DM865 – Spring 2018

Heuristics and Approximation Algorithms

Metaheuristics

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Outline

1. Stochastic Local Search
2. Simulated Annealing
3. Iterated Local Search
4. Tabu Search
5. Variable Neighborhood Search

Escaping Local Optima

Possibilities:

- Non-improving steps: in local optima, allow selection of candidate solutions with equal or worse evaluation function value, *e.g.*, using minimally worsening steps.
  (Can lead to long walks in *plateaus*, *i.e.*, regions of search positions with identical evaluation function.)
- Diversify the neighborhood
- Restart: re-initialize search whenever a local optimum is encountered.
  (Often rather ineffective due to cost of initialization.)

Note: None of these mechanisms is guaranteed to always escape effectively from local optima.

Diversification *vs* Intensification

- Goal-directed and randomized components of LS strategy need to be balanced carefully.
- Intensification: aims at greedily increasing solution quality, *e.g.*, by exploiting the evaluation function.
- Diversification: aims at preventing search stagnation, that is, the search process getting trapped in confined regions.

Examples:

- Iterative Improvement (II): *intensification* strategy.
- Uninformed Random Walk/Picking (URW/P): *diversification* strategy.

Balanced combination of intensification and diversification mechanisms forms the basis for advanced LS methods.

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Randomized Iterative Impr.

aka, Stochastic Hill Climbing

Key idea: In each search step, with a fixed probability perform an uninformed random walk step instead of an iterative improvement step.

Randomized Iterative Improvement (RII):
determine initial candidate solution s
while termination condition is not satisfied **do**
  With probability `wp`:
    choose a neighbor s' of s uniformly at random
  Otherwise:
    choose a neighbor s' of s such that $f(s') < f(s)$ or,
      if no such s' exists, choose s' such that $f(s')$ is minimal
  $s := s'$

Example: Randomized Iterative Improvement for SAT

procedure *RIISAT*($F, wp, maxSteps$)
    input: *a formula* F, *probability* `wp`, *integer* `maxSteps`
    output: *a model* φ *for* F **or** $\emptyset$
    choose assignment φ for F uniformly at random;
    steps := 0;
    while not(φ is not proper) **and** (*steps* $<$ *maxSteps*) **do**
        with probability `wp` **do**
            select x in X uniformly at random and flip;
        otherwise
            select x in X^c uniformly at random from those that
                maximally decrease number of clauses violated;
        change φ;
        steps := *steps*$+1$;
    end
    if φ is a model for F **then return** φ
    else return $\emptyset$
    end
end *RIISAT*

X^c set of variables in violated clauses

Note:

- No need to terminate search when local minimum is encountered

  Instead: Impose limit on number of search steps or CPU time, from beginning of search or after last improvement.

- Probabilistic mechanism permits arbitrary long sequences of random walk steps

  Therefore: When run sufficiently long, RII is guaranteed to find (optimal) solution to any problem instance with arbitrarily high probability.

- GWSAT [Selman et al., 1994], was at some point state-of-the-art for SAT.

Constraint Programming

Constraint Satisfaction Problem (CSP)

A CSP is a finite set of variables X, together with a finite set of constraints C, each on a subset of X. A **solution** to a CSP is an assignment of a value $d \in D(x)$ to each $x \in X$, such that all constraints are satisfied simultaneously.

Constraint Optimization Problem (COP)

A COP is a CSP P defined on the variables $x_1, \ldots, x_n$, together with an objective function $f : D(x_1) \times \cdots \times D(x_n) \to Q$ that assigns a value to each assignment of values to the variables. An **optimal solution** to a minimization (maximization) COP is a solution d to P that minimizes (maximizes) the value of $f(d)$.

$\leadsto$ Constraints in a CSP can be relaxed and their violations determine the objective function. This is the most common approach in LS

Min-Conflict Heuristic

procedure *MCH* (*P*, *maxSteps*)
  input: *CSP instance P, positive integer maxSteps*
  output: *solution of P or* "no solution found"

  a := randomly chosen assignment of the variables in P;
  for *step* := 1 **to** *maxSteps* **do**
    if a satisfies all constraints of P **then** **return** a **end**
    x := randomly selected variable from conflict set $K(a)$;
    v := randomly selected value from the domain of x such that
      setting x to v minimises the number of unsatisfied constraints;
    a := a with x set to v;
  end
  return "no solution found"
end *MCH*

Min-Conflict Heuristic for n-Queens Problem

```
var{int} queen[Size](m,Size) := distr.get();

ConstraintSystem 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));

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;
    }
    it = it + 1;
  }
}
cout << queen << endl;
```

Min-Conflict + Random Walk for SAT

```
procedure WalkSAT (F, maxTries, maxSteps, slc)
    input: CNF formula F, positive integers maxTries and maxSteps,
        heuristic function slc
    output: model of F or 'no solution found'
    for try := 1 to maxTries do
        a := randomly chosen assignment of the variables in formula F;
        for step := 1 to maxSteps do
            if a satisfies F then return a end
            c := randomly selected clause unsatisfied under a;
            x := variable selected from c according to heuristic function slc;
            a := a with x flipped;
        end
    end
    return 'no solution found'
end WalkSAT
```

Example of *slc* heuristic: with prob. *wp* select a random move, with prob. $1 - wp$ select the best

Probabilistic Iterative Improv.

Key idea: Accept worsening steps with probability that depends on respective deterioration in evaluation function value:
bigger deterioration $\cong$ smaller probability

Realization:

- Function $p(f, s)$: determines probability distribution over neighbors of s based on their values under evaluation function f.
- Let $\texttt{step}(s, s') := p(f, s, s')$.

Note:

- Behavior of PII crucially depends on choice of p.
- II and RII are special cases of PII.

Example: Metropolis PII for the TSP

- **Search space S:** set of all Hamiltonian cycles in given graph G.
- **Solution set:** same as S
- **Neighborhood relation $\mathcal{N}(s)$:** 2-edge-exchange
- **Initialization:** an Hamiltonian cycle uniformly at random.
- **Step function:** implemented as 2-stage process:

  1. select neighbor $s' \in N(s)$ uniformly at random;
  2. accept as new search position with probability:

$$p(T, s, s') := \begin{cases} 1 & \text{if } f(s') \leq f(s) \\ \exp \frac{-(f(s') - f(s))}{T} & \text{otherwise} \end{cases}$$

  (Metropolis condition), where *temperature* parameter T controls likelihood of accepting worsening steps.

- **Termination:** upon exceeding given bound on run-time.

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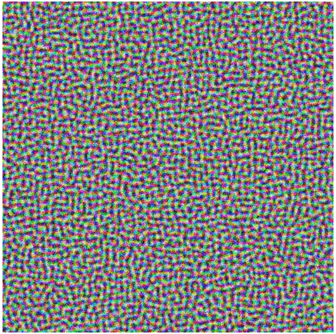
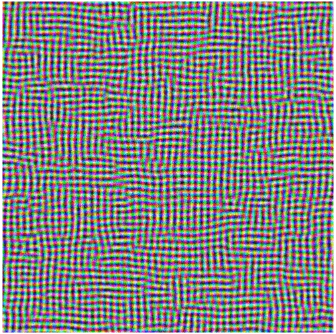
Inspired by statistical mechanics in matter physics:

- candidate solutions $\cong$ states of physical system
- evaluation function $\cong$ thermodynamic energy
- globally optimal solutions $\cong$ ground states
- parameter T $\cong$ physical temperature

Note: In physical process (*e.g.*, annealing of metals), perfect ground states are achieved by very slow lowering of temperature.





Simulated Annealing

Key idea: Vary temperature parameter, *i.e.*, probability of accepting worsening moves, in Probabilistic Iterative Improvement according to annealing schedule (aka *cooling schedule*).

Simulated Annealing (SA):

determine initial candidate solution s
set initial temperature T according to annealing schedule
while termination condition is not satisfied: **do**
    while maintain same temperature T according to annealing schedule **do**
        probabilistically choose a neighbor s' of s using proposal mechanism
        if s' satisfies probabilistic acceptance criterion (depending on T) **then**
            $s := s'$
    update T according to annealing schedule

- 2-stage step function based on
  - proposal mechanism (often uniform random choice from $N(s)$)
  - acceptance criterion (often *Metropolis condition*)

- Annealing schedule
  (function mapping run-time t onto temperature $T(t)$):
  - initial temperature T_0
    (may depend on properties of given problem instance)
  - temperature update scheme
    (*e.g.*, linear cooling: $T_{i+1} = T_0(1 - i/I_{max})$,
    geometric cooling: $T_{i+1} = \alpha \cdot T_i$)
  - number of search steps to be performed at each temperature
    (often multiple of neighborhood size)
  - may be *static* or *dynamic*
  - seek to balance moderate execution time with asymptotic behavior properties

- Termination predicate: often based on *acceptance ratio*,
  i.e., ratio accepted / proposed steps *or* number of idle iterations

Example: Simulated Annealing for TSP

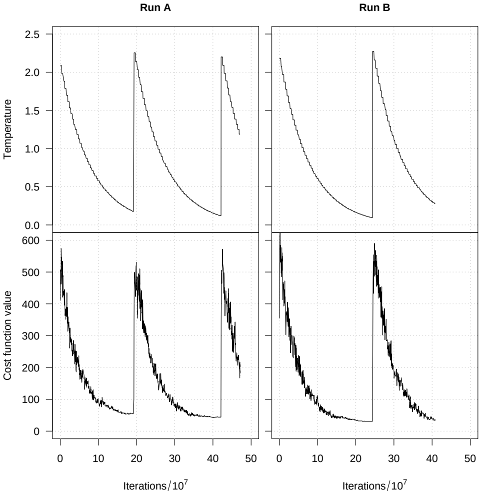
Extension of previous PII algorithm for the TSP, with

- proposal mechanism: uniform random choice from 2-exchange neighborhood;
- acceptance criterion: Metropolis condition (always accept improving steps, accept worsening steps with probability $\exp\left[-(f(s') - f(s))/T\right]$);
- annealing schedule: geometric cooling $T := 0.95 \cdot T$ with $n \cdot (n-1)$ steps at each temperature (n = number of vertices in given graph), T_0 chosen such that 97% of proposed steps are accepted;
- termination: when for five successive temperature values no improvement in solution quality and acceptance ratio $< 2\%$.

Improvements:

- neighborhood pruning (*e.g.*, candidate lists for TSP)
- greedy initialization (*e.g.*, by using NNH for the TSP)
- *low temperature starts* (to prevent good initial candidate solutions from being too easily destroyed by worsening steps)

Profiling


Run A
Run B
Temperature
Cost function value
2.5
2.0
1.5
1.0
0.5
0.0
600
500
400
300
200
100
0
0 10 20 30 40 50
Iterations/10^7

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Iterated Local Search

Key Idea: Use two types of LS steps:

- *subsidiary local search* steps for reaching local optima as efficiently as possible (intensification)
- perturbation steps for effectively escaping from local optima (diversification).

Also: Use acceptance criterion to control diversification *vs* intensification behavior.

Iterated Local Search (ILS):
determine initial candidate solution s
perform subsidiary local search on s
while termination criterion is not satisfied **do**
    $r := s$
    perform perturbation on s
    perform subsidiary local search on s
    based on acceptance criterion,
        keep s or revert to $s := r$

Note:

- *Subsidiary local search* results in a local minimum.
- ILS trajectories can be seen as walks in the space of local minima of the given evaluation function.
- *Perturbation phase* and *acceptance criterion* may use aspects of *search history* (*i.e.*, limited memory).
- In a high-performance ILS algorithm, *subsidiary local search*, *perturbation mechanism* and *acceptance criterion* need to complement each other well.

Components

Subsidiary local search:

- More effective subsidiary local search procedures lead to better ILS performance.
  Example: 2-opt *vs* 3-opt *vs* LK for TSP.

- Often, subsidiary local search = iterative improvement,
  but more sophisticated LS methods can be used.
  (*e.g.*, Tabu Search).

Components

Perturbation mechanism:

- Needs to be chosen such that its effect *cannot* be easily undone by subsequent local search phase.
  (Often achieved by search steps larger neighborhood.)
  Example: local search = 3-opt, perturbation = 4-exchange steps in ILS for TSP.
- A perturbation phase may consist of one or more perturbation steps.
- Weak perturbation $\Rightarrow$ short subsequent local search phase;
  but: risk of revisiting current local minimum.
- Strong perturbation $\Rightarrow$ more effective escape from local minima;
  but: may have similar drawbacks as random restart.
- Advanced ILS algorithms may change nature and/or strength of perturbation adaptively during search.

Components

Acceptance criteria:

- Always accept the best of the two candidate solutions

  $\Rightarrow$ ILS performs Iterative Improvement in the space of local optima reached by subsidiary local search.

- Always accept the most recent of the two candidate solutions

  $\Rightarrow$ ILS performs random walk in the space of local optima reached by subsidiary local search.

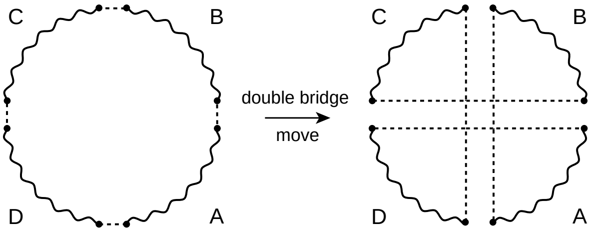
- Intermediate behavior: select between the two candidate solutions based on the *Metropolis criterion* (*e.g.*, used in *Large Step Markov Chains* [Martin et al., 1991].

- Advanced acceptance criteria take into account search history,
  e.g., by occasionally reverting to *incumbent solution*.

Examples

Example: Iterated Local Search for the TSP (1)

- **Given:** TSP instance π.
- **Search space:** Hamiltonian cycles in π.
- **Subsidiary local search:** Lin-Kernighan variable depth search algorithm
- **Perturbation mechanism:**
  'double-bridge move' = particular 4-exchange step:



- **Acceptance criterion:** Always return the best of the two given candidate round trips.

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Tabu Search

Key idea: Avoid repeating history (memory)
How can we remember the history without

- memorizing full solutions (space)
- computing hash functions (time)

$\rightsquigarrow$ use attributes

Tabu Search

Key idea: Use aspects of search history (memory) to escape from local minima.

- Associate tabu attributes with candidate solutions or solution components.
- Forbid steps to search positions recently visited by underlying iterative best improvement procedure based on tabu attributes.

Tabu Search (TS):

determine initial candidate solution s
While *termination criterion* is not satisfied:
    determine set N' of non-tabu neighbors of s
    choose a best candidate solution s' in N'

    update tabu attributes based on s'
    $s := s'$

Example: Tabu Search for CSP

- **Search space:** set of all complete assignments of X.
- **Solution set:** assignments that satisfy all constraints
- **Neighborhood relation:** one exchange
- **Memory:** Associate tabu status (Boolean value) with each pair (variable,value) (x, val).
- **Initialization:** a random assignment
- **Search steps:**
  - pairs (x, v) are tabu if they have been changed in the last `tt` steps;
  - neighboring assignments are admissible if they can be reached by changing a non-tabu pair or have fewer unsatisfied constraints than the best assignments seen so far (aspiration criterion);
  - choose uniformly at random admissible neighbors with minimal number of unsatisfied constraints.
- **Termination:** upon finding a feasible assignment *or*
  after given bound on number of search steps has been reached *or*
  after a number of idle iterations

Note:

- Admissible neighbors of s: Non-tabu search positions in $N(s)$
- Tabu tenure: a fixed number of subsequent search steps for which the last search position or the solution components just added/removed from it are declared tabu
- Aspiration criterion (often used): specifies conditions under which tabu status may be overridden (*e.g.*, if considered step leads to improvement in incumbent solution).
- Crucial for efficient implementation:
  - efficient best improvement local search
    $\rightsquigarrow$ pruning, delta updates, (auxiliary) data structures
  - efficient determination of tabu status:
    store for each variable x the number of the search step when its value was last changed it_x; x is tabu if $it - it_x < tt$, where it = current search step number.

Design Choices

Design choices:

- Neighborhood exploration:
  - no reduction
  - min-conflict heuristic
- Prohibition power for `move = <x,new_v,old_v>`
  - `<x,-,->`
  - `<x,-,old_v>`
  - `<x,new_v,old_v>`, `<x,old_v,new_v>`
- Tabu list dynamics:
  - Interval: $\texttt{tt} \in [t_b, t_b + w]$
  - Adaptive: $\texttt{tt} = \lfloor \alpha \cdot c \rfloor + \texttt{RandU}(0, t_b)$

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Variable Neighborhood Search

Variable Neighborhood Search is a method based on the systematic change of the neighborhood during the search.

Central observations

- a local minimum w.r.t. one neighborhood function is not necessarily locally minimal w.r.t. another neighborhood function
- a global optimum is locally optimal w.r.t. all neighborhood functions

Key principle: change the neighborhood during the search

- Several adaptations of this central principle
  - (Basic) Variable Neighborhood Descent (VND)
  - Variable Neighborhood Search (VNS)
  - Reduced Variable Neighborhood Search (RVNS)
  - Variable Neighborhood Decomposition Search (VNDS)
  - Skewed Variable Neighborhood Search (SVNS)
- Notation
  - N_k, $k = 1, 2, \ldots, k_m$ is a set of neighborhood functions
  - $N_k(s)$ is the set of solutions in the k-th neighborhood of s

How to generate the various neighborhood functions?

- for many problems different neighborhood functions (local searches) exist / are in use
- change parameters of existing local search algorithms
- use k-exchange neighborhoods; these can be naturally extended
- many neighborhood functions are associated with distance measures; in this case increase the distance

Basic Variable Neighborhood Descent

Procedure BVND
input : N_k, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for N_k, $k = 1, 2, \ldots, k_{max}$
$k \leftarrow 1$
repeat
    $s' \leftarrow$ FindBestNeighbor(s,N_k)
    if $f(s') < f(s)$ **then**
        $s \leftarrow s'$
        $(k \leftarrow 1)$
    else
        $k \leftarrow k + 1$
until $k = k_{max}$;

Variable Neighborhood Descent

Procedure VND
input : N_k, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for N_k, $k = 1, 2, \ldots, k_{max}$
$k \leftarrow 1$
repeat
  $s' \leftarrow$ IterativeImprovement(s,N_k)
  if $f(s') < f(s)$ **then**
    $s \leftarrow s'$
    $k \leftarrow 1$
  else
    $k \leftarrow k + 1$
until $k = k_{max}$;

- Final solution is locally optimal w.r.t. all neighborhoods
- First improvement may be applied instead of best improvement
- Typically, order neighborhoods from smallest to largest
- If iterative improvement algorithms II_k, $k = 1, \ldots, k_{max}$ are available as black-box procedures:
  - order black-boxes
  - apply them in the given order
  - possibly iterate starting from the first one
  - order chosen by: *solution quality* and *speed*

Basic Variable Neighborhood Search

Procedure BVNS
input : N_k, $k = 1, 2, \ldots, k_{max}$, and an initial solution s
output: a local optimum s for N_k, $k = 1, 2, \ldots, k_{max}$

```
repeat
    k ← 1
    repeat
        s′ ← RandomPicking(s, N_k)
        s″ ← IterativeImprovement(s′, N_k)
        if f(s″) < f(s) then
            s ← s″
            k ← 1
        else
            k ← k + 1
    until k = k_max;
until Termination Condition;
```

To decide:

- which neighborhoods
- how many
- which order
- which change strategy

- Extended version: parameters k_{min} and k_{step}; set $k \leftarrow k_{min}$ and increase by k_{step} if no better solution is found (achieves diversification)

Summary

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