DM811 Heuristics for Combinatorial Optimization

Stochastic Local Search and Metaheuristics

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Course Overview

- Combinatorial Optimization, Methods and Models
- CH and LS: overview
- ✓ Working Environment and Solver Systems
- Methods for the Analysis of Experimental Results
- ✓ Construction Heuristics
- ✓ Local Search: Components, Basic Algorithms
 - Efficient Local Search: Incremental Updates and Neighborhood Pruning
 - Local Search: Neighborhoods and Search Landscape
 - Stochastic Local Search & Metaheuristics
 - Configuration Tools: F-race
 - Very Large Scale Neighborhoods

Examples: GCP, CSP, TSP, SAT, MaxIndSet, SMTWP, Steiner Tree, Unrelated Parallel Machines, p-median, set covering, QAP, ...

Outline

1. Beyond Iterative Improvement

2. Trajectory Based Metaheuristics
Stochastic Local Search
Simulated Annealing
Iterated Local Search
Tabu Search
Variable Neighborhood Search
Guided Local Search

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Escaping Local Optima

Possibilities:

- Enlarge the neighborhood
- Restart: re-initialize search whenever a local optimum is encountered.
 (Often rather ineffective due to cost of initialization.)
- 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.)
 This is what Metaheuristics do.

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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- 2. Trajectory Based Metaheuristics
 Stochastic Local Search
 Simulated Annealing
 Iterated Local Search
 Tabu Search
 Variable Neighborhood Search
 Guided Local Search

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'
```

Taken from Hoos and Tsang. With infite time it reaches optimum with $\mathsf{p}>0$

Example: Randomized Iterative Improvement for SAT

```
procedure RIISAT(F, wp, maxSteps)
   input: a formula F, probability wp, integer maxSteps
   output: a model \varphi for F or \emptyset
   choose assignment \varphi for F uniformly at random;
   steps := 0;
   while not(\varphi 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 \varphi;
      steps := steps + 1;
   end
   if \varphi is a model for F then return \varphi
   else return 0
   end
end RIISAT
```

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.

Min-Conflict Heuristic

(Already encountered) **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

Taken from Hoos and Tsang. Does it converge? Is the search space in GCP connected?

Min-Conflict Heuristic

```
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;
```

Min-Conflict + Random Walk

```
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 := \text{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 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:

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

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

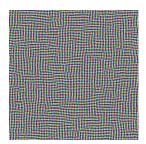
• **Termination:** upon exceeding given bound on run-time.

Inspired by statistical mechanics in matter physics:

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

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: \mathbf{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 $\bot s := s'$

update T according to annealing schedule

- 2-stage step function based on
 - ullet 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)):
 - ullet 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

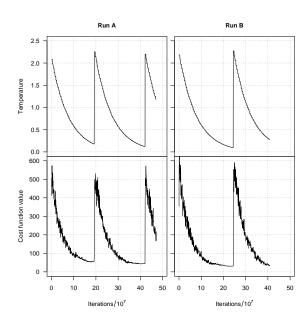
Extension of previous PII algorithm for the TSP, with

- proposal mechanism: uniform random choice from 2-exchange neighborhood;
- acceptance criterion: Metropolis condition (always accept improving steps, accept worsening steps with probability $\exp[-(f(s') f(s))/T]$);
- 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



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 = s
```

```
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 ⇒ short subsequent local search phase;
 but: risk of revisiting current local minimum.
- Strong perturbation ⇒ 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)

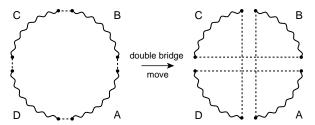
• **Given:** TSP instance π .

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

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

→ use attirbutes

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: feasible assignment of X.
- Neighborhood relation: one-exchange.
- **Memory:** Associate tabu status (Boolean value) with each pair (x, v).
- Initialization: a construction heuristic
- 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
 → 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.

Note: Performance of Tabu Search depends crucially on setting of tabu tenure tt:

- tt too low

 search stagnates due to inability to escape from local minima;
- tt too high

 search becomes ineffective due to overly restricted search
 path (admissible neighborhoods too small)

Advanced TS methods:

- Robust Tabu Search [Taillard, 1991]:
 repeatedly choose tt from given interval;
 also: force specific steps that have not been made for a long time.
- Reactive Tabu Search [Battiti and Tecchiolli, 1994]: dynamically adjust tt during search; also: use escape mechanism to overcome stagnation.

Further improvements can be achieved by using *intermediate-term* or *long-term memory* to achieve additional *intensification* or *diversification*.

Examples:

- Occasionally backtrack to elite candidate solutions, i.e., high-quality search positions encountered earlier in the search; when doing this, all associated tabu attributes are cleared.
- Freeze certain solution components and keep them fixed for long periods of the search.
- Occasionally force rarely used solution components to be introduced into current candidate solution.
- Extend evaluation function to capture frequency of use of candidate solutions or solution components.

Tabu search algorithms are state of the art for solving many combinatorial problems, including:

- SAT and MAX-SAT
- CSP and MAX-CSP
- GCP
- many scheduling problems
- → typically works well with small neighborhoods (because based on best improvement)

Crucial factors in many applications:

- choice of neighborhood relation
- efficient evaluation of candidate solutions (caching and incremental updating mechanisms)

Min-Conflict + Tabu Search

- After the value of a variable x is changed from v to v' with min-conflict heuristic, the variable/value pair (x_i,v) is declared tabu for the next tt steps
- \bullet tt = 2 is often a good choice
- ➡ Advantage: the neighborhood does not need to be searched exahustively

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: $\mathsf{tt} \in [t_b, t_b + w]$
 - Adaptive: $tt = [\alpha \cdot c] + RandU(0, t_b)$

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
 - ullet \mathcal{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: \mathcal{N}_k, k = 1, 2, \dots, k_{max}, and an initial solution s
output: a local optimum s for \mathcal{N}_k, k=1,2,\ldots,k_{max}
k \leftarrow 1
repeat
    s' \leftarrow \mathsf{FindBestNeighbor}(s, \mathcal{N}_k)
   if f(s') < f(s) then s \leftarrow s' (k \leftarrow 1)
   until k = k_{max}:
```

Variable Neighborhood Descent

```
Procedure VND
input : \mathcal{N}_k, k = 1, 2, \dots, k_{max}, and an initial solution s
output: a local optimum s for \mathcal{N}_k, k=1,2,\ldots,k_{max}
k \leftarrow 1
repeat
    s' \leftarrow \mathsf{IterativeImprovement}(s, \mathcal{N}_k)
   \lfloor k \leftarrow k+1 \rfloor
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

Example

VND for single-machine total weighted tardiness problem

- Candidate solutions are permutations of job indexes
- Two neighborhoods: interchange and insert
- Influence of different starting heuristics also considered

| initial | interchange | | insert | | interch.+insert | | insert+interch. | |
|----------|--------------|-------|--------------|--------------------|-----------------|--------------------|-----------------|------|
| solution | Δ avg | tavg | Δ avg | $oldsymbol{t}$ avg | Δ avg | $oldsymbol{t}$ avg | Δ avg | tavg |
| EDD | 0.62 | 0.140 | 1.19 | 0.64 | 0.24 | 0.20 | 0.47 | 0.67 |
| MDD | 0.65 | 0.078 | 1.31 | 0.77 | 0.40 | 0.14 | 0.44 | 0.79 |

 Δ avg deviation from best-known solutions, averaged over 100 instances

Basic Variable Neighborhood Search

```
Procedure BVNS
input : \mathcal{N}_k, k = 1, 2, \dots, k_{max}, and an initial solution s
output: a local optimum s for \mathcal{N}_k, k = 1, 2, \dots, k_{max}
repeat
     k \leftarrow 1
     repeat
         s' \leftarrow \mathsf{RandomPicking}(s, \mathcal{N}_k)
     s' \leftarrow \mathsf{RandomPicking}(s, \mathcal{N}_k)s'' \leftarrow \mathsf{IterativeImprovement}(s', \mathcal{N}_k)
      if f(s'') < f(s) then
     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)

Extensions (1)

Reduced Variable Neighborhood Search (RVNS)

- same as VNS except that no IterativeImprovement procedure is applied
- only explores different neighborhoods randomly
- can be faster than standard local search algorithms for reaching good quality solutions

Extensions (2)

Variable Neighborhood Decomposition Search (VNDS)

- same as in VNS but in IterativeImprovement all solution components are kept fixed except k randomly chosen
- IterativeImprovement is applied on the k unfixed components



• IterativeImprovement can be substituted by exhaustive search up to a maximum size b (parameter) of the problem

Extensions (3)

Skewed Variable Neighborhood Search (SVNS)

- Derived from VNS
- Accept $s \leftarrow s''$ when s'' is worse
 - according to some probability
 - skewed VNS: accept if

$$f(s'') - \alpha \cdot d(s, s'') < f(s)$$

 $d(s,s^{\prime\prime})$ measures the distance between solutions (underlying idea: avoiding degeneration to multi-start)

Guided Local Search

- Key Idea: Modify the evaluation function whenever a local optimum is encountered.
- Associate weights (penalties) with solution components; these determine impact of components on evaluation function value.
- Perform Iterative Improvement; when in local minimum, increase penalties of some solution components until improving steps become available.

Guided Local Search (GLS):

```
\begin{array}{ll} \mbox{determine } \mbox{\it initialize penalties} \\ \end{array}
```

```
while termination criterion is not satisfied do compute modified evaluation function g' from g based on penalties perform subsidiary local search on s using evaluation function g' update penalties based on s
```

Guided Local Search (continued)

• Modified evaluation function:

$$g'(s) := f(s) + \sum_{i \in SC(s)} \mathtt{penalty}(i),$$

where SC(s) is the set of solution components used in candidate solution s.

- Penalty initialization: For all i: penalty(i) := 0.
- **Penalty update** in local minimum s: Typically involves *penalty increase* of some or all solution components of s; often also occasional *penalty decrease* or *penalty smoothing*.
- Subsidiary local search: Often Iterative Improvement.

Potential problem:

Solution components required for (optimal) solution may also be present in many local minima.

Possible solutions:

A: Occasional decreases/smoothing of penalties.

B: Only increase penalties of solution components that are least likely to occur in (optimal) solutions.

Implementation of B:

Only increase penalties of solution components i with maximal utility [Voudouris and Tsang, 1995]:

$$\mathtt{util}(s,i) := \frac{f_i(s)}{1 + \mathtt{penalty}(i)}$$

where $f_i(s)$ is the solution quality contribution of i in s.

Example: Guided Local Search (GLS) for the TSP

[Voudouris and Tsang 1995; 1999]

- Given: TSP instance π
- **Search space:** Hamiltonian cycles in π with n vertices;
- Neighborhood: 2-edge-exchange;
- Solution components edges of π ;
- $f_e(G,p) := w(e);$
- Penalty initialization: Set all edge penalties to zero.
- Subsidiary local search: Iterative First Improvement.
- Penalty update: Increment penalties of all edges with maximal utility by

$$\lambda := 0.3 \cdot \frac{w(s_{2\text{-}opt})}{n}$$

where $s_{2-opt} = 2$ -optimal tour.

Lagrangian Method

ullet Change the objective function bringing constraints g_i into it

$$L(\vec{s}, \vec{\lambda}) = f(\vec{s}) + \sum_{i} \lambda_{i} g_{i}(\vec{s})$$

- ullet λ_i are continous variables called Lagrangian Multipliers
- $\bullet \ L(\vec{s}^*,\lambda) \leq L(\vec{s}^*,\vec{\lambda}^*) \leq L(\vec{s},\vec{\lambda}^*)$
- ullet Alternate optimizations in \vec{s} and in $\vec{\lambda}$