Metaheuristics and Local Search

Discrete optimization problems

- Variables $x_1, \dots, x_n$.
- Variable domains $D_1, \dots, D_n$, with $D_j \subseteq \mathbb{Z}$.
- Constraints $C_1, \dots, C_m$, with $C_i \subseteq D_1 \times \cdots \times D_n$.
- Objective function $f : D_1 \times \cdots \times D_n \to \mathbb{R}$, to be minimized.

Solution approaches

- Complete (exact) algorithms $\rightsquigarrow$ *systematic search*
  - Integer linear programming
  - Finite domain constraint programming
- Approximate algorithms
  - Heuristic approaches $\rightsquigarrow$ *heuristic search*
    - Constructive methods: construct solutions from partial solutions
    - **Local search:** improve solutions through neighborhood search
    - **Metaheuristics:** Combine basic heuristics in higher-level frameworks
  - Polynomial-time approximation algorithms for NP-hard problems

Metaheuristics

- Heuriskein ($\varepsilon\upsilon\rho\iota\sigma\kappa\varepsilon\iota\nu$): to find
- Meta: beyond, in an upper level
- *Survey paper:* C. Blum, A. Roli: Metaheuristics in Combinatorial Optimization, ACM Computing Surveys, Vol. 35, 2003. ȟttp://iridia.ulb.ac.be/ meta/newsite/downloads/ACSUR-blum-roli.pdf

Characteristics

- Metaheuristics are strategies that “guide” the search process.
- The goal is to efficiently explore the search space in order to find (near-) optimal solutions.
- Metaheuristics range from simple local search to complex learning procedures.
- Metaheuristic algorithms are approximate and usually non-deterministic.
- They may incorporate mechanisms to avoid getting trapped in confined areas of the search space.

Characteristics (2)

- The basic concepts of metaheuristics permit an abstract level description.
- Metaheuristics are not problem-specific.
- Metaheuristics may make use of domain-specific knowledge in the form of heuristics that are controlled by the upper level strategy.

- Today more advanced metaheuristics use search experience (embodied in some form of memory) to guide the search.

Intensification and diversification

Glover and Laguna 1997

The main difference between intensification and diversification is that during an intensification stage the search focuses on examining neighbors of elite solutions. ... The diversification stage on the other hand encourages the search process to examine unvisited regions and to generate solutions that differ in various significant ways from those seen before.

Classification of metaheuristics

- Single point search (trajectory methods) vs. population-based search
- Nature-inspired vs. non-nature inspired
- Dynamic vs. static objective function
- One vs. various neighborhood structures
- Memory usage vs. memory-less methods

I. Trajectory methods

- Basic local search: iterative improvement
- Simulated annealing
- Tabu search
- Explorative search methods
  - Greedy Randomized Adaptive Search Procedure (GRASP)
  - Variable Neighborhood Search (VNS)
  - Guided Local Search (GLS)
  - Iterated Local Search (ILS)

Local search

- Find an initial solution s
- Define a neighborhood $\mathcal{N}(s)$
- Explore the neighborhood
- Proceed with selected neighbor

Simple descent

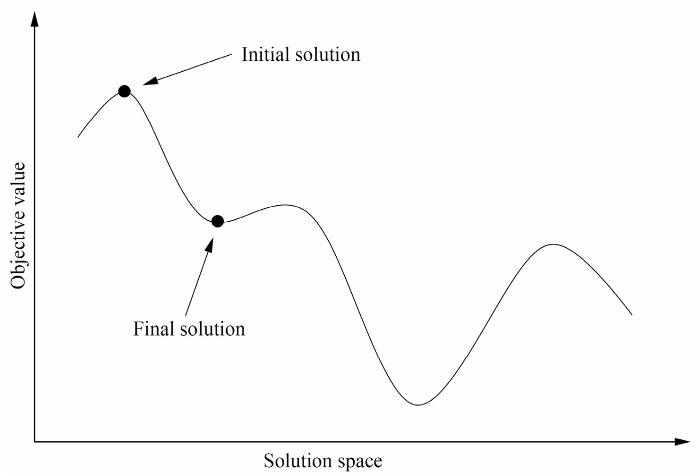
```
procedure SimpleDescent(solution s)
  repeat
    choose s' ∈ N(s)
    if f(s') < f(s) then
      s ← s'
    end if
  until f(s') ≥ f(s), ∀s' ∈ N(s)
end
```

Deepest descent

```
procedure DeepestDescent(solution s)
   repeat
      choose s' ∈ N(s) with f(s') ≤ f(s''), ∀s'' ∈ N(s)
      if f(s') < f(s) then
         s ← s'
      end if
   until f(s') ≥ f(s), ∀s' ∈ N(s)
end
```

Problem: Local minima

Local and global minima



Multistart and deepest descent

```
procedure Multistart
   iter ← 1
   f(Best) ← ∞
   repeat
      choose a starting solution s_0 at random
      s ← DeepestDescent(s_0)
      if f(s) < f(Best) then
         Best ← s
      end if
      iter ← iter + 1
   until iter = IterMax
end
```

Simulated annealing

Kirkpatrick 83

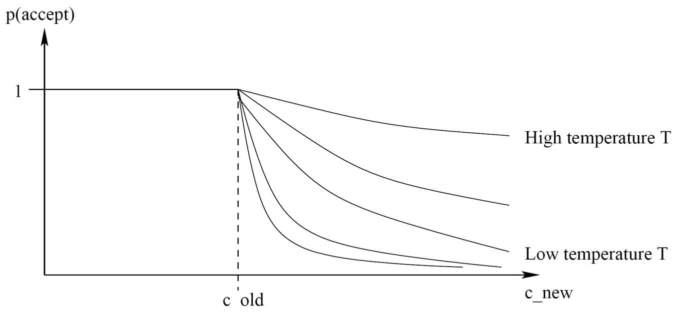
- *Anneal:* to heat and then slowly cool (esp. glass or metal) to reach minimal energy state
- Like standard local search, but sometimes accept worse solution.

- Select random solution from the neighborhood and accept it with probability ⇝ *Boltzmann distribution*

$$p = \begin{cases} 1, & \text{if } f(new) < f(old), \\ exp(-(f(new) - f(old))/T), & \text{else.} \end{cases}$$

- Start with high *temperature* T, and gradually lower it ⇝ *cooling schedule*

Acceptance probability



Algorithm

$s \leftarrow$ GenerateInitialSolution()
$T \leftarrow T_0$
while termination conditions not met **do**
  $s' \leftarrow$ PickAtRandom($\mathcal{N}(s)$)
  if $(f(s') < f(s))$ **then**
    $s \leftarrow s'$
  else
    Accept s' as new solution with probability $p(T, s', s)$
  endif
  Update(T)
endwhile

Tabu search

Glover 86

- Local search with short term memory, to escape local minima and to avoid cycles.
- *Tabu list:* Keep track of the last r moves, and don't allow going back to these.
- *Allowed set:* Solutions that do not belong to the tabu list.
- Select solution from allowed set, add to tabu list, and update tabu list.

Basic algorithm

$s \leftarrow$ GenerateInitialSolution()
$TabuList \leftarrow \emptyset$
while termination conditions not met **do**
  $s \leftarrow$ ChooseBestOf($\mathcal{N}(s) \setminus TabuList$)
  Update($TabuList$)
endwhile

Choices in tabu search

- Neighborhood
- Size of tabu list $\rightsquigarrow$ *tabu tenure* (static/dynamic)
- Kind of tabu to use (complete solutions vs. attributes) $\rightsquigarrow$ *tabu conditions*
- *Aspiration criteria* (exceptions to tabu conditions)
- Termination condition
- Long-term memory: recency, frequency, quality, influence

Refined algorithm

$s \leftarrow$ GenerateInitialSolution()
Initialize TabuLists ($TL_1, ..., TL_r$)
$k \leftarrow 0$
while termination conditions not met **do**
  $AllowedSet(s,k) \leftarrow \{s' \in \mathcal{N}(s) \mid$
    s' does not violate a tabu condition
    or satisfies at least one aspiration condition }
  $s \leftarrow$ ChooseBestOf($AllowedSet(s,k)$)
  UpdateTabuListsAndAspirationConditions()
  $k \leftarrow k+1$
endwhile

II. Population-based search

Use a set (i.e. a population) of solutions rather than a single solutions

- Evolutionary computation
- Ant colony optimization

Evolutionary computation

- Idea: Mimic evolution - obtain better solutions by combining current ones.
- Keep several current solutions, called *population* or *generation.*
- Create new generation:
  - select a pool of promising solutions, based on a *fitness function.*
  - create new solutions by combining solutions in the pool in various ways $\rightsquigarrow$ *recombination, crossover.*
  - add random *mutations.*

- *Variants:* Evolutionary programming, evolutionary strategies, genetic algorithms

Algorithm

$P \leftarrow$ GenerateInitialPopulation()
Evaluate(P)
while termination conditions not met **do**
  $P' \leftarrow$ Recombine(P)
  $P'' \leftarrow$ Mutate(P')
  Evaluate(P'')
  $P \leftarrow$ Select($P'' \cup P$)
endwhile

Crossover and mutations

- Individuals (solutions) often coded as bit or integer vectors
- *Crossover* operations provide new individuals, e.g.

101101	*0110*	$\rightsquigarrow$	101101	**1011**
000110	**1011**		000110	*0110*

- *Mutations* often helpful, e.g., swap random bit.

Further issues

- Individuals (“genotypes”) vs. solutions (“phenotypes”): individuals are not necessarily solutions
- Evolution process: generational replacement vs. steady state fixed vs. variable population size
- Use of neighborhood structure to define recombination partners
- Two-parent vs. multi-parent crossover
- Infeasible individuals: reject/penalize/repair
- Intensification by local search
- Diversification by mutations

Ant colony optimization

Dorigo 92

- Observation: Ants are able to find quickly the shortest path from their nest to a food source $\rightsquigarrow$ how ?
- Each ant leaves a *pheromone* trail.
- When presented with a path choice, they are more likely to choose the trail with higher pheromone concentration.
- The shortest path gets high concentrations because ants choosing it can return more often.

Ant colony optimization (2)

- Ants are simulated by individual (ant) agents $\rightsquigarrow$ *swarm intelligence*

- Artificial ants incrementally construct solutions by adding components to a partial solution.
- By dispatching a number of ants, the pheromone levels associated with the components are adjusted according to how useful they are.
- Pheromone levels may also *evaporate* to discourage suboptimal solutions.

Construction graph

- Complete graph $G = (C, L)$
  - C solution components
  - L connections
- Pheromone trail values $\tau_i, \tau_{ij} \in \mathcal{T}$, for $c_i \in C, l_{ij} \in L$
- Heuristic values $\eta_i, \eta_{ij} \in \mathcal{H}$
- Moves in the graph depend on transition probabilities (use only τ_i, η_i)

$$p(c_r \mid s_a[c_l]) = \begin{cases} \dfrac{[\eta_r]^\alpha [\tau_r]^\beta}{\sum_{c_u \in J(s_a[c_l])} [\eta_u]^\alpha [\tau_u]^\beta}, & \text{if } c_r \in J(s_a[c_l]), \\ 0, & \text{otherwise.} \end{cases}$$

s_a denotes the solution constructed by ant a, c_l its last component.
$J(s_a[c_l])$ denotes the set of components allowed to be added.

Algorithm: Ant System (AS)

InitializePheromoneValues
while termination conditions not met **do**
  for all ants $a \in \mathcal{A}$ **do**
    $s_a \leftarrow$ ConstructSolution($\mathcal{T}, \mathcal{H}$)
  endfor
  ApplyOnlineDelayedPheromoneUpdate($\mathcal{T}, \{s_a \mid a \in \mathcal{A}\}$)
endwhile

- ApplyOnlineDelayedPheromoneUpdate $\rightsquigarrow$ increase of pheromone on solutions components found in high-quality solutions
- The Ant System (AS) algorithm may be generalized to the Ant Colony Optimization (ACO) Metaheuristics.