DM841
Discrete Optimization

Part 2 – Heuristics
(Stochastic) Local Search Algorithms

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Outline

1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
   - Components

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1. Local Search Algorithms

2. Basic Algorithms

3. Local Search Revisited
    Components

Local Search Algorithms

Given a (combinatorial) optimization problem Π and one of its instances π:

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)

Local Search Algorithms (cntd)

2. evaluation function $f_\pi : S(\pi) \to \mathbf{R}$
   - 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 $N(s) \subseteq S(\pi)$ that are in some sense close to s.
     (*e.g.*, for SAT: neighboring variable assignments differ in the truth value of exactly one variable)

Local Search Algorithms (cntd)

Further components [according to [HS]]

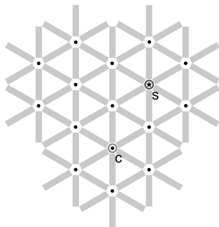
4. set of memory states $M(\pi)$
   (may consist of a single state, for LS algorithms that do not use memory)

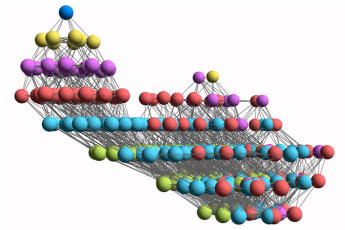
5. initialization function $\texttt{init} : \emptyset \to S(\pi)$
   (can be seen as a probability distribution $\Pr(S(\pi) \times M(\pi))$ over initial search positions and memory states)

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

7. termination predicate $\texttt{terminate} : S(\pi) \times M(\pi) \to \{\top, \bot\}$
   (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)

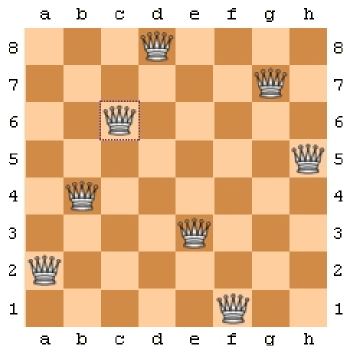
- **initialization:** uniform random choice from S, *i.e.*, $\texttt{init}(,\{a',m\}) := 1/|S|$ for all assignments a' and memory states m
- **step function:** uniform random choice from current neighborhood, *i.e.*, $\texttt{step}(\{a,m\},\{a',m\}) := 1/|N(a)|$ for all assignments a and memory states m, where $N(a) := \{a' \in S \mid \mathcal{N}(a,a')\}$ is the set of all neighbors of a.
- **termination:** when model is found, *i.e.*, $\texttt{terminate}(\{a,m\}) := \top$ if a is a model of F, and 0 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.



Local Search Examples
Random Walk

queensLS0a.co

```
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;
```

Local Search Examples

Another Random Walk

queensLS1.co

```
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 π:

1. search space S_π, solution representation: variables + implicit constraints
2. evaluation function $f_\pi : S \to \mathbf{R}$, soft constraints + objective
3. neighborhood relation $\mathcal{N}_\pi \subseteq S_\pi \times S_\pi$
4. set of memory states M_π
5. initialization function $\texttt{init} : \emptyset \to S_\pi \times M_\pi)$
6. step function $\texttt{step} : S_\pi \times M_\pi \to S_\pi \times M_\pi$
7. termination predicate $\texttt{terminate} : S_\pi \times M_\pi \to \{\top, \bot\}$

Decision vs Minimization

```
LS-Decision(π)
input: problem instance π ∈ Π
output: solution s ∈ S'(π) or ∅
(s, m) := init(π)

while not terminate(π, s, m) do
  └ (s, m) := step(π, s, m)

if s ∈ S'(π) then
  | return s
else
  └ return ∅
```

```
LS-Minimization(π')
input: problem instance π' ∈ Π'
output: solution s ∈ S'(π') or ∅
(s, m) := init(π');
s_b := s;
while not terminate(π', s, m) do
  | (s, m) := step(π', s, m);
  | if f(π', s) < f(π', ŝ) then
  |   └ s_b := s;
  └
if s_b ∈ S'(π') then
  | return s_b
else
  └ return ∅
```

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

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Iterative Improvement

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

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

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

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

  Note: Requires evaluation of all neighbors in each step!

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

  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.*, $\texttt{init}(\emptyset, \{a\}) := 1/|S|$ 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.*, $\texttt{step}(a, a') := 1/|I(a)|$ if $a' \in I(a)$, and 0 otherwise, where $I(a) := \{a' \mid \mathcal{N}(a, a') \wedge f(a') < f(a)\}$
- **termination**: when no improving neighbor is available *i.e.*, $\texttt{terminate}(a) := \top$ if $I(a) = \emptyset$, and 0 otherwise.

Examples

Random order first improvement for SAT

URW-for-SAT(F,$maxSteps$)
input: *propositional formula F, integer maxSteps*
output: *a model for F* **or** $\emptyset$

```
choose assignment φ of truth values to all variables in F
    uniformly at random;
steps := 0;
while ¬(φ satisfies F) and (steps < maxSteps) do
    select x uniformly at random from {x′|x′ is a variable in F and
    changing value of x′ in φ decreases the number of unsatisfied clauses}
    steps := steps+1;
if φ satisfies F then
    return φ
else
    return ∅
```

Local Search Algorithms

Iterative Improvement

queensLS00.co

```
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

queensLS0.co

```
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;
```

Local Search Algorithms
First Improvement

queensLS2.co

```
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

queensLS0b.co

```
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 $\mapsto$ 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

Resumé: Local Search Algorithms

A theoretical framework

For given problem instance π:

1. search space S_π, solution representation: variables + implicit constraints
2. evaluation function $f_\pi : S \to \mathbf{R}$, soft constraints + objective
3. neighborhood relation $\mathcal{N}_\pi \subseteq S_\pi \times S_\pi$
4. set of memory states M_π
5. initialization function $\texttt{init} : \emptyset \to S_\pi \times M_\pi)$
6. step function $\texttt{step} : S_\pi \times M_\pi \to S_\pi \times M_\pi$
7. termination predicate $\texttt{terminate} : S_\pi \times M_\pi \to \{\top, \bot\}$

Computational analysis on each of these components is necessay!

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 $v_1, v_2, \dots, v_n$.
- **Search space:** Hamiltonian cycles in G;
- **Neighborhood relation** N**:** standard 2-exchange neighborhood
- **Initialization:**

  search position := fixed canonical tour $< v_1, v_2, \dots, v_n, v_1 >$
  "mask" P := random permutation of $\{1, 2, \dots, n\}$

- **Search steps:** determined using first improvement w.r.t. $f(s)$ = 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* ;

$$\begin{aligned}\Delta_{ij} \quad = \quad & d(\pi_{P[i]}, \pi_{P[j]}) + d(\pi_{P[i]+1}, \pi_{P[j]+1}) + \\ & -d(\pi_{P[i]}, \pi_{P[i]+1}) - d(\pi_{P[j]}, \pi_{P[j]+1})\end{aligned}$$

    if $\Delta_{ij} < 0$ **then**
      $\texttt{UpdateTour}(s, P[i], P[j])$

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* $s \in S_\pi$

```
FoundImprovement:=TRUE;
while FoundImprovement do
    FoundImprovement:=FALSE;
    for i = 1 to n − 1 do
        for j = i + 1 to n do
            if P[i] + 1 ≥ n or P[j] + 1 ≥ n then continue ;
            if P[i] + 1 = P[j] or P[j] + 1 = P[i] then continue ;
            Δij = d(π_P[i], π_P[j]) + d(π_P[i]+1, π_P[j]+1) +
                  −d(π_P[i], π_P[i]+1) − d(π_P[j], π_P[j]+1)
            if Δij < 0 then
                UpdateTour(s, P[i], P[j])
                FoundImprovement=TRUE
```

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

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LS Algorithm Components

Search space

Search Space

Solution representations defined by the variables and the implicit constraints:

- permutations (implicit: alldiffrerent)
  - 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!

LS Algorithm Components

Evaluation function

Evaluation (or cost) function:

- function $f_\pi : S_\pi \to \mathbf{Q}$ that maps candidate solutions of a given problem instance π onto rational numbers (most often integer), such that global optima correspond to solutions of π;
- 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

Constrained Optimization Problems exhibit two issues:

- feasibility
  eg, treveling 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

Constraint-based local search

From Van Hentenryck and Michel

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 occurences of values
- arithmetic violations
- combinations of these

Constraint-based local search

From Van Hentenryck and Michel

Combinatorial constraints

- $\texttt{alldiff}(x_1, \ldots, x_n)$:
  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:
  - $\mathrm{viol} = \sum_{v \in V} I(\max\{c_v - 1, 0\} > 0)$ value-based
  - $\mathrm{viol} = \max_{v \in V} \max\{c_v - 1, 0\}$ value-based
  - $\mathrm{viol} = \sum_{v \in V} \max\{c_v - 1, 0\}$ value-based
  - # variables with same value, variable-based, here leads to same definitions as previous three

Arithmetic constraints

- $l \leq r \leadsto \mathrm{viol} = \max\{l - r, 0\}$
- $l = r \leadsto \mathrm{viol} = |l - r|$
- $l \neq r \leadsto \mathrm{viol} = 1$ if $l = r$, 0 otherwise