Optimization and Simulation

Optimization

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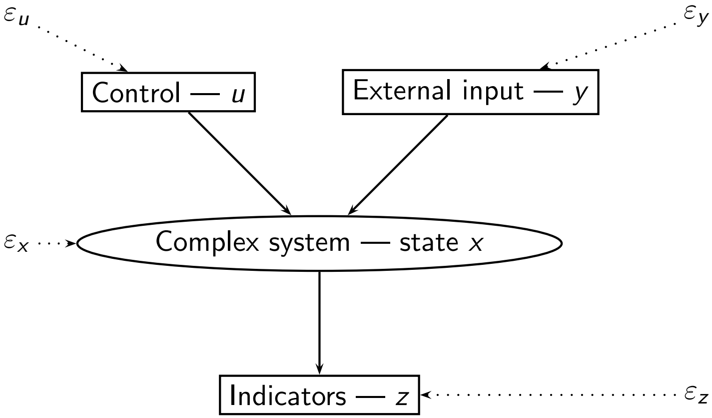
Outline

1. Introduction
2. Classical optimization problems
3. Greedy heuristics
4. Neighborhood and local search
5. Diversification
   - Variable Neighborhood Search
   - Simulated annealing
   - Comments

General framework

$$Z = h(X, Y, U) + \varepsilon_z$$



General framework

Assumptions

- Control U is deterministic.

$$Z(u) = h(X, Y, u) + \varepsilon_z$$

- Various features of Z are considered: mean, variance, quantile, etc.

$$(z_1(u), \ldots, z_m(u))$$

- They are combined in a single indicator:

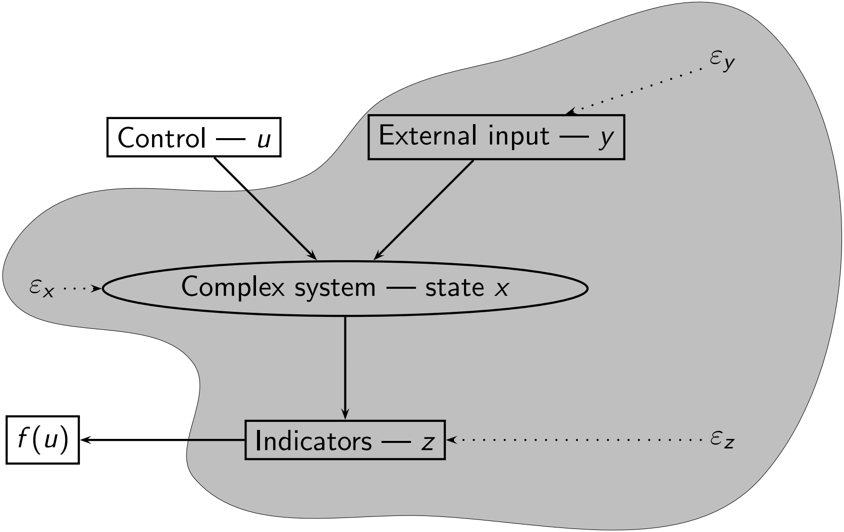
$$f(u) = g(z_1(u), \ldots, z_m(u))$$

General framework: example

Riccardo at Satellite

- X: number of customers in the bar
- Y: arrivals of customers
- u: service time of Riccardo
- $Z(u)$: waiting time of the customers
- $z_1(u)$: mean waiting time
- $z_2(u)$: maximum waiting time
- $f(u) = g(z_1(u), z_2(u)) = z_1 + z_2$

General framework: the black box



Optimization problem

$$\min_{u \in \mathbb{R}^n} f(u)$$

subject to

$$u \in \mathcal{U} \subseteq \mathbb{R}^n$$

- u: decision variables
- $f(u)$: objective function
- $u \in \mathcal{U}$: constraints
- $\mathcal{U}$: feasible set

If $\mathcal{U}$ is a finite set: **combinatorial optimization**.

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The knapsack problem

- Patricia prepares a hike in the mountain.
- She has a knapsack with capacity Wkg.
- She considers carrying a list of n items.
- Each item has a utility u_i and a weight w_i.
- What items should she take to maximize the total utility, while fitting in the knapsack?

Modeling

Decision variables

$$x_i = \begin{cases} 1 & \text{if item } i \text{ goes into the knapsack,} \\ 0 & \text{otherwise} \end{cases}$$

Objective function

$$\max f(x) = \sum_{i=1}^{n} u_i x_i$$

Constraints

$$\sum_{i=1}^{n} w_i x_i \leq W$$

$$x_i \in \{0,1\} \quad i = 1, \ldots, n$$

Brute force algorithm

Enumeration

- As $\mathcal{U}$ is finite, all solutions can be enumerated.
- Each object can be in or out, for a total of 2^n combinations.
- For each of them, we must:
  - Check that the weight is feasible.
  - If so, calculate the utility and check if it is the largest so far.

Computational time

- About $2n$ floating point operations per combination.
- Assume a 1 Teraflops processor: 10^{12} floating point operations per second.

Brute force algorithm

Computational time

- If $n = 34$, about 1 second to solve.
- If $n = 40$, about 1 minute.
- If $n = 45$, about 1 hour.
- If $n = 50$, about 1 day.
- If $n = 58$, about 1 year.
- If $n = 69$, about 2583 years, more than the Christian Era.
- If $n = 78$, about 1,500,000 years, time elapsed since Homo Erectus appeared on earth.
- If $n = 91$, about 10^{10} years, roughly the age of the universe.

Combinatorial optimization

- The set of feasible solutions is finite.
- But the number of feasible solutions grows exponentially with the size of the problem.
- No optimality condition can be exploited.

Traveling salesman problem

The problem

- Consider n cities.
- For any pair (i, j) of cities, the distance d_{ij} between them is known.
- Find the shortest possible itinerary that starts from the home town of the salesman, visit all other cities, and come back to the origin.

Feasible solutions

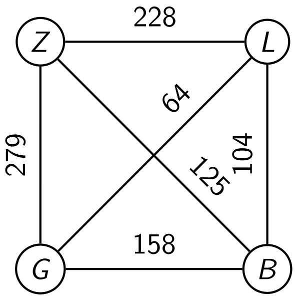
- Number of feasible solutions:

$$(n-1)! \approx \sqrt{2\pi/n-1)}\left(\frac{n-1}{e}\right)^{n-1}$$

- Again, the number of feasible solutions grows exponentially with the size of the problem.

TSP: example

Lausanne, Geneva, Zurich, Bern



Home town: Lausanne

3 possibilities:

- L → B → Z → G → L: 572 km
- L → B → G → Z → L: 769 km
- L → Z → B → G → L: 575 km

Integer linear optimization problem

Linear optimization

$$\min_{x \in \mathbb{R}^n} c^T x$$

subject to

$$Ax = b$$
$$x \geq 0.$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$.

Integer Linear optimization

$$\min_{x \in \mathbb{R}^n} c^T x$$

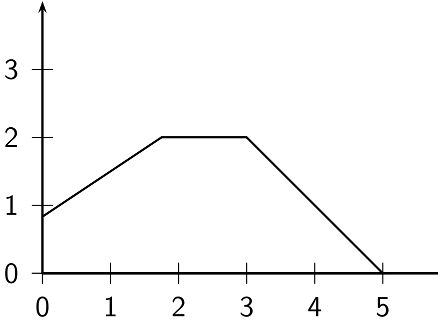
subject to

$$Ax = b$$
$$x \in \mathbb{N}.$$

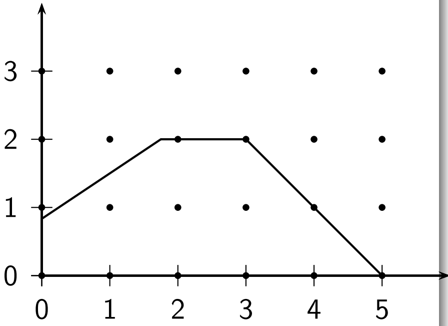
where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$.

Feasible set

Polyhedron



Intersection polyhedron/integer lattice



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Greedy heuristics

Principles

- Step by step construction of a feasible solution.
- At each step, a local optimization is performed.
- Decisions taken at previous steps are definitive.

Properties

- Easy to implement.
- Short computational time.
- May generate poor solutions.

Greedy heuristics

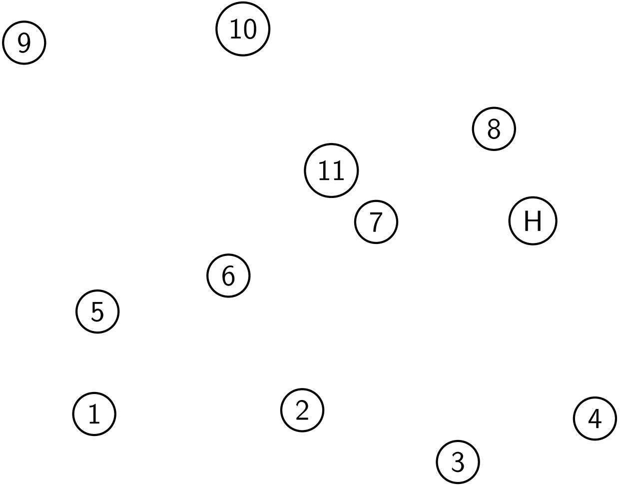
The knapsack problem

- Sort the items by decreasing order of u_i/w_i.
- For each item in this order, put it in the sack if it fits.

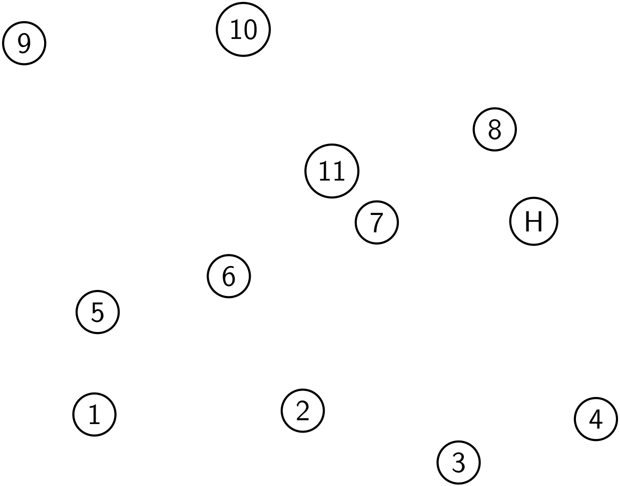
The traveling salesman problem

- Start from home.
- At each step, select the closest city as the next one.

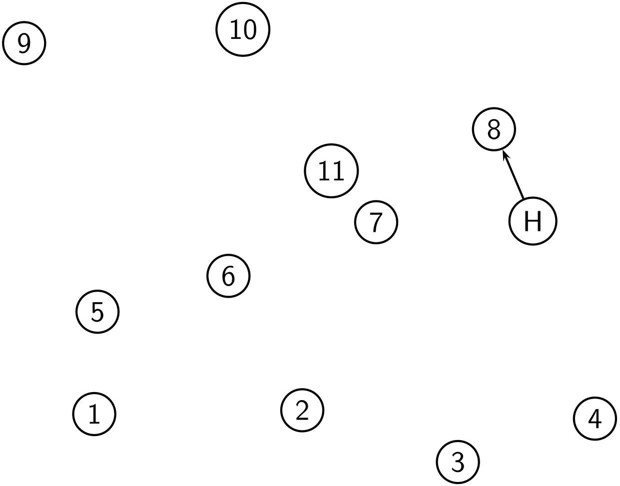
TSP: 12 cities (euclidean dist.)



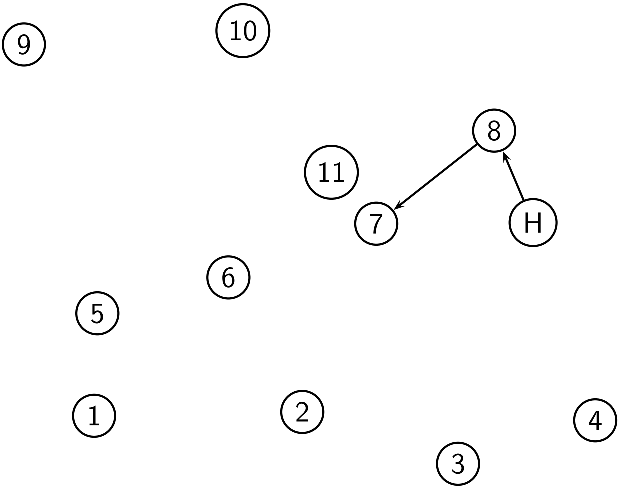
TSP: 12 cities



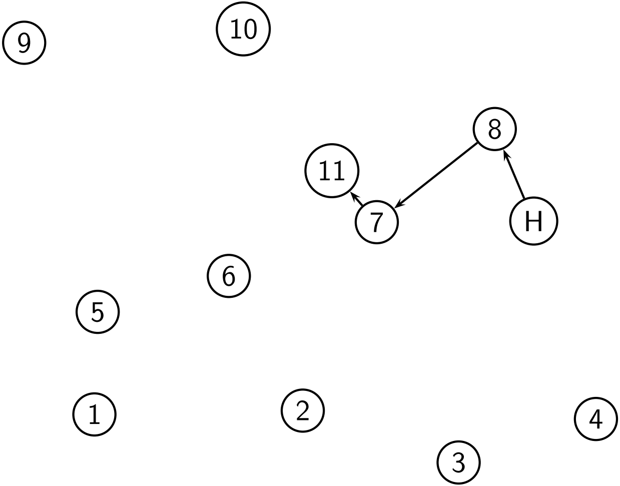
TSP: 12 cities



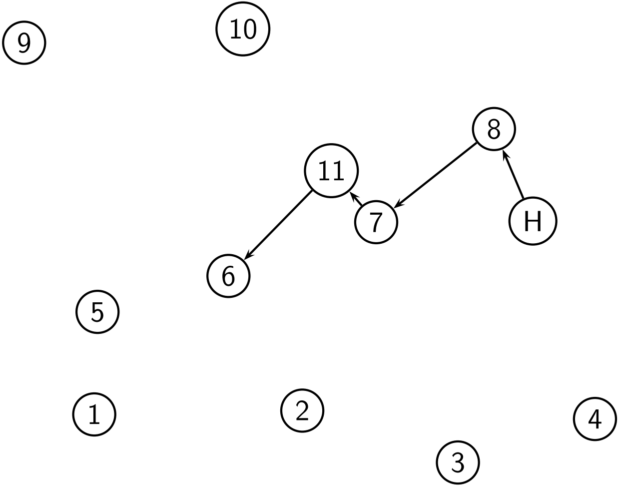
TSP: 12 cities



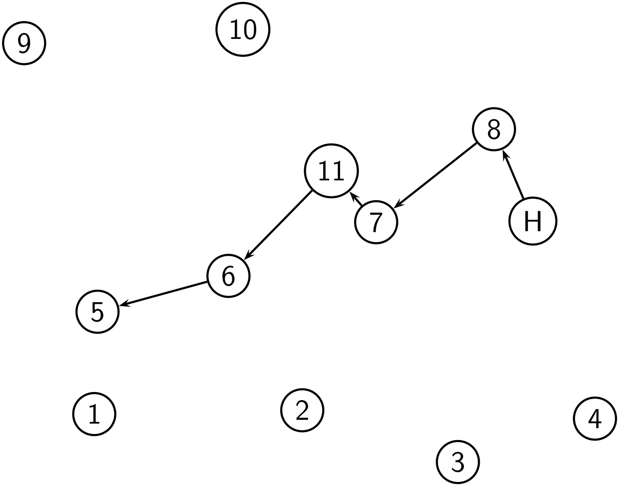
TSP: 12 cities



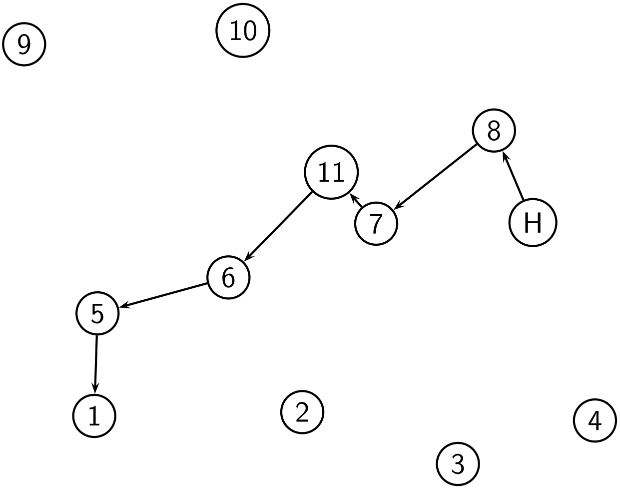
TSP: 12 cities



TSP: 12 cities



TSP: 12 cities



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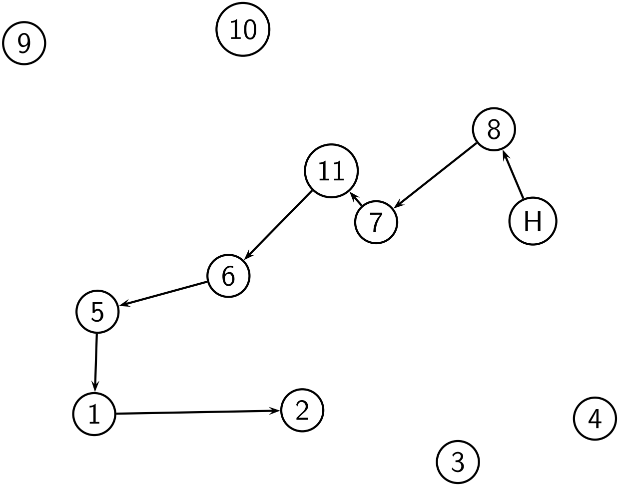
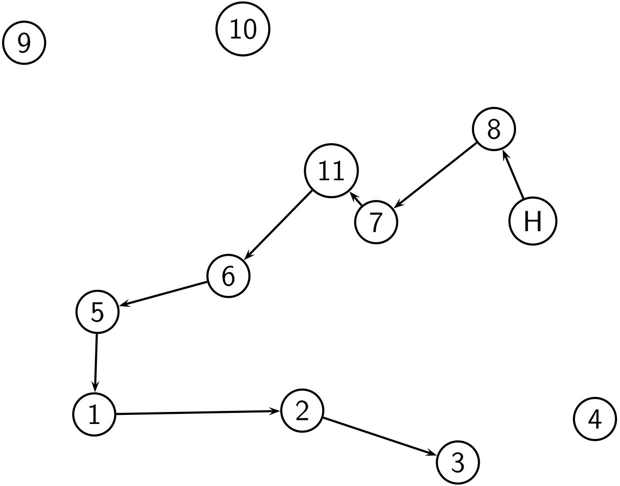
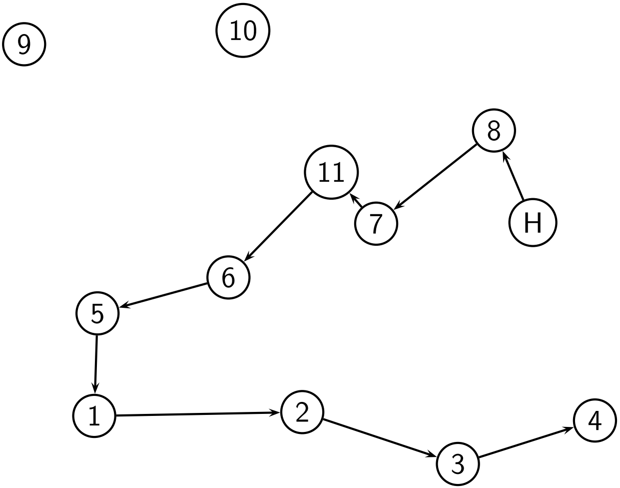


TSP: 12 cities



TSP: 12 cities



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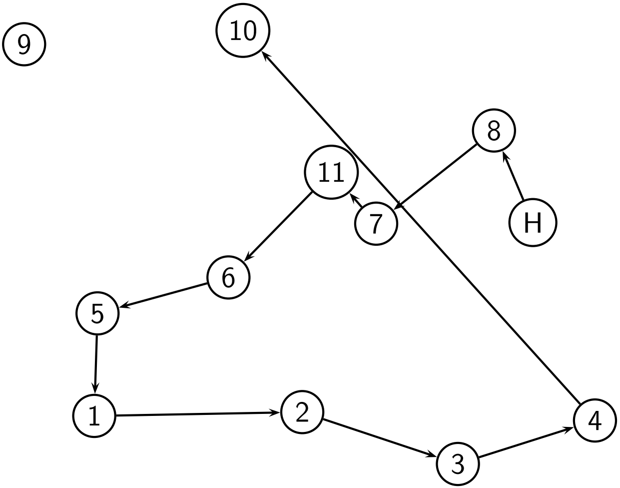
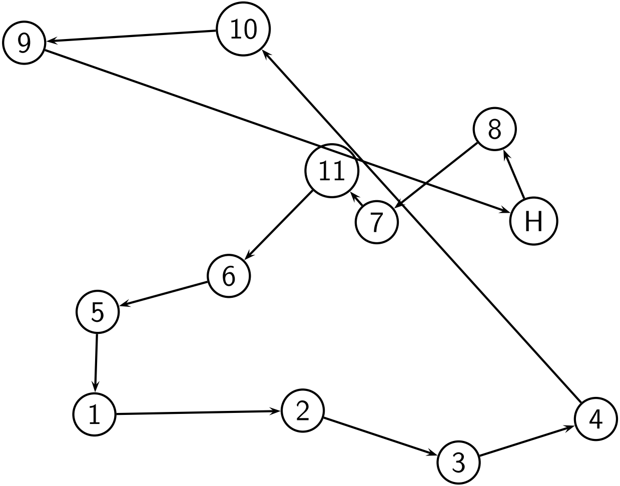
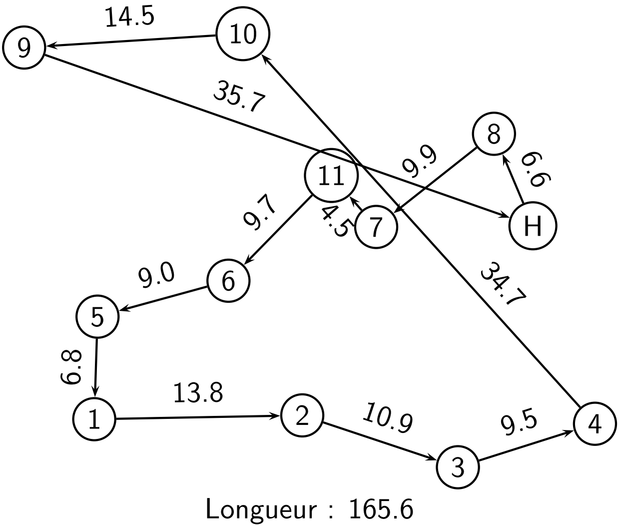


TSP: 12 cities



TSP: 12 cities



Integer optimization

Intuitive approach

- Solve the continuous relaxation.
- Round the solution.

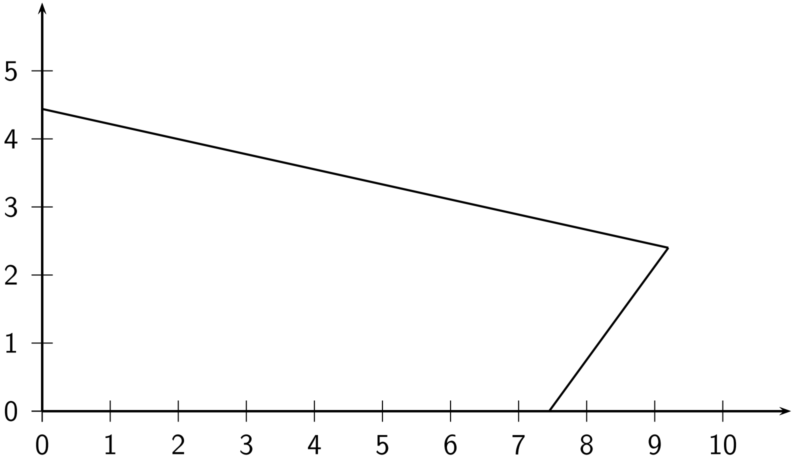
Example

$$\min_{x \in \mathbb{R}^2} -3x_1 - 13x_2$$

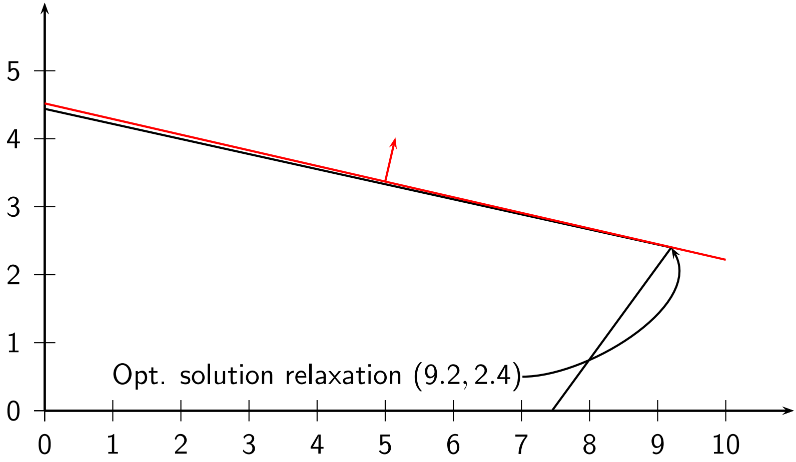
subject to

$$\begin{aligned} 2x_1 + 9x_2 &\leq 40 \\ 11x_1 - 8x_2 &\leq 82 \\ x_1, x_2 &\geq 0 \\ x_1, x_2 &\in \mathbb{N} \end{aligned}$$

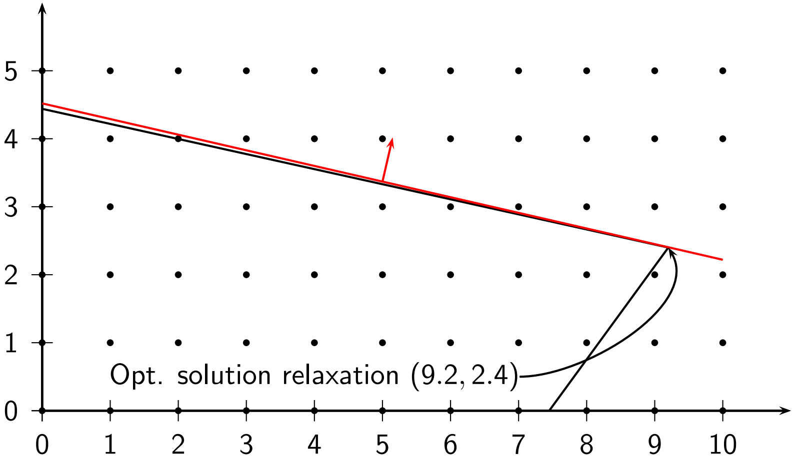
Relaxation: feasible set



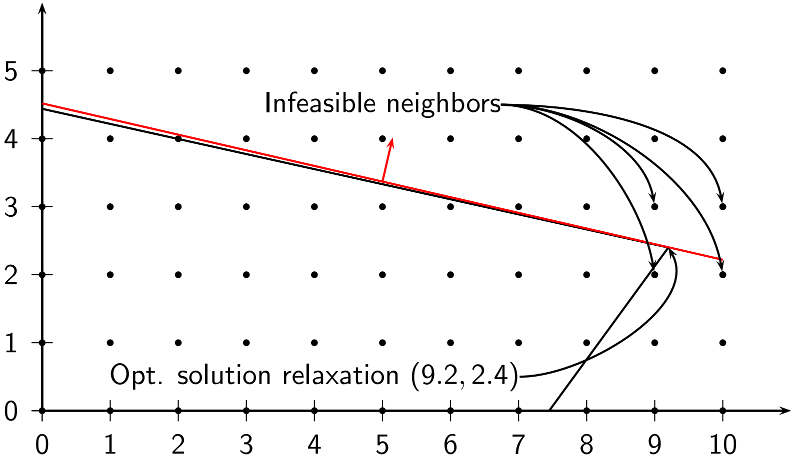
Optimal solution of the relaxation



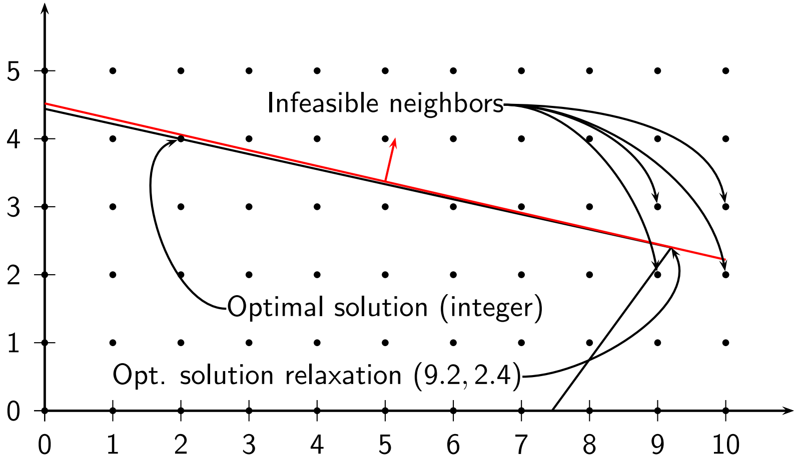
Integrality constraints



Infeasible neighbors



Solution of the integer optimization problem



Issues

- There are 2^n different ways to round. Which one to choose?
- Rounding may generate an infeasible solution.
- The rounded solution may be far from the optimal solution.

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Neighborhood and local search

Concept

- The feasible set is too large.
- At each iteration, restrict the optimization problem to a small feasible subset.
- Ideally, the small subset can be enumerated.
- Typically, it consists of solutions obtained from simple modifications of the current solution.
- The small subset is called a *neighborhood*.

Integer optimization: neighborhood

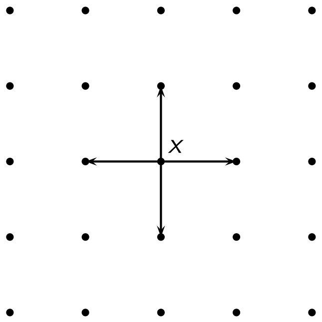
- Consider the current iterate $x \in \mathbb{Z}^n$.
- For each $k = 1, \ldots, n$, define 2 neighbors by increasing and decreasing the value of x_k by one unit.
- The neighbors y^{k+} and y^{k-} are defined as

$$y_i^{k+} = y_i^{k-} = x_i, \forall i \neq k, \quad y_k^{k+} = x_k + 1, \quad y_k^{k+} = x_k - 1.$$

- Example

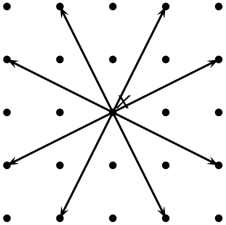
$$x = (3, 5, 2, 8) \quad y^{2+} = (3, 6, 2, 8) \quad y^{2-} = (3, 4, 2, 8)$$

Integer optimization: neighborhood



Integer optimization: neighborhood

- The concept of neighborhood is fairly general.
- It must be defined based on the structure of the problem.
- Creativity is required here.



Local search

- Consider the integer optimization problem

$$\min_{x \in \mathbb{Z}^n} f(x)$$

subject to

$$x \in \mathcal{F}.$$

- Consider the neighborhood structure $V(x)$, where $V(x)$ is the set of neighbors of x.
- At each iteration k, consider the neighbors in $V(x_k)$ one at a time.
- For each $y \in V(x_k)$, if $f(y) < f(x_k)$, then $x_{k+1} = y$ and proceed to the next iteration.
- If $f(y) \geq f(x_k)$, $\forall y \in V(x_k)$, x_k is a local minimum. Stop.

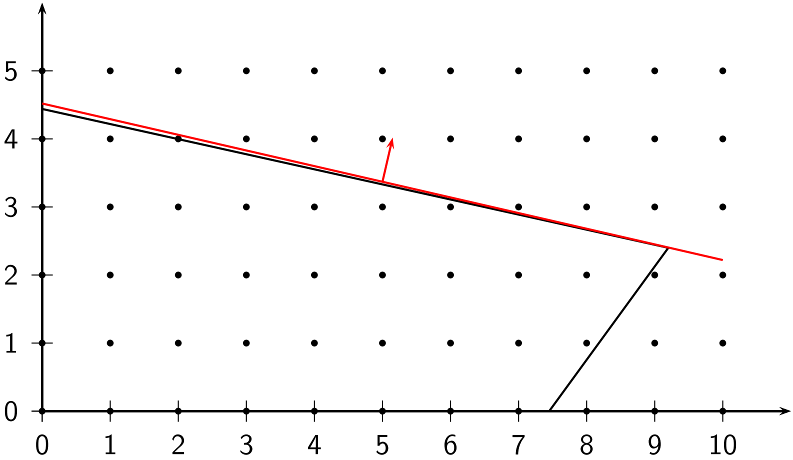
Local search: example

$$\min_{x \in \mathbb{R}^2} -3x_1 - 13x_2$$

subject to

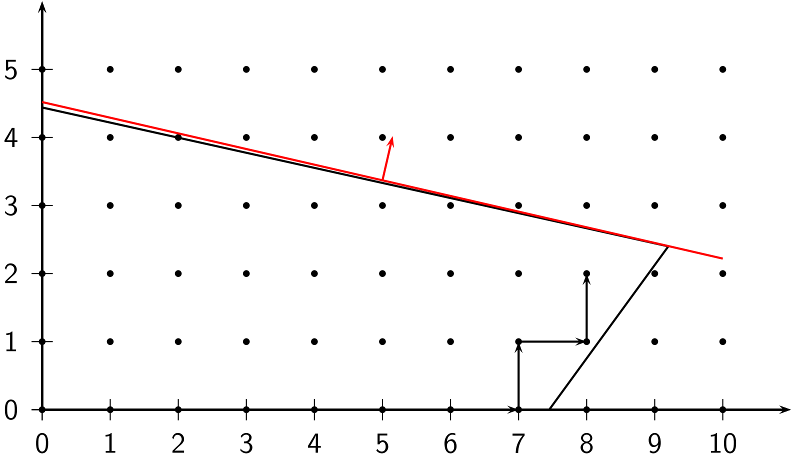
$$\begin{aligned} 2x_1 + 9x_2 &\leq 40 \\ 11x_1 - 8x_2 &\leq 82 \\ x_1, x_2 &\in \mathbb{N} \end{aligned}$$

Local search: example



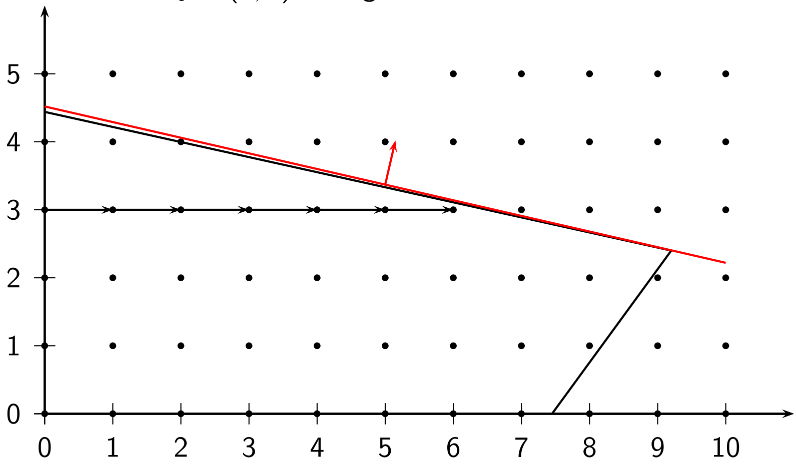
Local search: example

$x_0 = (6, 0)$ - Neighborhood: E - N - O - S



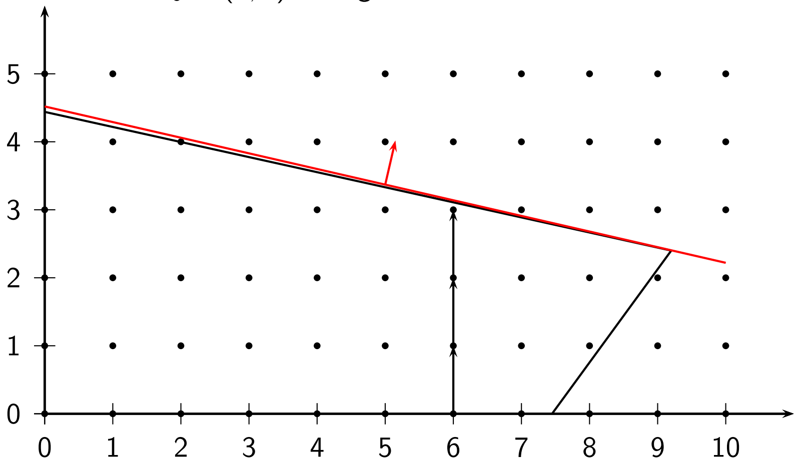
Local search: example

$x_0 = (0, 3)$ - Neighborhood: E - N - O - S



Local search: example

$x_0 = (6, 0)$ - Neighborhood : N - O - S - E



Local search: comments

- The algorithm stops at a local minimum, that is a solution better than all its neighbors.
- The outcome depends on the starting point and the structure of the neighborhood.
- The neighborhood must be sufficiently large to increase the chances of improvement, and sufficiently small to avoid a lengthy enumeration.
- Example of a neighborhood too small: one neighbor at the west.
- Example of a neighborhood too large: each feasible point is in the neighborhood.
- It is good practice to use symmetric neighborhoods:

$$y \in V(x) \iff x \in V(y).$$

The knapsack problem

$$\max_{x \in \{0,1\}^n} u^T x$$

subject to

$$w^T x \leq W.$$

The knapsack problem: neighborhood

- Current solution: for each item i, $x_i = 0$ or $x_i = 1$.
- Neighbor solution: select an item j, and change the decision: $x_j \leftarrow 1 - x_j$.
- Warning: check feasibility.
- Generalization: neighborhood of size k: select k items, and change the decision for them (checking feasibility).

The knapsack problem: neighborhood

- A neighborhood of size k modifies k variables.
- Number of neighbors:

$$\frac{n!}{k!(n-k)!}$$

- $k = 1$: n neighbors.
- $k = n$: 1 neighbor.

Example : $W = 300$.

i	1	2	3	4	5	6	7	8	9	10	11	12
U	80	31	48	17	27	84	34	39	46	58	23	67
W	84	27	47	22	21	96	42	46	54	53	32	78

First solution: empty sack.

The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0	0	0	0	0	84	80	0

The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
1	1	0	0	0	0	0	0	0	0	0	0	0	84		80
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	80
2	1	1	0	0	0	0	0	0	0	0	0	0	111	111	80

The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
2	1	1	0	0	0	0	0	0	0	0	0	0	111		111
	0	1	0	0	0	0	0	0	0	0	0	0	27	31	111
	1	0	0	0	0	0	0	0	0	0	0	0	84	80	111
3	1	1	1	0	0	0	0	0	0	0	0	0	158	159	111

The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
3	1	1	1	0	0	0	0	0	0	0	0	0	158		159
	0	1	1	0	0	0	0	0	0	0	0	0	74	79	159
	1	0	1	0	0	0	0	0	0	0	0	0	131	128	159
	1	1	0	0	0	0	0	0	0	0	0	0	111	111	159
4	1	1	1	1	0	0	0	0	0	0	0	0	180	176	159

The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
4	1	1	1	1	0	0	0	0	0	0	0	0	180		176
	0	1	1	1	0	0	0	0	0	0	0	0	96	96	176
	1	0	1	1	0	0	0	0	0	0	0	0	153	145	176
	1	1	0	1	0	0	0	0	0	0	0	0	133	128	176
	1	1	1	0	0	0	0	0	0	0	0	0	158	159	176
5	1	1	1	1	1	0	0	0	0	0	0	0	201	203	176

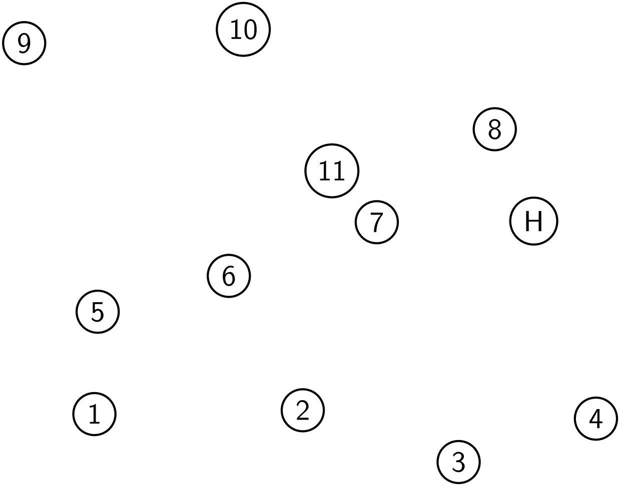
The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	$w^T x_c$	$u^T x_c$	$u^T x^*$
5	1	1	1	1	1	0	0	0	0	0	0	0	201		203
	0	1	1	1	1	0	0	0	0	0	0	0	117	123	203
	1	0	1	1	1	0	0	0	0	0	0	0	174	172	203
	1	1	0	1	1	0	0	0	0	0	0	0	154	155	203
	1	1	1	0	1	0	0	0	0	0	0	0	179	186	203
	1	1	1	1	0	0	0	0	0	0	0	0	180	176	203
6	1	1	1	1	1	1	0	0	0	0	0	0	297	287	203

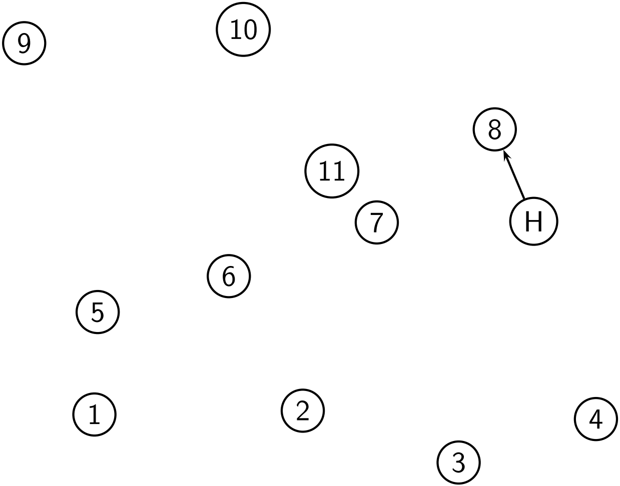
The knapsack problem: local search

k	1	2	3	4	5	6	7	8	9	10	11	12	w^Tx_c	u^Tx_c	u^Tx^*
6	1	1	1	1	1	1	0	0	0	0	0	0	297		287
	0	1	1	1	1	1	0	0	0	0	0	0	213	207	287
	1	0	1	1	1	1	0	0	0	0	0	0	270	256	287
	1	1	0	1	1	1	0	0	0	0	0	0	250	239	287
	1	1	1	0	1	1	0	0	0	0	0	0	275	270	287
	1	1	1	1	0	1	0	0	0	0	0	0	276	260	287
	1	1	1	1	1	0	0	0	0	0	0	0	201	203	287
	1	1	1	1	1	1	1	0	0	0	0	0	339	321	287
	1	1	1	1	1	1	0	1	0	0	0	0	343	326	287
	1	1	1	1	1	1	0	0	1	0	0	0	351	333	287
	1	1	1	1	1	1	0	0	0	1	0	0	350	345	287
	1	1	1	1	1	1	0	0	0	0	1	0	329	310	287
	1	1	1	1	1	1	0	0	0	0	0	1	375	354	287

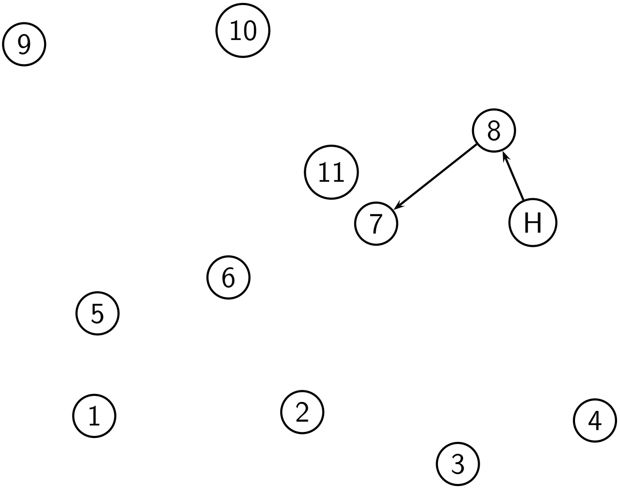
TSP: 12 cities



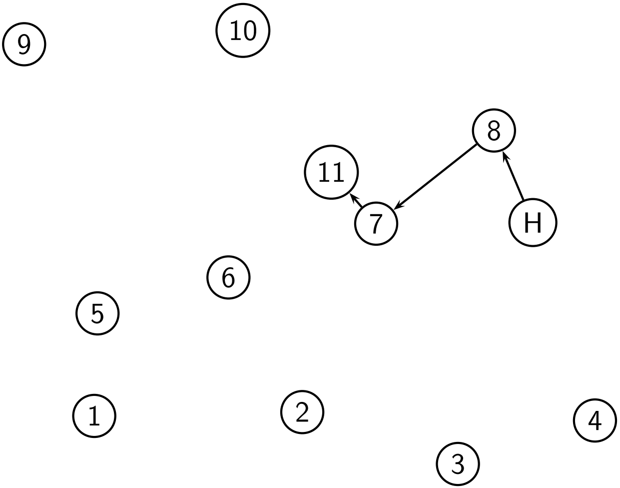
Initial solution from greedy algorithm



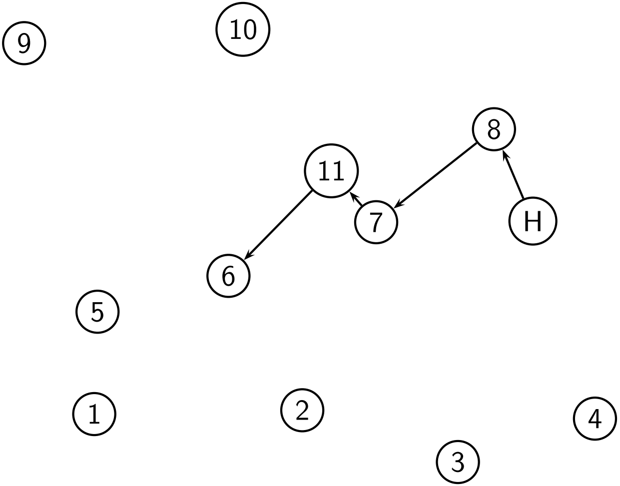
Initial solution from greedy algorithm



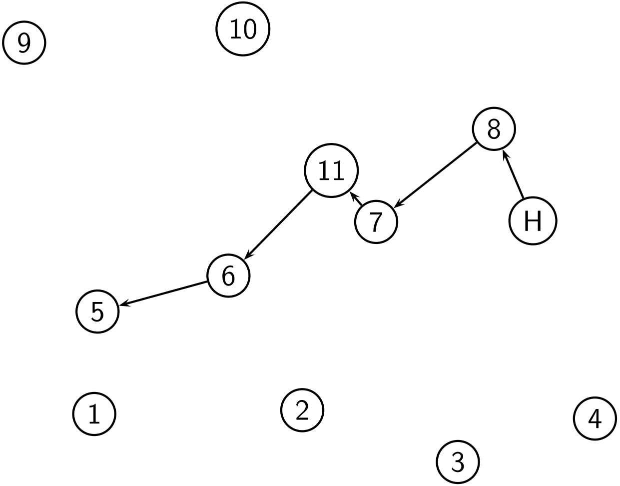
Initial solution from greedy algorithm



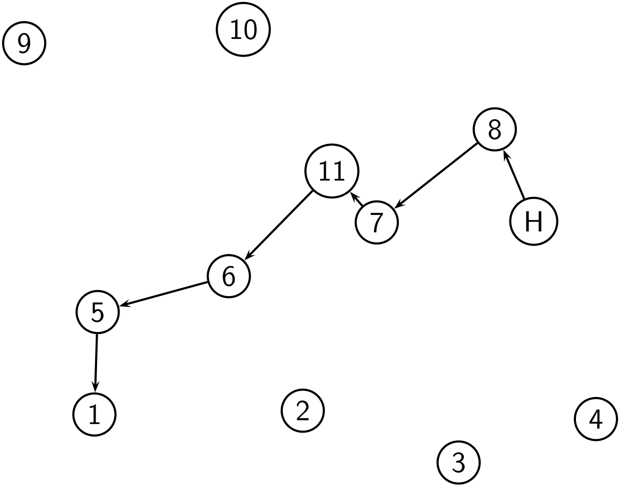
Initial solution from greedy algorithm



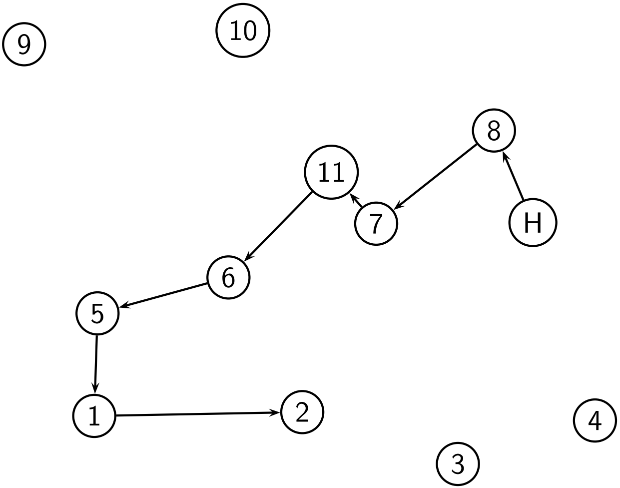
Initial solution from greedy algorithm



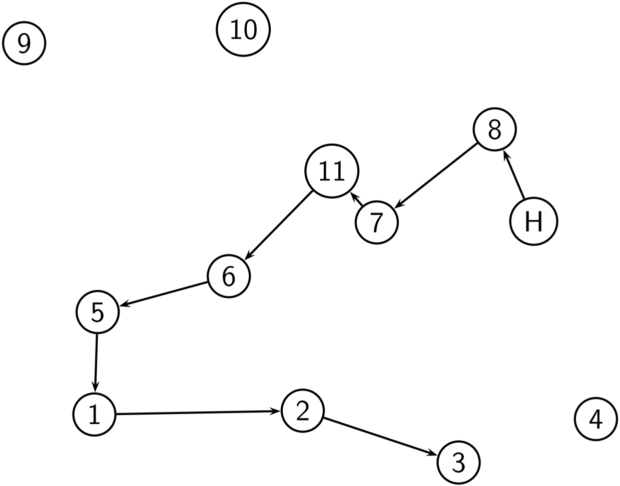
Initial solution from greedy algorithm



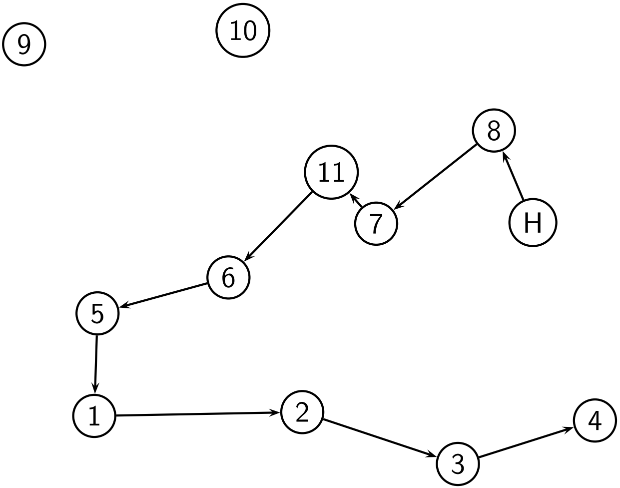
Initial solution from greedy algorithm



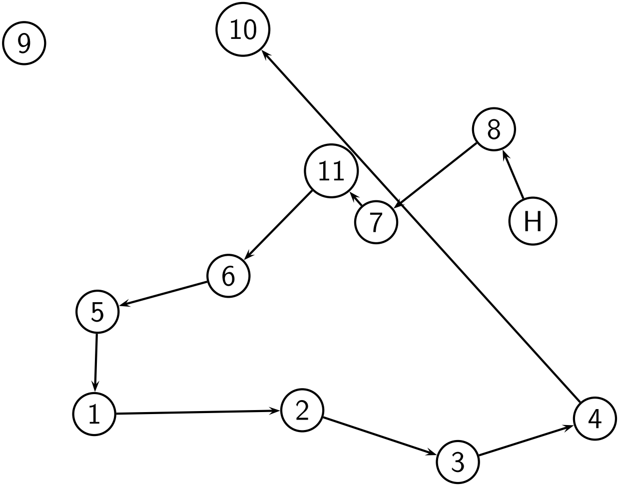
Initial solution from greedy algorithm



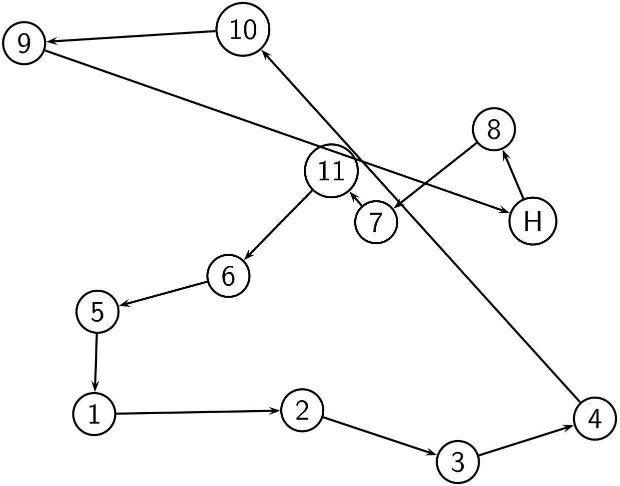
Initial solution from greedy algorithm



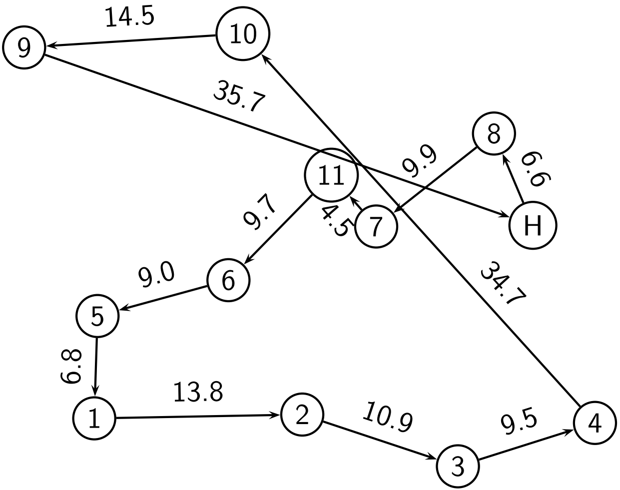
Initial solution from greedy algorithm



Initial solution from greedy algorithm



Initial solution from greedy algorithm



Length : 165.6

Neighborhood: 2-OPT

2-OPT

- Select two cities.
- Swap their position in the tour.
- Visit all intermediate cities in reverse order.

Example

Current tour:

A–B–C–D–E–F–G–H–A

Exchange C and G to obtain

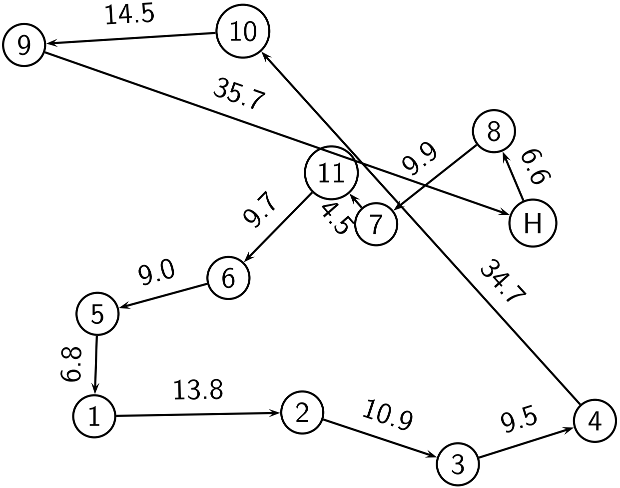
A–B–G–F–E–D–C–H–A.

Neighborhood: 2-OPT(1,9)

Example

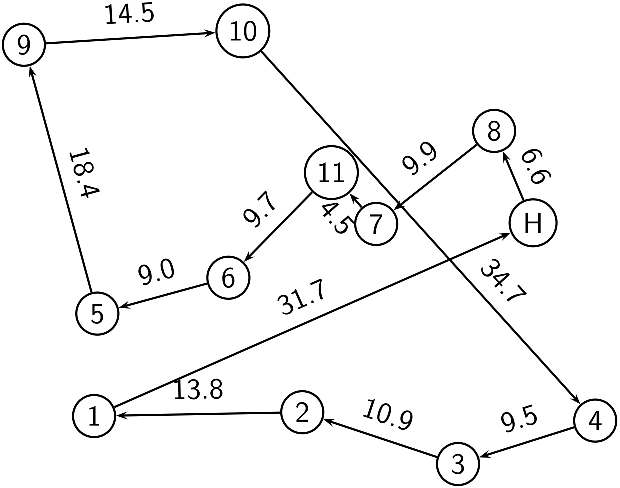
- Try to improve the solution using 2-OPT swapping 1 and 9.
- Before: H–8–7–11–6–5–1–2–3–4–10–9–H (length: 165.6)
- After : H–8–7–11–6–5–9–10–4–3–2–1–H (length: 173.3)
- No improvement.

Neighborhood: 2-OPT(1,9)



Length: 165.6

Neighborhood: 2-OPT(1,9)

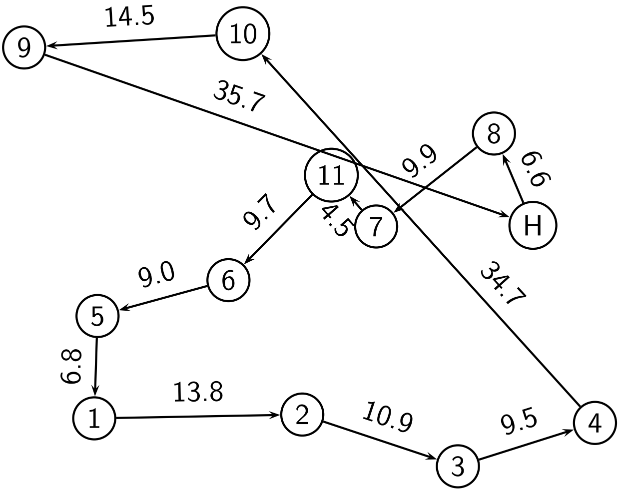


Length: 173.3

Local search

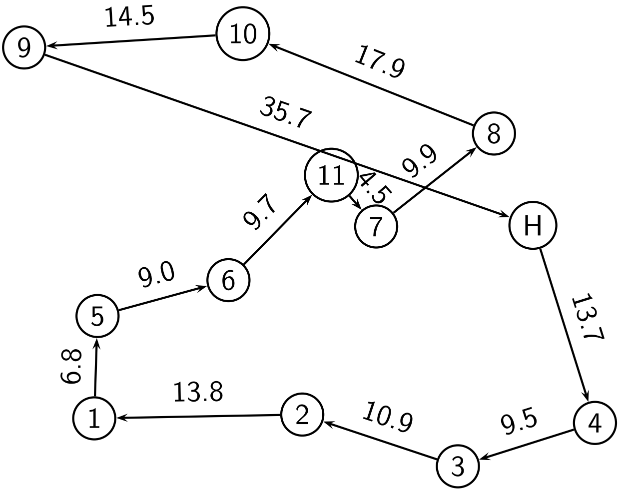
- Consider each pair of nodes.
- Apply 2-OPT.
- Select the best tour.

Current tour



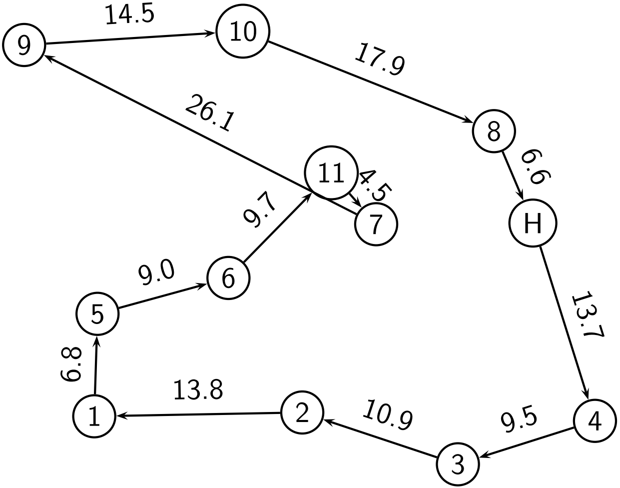
Length: 165.6

Best neighbor: 2-OPT(8,4)



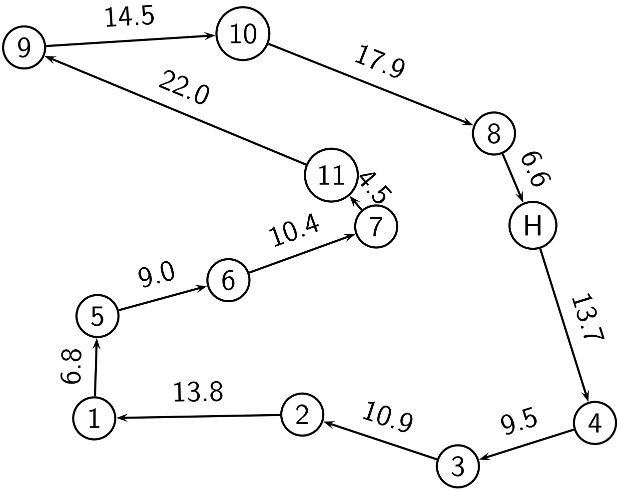
Length: 155.8

Best neighbor: 2-OPT(8,9)



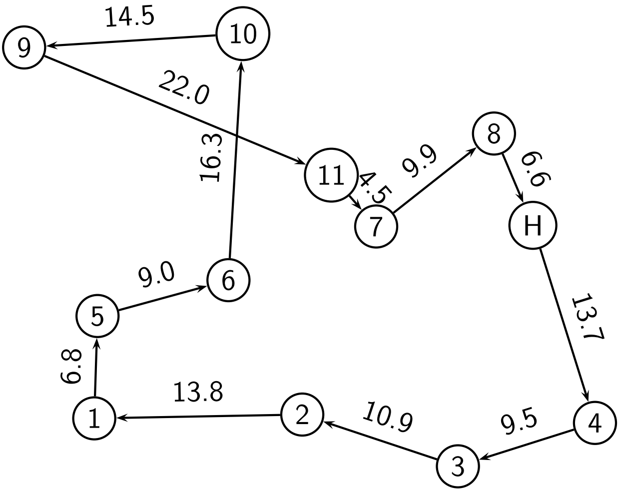
Length: 143.0

Best neighbor: 2-OPT(11,7)



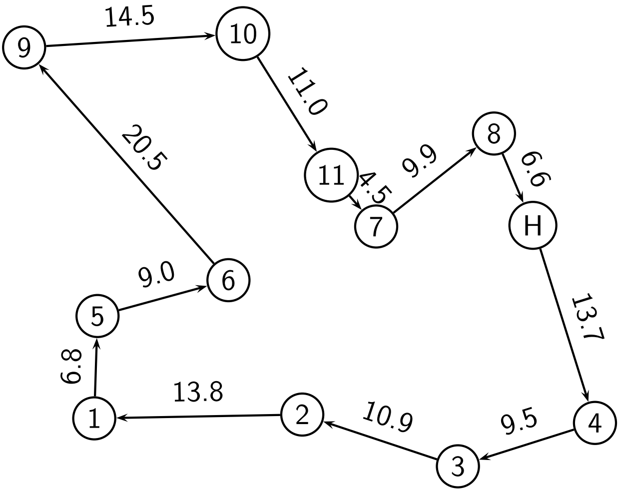
Length: 139.5

Best neighbor: 2-OPT(7,10)



Length: 137.5

Best neighbor: 2-OPT(10,9)



Length: 130.7

Outline

1. Introduction
2. Classical optimization problems
3. Greedy heuristics
4. Neighborhood and local search
5. Diversification
   - Variable Neighborhood Search
   - Simulated annealing
   - Comments

Variable Neighborhood Search

- aka VNS
- Idea: consider several neighborhood structures.
- When a local optimum has been found for a given neighborhood structure, continue with another structure.

VNS: method

Input
- $V_1, V_2, \ldots, V_K$ neighborhood structures.
- Initial solution x_0.

Initialization
- $x_c \leftarrow x_0$
- $k \leftarrow 1$

Iterations Repeat
- Apply local search from x_c using neighborhood V_k

$$x^+ \leftarrow LS(x_c, V_k)$$

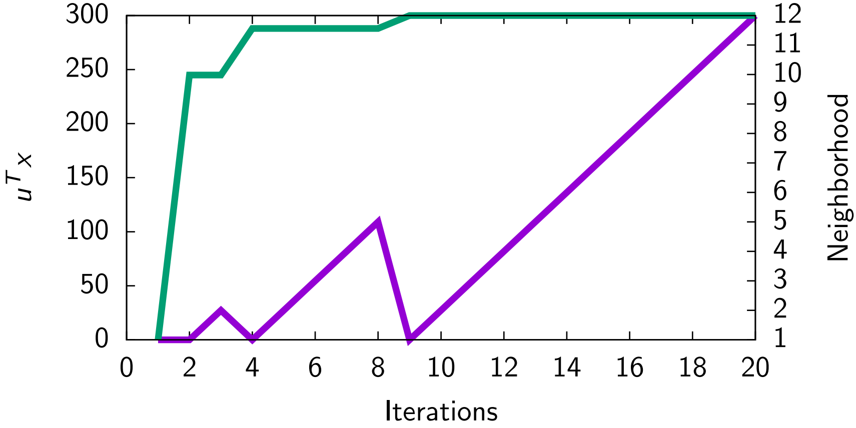
- If $f(x^+) < f(x_c)$, then $x_c \leftarrow x^+$, $k \leftarrow 1$.
- Otherwise, $k \leftarrow k + 1$.

Until $k = K$.

VNS: example for the knapsack problem

- Neighborhood of size k: modify k variables.
- Local search: current iterate: x_c
  - randomly select a neighbor x^+
  - if $w^T x^+ \leq W$ and $u^T x^+ > u^T x_c$, then $x_c \leftarrow x^+$
- Repeat 1000 times, for any k.
- The complexity is therefore independent of k.

VNS: example for the knapsack problem



Simulated annealing

Analogy with metallurgy

- Heating a metal and then cooling it down slowly improves its properties.
- The atoms take a more solid configuration.

In optimization:

- Local search can both decrease and increase the objective function.
- At "high temperature", it is common to increase.
- At "low temperature", increasing happens rarely.
- Simulated annealing: slow cooling = slow reduction of the probability to increase.

Simulated annealing

Modify the local search.

For the sake of simplicity: consider a neighborhood structure containing only feasible solutions.

Let x_k be the current iterate

- Select $y \in V(x_k)$.
- If $f(y) \leq f(x_k)$, then $x_{k+1} = y$.
- Otherwise, $x_{k+1} = y$ with probability

$$e^{-\frac{f(y)-f(x_k)}{T}}$$

with $T > 0$.

Concretely, draw r between 0 and 1.

Accept y as next iterate if

$$e^{-\frac{f(y)-f(x_k)}{T}} > r$$

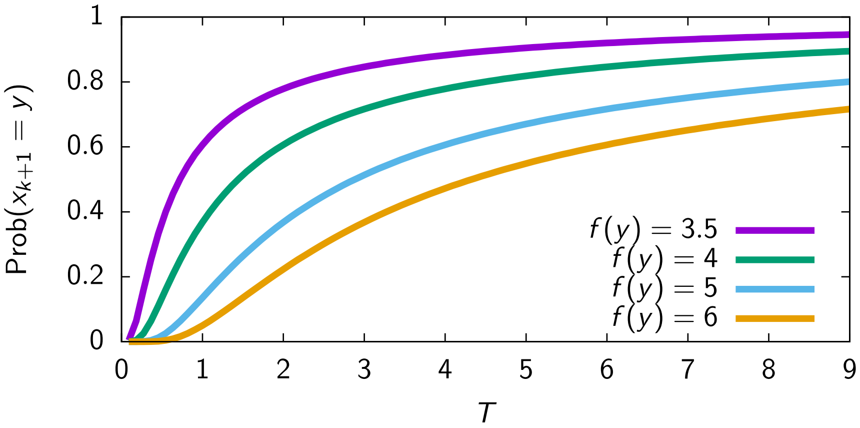
Simulated annealing

$$\text{Prob}(x_{k+1} = y) = \begin{cases} 1 & \text{if } f(y) \leq f(x_k) \\ e^{-\frac{f(y)-f(x_k)}{T}} & \text{if } f(y) > f(x_k) \end{cases}$$

- If T is high (hot temperature), high probability to increase.
- If T is low, almost only decreases.

Simulated annealing

Example : $f(x_k) = 3$



Simulated annealing

- In practice, start with high T for flexibility.
- Then, decrease T progressively.

Simulated annealing

Input
- Initial solution x_0
- Initial temperature T_0, minimum temperature T_f
- Neighborhood structure $V(x)$
- Maximum number of iterations K

Initialize $x_c \leftarrow x_0$, $x^* \leftarrow x_0$, $T \leftarrow T_0$

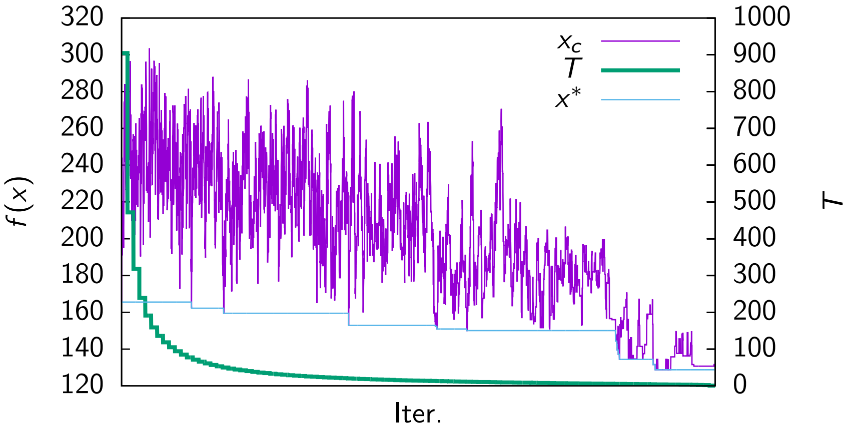
Simulated annealing

Repeat $k \leftarrow 1$

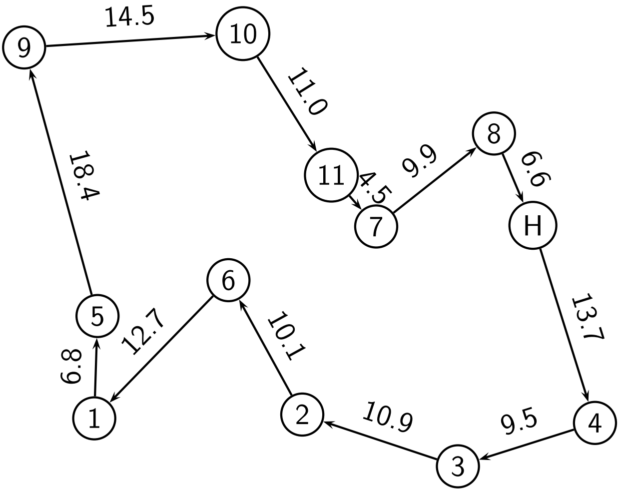
- While $k < K$
  - Randomly select a neighbor $y \in V(x_c)$
  - $\delta \leftarrow f(y) - f(x_c)$
  - If $\delta < 0$, $x_c = y$.
  - Otherwise, draw r between 0 and 1
    - If $r < exp(-\delta/T)$, then $x_c = y$
  - If $f(x_c) < f(x^*)$, $x^* = x_c$.
  - $k \leftarrow k + 1$
- Reduce T

Until $T \leq T_f$

Example: traveling salesman problem



Best solution found



Length : 128.8

Practical comments

- Parameters must be tuned.
- In particular, the reduction rate of the temperature must be specified.
  - Let δ_t be a typical increase of the objective function.
  - In the beginning, we want such an increase to be accepted with probability p_0 (e.g. $p_0 = 0.999$)
  - At the end, we want such an increase to be accepted with probability p_f (e.g. $p_f = 0.00001$)
  - We allow for M updates of the temperature. So, for $m = 0, \ldots, M$,

$$T = -\frac{\delta_t}{\ln(p_0 + \frac{p_f - p_0}{M} m)}$$

Heuristics: general framework

Exploration

Neighborhood

Intensification

Local search

Diversification

Escape from local minima

Exploration: comments

- Neighborhood structure
- It is a “vehicle” to explore the solution space.
- Must be able to (potentially) reach any solution
- Must be tailored to the problem

Intensification: comments

- Local search.
- Exploit the neighborhood structure to find better solutions.
- Many variants are possible:
  - exhaustive search: evaluate all neighbors
  - limited search: evaluate a given number of neighbors
  - randomized search: select the neighbors randomly

Diversification: comments

How to avoid being blocked in local minimum?

- Apply an algorithm from multiple starting points.
  - How to choose starting point?
  - How to avoid shooting in the dark?
- Allow the algorithm to proceed upwards: simulated annealing
  - Climb the mountain to find another valley.
  - How to decide when it is time to climb or to go down?
- Change the structure of the neighborhood: variable neighborhood search
  - How to choose the neighborhood structures?

Meta-heuristics

- Methods designed to escape from local optima are sometimes called "meta-heuristics".
- Plenty of variants are available in the literature.
- In general, success depends on exploiting well the properties of the problem at hand.
- VNS is one of the simplest to code.
- Additional bio-inspired methods have also been proposed and applied: genetic algorithms, ant colony optimization, etc.