# Optimization and Simulation

## Optimization

Michel Bierlaire

Transport and Mobility Laboratory
School of Architecture, Civil and Environmental Engineering
Ecole Polytechnique Fédérale de Lausanne

# Outline

# Optimization

### Procedure

- Mathematical modeling.
- Selection of an algorithm.
- Solving the problem.

# Optimization

## Mathematical modeling

- Decision variables $x$.
- Objective function $f$.
- Constraints $X$.

## Optimization problem

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

subject to

$$x \in X \subseteq \mathbb{R}^n.$$

# Optimization

## Selection of an algorithm

- Mathematical properties of the model.
- Linear optimization.
- Convex optimization.
- Mixed integer linear optimization.
- Differentiable optimization.

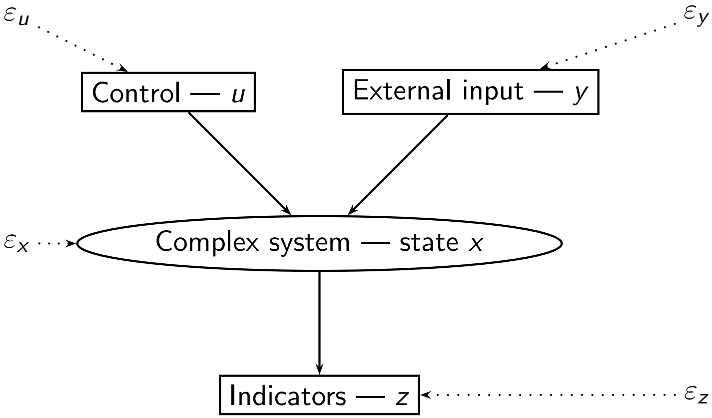
# Optimization

### Solving the problem

- Implement, or obtain the code of the algorithm.
- Import the data.
- Solve.

# 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:

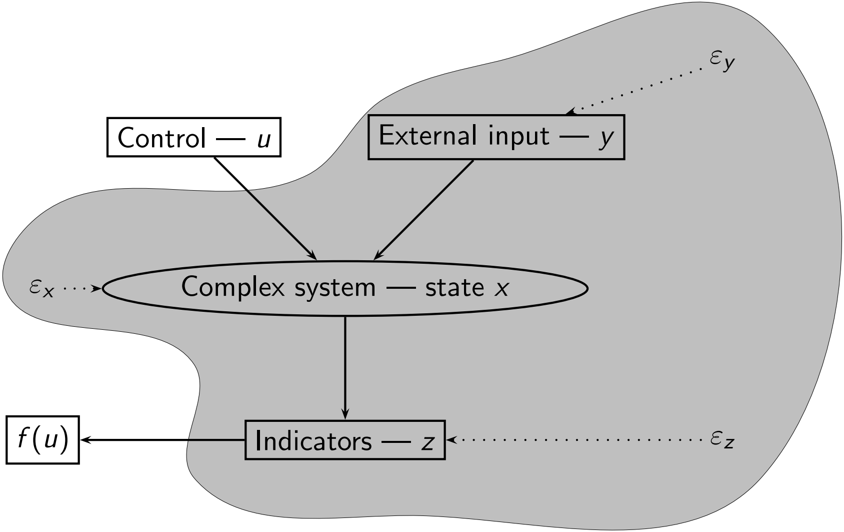
$$f(u) = g(z_1(u), \ldots, z_m(u))$$

# General framework: example

## Rico at Satellite

- $X$: number of customers in the bar
- $Y$: arrivals of customers
- $u$: service time of Rico
- $Z(u)$: 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

# Optimization problem

## Combinatorial optimization

- $f$ and $\mathcal{U}$ have no specific property.
- $f$ is a black box.
- $\mathcal{U}$ is a finite set of valid configurations.
- No optimality condition is available.

# Optimization methods

### Exact methods (branch and bound)

- Finds the optimal solution.
- Suffers from the curse of dimensionality.
- Requires the availability of valid and tight bounds.

### Approximation algorithms

- Finds a sub-optimal solution.
- Guarantees a bound on the quality of the solution.
- Mainly used for theoretical purposes.

### Heuristics

- Smart exploration of the solution space.
- No guarantee about optimality.
- Few assumptions about the problem.

# Outline

# The knapsack problem

- Patricia prepares a hike in the mountain.
- She has a knapsack with capacity $W$ kg.
- 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?

# Mathematical model

## 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

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

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

# Instance

$n = 12$

Maximum weight: 300.

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

# Real example

## Portfolio optimization

- Items: potential assets.
- Utility: return.
- Weight: risk.
- Capacity: maximum risk.

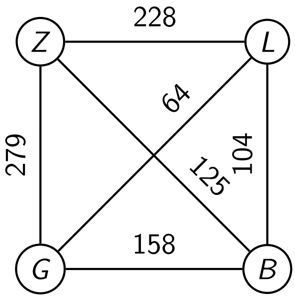
# Traveling salesman problem

### 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.

# TSP: example

Lausanne, Geneva, Zurich, Bern

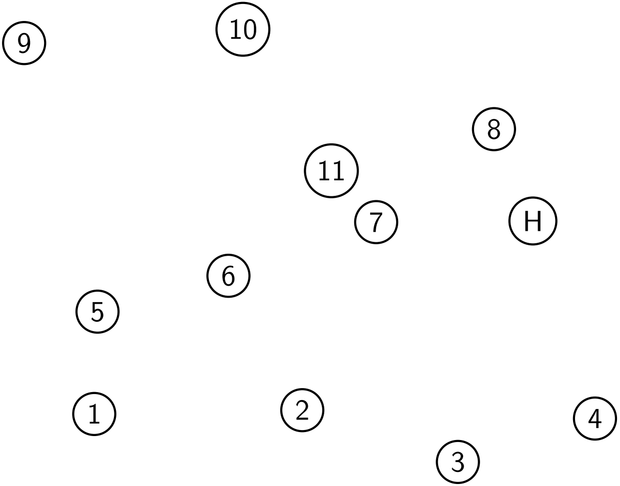



Home town: Lausanne

3 possibilities (+ their symmetric version):

- L $\rightarrow$ B $\rightarrow$ Z $\rightarrow$ G $\rightarrow$ L: 572 km
- L $\rightarrow$ B $\rightarrow$ G $\rightarrow$ Z $\rightarrow$ L: 769 km
- L $\rightarrow$ Z $\rightarrow$ B $\rightarrow$ G $\rightarrow$ L: 575 km

# TSP: 12 cities (euclidean dist.)



# 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

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

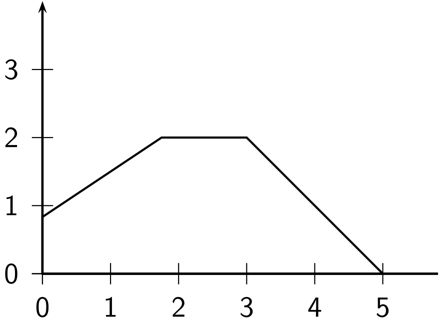
subject to

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

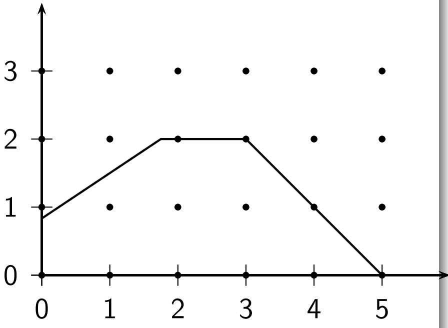
where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$.

# Feasible set

## Polyhedron




## Intersection polyhedron/integer lattice



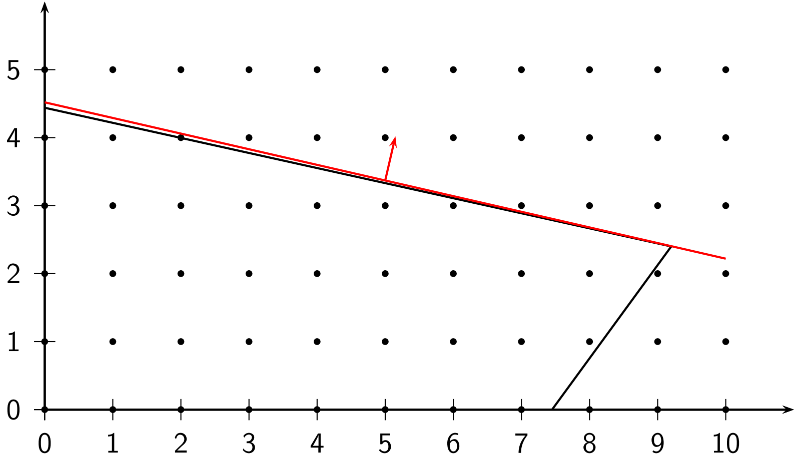
# Example

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

subject to

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

# Example



# Outline

# Outline

# Brute force algorithm

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

subject to

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

## Brute force algorithm

- $f^* = +\infty$
- For each $x \in \mathcal{U}$, if $f(x) < f^*$ then $x^* = x$, $f^* = f(x^*)$.

# Knapsack problem

### Enumeration

- 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 better than $f^*$.

# Python implementation

```
import numpy as np
import itertools
utility = np.array([80, 31, 48, 17, 27, 84, 34, 39, 46, 58, 23, 67])
weight = np.array([84, 27, 47, 22, 21, 96, 42, 46, 54, 53, 32, 78])
capacity = 300
n = len(utility)
fstar = -np.inf
xstar = None
for c in itertools.product([0, 1], repeat = n):
    w = np.inner(c, weight)
    if w <= capacity:
        u = np.inner(c, utility)
        if u > fstar:
            xstar = c
            fstar = u
```

Solution: (1, 1, 1, 1, 1, 0, 0, 1, 0, 1, 0, 0). Weight: 300. Utility: 300.

# Knapsack problem

## Computational time

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

# Knapsack problem

## 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.

# Traveling salesman problem

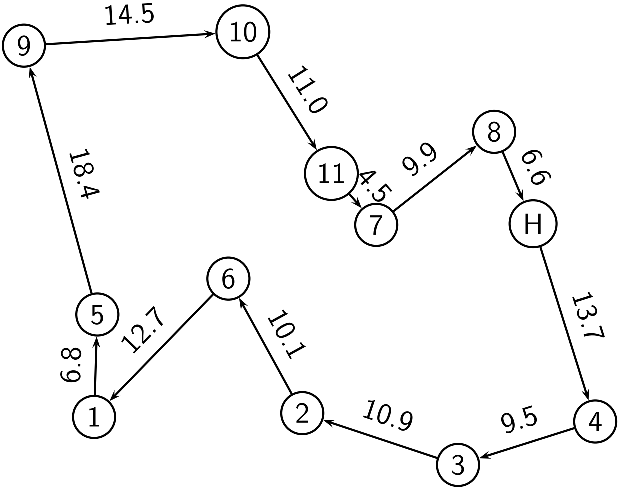
## Python code

```
fstar = np.inf
xstar = None
for t in itertools.permutations(names[1:]):
    tour = ['0']+list(t)
    tl = tsp.tourLength(tour)
    if tl < fstar:
        xstar = tour
        fstar = tl
```

## TSP with 12 cities

- $11! = 39916800$ permutations.
- Running time: about 5 minutes.
- Solution: H–4–3–2–6–1–5–9–10–11–7–8
- Tour length: 128.762

# Optimal solution




Length : 128.762

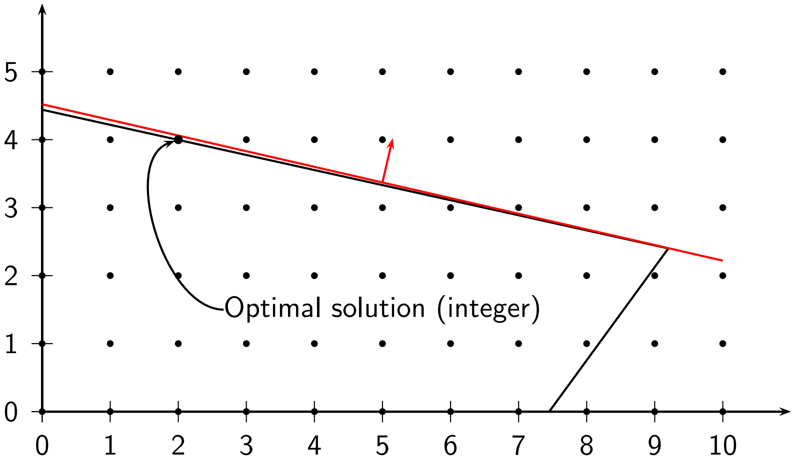
# Integer optimization

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

subject to

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

# Feasible set: 36 solutions



# Brute force algorithm

## Comments

- Very simple to implement.
- Works only for small instances.
- Curse of dimensionality.
- Running time increases exponentially with the size of the problem.
- Not a reasonable option.

# Outline

# 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.
- Used to generate initial solutions.

# The knapsack problem

### Greedy heuristic

- 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 knapsack problem

| Item | Utility | Weight | Ratio |
|---|---|---|---|
| 1 | 80 | 84 | 0.952 |
| 2 | 31 | 27 | 1.148 |
| 3 | 48 | 47 | 1.021 |
| 4 | 17 | 22 | 0.773 |
| 5 | 27 | 21 | 1.286 |
| 6 | 84 | 96 | 0.875 |
| 7 | 34 | 42 | 0.810 |
| 8 | 39 | 46 | 0.848 |
| 9 | 46 | 54 | 0.852 |
| 10 | 58 | 53 | 1.094 |
| 11 | 23 | 32 | 0.719 |
| 12 | 67 | 78 | 0.859 |

# The knapsack problem

| Item | Utility | Weight | Ratio | Order | Remaining capacity |
|---|---|---|---|---|---|
| 1 | 80 | 84 | 0.952 | 5 | 68 |
| 2 | 31 | 27 | 1.148 | 2 | 252 |
| 3 | 48 | 47 | 1.021 | 4 | 152 |
| 4 | 17 | 22 | 0.773 | | |
| 5 | 27 | 21 | 1.286 | 1 | 279 |
| 6 | 84 | 96 | 0.875 | 6 | -28 |
| 7 | 34 | 42 | 0.810 | | |
| 8 | 39 | 46 | 0.848 | | |
| 9 | 46 | 54 | 0.852 | | |
| 10 | 58 | 53 | 1.094 | 3 | 199 |
| 11 | 23 | 32 | 0.719 | | |
| 12 | 67 | 78 | 0.859 | | |

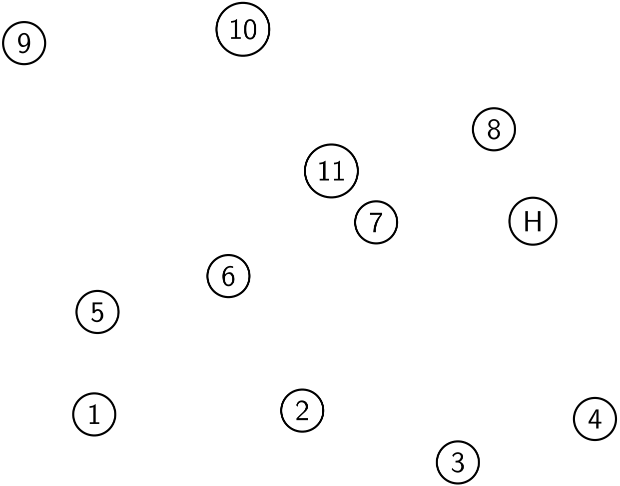
Utility: 244 (Opt: 300). Weight: 232.

# The traveling salesman problem

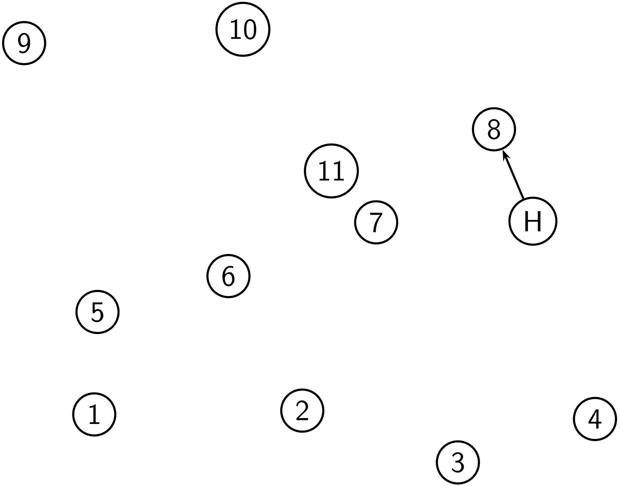
## Greedy heuristic

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

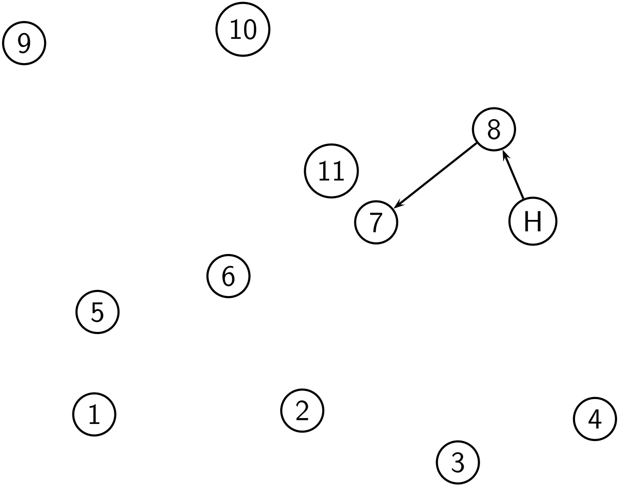
# TSP: 12 cities



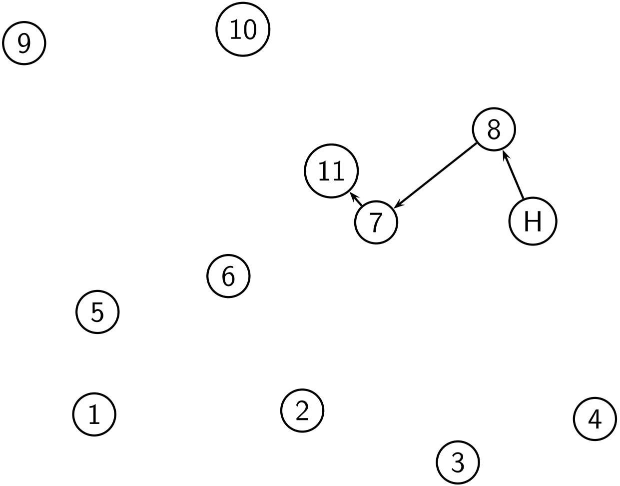
# TSP: 12 cities



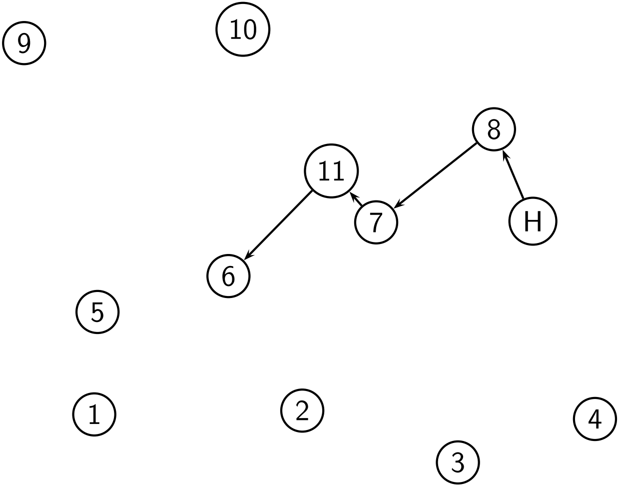
# TSP: 12 cities



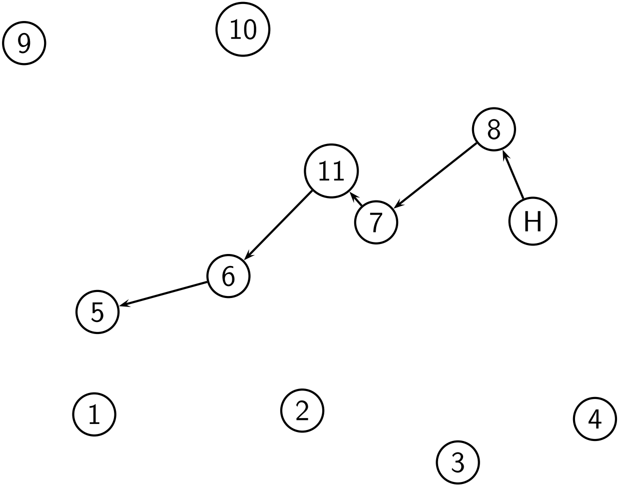
# TSP: 12 cities



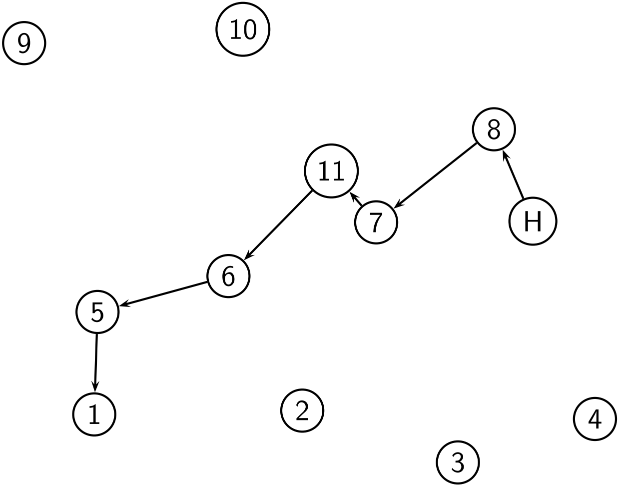
# TSP: 12 cities



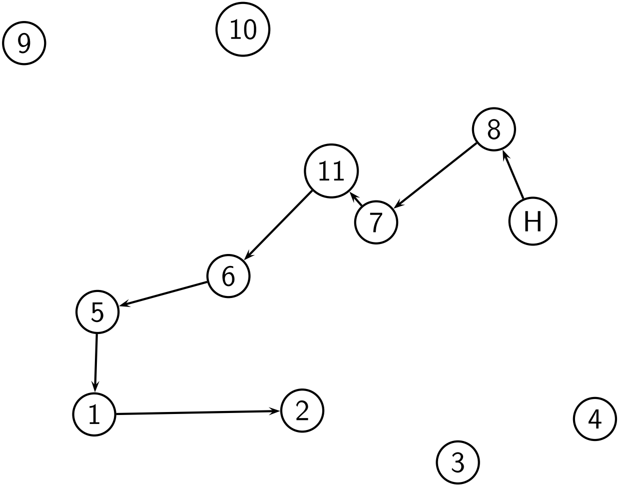
# TSP: 12 cities



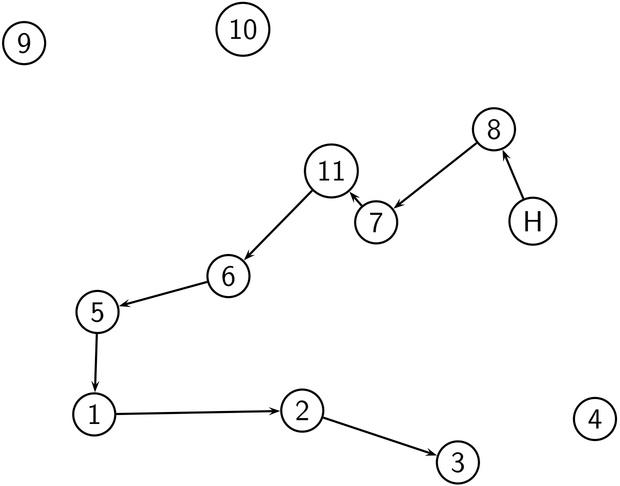
# TSP: 12 cities



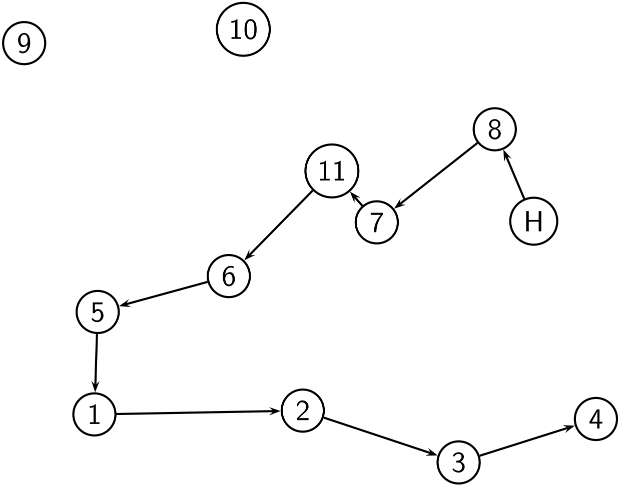
# TSP: 12 cities



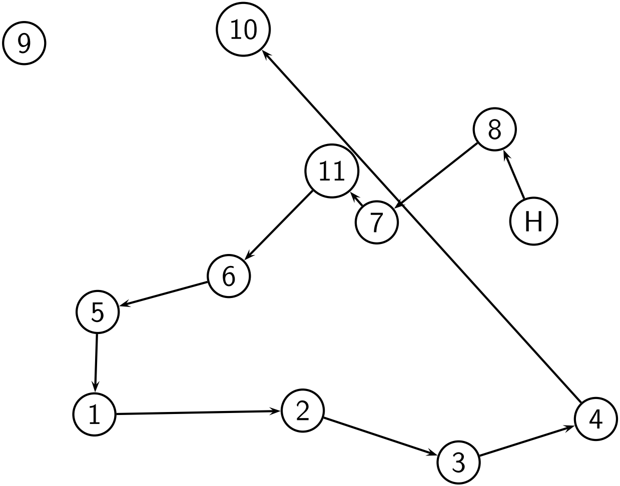
# TSP: 12 cities



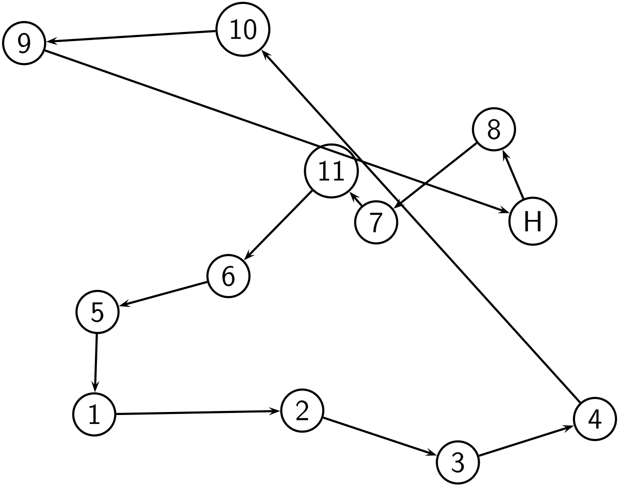
# TSP: 12 cities



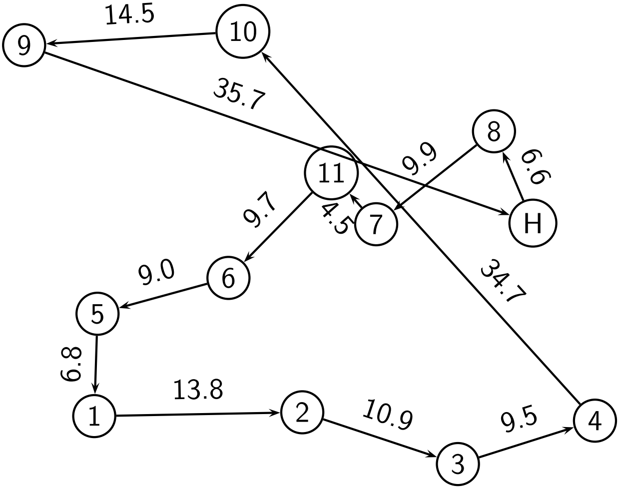
# TSP: 12 cities



# TSP: 12 cities



# TSP: 12 cities




Length: 165.6 [Optimal: 128.762]

# Integer optimization

### Intuitive approach

- Solve the continuous relaxation.
- Round the solution.

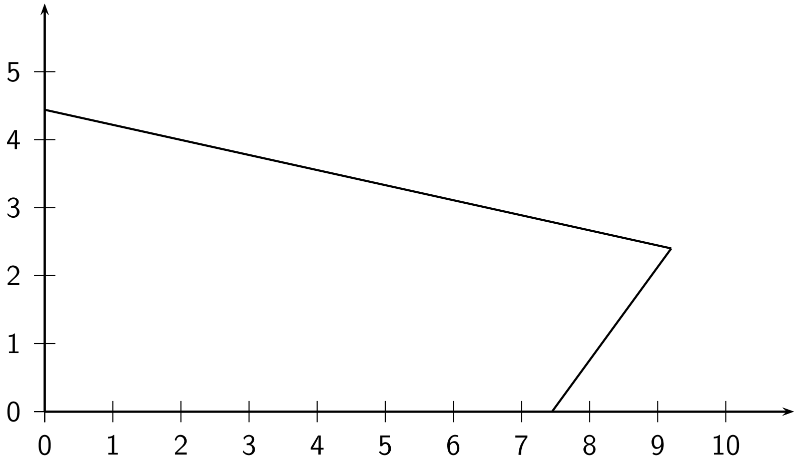
# Example

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

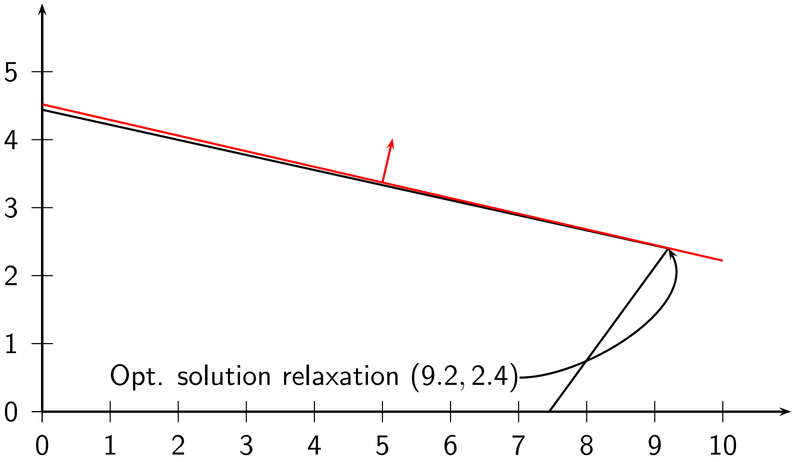
subject to

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

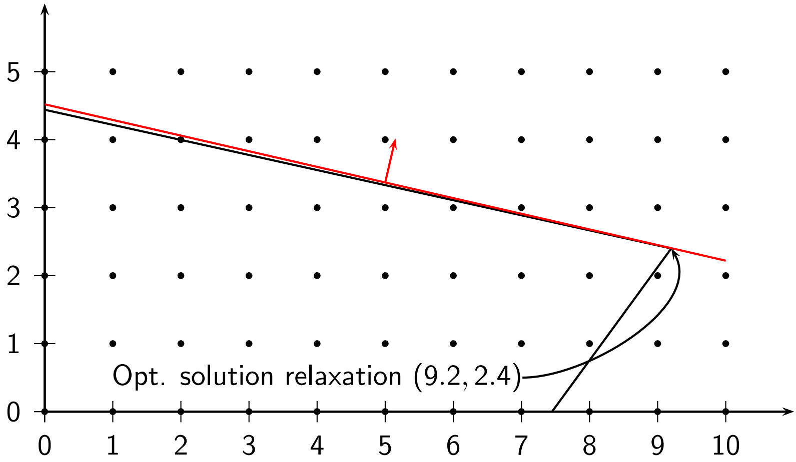
# Relaxation: feasible set



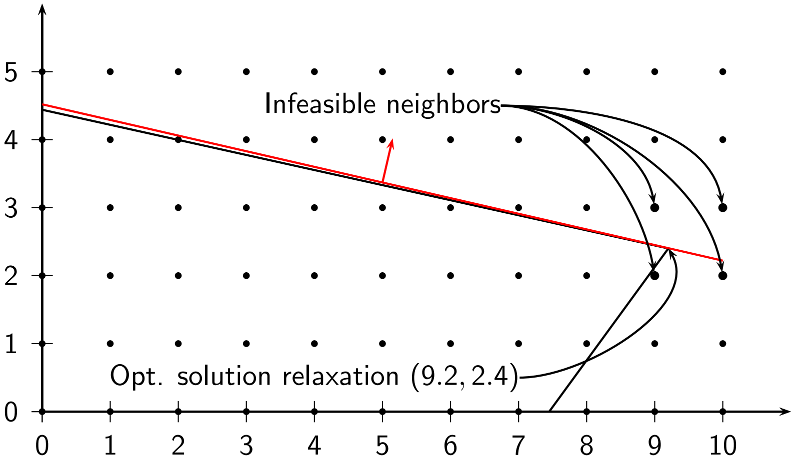
# Optimal solution of the relaxation



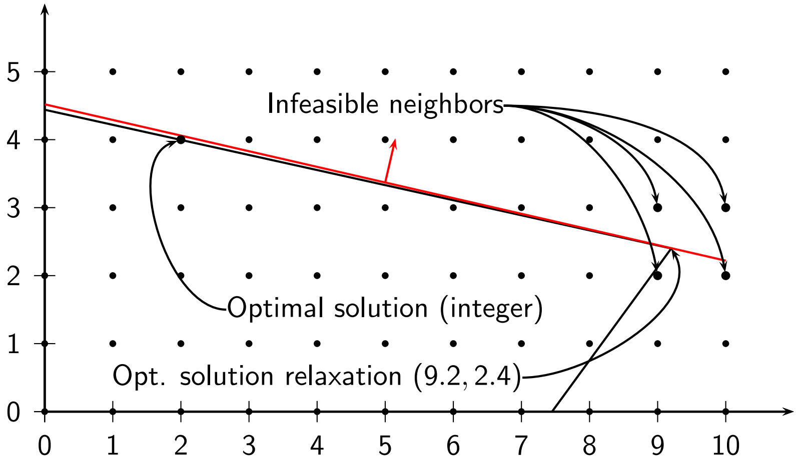
# Integrality constraints



# 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.

# Greedy heuristics

## Comments

- Fast.
- Easy to implement.
- Useful to find an initial solution.
- Feasibility is usually the main issue (rounding issues with ILP).

# Outline

1. Motivation
2. Classical problems
3. Algorithms
   - Brute force
   - Greedy heuristics
   - Exploration
   - Intensification
   - Diversification
4. Summary

# Heuristics: general framework

**Exploration**

Neighborhood

**Intensification**

Local search

**Diversification**

Escape from local minima

# Neighborhood

## Concept

- The feasible set is too large.
- We need to explore it in a smart way.
- Idea: at each iteration, restrict the optimization problem to a small feasible subset that can be enumerated.
- The small subset is called a *neighborhood*.
- It is a sorted list of solutions.
- Ideally, all these solutions must be feasible.
- Neighborhoods can be constructed incrementally during the algorithms.

# Neighborhood types

## Fundamental neighborhood structure

- Obtained from simple modifications of the current solution.
- These modifications must be designed based on the properties of the problem.

## Shuffled neighborhood structure

- Obtained from shuffling the solutions from another neighborhood.
- The shuffling can be deterministic or random.

## Feasible neighborhood structure

- Useful when a potential neighborhood structure contains infeasible solutions.
- Feasibility checks can also be done while generating the neighbors.

# Neighborhood types

### Truncated neighborhood structure

- Useful when a potential neighborhood structure is too large.
- The size of the neighborhood is controlled.

### Combined neighborhood structure

- Union, intersection, or any combination of other structures.
- Use building blocks to construct more complex structures.

# Neighborhoods

## Important properties

- Neighborhood structures are used to explore the solution space.
- Algorithms will move from $x$ to an element of $V(x)$.
- They can be seen as "vehicles".
- Symmetry: it is good practice to use symmetric neighborhoods:

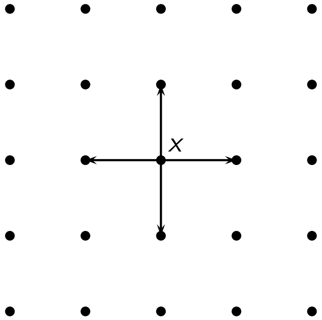
$$y \in V(x) \Longleftrightarrow x \in V(y).$$

- Reachability: a neighborhood $V$ must be rich enough to reach any feasible solution, from another feasible solution. For each $x_1, x_K \in \mathcal{U}$, there exists a sequence $x_2, \ldots, x_{K-1} \in \mathcal{U}$ such that

$$x_{k+1} \in V(x_k),\ k = 1, \ldots, K-1.$$

- Analogy with Markov chains: irreducibility.

# Integer optimization



# Integer optimization

- 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

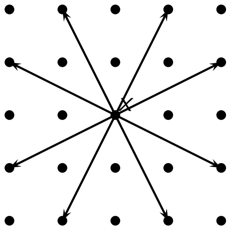
$$x = (3, 5, 2, 8) \quad y^{2+} = (3, 6, 2, 8) \quad y^{2-} = (3, 4, 2, 8)$$

- Size of the neighborhood: $2n$.
- Feasibility should also be enforced.
- If $n$ is large, truncation may be useful.
- The order is arbitrary, but must be specified.
- Shuffling may be useful.

# Integer optimization

## Creativity

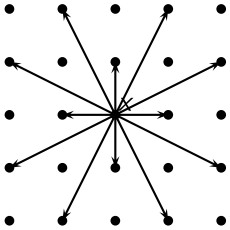
- The concept of neighborhood is fairly general.
- It must be defined based on the structure of the problem.
- Creativity is required here.



# Integer optimization

## Combinations

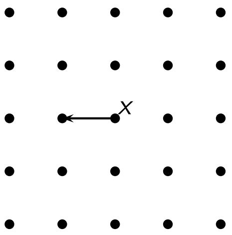
- Combining neighborhoods is easy.
- Trade-off between flexibility and complexity.



# Integer optimization

## Properties

- Verify the properties.
- Symmetry and reachability.



# The knapsack problem

## Fundamental 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).
- Order: based on the utility/weight ratio, for instance.

# The knapsack problem

## Truncated 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.
- Useful to truncate to $M$.
- Size of the neighborhood:

$$\min\left(\frac{n!}{k!(n-k)!}, M\right).$$

# Python code

```
def neighborhood(sack, size = 1, random = True, truncated = None):
    n = len(sack)
    combinations = np.array(list(itertools.combinations(range(n), size)))
    if random:
        np.random.shuffle(combinations)
    if truncated is not None:
        combinations = combinations[:truncated]
    theNeighborhood = []
    for c in combinations:
        s = np.array(sack)
        s[c] = 1 - sack[c]
        theNeighborhood.append(s)
    return theNeighborhood
```

# Traveling salesman problem

## 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

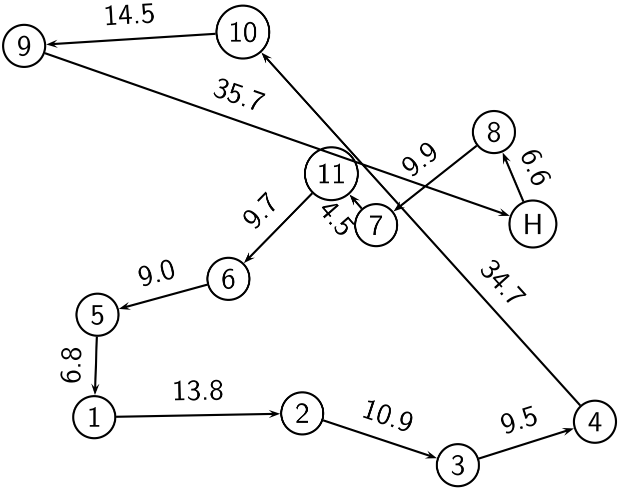
A–B–G–F–E–D–C–H–A.

# Traveling salesman problem

Example: 2-OPT(1,9)

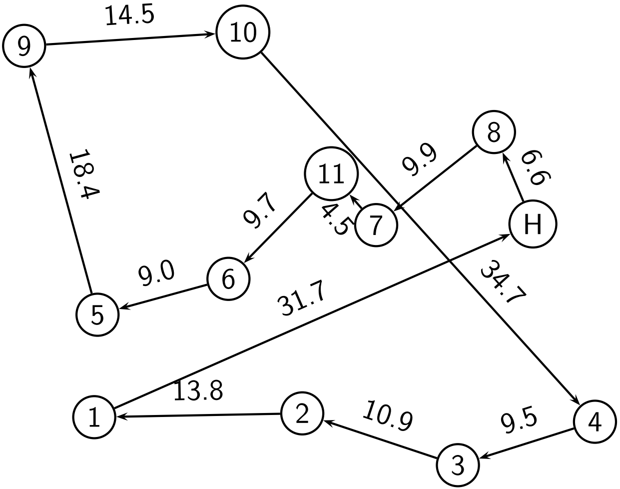
- Try to improve the solution using 2-OPT swapping 1 and 9.
- Before: H–8–7–11–6–5–1–2–3–4–10–9–H (length: 165.6)
- After : H–8–7–11–6–5–9–10–4–3–2–1–H (length: 173.3)
- No improvement.

# Neighborhood: 2-OPT(1,9)




Length: 165.6

# Neighborhood: 2-OPT(1,9)




Length: 173.3

# Exploration

## Comments

- Design of "vehicles" to explore the solution space.
- Fundamental neighborhoods exploit the structure of the problem.
- Various operations allow to modify and combine neighborhoods.
- Trade-off between flexibility and complexity.
- 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.

# Outline

# Local search: version one

- Consider the combinatorial optimization problem

$$\min f(x)$$

subject to

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

- Consider the neighborhood structure $V(x)$, where $V(x)$ is the set of feasible 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: version two

- Consider the combinatorial optimization problem

$$\min f(x)$$

subject to

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

- Consider the neighborhood structure $V(x)$, where $V(x)$ is the set of neighbors of $x$.
- At each iteration $k$, find $y$ such that

$$f(y) \leq f(x_k), \ \forall y \in V(x_k).$$

- If $f(y) = f(x_k)$, $x_k$ is a local minimum. Stop.
- Otherwise, proceed to the next iteration.

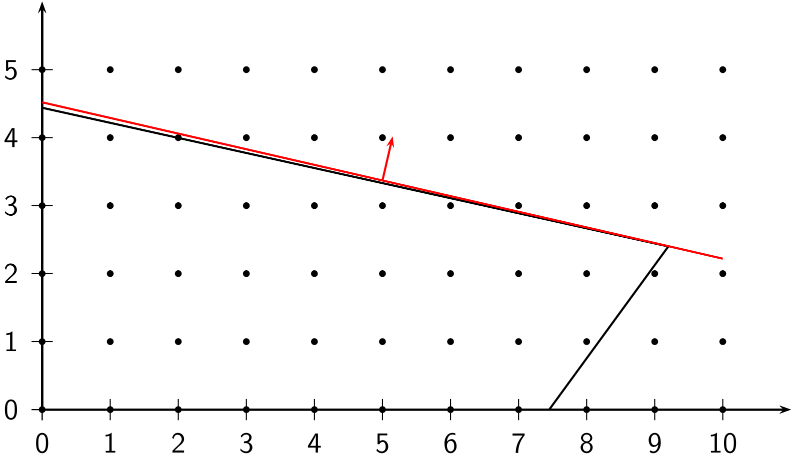
# Local search: example

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

subject to

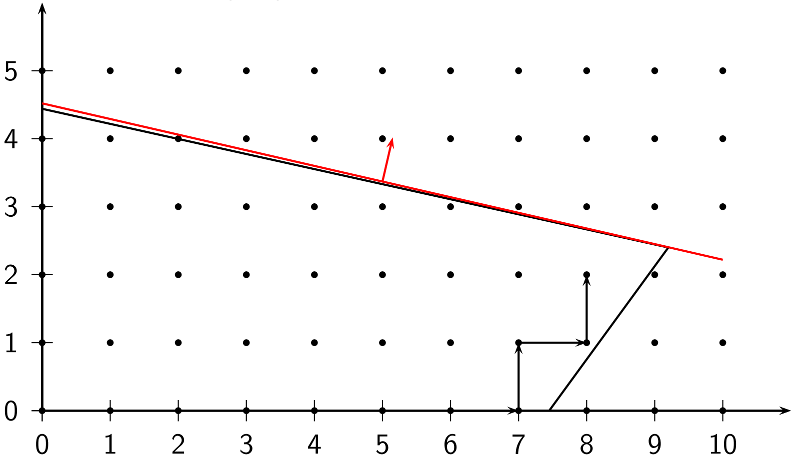
$$\begin{array}{rcl} 2x_1 + 9x_2 & \leq & 40 \\ 11x_1 - 8x_2 & \leq & 82 \\ x_1, x_2 & \in & \mathbb{N} \end{array}$$

# Local search: example



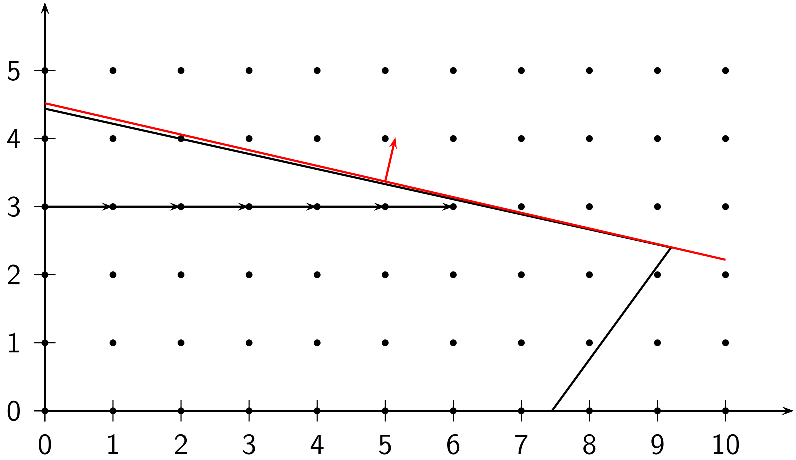
# Local search: example

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



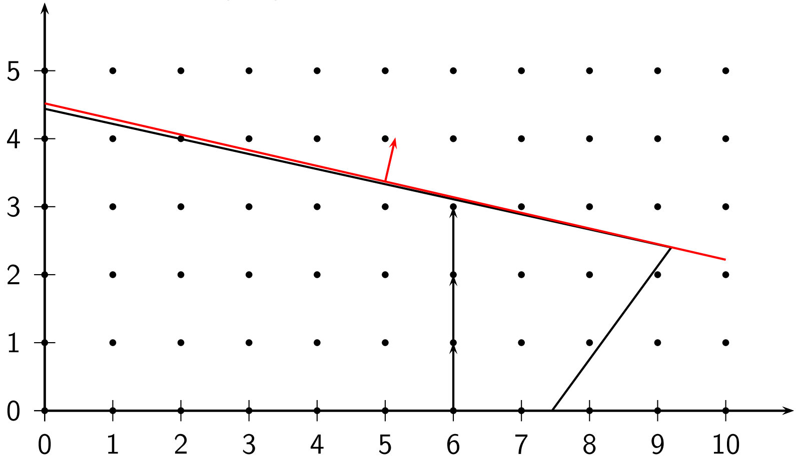
# Local search: example

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



# Local search: example

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



# The knapsack problem

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

subject to

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

# The knapsack problem

```
def localSearch(u, w, capacity, initSolution, neighborhood):
    x = initSolution
    ux = np.inner(u, x)
    wx = np.inner(w, x)
    if wx > capacity:
        Exception(f'Infeasible weight {wx} > {capacity}')
    localOptimum = False
    while not localOptimum:
        neighbors = neighborhood(x)
        localOptimum = True
        for y in neighbors:
            wy = np.inner(w, y)
            if wy <= capacity:
                uy = np.inner(u, y)
                if uy > ux:
                    localOptimum = False
                    x = y
                    ux = uy
                    wx = wy
```

# The knapsack problem

```
def neighborhood1(sack):
    return neighborhood(sack, size = 1, random = False, truncated = None)
firstSack = np.array([0]*n)

localSearch(utility, weight, capacity, firstSack, neighborhood1)
First sack: [0 0 0 0 0 0 0 0 0 0 0 0] U=0 W=0
New sack  : [1 0 0 0 0 0 0 0 0 0 0 0] U=80 W=84
New sack  : [0 0 0 0 0 1 0 0 0 0 0 0] U=84 W=96
New sack  : [1 0 0 0 0 1 0 0 0 0 0 0] U=164 W=180
New sack  : [1 1 0 0 0 1 0 0 0 0 0 0] U=195 W=207
New sack  : [1 0 1 0 0 1 0 0 0 0 0 0] U=212 W=227
New sack  : [1 0 0 0 0 1 0 0 0 1 0 0] U=222 W=233
New sack  : [1 0 0 0 0 1 0 0 0 0 0 1] U=231 W=258
New sack  : [1 1 0 0 0 1 0 0 0 0 0 1] U=262 W=285
New sack  : [1 0 0 0 0 1 1 0 0 0 0 1] U=265 W=300
```

# The knapsack problem

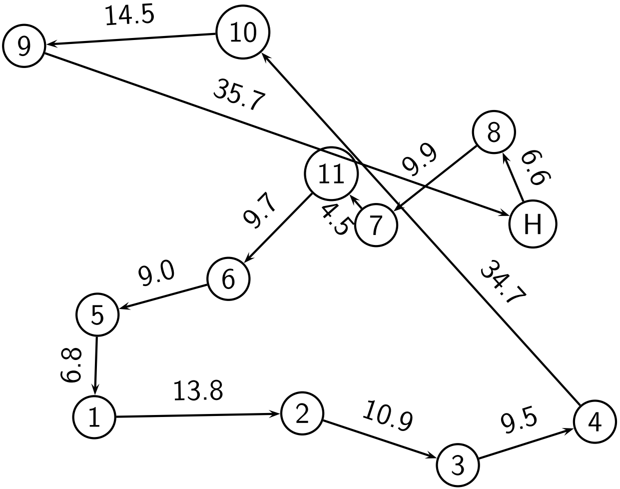
```
def neighborhood2(sack):
    return neighborhood(sack, size = 3, random = False, truncated = None)

firstSack = np.array([0]*n)
localSearch(utility, weight, capacity, firstSack, neighborhood2)
First sack: [0 0 0 0 0 0 0 0 0 0 0 0] U=0 W=0
New sack  : [1 1 1 0 0 0 0 0 0 0 0 0] U=159 W=158
New sack  : [1 1 0 0 0 1 0 0 0 0 0 0] U=195 W=207
New sack  : [1 0 1 0 0 1 0 0 0 0 0 0] U=212 W=227
New sack  : [1 0 0 0 0 1 0 0 0 1 0 0] U=222 W=233
New sack  : [1 0 0 0 0 1 0 0 0 0 0 1] U=231 W=258
New sack  : [0 1 0 0 0 1 0 0 0 1 0 1] U=240 W=254
New sack  : [0 0 1 0 0 1 0 0 1 0 0 1] U=245 W=275
New sack  : [0 0 1 0 0 1 0 0 0 1 0 1] U=257 W=274
New sack  : [1 0 1 0 0 1 0 0 1 0 0 0] U=258 W=281
New sack  : [1 0 1 0 0 1 0 0 0 1 0 0] U=270 W=280
New sack  : [0 0 1 1 0 1 0 0 0 1 0 1] U=274 W=296
New sack  : [0 0 1 0 1 1 0 0 0 1 0 1] U=284 W=295
New sack  : [1 0 0 0 1 1 0 1 0 1 0 0] U=288 W=300
```

# Traveling salesman problem

**Procedure**

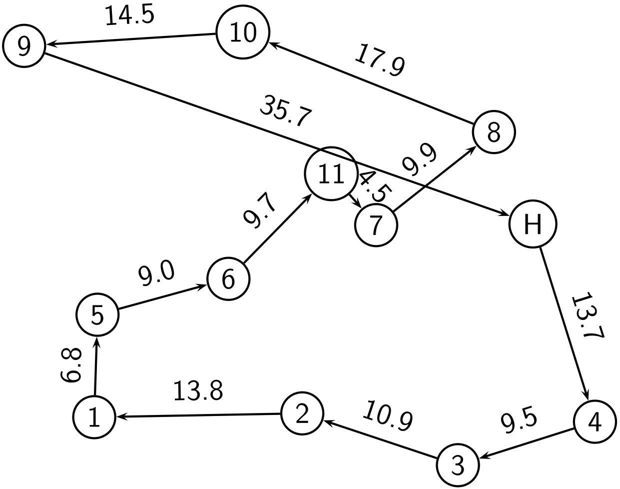
- Start with the outcome of the greedy algorithm.
- Use the 2-OPT neighborhood.
- Use version two of the local search.

# Current tour



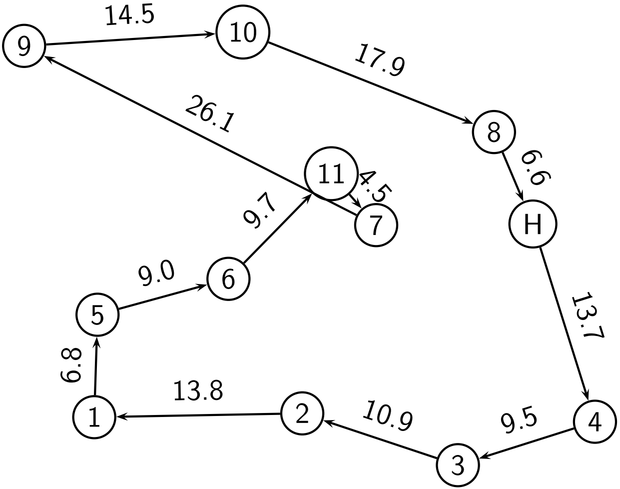

Length: 165.6

# Best neighbor: 2-OPT(8,4)



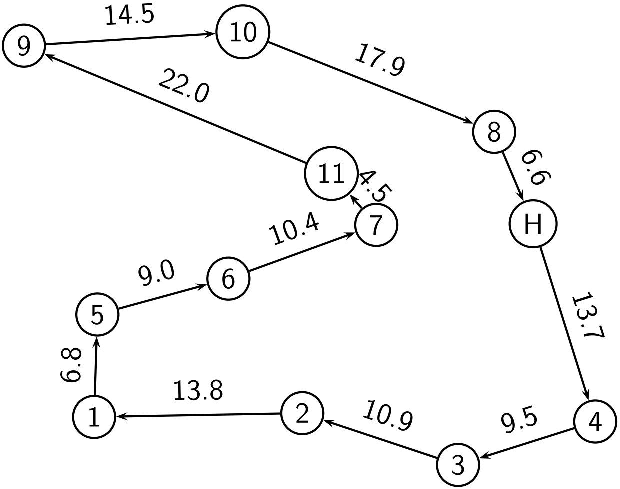

Length: 155.8

# Best neighbor: 2-OPT(8,9)



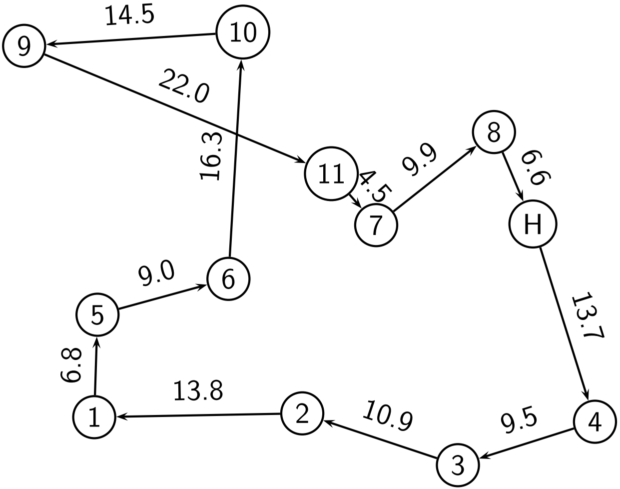

Length: 143.0

# Best neighbor: 2-OPT(11,7)



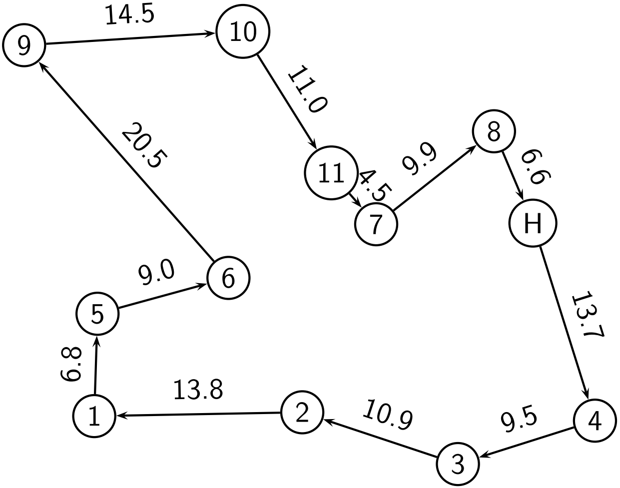

Length: 139.5

# Best neighbor: 2-OPT(7,10)




Length: 137.5

# Best neighbor: 2-OPT(10,9)




Length: 130.7 [Opt: 128.762]

# 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.
- Several variants are possible.

# Outline

1. Motivation
2. Classical problems
3. Algorithms
   - Brute force
   - Greedy heuristics
   - Exploration
   - Intensification
   - Diversification
4. Summary

# Changing the starting point

### Idea

- Launch the local search from several starting points.
- Select the best local optimum.

### Issues

- Feasibility.
- Same local optimum may be generated many times.
- Shooting in the dark.

# 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 $V_k$

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

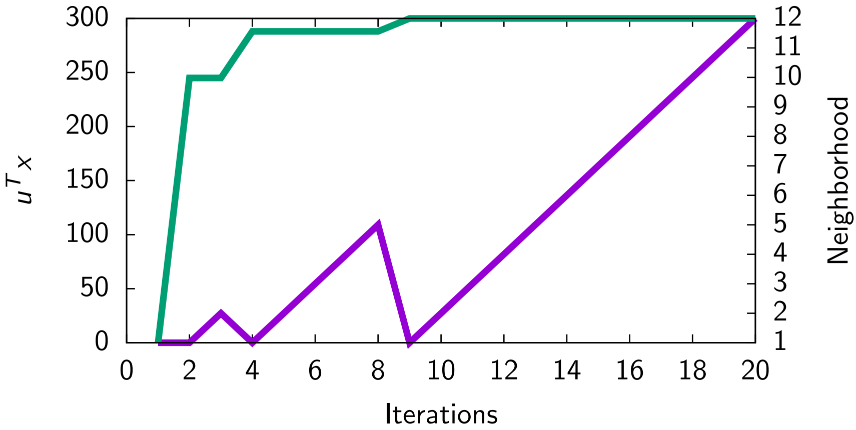
- If $f(x^+) < f(x_c)$, then $x_c \leftarrow x^+$, $k \leftarrow 1$.
- Otherwise, $k \leftarrow k + 1$.

**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 $x_c \leftarrow x^+$

# 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

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

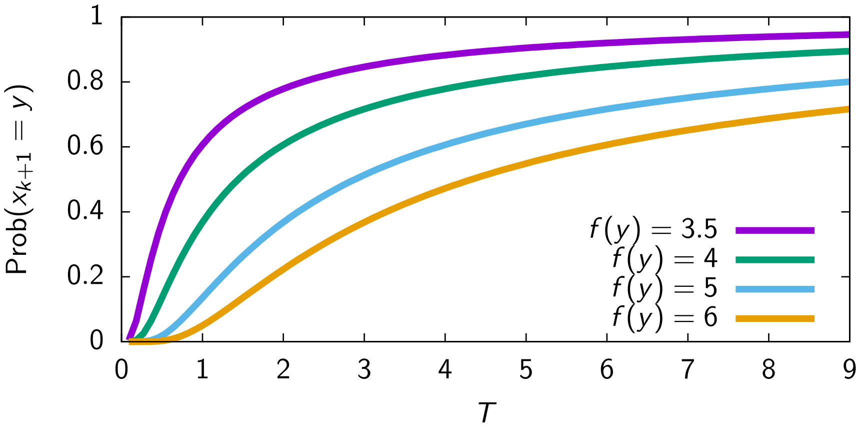
# Simulated annealing

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

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

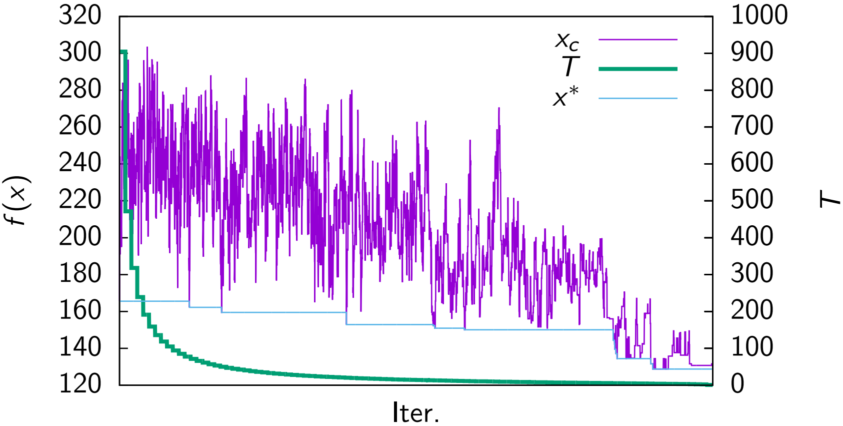
# Simulated annealing

Repeat $k \leftarrow 1$

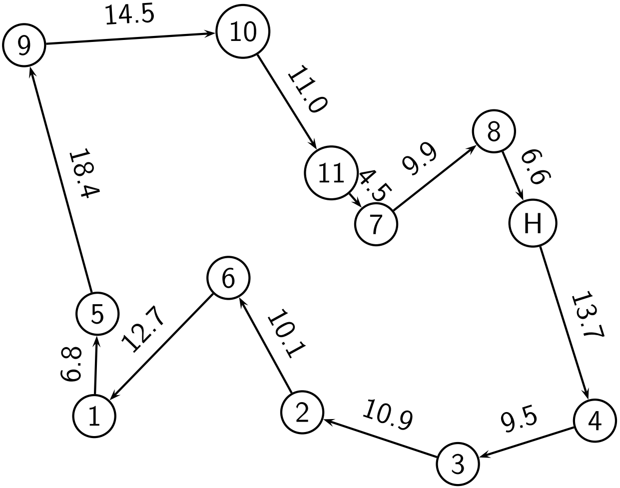
- While $k < K$
  - Randomly select a neighbor $y \in V(x_c)$
  - $\delta \leftarrow f(y) - f(x_c)$
  - If $\delta < 0$, $x_c = y$.
  - Otherwise, draw $r$ between 0 and 1
    - If $r < exp(-\delta/T)$, then $x_c = y$
  - If $f(x_c) < f(x^*)$, $x^* = x_c$.
  - $k \leftarrow k + 1$
- Reduce $T$

Until $T \leq T_f$

# Example: traveling salesman problem



# Best solution found




Length : 128.8 [Optimal!]

# Practical comments

- Parameters must be tuned.
- In particular, the reduction rate of the temperature must be specified.
  - Let $\delta_t$ 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 $m = 0, \ldots, M$,

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

# Comments

How to avoid being blocked in local minimum?

- Apply an algorithm from multiple starting points.
    - How to find feasible starting point?
    - How to avoid shooting in the dark?
- Change the structure of the neighborhood: variable neighborhood search
    - How to choose the neighborhood structures?
- 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?

# Outline

# Combinatorial optimization

### Chacteristics

- $f$ and $\mathcal{U}$ have no specific property.
- $f$ is a black box.
- $\mathcal{U}$ is a finite set of valid configurations.
- No optimality condition is available.

# Optimization methods

## Exact methods (branch and bound)

- Finds the optimal solution.
- Suffers from the curse of dimensionality.
- Requires the availability of valid and tight bounds.

## Approximation algorithms

- Finds a sub-optimal solution.
- Guarantees a bound on the quality of the solution.
- Mainly used for theoretical purposes.

## Heuristics

- Smart exploration of the solution space.
- No guarantee about optimality.
- Few assumptions about the problem.

# Heuristics: general framework

**Exploration**

Neighborhood

**Intensification**

Local search

**Diversification**

Escape from local minima

# 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.