v0.1: Seth Gilbert
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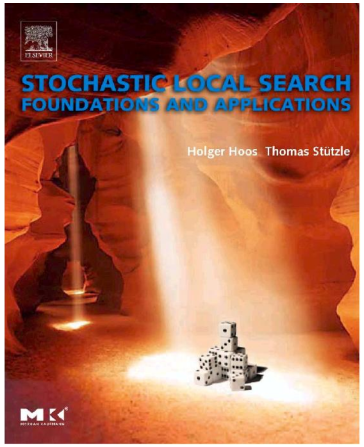
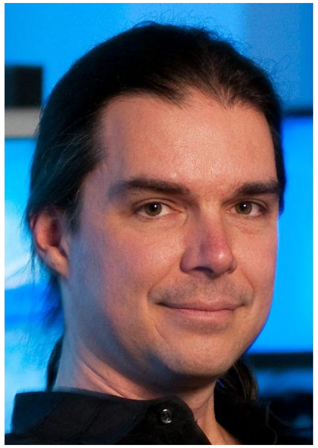
CS4234
Optimiz(s)ation Algorithms





← Steven's external PhD thesis evaluator

L9 – Stochastic Local Search

Many parts of the material is based on slides provided with the book 'Stochastic Local Search: Foundations and Applications' by Holger H. Hoos and Thomas Stützle (Morgan Kaufmann, 2004) – see http://www.sls-book.net for further information.

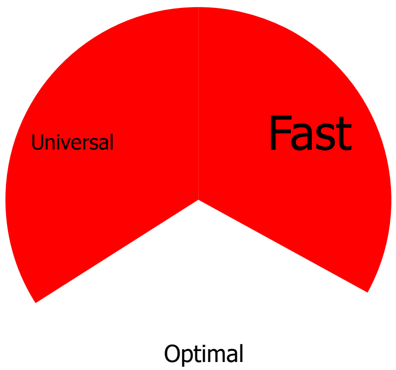
Outline

- A New Search Paradigm
- SLS Definitions
- Basic Hill Climbing (example on M/G-**NR**-TSP)
- Various SLS Ideas (all on TSP)
- Small Experiments throughout the Lecture

Back to NP-hard COP

Recall: Lecture 1

- COP = Combinatorial Optimization Problem
- Many of them are NP-hard
- Still remember the ${}_3C_2$ reality?
- This time, we will also sacrifice optimality
  - But unlike Approximation Algorithms, this time we will **NOT** have any guarantee of the solution quality…
  - Theoretical Computer Scientists won't like this…



Search Paradigm

Solving NP-hard Combinatorial Optimization Problems (COPs) through **Complete Search** that **sacrifices speed** is usually by iteratively (or recursively) generate and evaluate (all) candidate solutions

- e.g. Try all (**N**-1)! possible TSP tours one by one, evaluate them, and report the best (minimal one)
- Note: Evaluating one candidate solution (e.g. compute the cost of a given TSP tour) is typically computationally much cheaper than finding one (out of possibly many) optimal solutions (e.g. find the optimal TSP tour)

A New Search Paradigm

What you already know: **Systematic Search**:

- Traverse search space for given problem instance in a *systematic manner*
- **Complete**: Guaranteed to eventually find (optimal) solution, or to determine that no solution exists

A New Paradigm: **Local Search**:

- Start at a (random) position in search space
- Iteratively move from a position to its neighbouring position, usually (but not always) perturbative (next slide)
- **Typically incomplete**: Not guaranteed to find (optimal) solutions, cannot determine insolubility with certainty…

A New Search Paradigm, Continued

- Perturbative Search
  - search space = complete candidate solutions
  - search step = modification of one/more sol. components
  - e.g. swap two edges (2-exchange) in a TSP tour
- Constructive Search (aka construction heuristics)
  - search space = partial candidate solutions
  - search step = extension with one/more sol. components
  - e.g. from one vertex, go to nearest neighbor vertex, the Greedy Nearest Neighbor heuristic

Systematic versus Local Search

- **Completeness**: Advantage of systematic search, but not always relevant, e.g., when existence of solutions is guaranteed by construction or in real-time situations (e.g. TSP when input is a complete graph).
- **Any-time property**: Positive correlation between run-time and solution quality or probability; typically more readily achieved by Local Search.
- **Complementarity**: Local and Systematic Search can be fruitfully combined, e.g., by using Local Search for finding solutions whose optimality is proven using Systematic Search.

When to use?

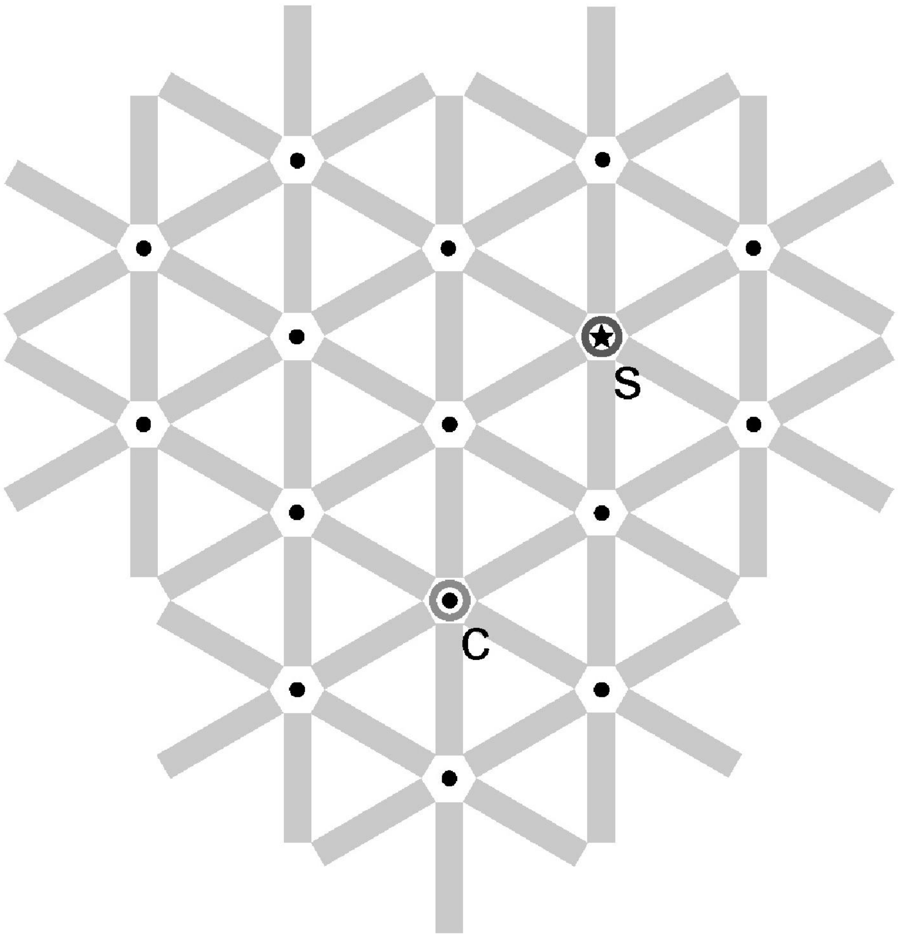
- **Systematic search** is often better suited when ...
  - proofs of insolubility or optimality are required;
  - time constraints are not critical;
- **Local search** is often better suited when ...
  - reasonably good solutions are required within a short time;
  - parallel processing is used;

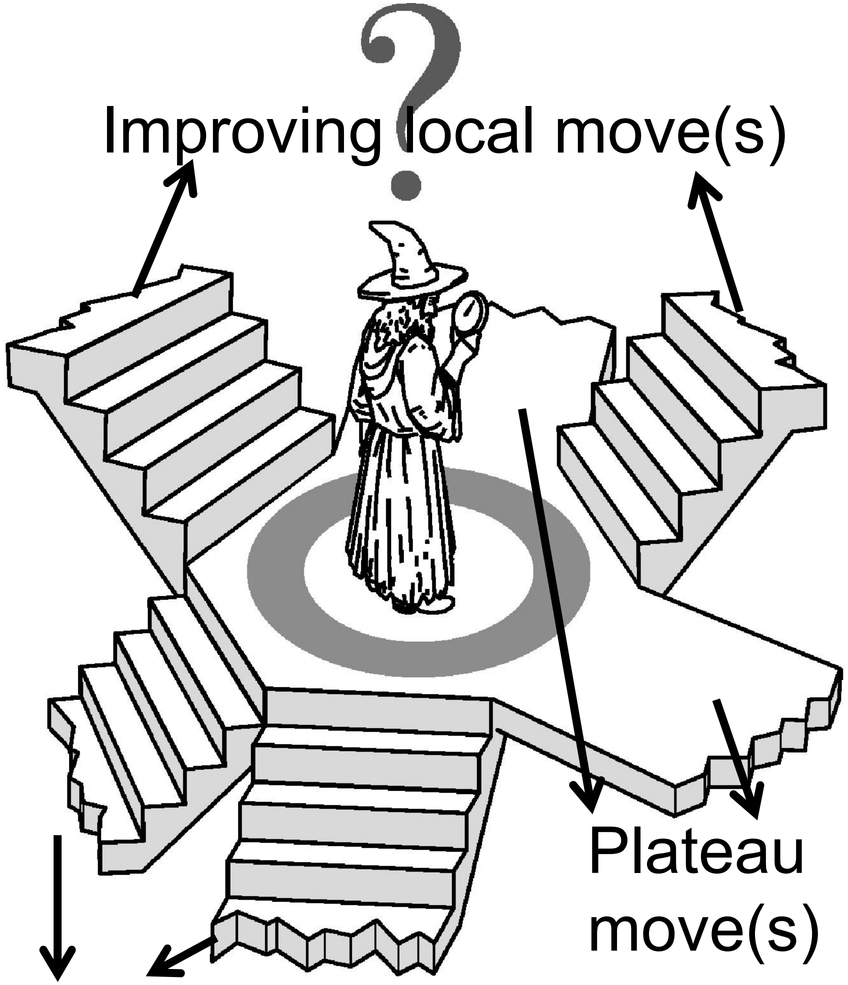
The term Stochastic in SLS

- Many prominent local search algorithms use **randomised** (stochastic) choices in generating and modifying candidate solutions.
- These Stochastic Local Search (SLS) algorithms are one of the most successful and widely used approaches for solving hard combinatorial problems.
- Some well-known SLS methods and algorithms:
  - Evolutionary (Genetic) Algorithms
  - Simulated Annealing
  - Tabu Search (Steven's old favourite due to his PhD)

SLS — global versus local view

- S = solution, C = current search position





Definitions (1/6)

For a given problem instance π of a COP:

- **search space $S(\pi)$**
  - e.g., for TSP: set of all possible TSP tours
- **solution set $S'(\pi) \subseteq S(\pi)$**
  - e.g., for TSP: TSP tours of minimum length
- **neighbourhood relation $N(\pi) \subseteq S(\pi) \times S(\pi)$**
  - e.g., for TSP: 2-exchange neighbourhood
- **set of memory states $M(\pi)$**
  - May be not used in some memoryless SLS algorithms
  - e.g., tabu list in Tabu Search algorithm (next lecture)

Definitions (2/6)

Continued:

- **(init)ialization function: $\emptyset \rightarrow D(S(\pi) \times M(\pi))$**
  - Specifies probability distribution over initial search positions and memory states
- **step function: $S(\pi) \times M(\pi) \rightarrow D(S(\pi) \times M(\pi))$**
  - Maps each search position and memory state onto probability distribution over subsequent, neighbouring search positions and memory states
- **termination function: $S(\pi) \times M(\pi) \rightarrow D(\{T, F\})$**
  - Determines the termination probability for each search position and memory state

Generic SLS Algorithm

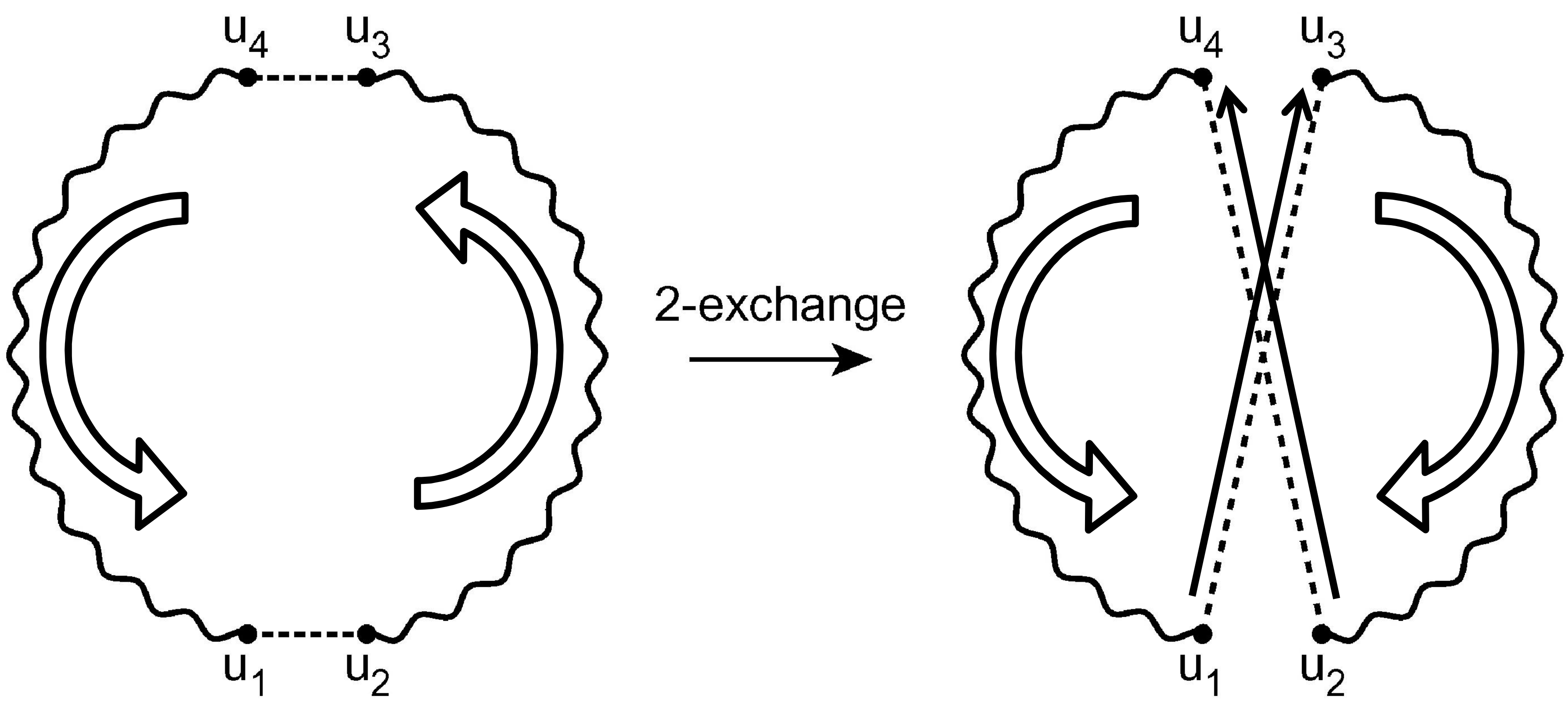
```
procedure SLS-Minimisation(π′)
   input: problem instance π′ ∈ Π′
   output: solution s ∈ S′(π′) or ∅
   (s, m) := init(π′);
   ŝ := s;
   while not terminate(π′, s, m) do
      (s, m) := step(π′, s, m);
      if f(π′, s) < f(π′, ŝ) then
         ŝ := s;
      end
   end
   if ŝ ∈ S′(π′) then
      return ŝ
   else
      return ∅
   end
end SLS-Minimisation
```

Definitions (3/6)

Continued:

- **neighborhood (set)** of candidate solution **s**:
  N(s) := {s' ∈ S | N(s, s')}
- **neighborhood graph** of problem instance π:
  $\mathbf{G_N(\pi) := (S(\pi), N(\pi))}$
  - We will discuss more of "Fitness Landscape" in next two lectures
- **k-exchange neighbourhood**: candidate solutions **s** and **s'** are called neighbours iff **s** differs from **s'** in at most **k** solution components
  - 2-exchange neighbourhood for TSP
    (solution components = edges in given graph)

Search steps in the 2-exchange neighbourhood for the TSP



Definitions (4/6)

Continued:

- **search step** (or **move**): Pair of search positions **s**, **s'** for which **s'** can be reached from **s** in <u>one step</u>, i.e., **N(s, s')** and **step(s, m)(s', m') > 0** for some memory states **m, m'** ∈ **M**.
- **search trajectory**: Finite sequence of search positions $(s_0, s_1, \ldots, s_k)$ such that (s_{i-1}, s_i) is a search step for any $i \in \{1, \ldots, k\}$.
  - We will see more about animation of search trajectory that I did during my PhD days in the next two lectures
- **search strategy**: Specified by **init** and **step** function; to some extent independent of problem instance and other components of SLS algorithm.

Definitions (5/6)

Continued:

- Evaluation function $\mathbf{g(\pi) : S(\pi) \rightarrow R}$ that maps candidate solutions of a given problem instance π onto real numbers, such that global optima correspond to solutions of π;
  - used for ranking or assessing neighbors of current search position to provide guidance to search process.
- Evaluation versus objective functions:
  - Evaluation function: Part of SLS algorithm.
  - Objective function: Integral part of optimization problem.

Hill-Climbing for (M/G-NR-)TSP

Also known as **Iterative Improvement/Descent**

- **search space S:** set of all possible TSP tours
- **solution set S':** set of TSP tours of minimum length
- **neighbourhood relation N:** 2-exchange neighbourhood
- **set of memory states M:** {0}, not used
- **init**: classic greedy nearest neighbour heuristic
- **step**: uniform random choice from improving neighbors, i.e., **step(s)(s') := 1/#I(s)** if **s'** ∈ **I(s)**, and **0** otherwise, where **I(s) := {s'** ∈ **S | N(s, s') and g(s') < g(s)}**
- **terminates** when no improving neighbor available

Intermezzo: Experiments (1/2)

SLS Ideas: Delta Evaluations (1/2)

Incremental updates (aka delta evaluations)

- **Key idea**: Calculate effects of differences between the current search position **s** and its neighbours **s'** on evaluation function value.
- Evaluation function values often consist of *independent contributions of solution components*; hence, **g(s)** can be efficiently calculated from **g(s')** by differences between **s** and **s'** in terms of solution components.
  - That is, we do not re-compute everything from scratch
- Typically crucial for the efficient implementation of various SLS algorithms.

SLS Ideas: Delta Evaluations (2/2)

Example: Incremental updates for TSP

- solution components = edges of a given graph **G**
- standard 2-exchange neighbourhood, i.e., neighbouring round trips **p** and **p'** differ only in <u>two edges</u>
- **w(p') = w(p)**
  – 2 edges in **p** but not in **p**
  + 2 edges in **p'** but not in **p**
- This can be done in Constant time (i.e. 4 arithmetic operations), compared to Linear time (i.e. **n** arithmetic operations for graph with **n** vertices) for computing **w(p')** from scratch.

Definitions (6/6)

Continued:

- **Local minimum**: Search position without improving neighbours w.r.t. given evaluation function **g** and neighbourhood **N**, i.e., position $\mathbf{s} \in \mathbf{S}$ such that $\mathbf{g(s)} \leq \mathbf{g(s')}$ for all $\mathbf{s'} \in \mathbf{N(s)}$.
- **Strict local minimum**: Search position $\mathbf{s} \in \mathbf{S}$ such that $\mathbf{g(s)} < \mathbf{g(s')}$ for all $\mathbf{s'} \in \mathbf{N(s)}$.
- **Local maximum** and **strict local maximum** are defined analogously
- **Local minimum/maximum** is also called as **local optima**
- What we want: **Global optima**

SLS Ideas: Escaping Local Optima

Main Problem of simple Hill-Climbing:

- (Quick) stagnation in local optima of evaluation function **g**.

So, some simple mechanisms to improve it:

- **Restart**: Re-initialize search whenever a local optima is encountered.
  - Often rather ineffective due to cost of initialization.
- **Non-improving steps**: In local optima, allow selection of candidate solutions with *equal* or *worse* evaluation function value, e.g., using minimally worsening steps.
  - Can lead to long walks in plateaus,
    i.e., regions of search positions with identical evaluation function.
- Neither of these mechanisms is guaranteed to always escape effectively from local optima.

SLS Ideas: Search Strategy

Diversification vs Intensification

- Goal-directed and randomized components of SLS strategy need to be balanced carefully.
- **Intensification**: Aims to greedily increase solution quality or probability, e.g., by exploiting the evaluation function.
- **Diversification**: Aims to prevent search stagnation by preventing search from getting trapped in confined regions.
- Examples:
  - Iterative Improvement (II): intensification strategy.
  - Uninformed Random Walk (URW): diversification strategy.
- Balanced combination of intensification and diversification mechanisms forms the basis for advanced SLS methods.

Note about Local Optima

Note:

- Local minima depend on **g** and neighborhood relation **N**.
- Larger neighborhoods **N(s)** induce:
  - Neighborhood graphs with smaller diameter,
  - Fewer local minima.
- Ideal case is the exact neighborhood, i.e., neighborhood relation for which any local optimum is also guaranteed to be a global optimum.
  - Typically, exact neighborhoods are too large to be searched effectively (exponential in size of problem instance).

SLS Ideas: Neighborhood Size

We face a trade-off situation here:

- Using larger neighborhoods can improve performance of Hill-Climbing (and other SLS methods).
  - Example: 2-exchange neighborhood to 3-exchange neighborhood :O
- But the time required for determining improving search steps increases (sometimes significantly) with neighborhood size.
- So we have to decide if the effectiveness of larger neighborhoods worth the additional time complexity of search steps.

SLS Ideas: Neighborhood Pruning

Neighborhood Pruning:

- Idea: Reduce size of neighborhoods by excluding neighbors that are likely/guaranteed not to yield improvements in **g**.
- Note: Crucial for large neighborhoods, but can be also very useful for small neighborhoods.
- Example: *Candidate lists* for the TSP
  - Problem intuition: High-quality solutions likely include short edges.
  - Candidate list of vertex v: list of v's nearest neighbours (limited number), sorted according to increasing edge weights.
  - Search steps (e.g., 2-exchange moves) always involve edges to elements of candidate lists.
  - Significant impact on performance of SLS algorithms for the TSP.

SLS Ideas: Pivoting Rules

How to choose improving neighbor in each step?

- **Best Improvement** (a.k.a. gradient descent, greedy Hill-Climbing): Choose maximally improving neighbor, i.e., randomly select from $\mathbf{I^*(s) := \{s' \in N(s) \mid g(s') = g^*\}}$, where $\mathbf{g^* := \min\{g(s') \mid s' \in N(s)\}}$.
  - Notice that this requires evaluation of <u>all neighbors</u> in each step.
- Alternative: **First Improvement**: Evaluate neighbors in fixed order, choose the first improving step encountered.
  - Note: Can be much faster than Best Improvement,
  - Overall quality may be weaker overall (but can also be better due to faster evaluation time per iteration on fixed time limit),
  - Order of evaluation can have significant impact on performance.

SLS Ideas: Variable Neighborhood

Recall: Local minima are relative to neighborhood.

- Key idea: To escape from local minima of a given neighborhood relation, we can switch to a *different neighborhood relation*.
- Use **k** neighborhood relations N_1, N_2, …, N_k, (typically) ordered according to increasing neighborhood size.
- Always use smallest neighborhood that facilitates improving steps.
- Upon termination, candidate solution is locally optimal w.r.t. all neighborhoods

SLS Time Complexity

- (Very) hard to analyze
- Usually O(#iterations*polynomial_cost_per_iteration)
  - But if we use techniques like variable neighborhood, the cost per iteration can be different :S…
- Others just set execution time limit and just run the SLS until the execution time limit has elapsed
  - Like in our experiment so far…

Some More Experiments (2/2)

Summary

- Introducing a new search paradigm: Stochastic Local Search (SLS)
- SLS Definitions
- Hill-Climbing SLS on an example NP-hard COP: The M/G-**NR**-TSP
- Various SLS Ideas
  - No proof, all "heuristics" :O…
- (Most) ideas are experimented directly on a certain M/G-NR-TSP problem