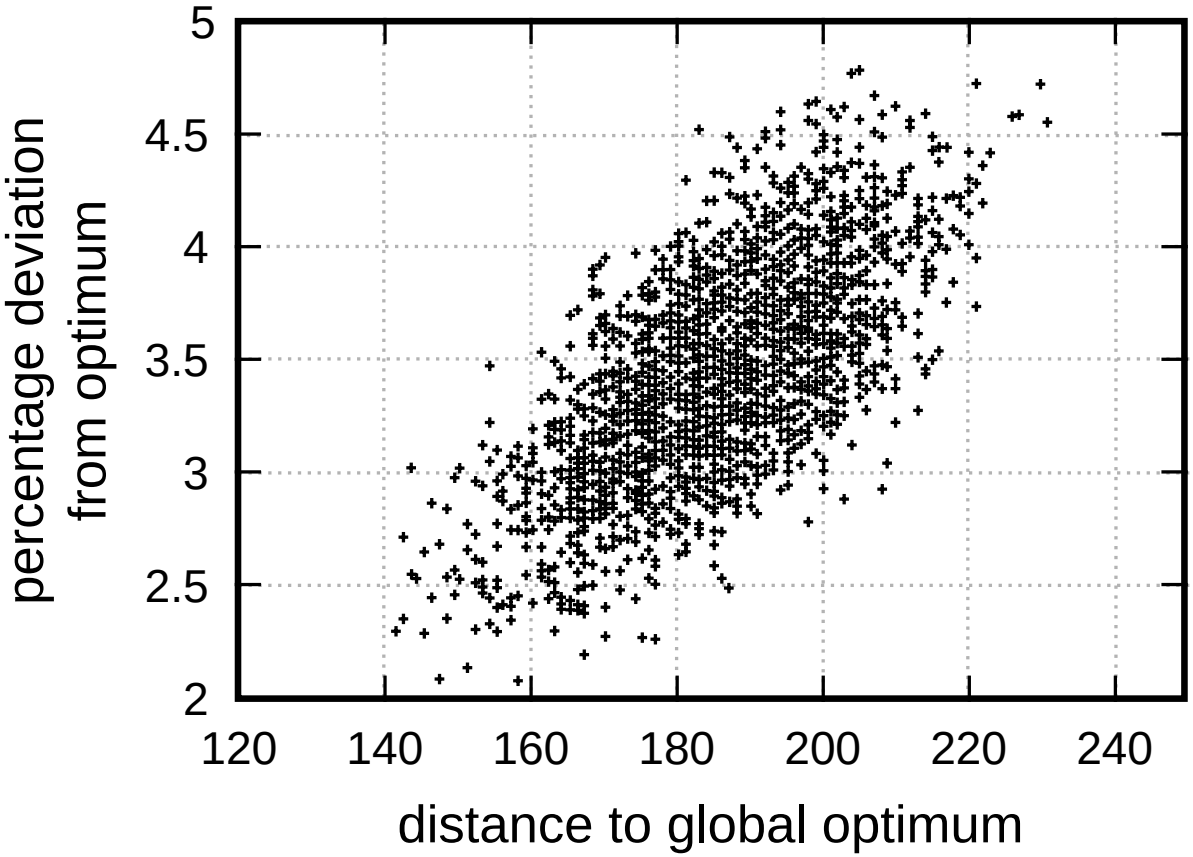
Fitness Distance Plots:

Graphical representation of fitness–distance correlation;
distance from (closest) optimal solution *vs* relative solution quality.

Measuring FDC:

Sample locally optimal candidate solutions, as determined
by a (simple) SLS algorithm, *e.g.*, iterative improvement.

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



Implications of FDC for SLS behaviour:

- High FDC (close to one):
  - 'Big valley' structure of landscape provides guidance for local search;
  - high-quality local minima provide good starting points;
  - search diversification: perturbation is better than restart;
  - search initialisation: high quality starting points help;
  - typical for TSP.
- FDC close to zero:
  - global structure of landscape does not provide guidance for local search;
  - indicative of harder problems, such as certain instance types of QAP (Quadratic Assignment Problem)

Ruggedness

Idea: Rugged landscapes, *i.e.*, landscapes with with many local minima, are hard to seach.

Measures for landscape ruggedness:

- autocorrelation function [Weinberger, 1990; Stadler, 1995]
- correlation length [Stadler, 1995]
- autocorrelation coefficient [Angel & Zissimopoulos, 1997]

Empirical autocorrelation function $r(i)$:

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

Empirical autocorrelation coefficient (ACC) ξ:

$$\xi = 1/(1 - r(1))$$

Note: $r(i)$ and ξ depend on the given neighbourhood relation.

Implications of ACC on SLS behaviour:

- High ACC (close to one):
  - "smooth" landscape;
  - evaluation function values for neighbouring candidate solutions are close on average;
  - low local minima density;
  - problem typically relative easy for local search.

- Low ACC (close to zero):
  - very rugged landscape;
  - evaluation function values for neighbouring candidate solutions are almost uncorrelated;
  - high local minima density;
  - problem typically relatively hard for local search.

Measuring ACC:

- measure series $\mathbf{g} = (g_1, \ldots, g_m)$ of evaluation function values along uninformed random walk;
- estimate ACC based on autocorrelation function on $\mathbf{g}$, where distance is measured in search steps.

$\rightsquigarrow$ computationally cheap compared to, *e.g.*, FDC analysis.

Note: (Bounds on) ACC can be theoretically derived in many cases, including TSP with 2-exchange neighbourhood.

Plateaus

Intuition: Plateaus, *i.e.*, 'flat' regions in the search landscape, can impede search progress due to lack of guidance by the evaluation function.

Definition

- *region:* connected subgraph of G_N.
- *border of region R:* set of $s \in S$ with direct neighbours that are not contained in R (border positions).

Definition (continued)

- *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 neighbours at the plateau level l.
- *exit of plateau region R:* direct neighbour 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_N
- *plateau width* = maximal distance of any plateau position to the respective closest border position
- *plateau branching factor* = fraction of neighbours of a plateau position that are also on the plateau.
- *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:

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

Barriers and Basins

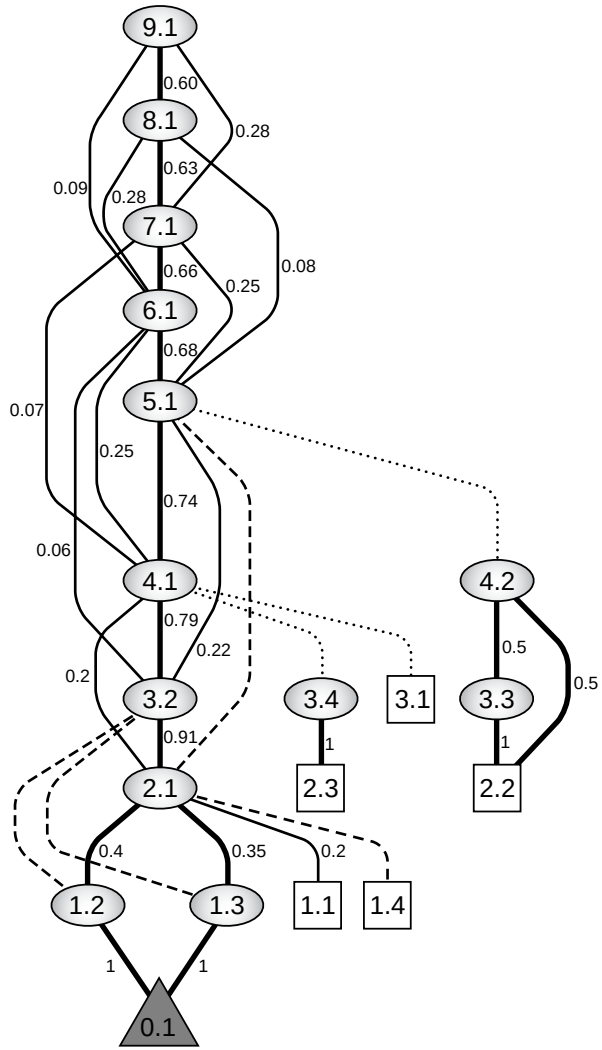
- positions s, s' are *mutually accessible at level l*
  iff there is a path connecting s' and s in the neighbourhood graph that visits only positions t with $g(t) \leq l$
- The *barrier level between positions s, s'*
  is the lowest level l at which s' and s' are mutually accessible.
- *Basin below position s* = set of search positions s' at level $g(s') < g(s)$ such that s and s' are mutually accessible at level $g(s)$.

- A *gradient walk from position s to s'* is a possible trajectory of iterative best improvement (= gradient descent) from s to s'.
- The *gradient basin of position s* is the sets of all positions s' such that there is a gradient walk from s' to s.

Barries trees and plateau connection graphs

- *Barrier trees* and *plateau connection graphs* are based on collapsing positions on the same plateau or in the same basin into 'macro positions' and illustrate connections between these regions.
- This type of search space analysis can give much deeper insights into SLS behaviour and problem hardness than global measures, such as FDC or ACC.
- This type of analysis is computationally expensive and requires enumeration of large parts of the search space.

Example: Search space structure (plateau connection graph) of *easy* Random 3-SAT instance



Example: Search space structure (plateau connection graph) of *hard* Random 3-SAT instance