Part 2 – Heuristics
(Stochastic) Local Search Algorithms

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark
Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   Components
Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   Components
Local Search Algorithms

Given a (combinatorial) optimization problem $\Pi$ and one of its instances $\pi$:

1. search space $S(\pi)$
   - specified by the definition of (finite domain, integer) variables and their values handling implicit constraints
   - all together they determine the representation of candidate solutions
   - common solution representations are discrete structures such as: sequences, permutations, partitions, graphs
     (e.g., for SAT: array, sequence of truth assignments to propositional variables)

Note: solution set $S'(\pi) \subseteq S(\pi)$
(e.g., for SAT: models of given formula)
2. evaluation function $f_\pi : S(\pi) \to \mathbb{R}$

   - it handles the soft constraints and the objective function (e.g., for SAT: number of false clauses)

3. neighborhood function, $\mathcal{N}_\pi : S \to 2^{S(\pi)}$

   - defines for each solution $s \in S(\pi)$ a set of solutions $\mathcal{N}(s) \subseteq S(\pi)$ that are in some sense close to $s$. (e.g., for SAT: neighboring variable assignments differ in the truth value of exactly one variable)
4. set of memory states $M(\pi)$
   (may consist of a single state, for LS algorithms that do not use memory)

5. initialization function $\text{init} : \emptyset \to S(\pi)$
   (can be seen as a probability distribution $\Pr(S(\pi) \times M(\pi))$ over initial search positions and memory states)

6. step function $\text{step} : S(\pi) \times M(\pi) \to S(\pi) \times M(\pi)$
   (can be seen as a probability distribution $\Pr(S(\pi) \times M(\pi))$ over subsequent, neighboring search positions and memory states)

7. termination predicate $\text{terminate} : S(\pi) \times M(\pi) \to \{\top, \bot\}$
   (determines the termination state for each search position and memory state)
Local search — global view

Neighborhood graph

- vertices: candidate solutions (search positions)
- vertex labels: evaluation function
- edges: connect “neighboring” positions
- s: (optimal) solution
- c: current search position
Iterative Improvement

**Iterative Improvement (II):**
determine initial candidate solution \( s \)

while \( s \) has better neighbors do

  choose a neighbor \( s' \) of \( s \) such that \( f(s') < f(s) \)

  \( s := s' \)

▶ If more than one neighbor have better cost then need to choose one (heuristic pivot rule)

▶ The procedure ends in a local optimum \( \hat{s} \):
  Def.: Local optimum \( \hat{s} \) w.r.t. \( N \) if \( f(\hat{s}) \leq f(s) \) \( \forall s \in N(\hat{s}) \)

▶ Issue: how to avoid getting trapped in bad local optima?
  ▶ use more complex neighborhood functions
  ▶ restart
  ▶ allow non-improving moves
Example: Local Search for SAT

Example: Uninformed random walk for SAT (1)

- **solution representation and search space** $S$: array of boolean variables representing the truth assignments to variables in given formula $F$  
  no implicit constraint  
  (solution set $S'$: set of all models of $F$)

- **neighborhood relation** $\mathcal{N}$: 1-flip neighborhood, i.e., assignments are neighbors under $\mathcal{N}$ iff they differ in the truth value of exactly one variable

- **evaluation function** handles clause and proposition constraints  
  $f(s) = 0$ if model $f(s) = 1$ otherwise

- **memory**: not used, i.e., $M := \emptyset$
Example: Uninformed random walk for SAT (2)

- **initialization:** uniform random choice from \( S \), i.e.,
  \[
  \text{init}(\{a', m\}) := \frac{1}{|S|}
  \]
  for all assignments \( a' \) and memory states \( m \)

- **step function:** uniform random choice from current neighborhood, i.e.,
  \[
  \text{step}(\{a, m\}, \{a', m\}) := \frac{1}{|N(a)|}
  \]
  for all assignments \( a \) and memory states \( m \),
  where \( N(a) := \{a' \in S \mid N(a, a')\} \) is the set of all neighbors of \( a \).

- **termination:** when model is found, i.e.,
  \[
  \text{terminate}(\{a, m\}) := \top \text{ if } a \text{ is a model of } F, \text{ and } 0 \text{ otherwise.}
  \]
N-Queens Problem

**N-Queens problem**

**Input:** A chessboard of size $N \times N$

**Task:** Find a placement of $n$ queens on the board such that no two queens are on the same row, column, or diagonal.
import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    select(q in Size, v in Size) {
        queen[q] := v;
        cout << "chng @ " << it << ": queen["<<q<<"]=" << v << " viol: " << S.violations() << endl;
    }
    it = it + 1;
}
cout << queen << endl;
import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    select(q in Size : S.violations(queen[q])>0, v in Size) {
        queen[q] := v;
        cout<<"chng @ "<<it<<": queen["<<q<<"]:="<<v<<" viol: "<<S.
        violations()<<endl;
    }
    it = it + 1;
}

cout << queen << endl;
Metaheuristics

- Variable Neighborhood Search and Large Scale Neighborhood Search
diversified neighborhoods + incremental algorithmics ("diversified" ≡
multiple, variable-size, and rich).

- Tabu Search: Online learning of moves
  Discard undoing moves,
  Discard inefficient moves
  Improve efficient moves selection

- Simulated annealing
  Allow degrading solutions

- “Restart” + parallel search
  Avoid local optima
  Improve search space coverage
Summary: Local Search Algorithms

For given problem instance $\pi$:

1. search space $S_\pi$, solution representation: variables + implicit constraints
2. evaluation function $f_\pi : S \rightarrow \mathbb{R}$, soft constraints + objective
3. neighborhood relation $N_\pi \subseteq S_\pi \times S_\pi$
4. set of memory states $M_\pi$
5. initialization function $\text{init} : \emptyset \rightarrow S_\pi \times M_\pi$
6. step function $\text{step} : S_\pi \times M_\pi \rightarrow S_\pi \times M_\pi$
7. termination predicate $\text{terminate} : S_\pi \times M_\pi \rightarrow \{\top, \bot\}$
**Decision vs Minimization**

**LS-Decision** ($\pi$)
input: problem instance $\pi \in \Pi$
output: solution $s \in S'(\pi)$ or $\emptyset$

$$(s, m) := \text{init}(\pi)$$

while not $\text{terminate}(\pi, s, m)$ do
  $$(s, m) := \text{step}(\pi, s, m)$$

if $s \in S'(\pi)$ then
  return $s$
else
  return $\emptyset$

**LS-Minimization** ($\pi'$)
input: problem instance $\pi' \in \Pi'$
output: solution $s \in S'(\pi')$ or $\emptyset$

$$(s, m) := \text{init}(\pi');$$

$s_b := s$;

while not $\text{terminate}(\pi', s, m)$ do
  $$(s, m) := \text{step}(\pi', s, m);$$
  if $f(\pi', s) < f(\pi', \hat{s})$ then
    $s_b := s$

if $s_b \in S'(\pi')$ then
  return $s_b$
else
  return $\emptyset$

However, the algorithm on the left has little guidance, hence most often
decision problems are transformed in optimization problems by, eg, counting
number of violations.
Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   Components
Iterative Improvement

- does not use memory
- **init**: uniform random choice from $S$ or construction heuristic
- **step**: uniform random choice from improving neighbors

$$\Pr(s, s') = \begin{cases} 
\frac{1}{|I(s)|} & \text{if } s' \in I(s) \\
0 & \text{otherwise}
\end{cases}$$

where $I(s) := \{s' \in S \mid N(s, s') \text{ and } f(s') < f(s)\}$

- terminates when no improving neighbor available

**Note**: Iterative improvement is also known as iterative descent or hill-climbing.
Iterative Improvement (cntd)

Pivoting rule decides which neighbors go in $I(s)$

- **Best Improvement** (aka \textit{gradient descent}, \textit{steepest descent}, \textit{greedy hill-climbing}): Choose maximally improving neighbors, i.e., $I(s) := \{s' \in N(s) \mid f(s') = g^*\}$, where $g^* := \min\{f(s') \mid s' \in N(s)\}$.

  \textit{Note}: Requires evaluation of all neighbors in each step!

- **First Improvement**: Evaluate neighbors in fixed order, choose first improving one encountered.

  \textit{Note}: Can be more efficient than Best Improvement but not in the worst case; order of evaluation can impact performance.
Examples

Iterative Improvement for SAT

- **search space** $S$: set of all truth assignments to variables in given formula $F$ (solution set $S'$: set of all models of $F$)
- **neighborhood relation** $\mathcal{N}$: 1-flip neighborhood
- **memory**: not used, i.e., $M := \{0\}$
- **initialization**: uniform random choice from $S$, i.e., $\text{init}(\emptyset, \{a\}) := 1/|S|$ for all assignments $a$
- **evaluation function**: $f(a) :=$ number of clauses in $F$ that are unsatisfied under assignment $a$  
  (Note: $f(a) = 0$ iff $a$ is a model of $F$.)
- **step function**: uniform random choice from improving neighbors, i.e., $\text{step}(a, a') := 1/|I(a)|$ if $a' \in I(a)$, and 0 otherwise, where $I(a) := \{a' | \mathcal{N}(a, a') \land f(a') < f(a)\}$
- **termination**: when no improving neighbor is available i.e., $\text{terminate}(a) := \top$ if $I(a) = \emptyset$, and 0 otherwise.
Examples

Random order first improvement for SAT

\[ URW\text{-for-SAT}(F,\text{maxSteps}) \]

**input:** propositional formula \( F \), integer \( \text{maxSteps} \)

**output:** a model for \( F \) or \( \emptyset \)

choose assignment \( \varphi \) of truth values to all variables in \( F \)
uniformly at random;

\( \text{steps} := 0; \)

while \( \neg (\varphi \text{ satisfies } F) \) and \( (\text{steps} < \text{maxSteps}) \) do

- select \( x \) uniformly at random from \( \{x'|x' \text{ is a variable in } F \text{ and changing value of } x' \text{ in } \varphi \text{ decreases the number of unsatisfied clauses}\} \)

- \( \text{steps} := \text{steps} + 1; \)

if \( \varphi \text{ satisfies } F \) then

- return \( \varphi \)

else

- return \( \emptyset \)
Local Search Algorithms
Iterative Improvement

import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    select(q in Size, v in Size : S.getAssignDelta(queen[q],v) < 0) {
        queen[q] := v;
        cout << "chng @ " <<it<<": queen["<<q<<"]:"<<v<<" viol: "<<S.violations() << endl;
    }
    it = it + 1;
}
cout << queen << endl;
Local Search Algorithms

Best Improvement

```cpp
import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    selectMin(q in Size,v in Size)(S.getAssignDelta(queen[q],v)) {
        queen[q] := v;
        cout<<"chng @ "<<it<<": queen["<<q<<"] := "<<v<<" viol: "<<S.
        violations() <<endl;
    }
    it = it + 1;
}
cout << queen << endl;
```
import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    selectFirst(q in Size, v in Size: S.getAssignDelta(queen[q],v) < 0) {
        queen[q] := v;
        cout << "chng @ " << it << ": queen["" << q << "] := "" << v << " viol: "" << S.violations() << endl;
    }
    it = it + 1;
}
cout << queen << endl;
Local Search Algorithms

Min Conflict Heuristic

```python
import cotls;
int n = 16;
range Size = 1..n;
UniformDistribution distr(Size);

Solver<LS> m();
var{int} queen[Size](m,Size) := distr.get();
ConstraintSystem<LS> S(m);

S.post(alldifferent(queen));
S.post(alldifferent(all(i in Size) queen[i] + i));
S.post(alldifferent(all(i in Size) queen[i] - i));
m.close();

int it = 0;
while (S.violations() > 0 && it < 50 * n) {
    select(q in Size : S.violations(queen[q])>0) {
        selectMin(v in Size)(S.getAssignDelta(queen[q],v)) {
            queen[q] := v;
            cout<<"chng @ "<<it<<": queen["<<q<<"] := "<<v<<" viol: "<<S.
            violations() <<endl;
        }
        it = it + 1;
    }
}
cout << queen << endl;
```
Resumé: Constraint-Based Local Search

Constraint-Based Local Search = Modelling + Search
Resumé: Local Search Modelling

Optimization problem (decision problems $\rightarrow$ optimization):

- Parameters

- Variables and Solution Representation
  implicit constraints

- Soft constraint violations

- Evaluation function: soft constraints + objective function

Differentiable objects:

- Neighborhoods

- Delta evaluations
  Invariants defined by one-way constraints
For given problem instance $\pi$:

1. search space $S_\pi$, solution representation: variables + implicit constraints

2. evaluation function $f_\pi : S \rightarrow \mathbb{R}$, soft constraints + objective

3. neighborhood relation $N_\pi \subseteq S_\pi \times S_\pi$

4. set of memory states $M_\pi$

5. initialization function $\text{init} : \emptyset \rightarrow S_\pi \times M_\pi$

6. step function $\text{step} : S_\pi \times M_\pi \rightarrow S_\pi \times M_\pi$

7. termination predicate $\text{terminate} : S_\pi \times M_\pi \rightarrow \{\top, \bot\}$

Computational analysis on each of these components is necessary!
Resumé: Local Search Algorithms

- Random Walk
- First/Random Improvement
- Best Improvement
- Min Conflict Heuristic

The step is the component that changes. It is also called: pivoting rule (for allusion to the simplex for LP)
Examples: TSP

Random-order first improvement for the TSP

- **Given:** TSP instance $G$ with vertices $v_1, v_2, \ldots, v_n$.
- **Search space:** Hamiltonian cycles in $G$;
- **Neighborhood relation $N$:** standard 2-exchange neighborhood
- **Initialization:**
  
  search position := fixed canonical tour $< v_1, v_2, \ldots, v_n, v_1 >$
  
  “mask” $P$ := random permutation of $\{1, 2, \ldots, n\}$

- **Search steps:** determined using first improvement w.r.t. $f(s) = \text{cost of tour } s$, evaluating neighbors in order of $P$ (does not change throughout search)

- **Termination:** when no improving search step possible (local minimum)
Examples: TSP

Iterative Improvement for TSP

\( TSP-2opt-first(s) \)

**input:** an initial candidate tour \( s \in S(\in) \)

**output:** a local optimum \( s \in S_\pi \)

for \( i = 1 \) to \( n - 1 \) do

for \( j = i + 1 \) to \( n \) do

if \( P[i] + 1 \geq n \) or \( P[j] + 1 \geq n \) then continue;

if \( P[i] + 1 = P[j] \) or \( P[j] + 1 = P[i] \) then continue;

\[ \Delta_{ij} = d(\pi_{P[i]}, \pi_{P[j]}) + d(\pi_{P[i]+1}, \pi_{P[j]+1}) + d(\pi_{P[j]}, \pi_{P[i]+1}) - d(\pi_{P[j]}, \pi_{P[i]+1}) \]

if \( \Delta_{ij} < 0 \) then

UpdateTour\( (s, P[i], P[j]) \)

is it really?
Examples

Iterative Improvement for TSP

**TSP-2opt-first(s)**

input: an initial candidate tour $s \in S(\in)$

output: a local optimum $s \in S_\pi$

$\text{FoundImprovement:=TRUE;}$

while FoundImprovement do

\hspace{1cm} $\text{FoundImprovement:=FALSE;}$

\hspace{1cm} for $i = 1$ to $n - 1$ do

\hspace{2cm} for $j = i + 1$ to $n$ do

\hspace{3cm} if $P[i] + 1 \geq n$ or $P[j] + 1 \geq n$ then continue ;

\hspace{3cm} if $P[i] + 1 = P[j]$ or $P[j] + 1 = P[i]$ then continue ;

\hspace{3cm} $\Delta_{ij} = d(\pi_{P[i]}, \pi_{P[j]}) + d(\pi_{P[i]+1}, \pi_{P[j]+1}) +$

\hspace{3cm} $-d(\pi_{P[i]}, \pi_{P[i]+1}) - d(\pi_{P[j]}, \pi_{P[j]+1})$

\hspace{3cm} if $\Delta_{ij} < 0$ then

\hspace{4cm} $\text{UpdateTour}(s, P[i], P[j])$

\hspace{4cm} $\text{FoundImprovement=TRUE}$
Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   Components
Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   Components
Search Space

Solution representations defined by the variables and the implicit constraints:

- permutations (implicit: all different)
  - linear (scheduling problems)
  - circular (traveling salesman problem)

- arrays (implicit: assign exactly one, assignment problems: GCP)

- sets (implicit: disjoint sets, partition problems: graph partitioning, max indep. set)

Multiple viewpoints are useful also in local search!
Evaluation (or cost) function:

- function \( f_\pi : S_\pi \rightarrow \mathbb{Q} \) that maps candidate solutions of a given problem instance \( \pi \) onto rational numbers (most often integer), such that global optima correspond to solutions of \( \pi \);
- used for assessing or ranking neighbors of current search position to provide guidance to search process.

Evaluation vs objective functions:

- **Evaluation function**: part of LS algorithm.
- **Objective function**: integral part of optimization problem.
- Some LS methods use evaluation functions different from given objective function (e.g., guided local search).
Constrained Optimization Problems exhibit two issues:

- feasibility
eg, traveling salesman problem with time windows: customers must be visited within their time window.
- optimization
  minimize the total tour.

How to combine them in local search?

- sequence of feasibility problems
- staying in the space of feasible candidate solutions
- considering feasible and infeasible configurations
If infeasible solutions are allowed, we count violations of constraints.

What is a violation?
Constraint specific:

- decomposition-based violations
  number of violated constraints, eg: alldiff

- variable-based violations
  min number of variables that must be changed to satisfy $c$.

- value-based violations
  for constraints on number of occurrences of values

- arithmetic violations

- combinations of these
Combinatorial constraints

- `alldiff(x_1, \ldots, x_n)`: Let \( a \) be an assignment with values \( V = \{ a(x_1), \ldots, a(x_n) \} \) and \( c_v = \#_a(v, x) \) be the number of occurrences of \( v \) in \( a \).

Possible definitions for violations are:

- \( \text{viol} = \sum_{v \in V} I(\max\{c_v - 1, 0\} > 0) \) value-based
- \( \text{viol} = \max_{v \in V} \max\{c_v - 1, 0\} \) value-based
- \( \text{viol} = \sum_{v \in V} \max\{c_v - 1, 0\} \) value-based
- \( \# \) variables with same value, variable-based, here leads to same definitions as previous three

Arithmetic constraints

- \( l \leq r \leadsto \text{viol} = \max\{l - r, 0\} \)
- \( l = r \leadsto \text{viol} = |l - r| \)
- \( l \neq r \leadsto \text{viol} = 1 \) if \( l = r \), 0 otherwise