Optimization and Simulation

Optimization

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Outline

Optimization

Procedure

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

Optimization

Mathematical modeling

- Decision variables x.
- Objective function f.
- Constraints $\mathcal{F}$.

Optimization problem

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

subject to

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

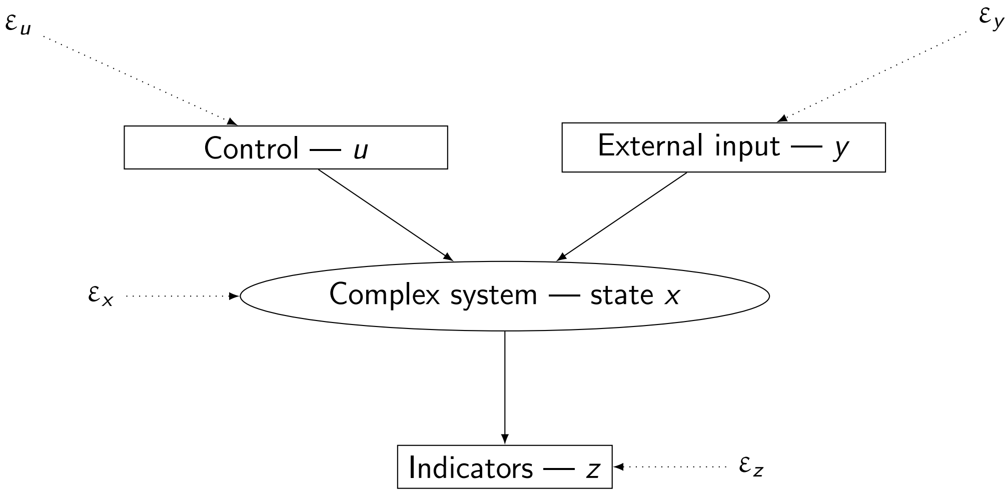
Optimization

Selection of an algorithm

- **Problem class:** linear / convex / mixed-integer / black-box.
- **Available structure:** derivatives, convexity, integrality, decomposability.
- **Computational budget:** cheap objective vs expensive simulation.
- **Desired guarantee:** exact optimum vs good feasible solution.

Simulation

$$Z = h(X, Y, U; \widehat{\theta}) + \varepsilon_z$$



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:

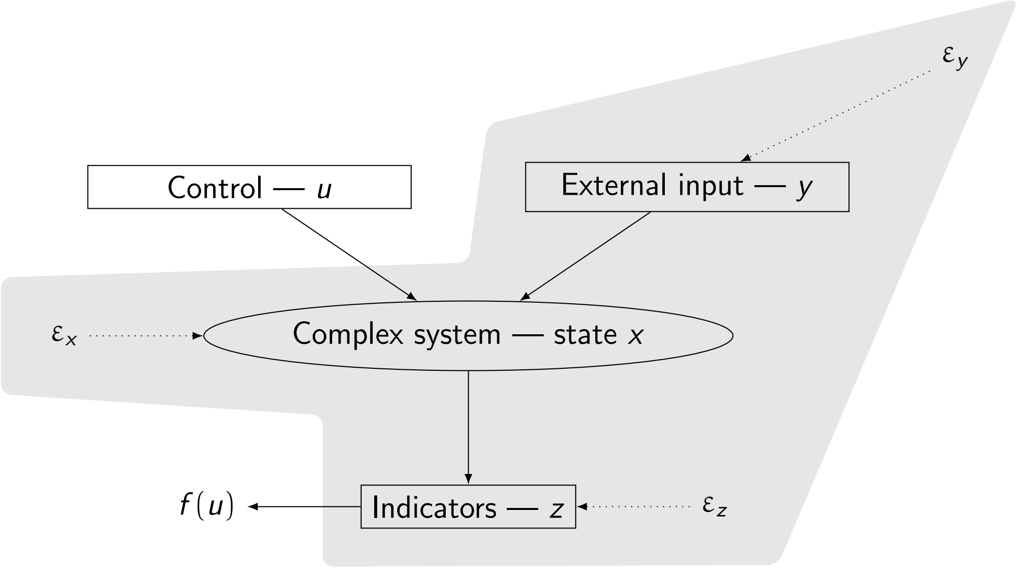
$$f(u) = g(z_1(u), \ldots, z_m(u))$$

General framework: example

Pavel at Satellite

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

Deterministic vs simulation-based objective

Deterministic optimization

- The objective can be evaluated exactly: $f(u)$.
- Re-evaluating $f(u)$ returns the same value.
- Comparisons between solutions are unambiguous.

Simulation-based optimization

- The objective is defined as an expectation:

$$f(u) = \mathbb{E}[Z(u)].$$

- It is evaluated using simulation:

$$\widehat{f}(u) \approx f(u).$$

- Each evaluation is noisy: repeated runs give different values.

Coping with Monte Carlo noise

Key difficulty

When $\widehat{f}(u)$ is noisy,

- small differences between solutions may be meaningless,
- comparisons may be unreliable,
- naive optimization can be misled by randomness.

Pragmatic strategies

In practice, one often:

- uses the <u>same random inputs</u> to compare candidate solutions,
- increases the number of simulation runs for promising solutions,
- applies variance reduction techniques,
- relies on algorithms that tolerate noise.

Scope of this lecture

What we do

- Focus on algorithmic ideas for exploring large solution spaces.
- Assume simulation noise is moderate or controlled.
- Use heuristics that are empirically robust to noise.

What we do not cover

- Statistical guarantees for noisy optimization.
- Optimal allocation of simulation budget.
- Formal convergence results for stochastic optimization.

Takeaway

Heuristic optimization and variance reduction are complementary tools for simulation-based problems.

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.
- Designed to mimic manual interventions.

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

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

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

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.

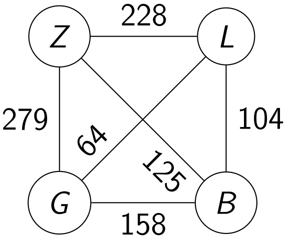
Traveling salesman problem

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

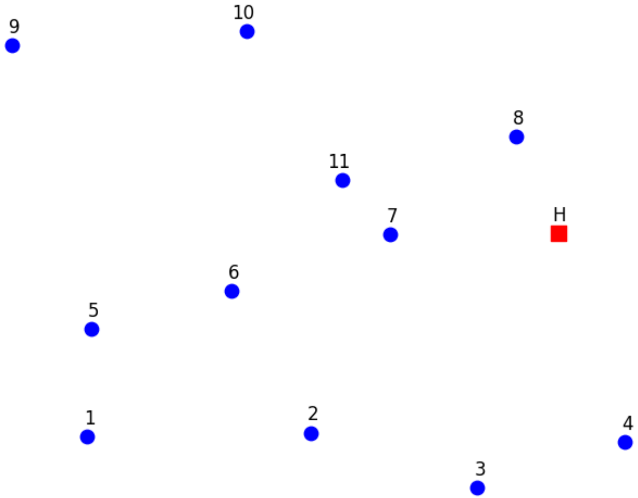


Home town: Lausanne

3 possibilities (+ their symmetric version):

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

$$Ax = b$$

$$x \geqslant 0.$$

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

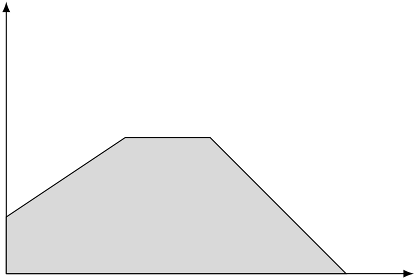
$$Ax = b$$

$$x \in \mathbb{N}.$$

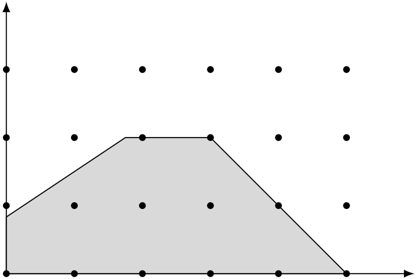
where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$.

Feasible set

Polyhedron



Intersection polyhedron/integer lattice



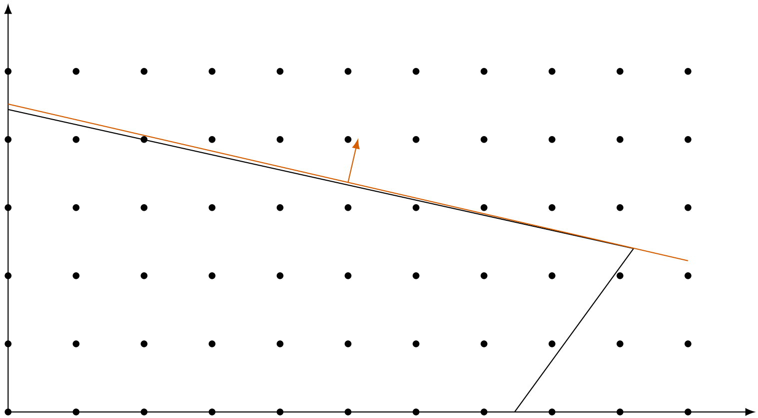
Example

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

subject to

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

Example



Outline

Motivation

Classical problems

Algorithms
- Brute force
- Greedy heuristics
- Exploration
- Intensification
- Diversification

Summary

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

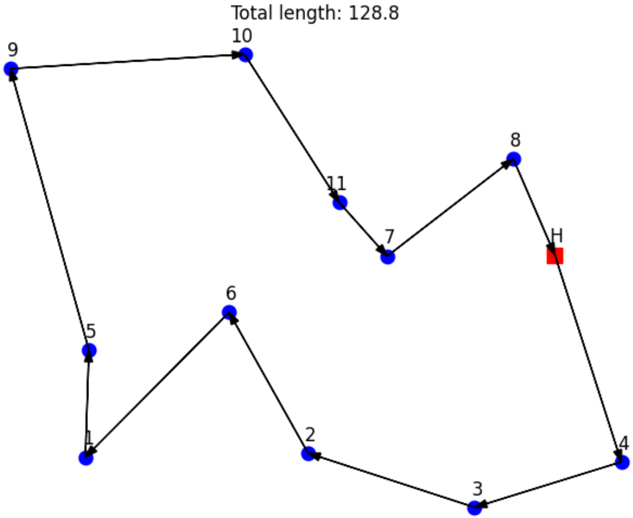
Python code

```
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! = $ 39'916'800 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



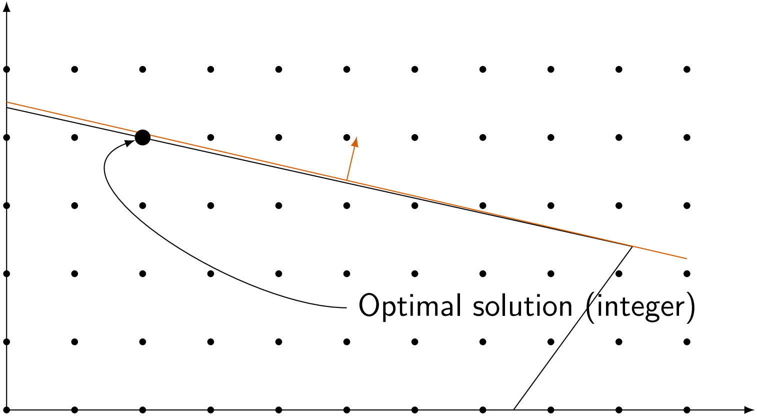
Integer optimization

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

subject to

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

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		

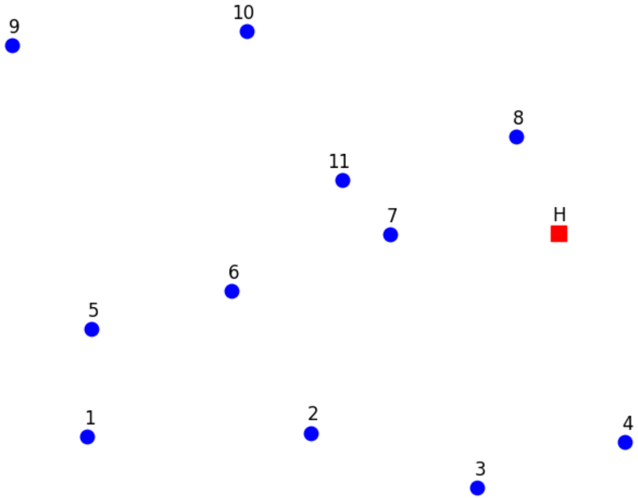
Utility: 244 (Opt: 300). Weight: 232.

The traveling salesman problem

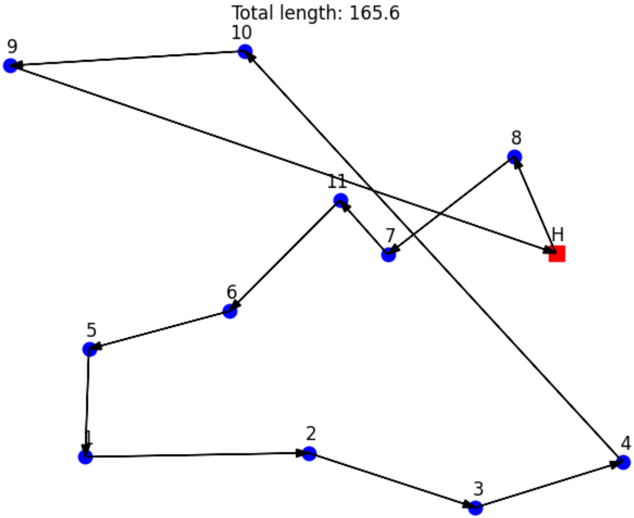
Greedy heuristic

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

TSP: 12 cities



TSP: 12 cities



TSP: 12 cities

Greedy solution

- Easy to generate.
- No combinatorial complexity.
- Not necessarily good.
- Length: 165.6.
- Optimal tour: 128.762.

Integer optimization

Intuitive approach

- Solve the continuous relaxation.
- Round the solution.

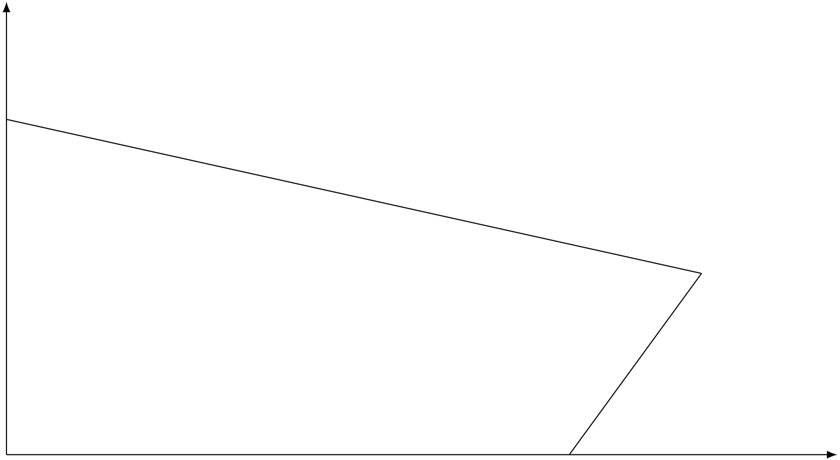
Example

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

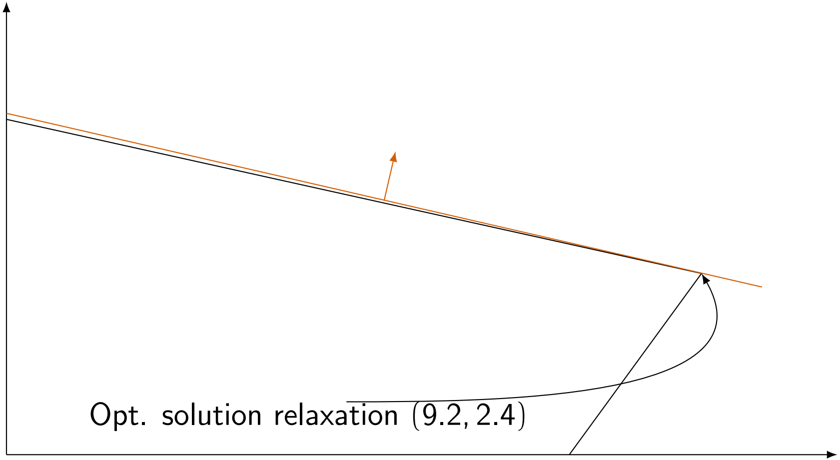
subject to

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

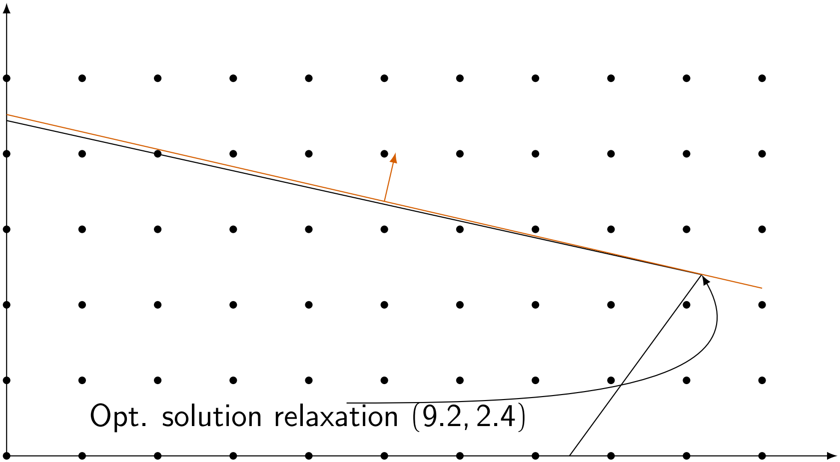
Relaxation: feasible set



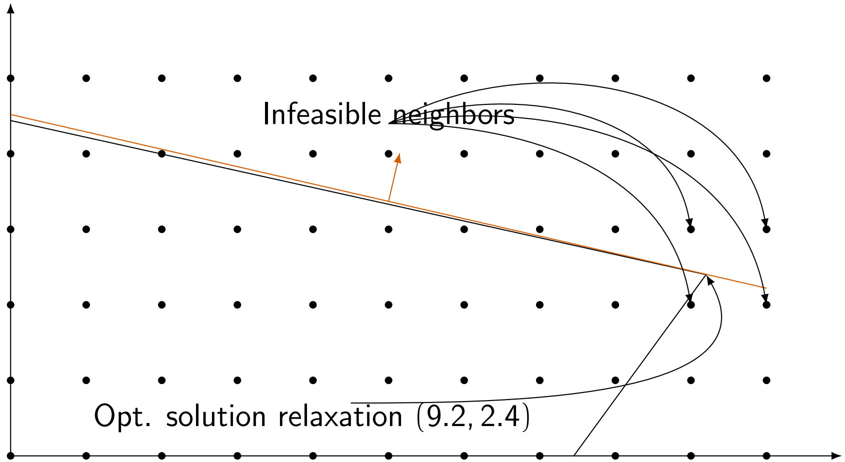
Optimal solution of the relaxation



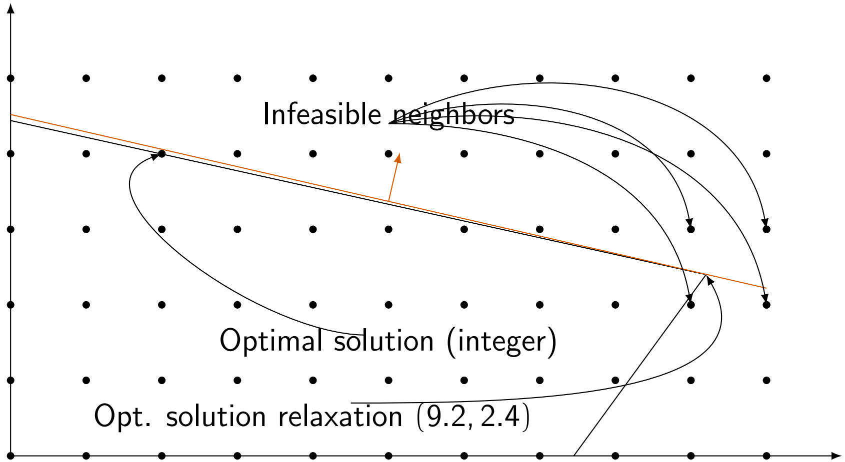
Integrality constraints



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.

Greedy heuristics

Comments

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

Outline

Heuristics: general framework

Exploration

Neighborhood

Intensification

Local search

Diversification

Escape from local minima

Optimization vs sampling: a useful analogy

Sampling (MCMC)

- Goal: explore the state space according to a target distribution.
- Moves are accepted to preserve the stationary distribution.

Optimization (heuristics)

- Goal: explore the same type of space to find low values of $f(x)$.
- Moves are designed to favor improvement, with mechanisms to escape local minima.

Key message

Both rely on neighborhood moves; the difference is whether we aim to sample or to optimize.

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.
- 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:

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

- 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.

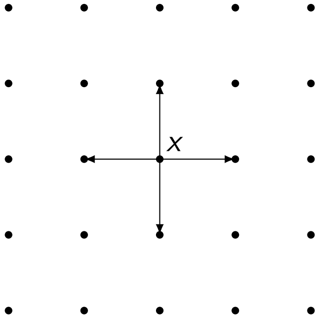
What makes a good neighborhood?

Design checklist

- **Reachability:** can we reach all feasible solutions (in principle)?
- **Feasibility handling:** generate only feasible neighbors or repair/filter infeasible ones.
- **Cost of evaluation:** neighbors should be cheap to evaluate (use incremental updates when possible).
- **Balance:** too small $\Rightarrow$ stuck; too large $\Rightarrow$ expensive enumeration.
- **Symmetry (often useful):**

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

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

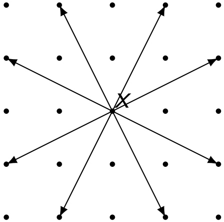
$$x = (3, 5, 2, 8) \quad y^{2+} = (3, 6, 2, 8) \quad y^{2-} = (3, 4, 2, 8)$$

- 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

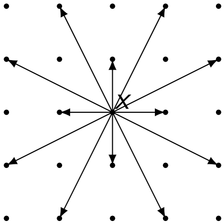
- The concept of neighborhood is fairly general.
- It must be defined based on the structure of the problem.
- Creativity is required here.



Integer optimization

Combinations

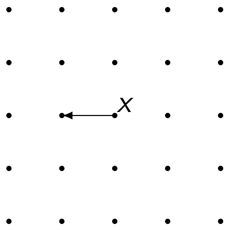
- Combining neighborhoods is easy.
- Trade-off between flexibility and complexity.



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

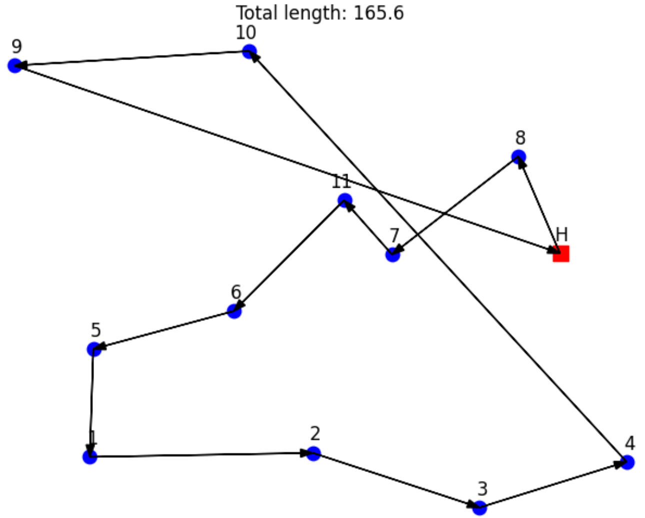
A–B–G–F–E–D–C–H–A.

Traveling salesman problem

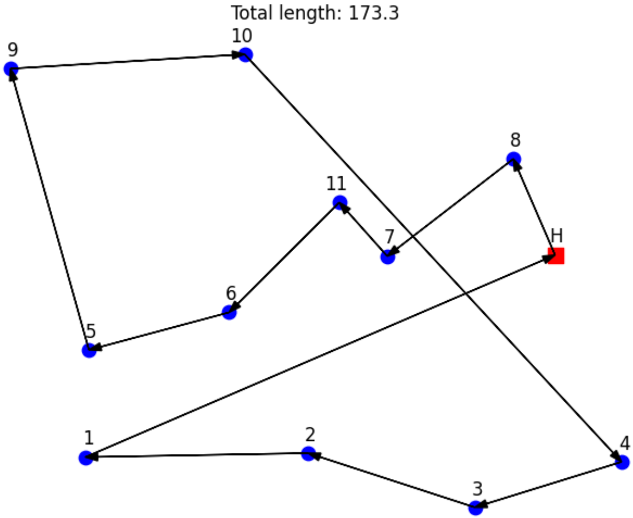
Example: 2-OPT(1,9)

- 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) before



Neighborhood: 2-OPT(1,9) after



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 $f(y) \geqslant f(x_k)$, $\forall y \in V(x_k)$, 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 $V(x)$ (set of neighbors of x).
- At iteration k, select a best neighbor

$$y \in \arg\min_{v \in V(x_k)} f(v).$$

- If $f(y) \geqslant f(x_k)$, then x_k is a local minimum. Stop.
- Otherwise, set $x_{k+1} = y$ and continue.

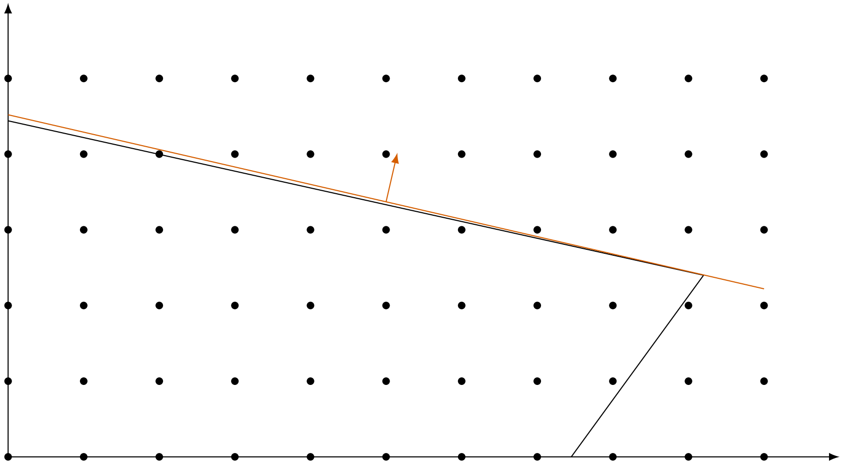
Local search: example

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

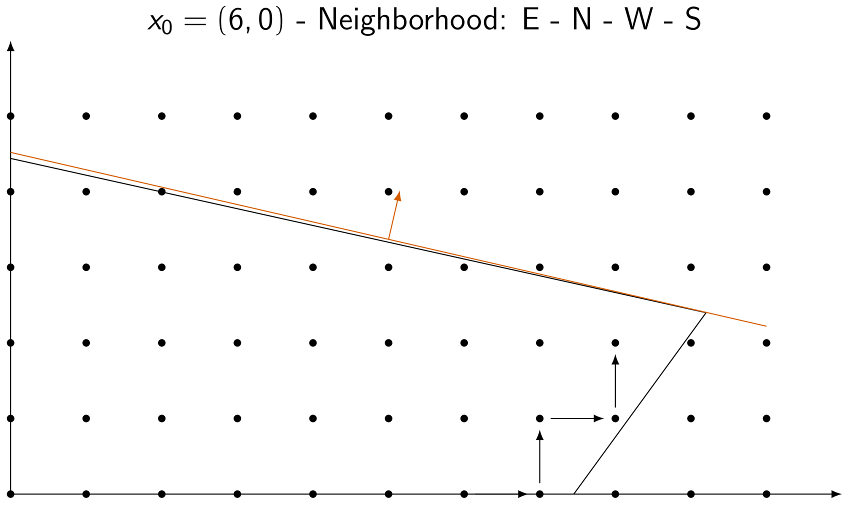
subject to

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

Local search: example

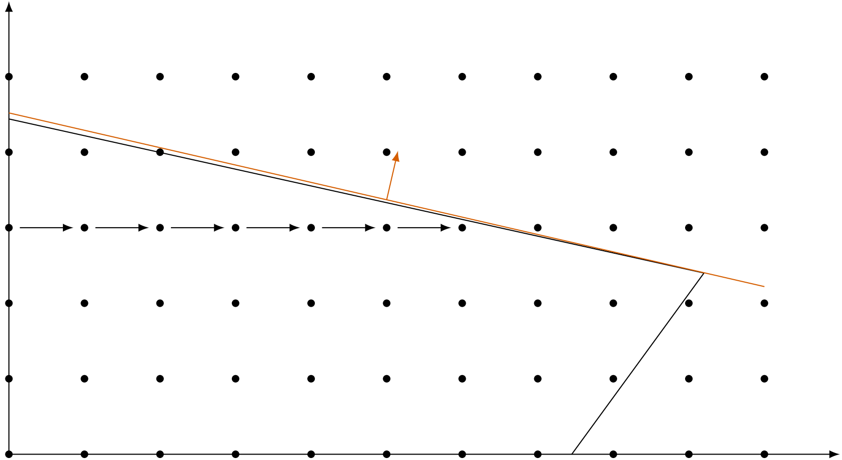


Local search: example



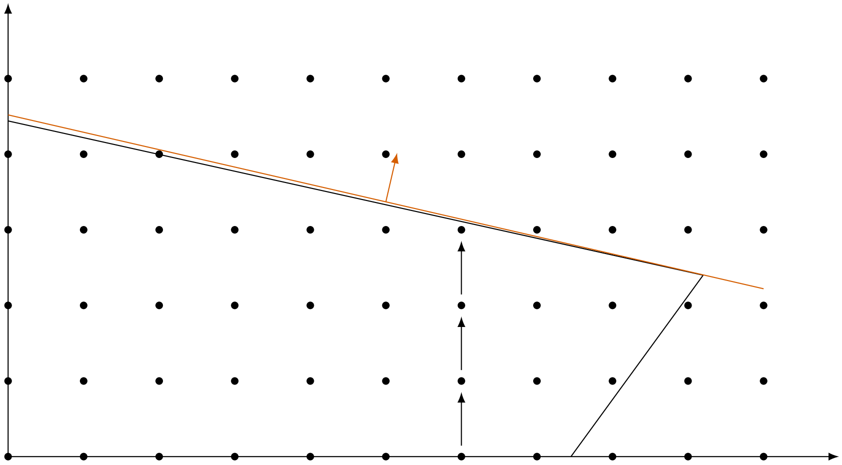
Local search: example

$x_0 = (0, 3)$ - 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

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

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

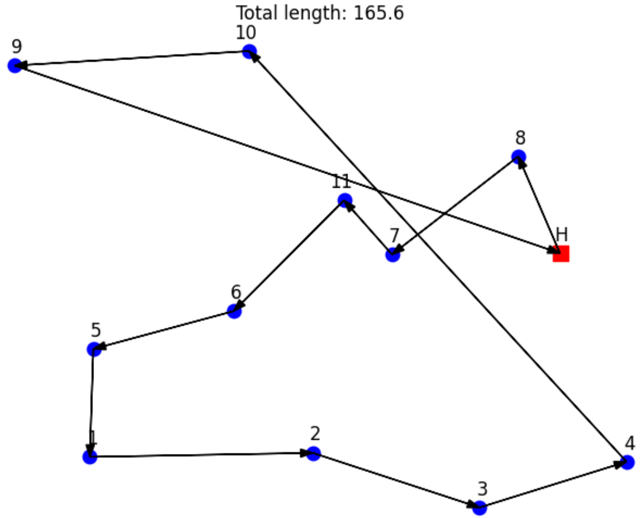
```
def neighborhood2(sack):
    return neighborhood(sack, size = 3, random = False, truncated = None)

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

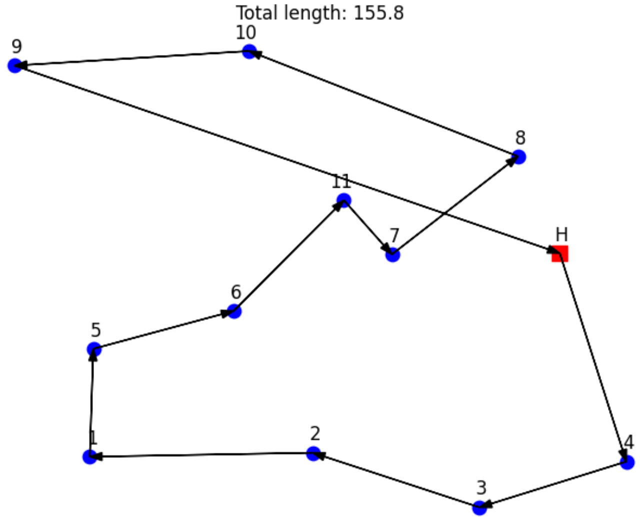
Procedure

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

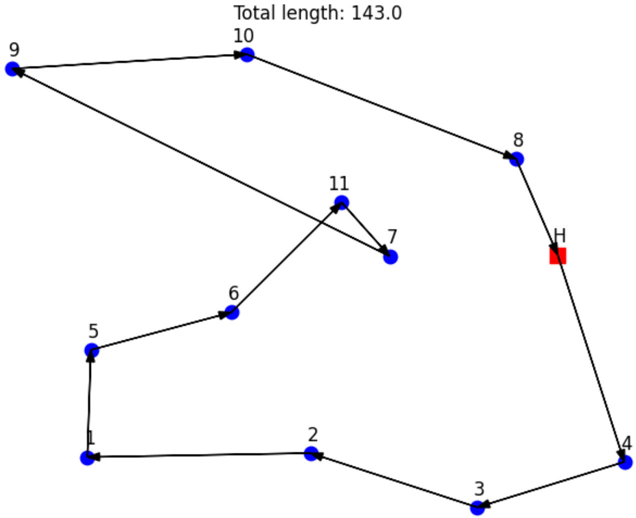
Current tour



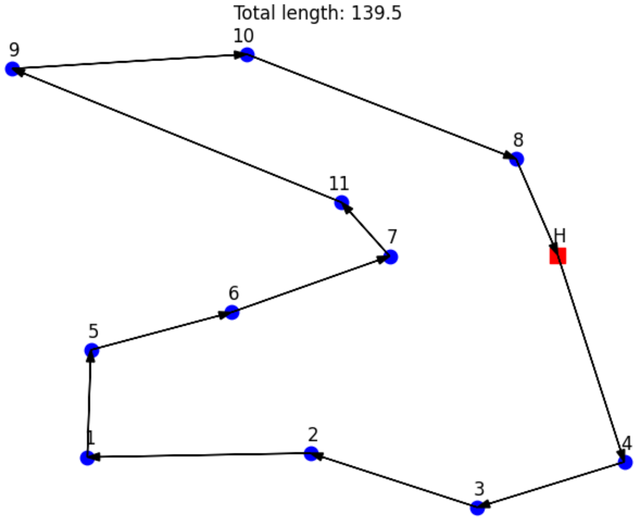
Best neighbor: 2-OPT(8,4)



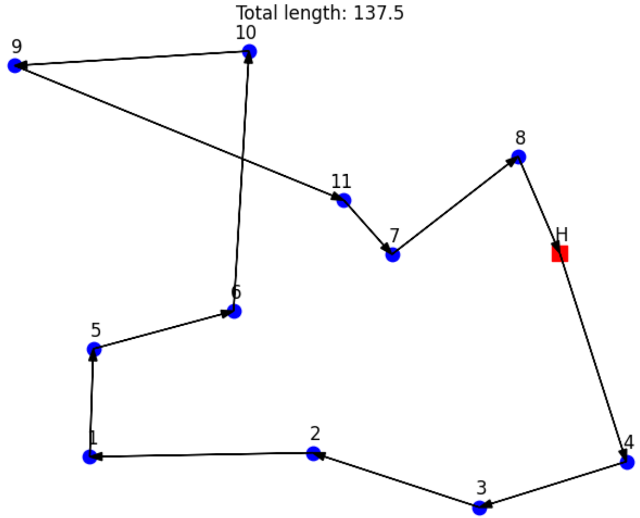
Best neighbor: 2-OPT(8,9)



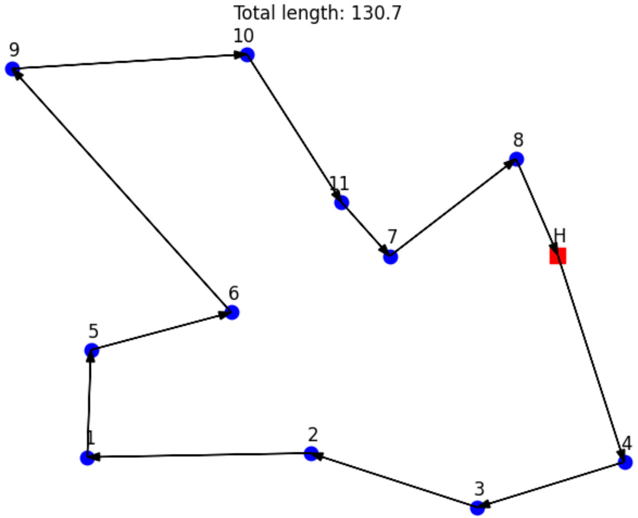
Best neighbor: 2-OPT(11,7)



Best neighbor: 2-OPT(7,10)



Best neighbor: 2-OPT(10,9)



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

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

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

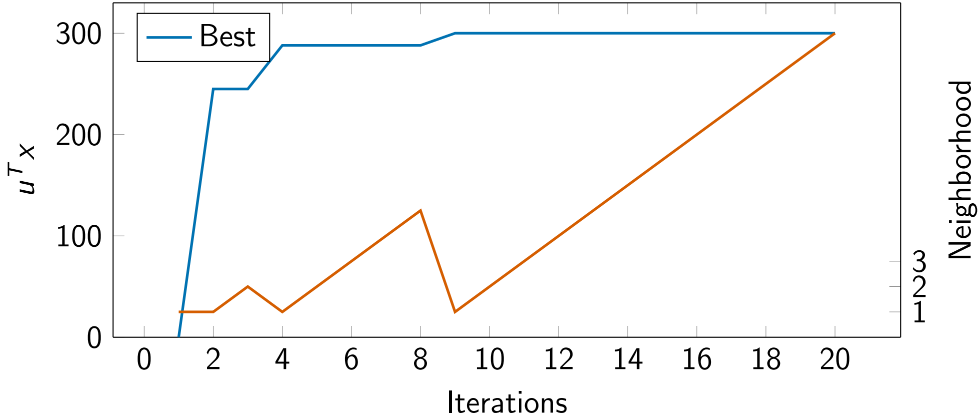
- If $f(x^+) < f(x_c)$, then $x_c \leftarrow x^+$, $k \leftarrow 1$.
- Otherwise, $k \leftarrow k + 1$.

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 $w^T x^+ \leqslant W$ 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 $f(y) \leqslant f(x_k)$, 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

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

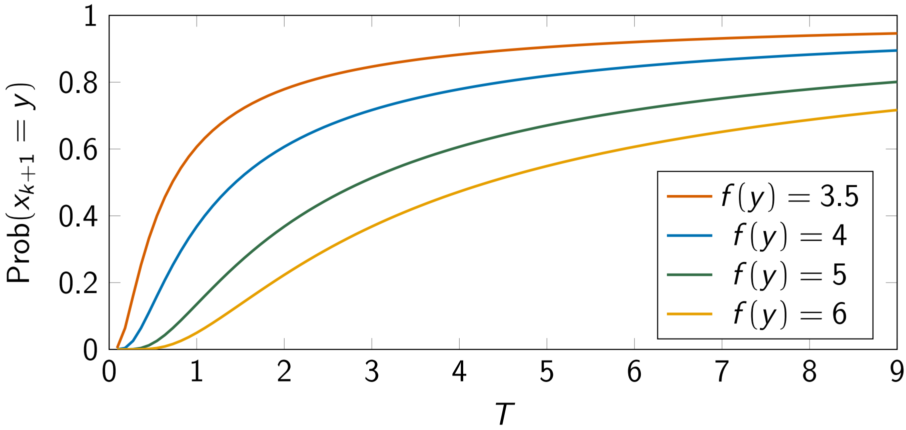
Simulated annealing

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

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

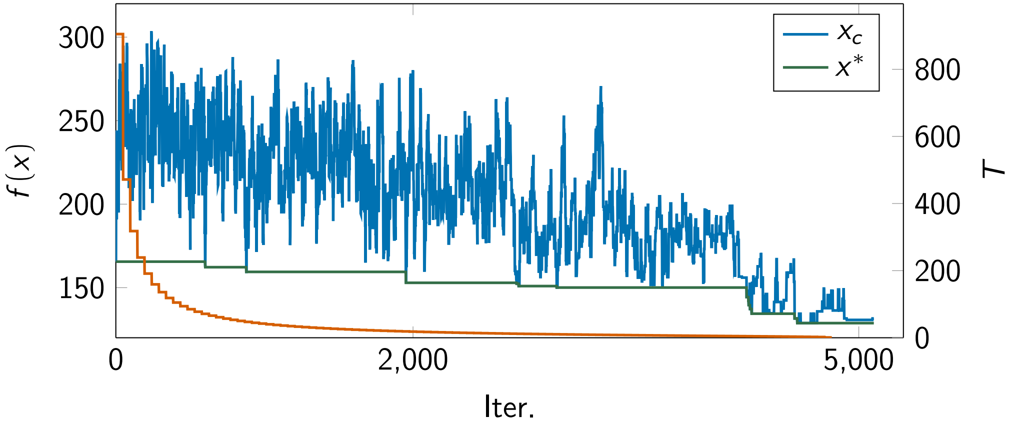
Simulated annealing

Repeat $k \leftarrow 1$

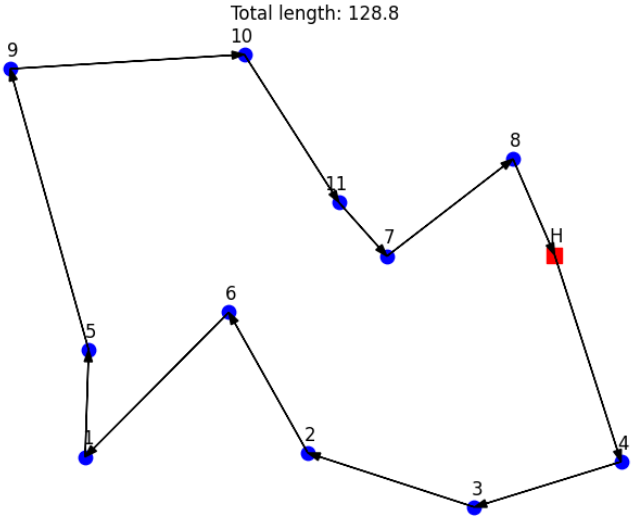
- While $k < K$
  - Randomly select a neighbor $y \in V(x_c)$
  - $\delta \leftarrow f(y) - f(x_c)$
  - If $\delta < 0$, $x_c = y$.
  - Otherwise, draw r between 0 and 1
    - If $r < exp(-\delta/T)$, then $x_c = y$
  - If $f(x_c) < f(x^*)$, $x^* = x_c$.
  - $k \leftarrow k + 1$
- Reduce T

Until $T \leqslant T_f$

Example: traveling salesman problem



Best solution found (optimal!)



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 $m = 0, \ldots, M$,

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

Simulated annealing and MCMC

Key connection

Simulated annealing applies Metropolis–Hastings to the distribution

$$\pi_T(x) \propto \exp\left(-\frac{f(x)}{T}\right),$$

where $T > 0$ is the temperature.

Interpretation

- High T: exploration (many uphill moves accepted).
- Low T: exploitation (mostly downhill moves).
- Cooling schedule: gradually shifts from exploration to exploitation.

Takeaway

Annealing is a meta-heuristic that uses an MCMC mechanism to escape local minima.

Comments

How to avoid being blocked in a 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

Characteristics

- 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.
- Designed to mimic manual interventions.

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.