STOCHASTIC LOCAL SEARCH FOUNDATIONS AND APPLICATIONS

Generalised Local Search Machines

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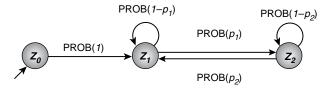
Stochastic Local Search: Foundations and Applications

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:

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

Key idea underlying Generalised Local Search Machines: Explicitly represent higher-level search control mechanism in the form of a *finite state machine*. Example: Simple 3-state GLSM



- States z₀, z₁, z₂ represent simple search strategies, such as Random Picking (for initialisation), Iterative Best Improvement and Uninformed Random Walk.
- PROB(p) refers to a probabilistic state transition with probability p after each search step.

Generalised Local Search Machines (GLSMs)

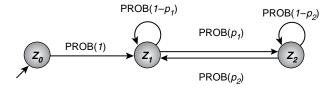
- States \cong simple search strategies.
- State transitions \cong search control.
- GLSM *M* starts in initial state.
- In each iteration:
 - ► *M* executes one search step associated with its current state *z*;
 - ► *M* selects a new state (which may be the same as *z*) in a nondeterministic manner.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

Formal definition of a GLSM

A Generalised Local Search Machine is defined as a tuple $\mathcal{M} := (Z, z_0, M, m_0, \Delta, \sigma_Z, \sigma_\Delta, \tau_Z, \tau_\Delta)$ where:

- Z is a set of states;
- $z_0 \in Z$ 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);
- $\Delta \subseteq Z \times Z$ is the *transition relation*;
- σ_Z and σ_Δ are sets of *state types* and *transition types*;
- $\tau_Z : Z \mapsto \sigma_Z$ and $\tau_\Delta : \Delta \mapsto \sigma_\Delta$ associate every state zand transition (z, z') with a state type $\sigma_Z(z)$ and transition type $\tau_\Delta((z, z'))$, respectively.

Example: Simple 3-state GLSM (formal definition)



• $Z := \{z_0, z_1, z_2\}$; $z_0 = initial machine state$

• no memory $(M := \{m_0\}; m_0 = \text{initial and only memory state})$

•
$$\Delta := \{(z_0, z_1), (z_1, z_2), (z_1, z_1), (z_2, z_1), (z_2, z_2)\}$$

•
$$\sigma_Z := \{z_0, z_1, z_2\}$$

• $\sigma_\Delta := \{\mathsf{PROB}(p) \mid p \in \{1, p_1, p_2, 1 - p_1, 1 - p_2\}\}$

•
$$\tau_Z(z_i) := z_i, \quad i \in \{0, 1, 2\}$$

• $\tau_{\Delta}((z_0, z_1)) := \mathsf{PROB}(1), \ \tau_{\Delta}((z_1, z_2)) := \mathsf{PROB}(p_1), \ \dots$

Example: Simple 3-state GLSM (semantics)

- Start in initial state z_0 , memory state m_0 (never changes).
- Perform one search step according to search strategy associated with state type z₀ (e.g., random picking).
- With probability 1, switch to state z_1 .
- Perform one search step according to state z₁; switch to state z₂ with probability p₁, otherwise, remain in state z₁.
- In state z₂, perform one search step according to z₂; switch back to state z₁ with probability p₂, otherwise, remain in state z₂.
- \rightsquigarrow After one z_0 step (initialisation), repeatedly and nondeterministically switch between phases of z_1 and z_2 steps until termination criterion is satisfied.

Note:

- States types formally represent (subsidiary) search strategies, whose definition is not part of the GLSM definition.
- Transition types formally represent mechanisms used for switching between GLSM states.
- Multiple states / transitions can have the same type.
- 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.

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;
- termination predicate for overall search process.

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* from *current machine state*, possibly depending on *search position* and *current memory state*; this may change the *current memory state*

Note:

- The current search position is only changed by the subsidiary search strategies associated with states, not as side-effect of machine state transitions.
- The machine state and memory state are only changed by state-transitions, not as side-effect of search steps. (Memory state is viewed as part of higher-level search control.)
- The operation of *M* is uniquely characterised by the evolution of *machine state*, *memory state* and *search position* over time.

GLSMs are factored representations of SLS strategies:

- Given 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).
- Termination of subsidiary search strategies are often reflected in conditional transitions leaving respective GLSM states.

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;
- the semantics of each transition type, i.e., under which conditions respective transitions are executed, and how they effect the memory state.

State types

- State type semantics are often most conveniently specified procedurally (see algorithm outlines for 'simple SLS methods' from Chapter 2).
- 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.
- parametric state type = state type τ whose semantics depends on memory state.

parametric state = state of parametric type.

Transitions types (1)

- 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):
 - executed with probability p, independently of memory state or search position;
 - probabilities of PROB transitions leaving any given state must sum to one.

Note:

- DET transitions are a special case of PROB transitions.
- For a GLSM *M* any state that can be reached from initial state z₀ by following a chain of PROB(p) transitions with p > 0 will eventually be reached with arbitrarily high probability in any sufficiently long run of *M*.
- In any state z with a 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.

Transitions types (2)

- Conditional probabilistic transitions type CPROB(C, p):
 - 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.

Note:

- ► Special cases of CPROB(*C*, *p*) transitions:
 - PROB(p) transitions;
 - conditional deterministic transitions, type CDET(C).
- Condition predicates should be efficiently computable (ideally: ≤ linear time w.r.t. size of given problem instance).

Commonly used simple condition predicates:

 \top always true

count(k) countm(k)	total number of GLSM steps $\geq k$ total number of GLSM steps modulo $k = 0$
<pre>scount(k) scountm(k)</pre>	number of GLSM steps in current state $\geq k$ 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
evalf(y)	current evaluation function value $\leq y$
noimpr(k)	incumbent candidate solution has not been improved within the last k steps

All based on local information; can also be used in negated form.

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, *e.g.*, to memorise current candidate solution.
- Can be added to any of the previously defined transition types.

Machine types:

Capture *structure of search control mechanism*, obtained by abstracting from state and transition types of GLSMs.

- 1-state machines:
 - simplest machine type, single initialising state only;
 - realises iterated sampling processes, such as Uninformed Random Picking.
- ► 1-state+init machines:
 - one initialising + one working state;
 - good model for many simple SLS methods.

sequential 1-state machines:



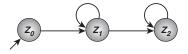
visit initialising state z₀ only on once.

alternating 1-state+init machines:



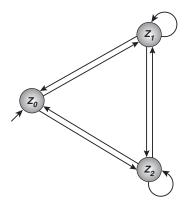
- may visit initialising state z₀ multiple times;
- good model for simple SLS methods with restart mechanism.

- 2-state+init sequential machines:
 - one initialising state (visited only once), two working states;



 any search trajectory can be partitioned into three phases: one initialisation step, a sequence of z₁ steps and a sequence of z₂ steps.

- ► 2-state+init alternating machines:
 - one initialising state, two working states;
 - arbitrary transitions between any states are possible.

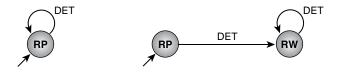


Generalisations:

- ► *k*-state+init sequential machines:
 - one initialising state (visited only once), k working states;
 - every search trajectory consists of 1+k phases.
- k-state+init alternating machines:
 - one initialising state, k working states;
 - arbitrary transitions between states;
 - may have multiple initialising states (*e.g.*, to realise alternative restart mechanisms).

Modelling SLS Methods Using GLSMs

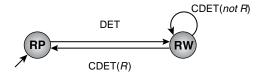
Uninformed Picking and Uninformed Random Walk



procedure step- $RP(\pi, s)$ input: problem instance $\pi \in \Pi$, candidate solution $s \in S(\pi)$ output: candidate solution $s \in S(\pi)$ s' := selectRandom(S); return s'end step-RP

procedure step- $RW(\pi, s)$ input: problem instance $\pi \in \Pi$, candidate solution $s \in S(\pi)$ output: candidate solution $s \in S(\pi)$ s' := selectRandom(N(s));return s'end step-RW

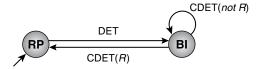
Uninformed Random Walk with Random Restart



 $R = \text{restart predicate, } e.g., \operatorname{countm}(k)$

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Iterative Best Improvement with Random Restart



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procedure step-Bl(\pi, s)

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

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

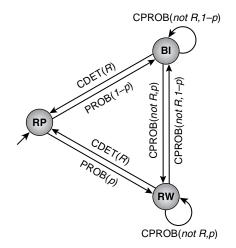
g^* := \min\{g(s') \mid s' \in N(s)\};

s' := selectRandom(\{s' \in N(s) \mid g(s') = g^*\});

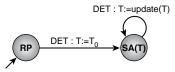
return s'

end step-Bl
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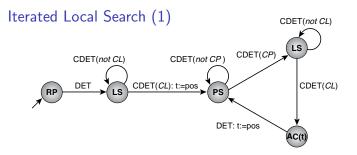
Randomised Iterative Best Improvement with Random Restart



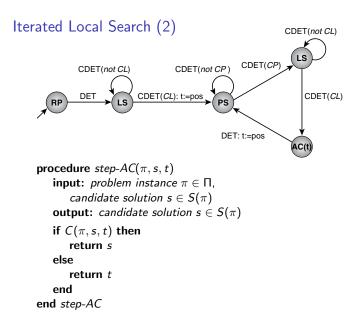
Simulated Annealing



- Note the use of transition actions and memory for temperature T.
- The parametric state SA(T) implements probabilistic improvement steps for given temperature T.
- ► The initial temperature *T*₀ and function *update* implement the annealing schedule.



- The acceptance criterion is modelled as a state type, since it affects the search position.
- Note the use of transition actions for memorising the current candidate solution (pos) at the end of each local search phase.
- Condition predicates CP and CL determine the end of perturbation and local search phases, respectively; in many ILS algorithms, CL := Imin.



Ant Colony Optimisation (1)

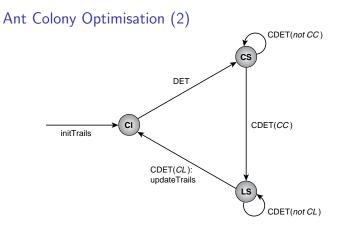
 General approach for modelling population-based SLS methods, such as ACO, as GLSMs:

Define search positions as *sets of candidate solutions*; search steps manipulate some or all elements of these sets.

Example: In this view, Iterative Improvement (II) applied to a population *sp* in each step performs one II step on each candidate solution from *sp* that is not already a local minimum.

(Alternative approaches exist.)

Pheromone levels are represented by memory states and are initialised and updated by means of transition actions.



- 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 ACO algorithms, *CL* := lmin.

Stochastic Local Search: Foundations and Applications

The basic GLSM model can be generalised and extended in various rather straightforward ways, such as:

- Co-operative GLSM models
- Learning GLSM models
- Evolutionary GLSM models
- Continuous GLSM models

Note: So far, these extensions remain mostly unexplored — lots of opportunities for interesting research!

Co-operative GLSM models

- Key idea: Apply multiple GLSMs simultaneously to the same problem instance
- Naturally captures population-based SLS approaches.
- Homogeneous co-operative GLSM models:
 Population of identical GLSMs; equivalent to performing multiple independent runs of the respective SLS method.
- Heterogenous co-operative GLSM models: Population of different GLSMs; model algorithm portfolios.

Co-operative GLSM models with communication

- GLSMs in population exchange information about their search trajectories, *e.g.*, via message passing or blackboard mechanism.
- Communication can be modelled via shared memory state or special transition actions (*e.g.*, *send*, *receive*).
- These models are naturally suited for representing population-based algorithms that use communication between individual search agents, such as ACO.

Learning via dynamic transition probabilities

- Key idea: In a GLSM with probabilistic transitions, let transition probabilities evolve over time to adaptively optimise search control strategy.
- Can build on concepts from learning automata theory.
- Single-instance learning:

Optimise control strategy on one problem instance during search process.

Multi-instance learning:

Adapt control strategies to features common to a class of problem instances.

 Transition probabilities can be adapted via external mechanism or via specialised transition actions.

Evolutionary GLSM models

- Key idea: Achieve learning/adaptation in co-operative GLSM models by varying number or type of individual GLSMs over time.
- Distinction between *single-* and *multi-instance learning* as before; similar mechanisms for controlling adaptation process.
- Can easily model, for example, self-optimising portfolios of SLS algorithms.
- Further extensions:
 - support mutation / recombination operations on GLSMs;
 - ► additionally support learning in individual GLSMs ~> evolving ensembles of dynamic GLSMs;
 - include communication between GLSMs in population.

Continuous GLSM models

- Note: Many previously discussed hybrid SLS methods can be extended to continuous optimisation problems and give rise to high-performance algorithms for solving these.
- The main feature of the GLSM model, namely its clear distinction between *lower-level, simple search strategies* and *higher-level search control*, equally applies to continuous SLS algorithms.
- Key idea: Model complex continuous SLS methods by using continuous optimisation procedures as subsidiary local search strategies.

Note: The GLSM model is well-suited for modelling algorithms for *hybrid combinatorial problems* that involve discrete as well as continuous solution components.