STOCHASTIC LOCAL SEARCH
FOUNDATIONS AND APPLICATIONS

Generalised Local Search Machines

Holger H. Hoos & Thomas Stützle
Outline

1. The Basic GLSM Model
2. State, Transition and Machine Types
3. Modelling SLS Methods Using GLSMs
4. Extensions of the Basic GLSM Model
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 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 $z_0, z_1, z_2$ 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.
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;
- \( \sigma_Z \) and \( \sigma_\Delta \) are sets of state types and transition types;
- \( \tau_Z : Z \mapsto \sigma_Z \) 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.
Example: Simple 3-state GLSM (formal definition)

- $Z := \{z_0, z_1, z_2\}$; $z_0 =$ initial machine state
- no memory ($M := \{m_0\}$; $m_0 =$ initial and only memory state)
- $\Delta := \{(z_0, z_1), (z_1, z_2), (z_1, z_1), (z_2, z_1), (z_2, z_2)\}$
- $\sigma_Z := \{z_0, z_1, z_2\}$
- $\sigma_\Delta := \{\text{PROB}(p) \mid p \in \{1, p_1, p_2, 1 - p_1, 1 - p_2\}\}$
- $\tau_Z(z_i) := z_i$, $i \in \{0, 1, 2\}$
- $\tau_\Delta((z_0, z_1)) := \text{PROB}(1)$, $\tau_\Delta((z_1, z_2)) := \text{PROB}(p_1)$, $\ldots$
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 $z_0$ (e.g., random picking).
- With probability 1, switch to state $z_1$.
- Perform one search step according to state $z_1$; switch to state $z_2$ with probability $p_1$, otherwise, remain in state $z_1$.
- In state $z_2$, perform one search step according to $z_2$; switch back to state $z_1$ with probability $p_2$, otherwise, remain in state $z_2$.

$\Rightarrow$ 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.
- $\sigma_Z, \sigma_\Delta$ 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 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 $\mathcal{M}$ 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.
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;

- 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* $\tau =$ state type $\tau$ for which search position after one $\tau$ step is independent of search position before step.

*initialising state* $\equiv$ state of initialising type.

▶ *parametric state type* $\tau =$ state type $\tau$ whose semantics depends on memory state.

*parametric state* $\equiv$ 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.

- Given GLSM $\mathcal{M}$ any state that can be reached from initial state $z_0$ by following a chain of $\text{PROB}(p)$ transitions with $p > 0$ with 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 $1/p$. 
Transitions types (2)

- **Conditional probabilistic transitions** – type $\text{CPROB}(C, p)$:
  - 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 $\text{CDET}(C)$.

- Condition predicates should be efficiently computable (ideally: $\leq$ linear time w.r.t. size of given problem instance).
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 \( k = 0 \)
- \( \text{lmin} \) current candidate solution is a local minimum w.r.t. the given neighbourhood relation
- \( \text{evalf}(y) \) current evaluation function value \( \leq y \)
- \( \text{noimpr}(k) \) 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 from 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 $z_0$ only once.

- **alternating 1-state+init machines:**

  - may visit initialising state $z_0$ 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 $z_1$ steps and a sequence of $z_2$ 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(π, s)
    input: problem instance π ∈ Π,
           candidate solution s ∈ S(π)
    output: candidate solution s ∈ S(π)
    s' := selectRandom(S);
    return s'
end step-RP

procedure step-RW(π, s)
    input: problem instance π ∈ Π,
           candidate solution s ∈ S(π)
    output: candidate solution s ∈ S(π)
    s' := selectRandom(N(s));
    return s'
end step-RW
Uninformed Random Walk with Random Restart

\[ R = \text{restart predicate, e.g., countm}(k) \]
Iterative Best Improvement with Random Restart

procedure step-BI(\( \pi, s \) )

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

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

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

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

return \( s' \)

end step-BI
Randomised Iterative Best Improvement with Random Restart

\[
\text{CPROB}(\text{not } R, 1-p)
\]

\[
\text{CDET}(R)
\]

\[
\text{PROB}(p)
\]

\[
\text{CPROB}(\text{not } R, p)
\]

\[
\text{CPROB}(\text{not } R, 1-p)
\]
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.
Iterated Local Search (1)

- 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 \((\text{pos})\) 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, \(CL := \text{lmin}\).
Iterated Local Search (2)

**procedure** `step-AC(π, s, t)`

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

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

if $C(\pi, s, t)$ then
  return $s$
else
  return $t$
end
end `step-AC`
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, $CL := l\text{min}$. 
Extensions of the Basic GLSM Model

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 \( \leadsto \) 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.