Course Overview

1. Combinatorial Optimization, Methods and Models
2. General overview
3. Solver System and Working Environment
4. Construction Heuristics
5. Local Search: Components, Basic Algorithms
6. Local Search: Neighborhoods and Search Landscape
7. Efficient Local Search: Incremental Updates and Neighborhood Pruning
8. Stochastic Local Search & Metaheuristics
9. Methods for the Analysis of Experimental Results
10. Configuration Tools: F-race
11. Very Large Scale Neighborhoods

Examples: GCP, CSP, TSP, SAT, MaxIndSet, SMTWP, Steiner Tree

Outline

1. Trajectory Based Metaheuristics
   Stochastic Local Search
   Simulated Annealing
   Iterated Local Search
   Tabu Search
   Variable Neighborhood Search
   Guided Local Search
Randomized Iterative Impr.  
a.k.a. 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

```plaintext
procedure RII SAT(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 \( X' \) 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 \( \emptyset \)
end RII SAT
```

**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, 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

Min-Conflict Heuristic

In Comet

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

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

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

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

**Key idea:** Accept worsening steps with probability that depends on respective deterioration in evaluation function value: bigger deterioration \(\Rightarrow\) smaller probability

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

**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 \(s' \in \mathcal{N}(s)\) uniformly at random;
  2. accept as new search position with probability:

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

(Metropolis condition), where temperature parameter \(T\) controls likelihood of accepting worsening steps.
- **Termination:** upon exceeding given bound on run-time.

**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
Metaheuristics

- 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

- 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)

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.

**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).

**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.

**Acceptance criteria:**

- Always accept the best of the two candidate solutions
  ⇒ 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
  ⇒ 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 \( G \).
- **Search space**: Hamiltonian cycles in \( G \).
- **Subsidiary local search**: Lin-Kernighan variable depth search algorithm
- **Perturbation mechanism**: 'double-bridge move' = particular 4-exchange step:

```
A
BC
D
```

- **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)

\( \Rightarrow \) 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:

1. determine set \( N' \) of non-tabu neighbors of \( s \)
2. choose a best candidate solution \( s' \) in \( N' \)
3. update tabu attributes based on \( s' \)

\( s := s' \)

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**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**:
  1. pairs \( (x,v) \) are tabu if they have been changed in the last \( tt \) steps;
  2. 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**);
  3. 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 $i_{tx}$; $x$ is tabu if $it - i_{tx} < tt$, where $it =$ current search step number.

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.

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

- $tt$ too low $\Rightarrow$ search stagnates due to inability to escape from local minima;

- $tt$ too high $\Rightarrow$ 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.

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

$\Rightarrow$ 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.

- $tt = 2$ is often a good choice

- Advantage: the neighborhood does not need to be searched exhaustively

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.

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

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

### Variable Neighborhood Descent

**Procedure VND**

**input**: $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{\text{max}}$, and an initial solution $s$

**output**: a local optimum $s$ for $\mathcal{N}_k$, $k = 1, 2, \ldots, k_{\text{max}}$

$k \leftarrow 1$

repeat

$s' \leftarrow \text{Iterative Improvement}(s, \mathcal{N}_k)$

if $f(s') < f(s)$ then

$s \leftarrow s'$

$k \leftarrow 1$

else

$k \leftarrow k + 1$

until $k = k_{\text{max}}$;

- 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 $II_k$, $k = 1, \ldots, k_{\text{max}}$ 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
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

<table>
<thead>
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<th>initial solution</th>
<th>interchange</th>
<th>insert</th>
<th>interch.+insert</th>
<th>insert+interch.</th>
</tr>
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<td></td>
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<td>$\Delta_{avg}$</td>
<td>$\Delta_{avg}$</td>
<td>$\Delta_{avg}$</td>
</tr>
<tr>
<td>EDD</td>
<td>0.62</td>
<td>0.140</td>
<td>1.19</td>
<td>0.64</td>
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<tr>
<td>MDD</td>
<td>0.65</td>
<td>0.078</td>
<td>1.31</td>
<td>0.77</td>
</tr>
</tbody>
</table>

$\Delta_{avg}$ deviation from best-known solutions, averaged over 100 instances

**Procedure BVNS**

- **input**: $N_k$, $k=1,2,...,k_{max}$, and an initial solution $s$
- **output**: a local optimum $s$ for $N_k$, $k=1,2,...,k_{max}$

```
repeat
  $k \leftarrow 1$
  repeat
    $s' \leftarrow \text{RandomPicking}(s,N_k)$
    $s'' \leftarrow \text{IterativeImprovement}(s',N_k)$
    if $f(s'')<f(s)$ then
      $s \leftarrow s''$
      $k \leftarrow 1$
    else
      $k \leftarrow k + 1$
  until $k = k_{max}$;
until Termination Condition;
```

**Extensions (1)**

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)

**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
Variable Neighborhood Decomposition Search (VNDS)
- Same as in VNS but in Iterative Improvement all solution components are kept fixed except \( k \) randomly chosen
- Iterative Improvement is applied on the \( k \) unfixed components

Iterative Improvement can be substituted by exhaustive search up to a maximum size \( b \) (parameter) of the problem

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Skewed Variable Neighborhood Search (SVNS)
- Derived from VNS
- Accepts \( s \leftarrow s'' \) when \( s'' \) is worse
  - According to some probability
  - Skewed VNS: accept if
    \[
    g(s'') - \alpha \cdot d(s, s'') < g(s)
    \]
    where \( d(s, s'') \) 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):**
- Determine initial candidate solution \( s \)
- Initialize penalties

**Guided Local Search (continued):**
- 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 \( s \)

**Modified evaluation function:**
\[
g'(s) := g(s) + \sum_{i \in SC(s)} \text{penalty}(i),
\]
where \( SC(s) \) is the set of solution components used in candidate solution \( s \).

**Penalty initialization:** For all \( i \): \( \text{penalty}(i) := 0 \).

**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.
Metaheuristics

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]:

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

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

Lagrangian Method

- Change the objective function bringing constraints $g_i$ into it

$$L(\bar{s}, \bar{\lambda}) = f(\bar{s}) + \sum_i \lambda_i g_i(\bar{s})$$

- $\lambda_i$ are continuous variables called Lagrangian Multipliers

- $L(\bar{s}^*, \lambda) \leq L(\bar{s}^*, \bar{\lambda}^*) \leq L(\bar{s}, \bar{\lambda}^*)$

- Alternate optimizations in $\bar{s}$ and in $\bar{\lambda}$

Example: Guided Local Search (GLS) for the TSP
[Voudouris and Tsang 1995; 1999]

- **Given**: TSP instance $G$
- **Search space**: Hamiltonian cycles in $G$ with $n$ vertices;
- **Neighborhood**: 2-edge-exchange;
- **Solution components** edges of $G$;
- $g_e(G,p) := w(e)$;
- **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 $\lambda := 0.3 \cdot \frac{w(s_{2-opt})}{n}$

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