STOCHASTIC LOCAL SEARCH FOUNDATIONS AND APPLICATIONS

Generalised Local Search Machines

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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).

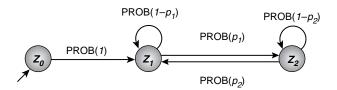
These hybrid SLS methods operate on two levels:

- ▶ 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.
- ▶ PROB(p) refers to a probabilistic state transition with probability p after each search step.

Generalised Local Search Machines (GLSMs)

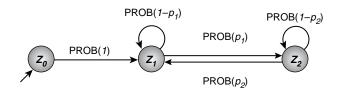
- States \cong simple search strategies.
- ▶ State transitions ≅ search control.
- GLSM M starts in initial state.
- In each iteration:
 - M executes one search step associated with its current state z;
 - M selects a new state (which may be the same as z) in a nondeterministic manner.
- M terminates 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);
- ▶ m₀ 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 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)



- $ightharpoonup Z := \{z_0, z_1, z_2\}; z_0 = \text{initial machine state}$
- ▶ 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 z_0 (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.
- \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.
- ▶ 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 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,
- neighbhourhood 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 Chaper 2).
- initialising state type = state type τ for which search position after one τ step is independ 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.
- Given GLSM \mathcal{M} any state that can be reached from initial state z_0 by following a chain of 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 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:

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 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:



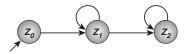
- ightharpoonup visit initialising state z_0 only on once.
- ► alternating 1-state+init machines:



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

► 2-state+init sequential machines:

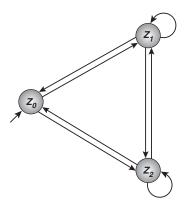
one initialising state (visited only once), two working states;



▶ 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.

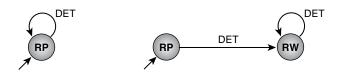


Generalisations:

- ► *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).

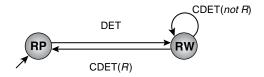
Modellig SLS Methods Using GLSMs

Uninformed Picking and Uninformed Random Walk



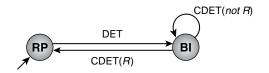
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\begin{array}{lll} \textbf{procedure} \ step\text{-}RP(\pi,s) & \textbf{procedure} \ step\text{-}RW(\pi,s) \\ \textbf{input:} \ problem \ instance} \ \pi \in \Pi, \\ \quad candidate \ solution \ s \in S(\pi) & candidate \ solution \ s \in S(\pi) \\ \textbf{output:} \ candidate \ solution \ s \in S(\pi) \\ s' := selectRandom(S); & s' := selectRandom(N(s)); \\ \textbf{return} \ s' & \textbf{return} \ s' \\ \textbf{end} \ step\text{-}RP & \textbf{end} \ step\text{-}RW \end{array}
```

Uninformed Random Walk with Random Restart



R = restart predicate, e.g., countm(k)

Iterative Best Improvement with Random Restart



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procedure step-BI(\pi,s)

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

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

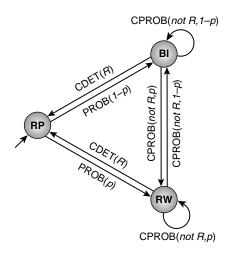
g^* := \min\{g(s') \mid s' \in N(s)\};

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

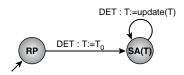
return s'

end step-BI
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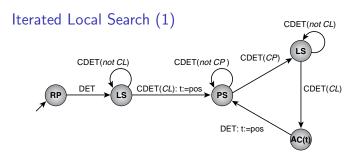
Randomised Iterative Best Improvement with Random Restart



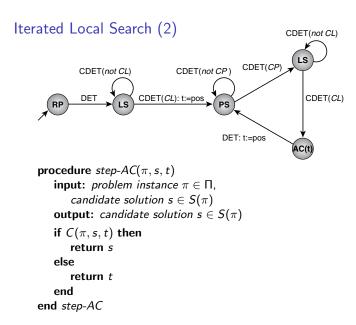
Simulated Annealing



- 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:

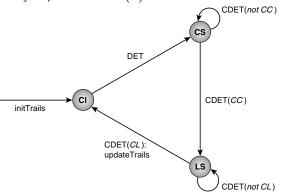
Define search positions as *sets of candidate solutions*; search steps manipulate some or all elements of these sets.

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.

Ant Colony Optimisation (2)



- ► 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* := Imin.

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 simultanously 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;

 - ▶ 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.