Metaheuristic Optimization

2. The Structure of Optimization

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Section Outline

- Goal 1: Learn how to solve different kinds of (optimization) problems.
- Goal 2: Learn to use optimization algorithms for that purpose.

Introduction

- Goal 1: Learn how to solve different kinds of (optimization) problems.
- Goal 2: Learn to use optimization algorithms for that purpose.
- Need to understand
  1. How to define an optimization problem formally.
  2. How an optimization algorithm works and what components it has.

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- Goal 2: Learn to use optimization algorithms for that purpose.
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  1. How to define an optimization problem formally.
  2. How an metaheuristic optimization algorithm works and what components it has.

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Components of an Optimization Problem

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1. a data type $\mathbb{X}$ for the possible solutions (candidate solutions),
2. one (or multiple) functions $f \in \vec{f}$ which rate "how good" a candidate solution is, and
3. a notion of what "good" actually means.

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Definition (Candidate Solution x)

A candidate solution x of an optimization problem is an element of the solution space $\mathbb{X}$ of the problem, i.e., a potential solution of the problem.

From the programmer's perspective, we can say:

Listing: Solution space $\mathbb{X}$

```
public class MySolutionSpace extends Object {
  ...
  }

//or, instead, maybe a simple or primitive type
//or an array...
```

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- solution space $=$ data structure for candidate solution

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- Usually subject to minimization $f(x_1) < f(x_2)$ means that x_1 is better than x_2
- Not necessarily a function as you know it from Maths like $f(x) = x^2 + \dots$, but may be arbitrary complex, involve complicated simulations, etc.

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- as you see: $f(x)$ could be anything, could be deterministic or randomized, a simple formula, or involve running large programs like simulations

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    - Objective function with human interaction! Why not!

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Solution Space and Objective

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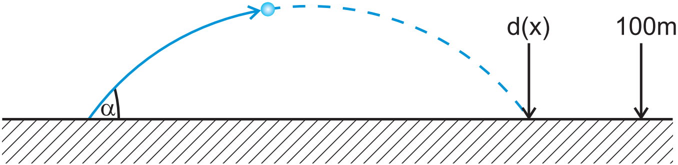
4. These steps are independent of how we will finally solve the problem
5. If you develop an optimization software for a client, it is very important to discuss these issues with the client and to formally write them down on paper! The client often does not know exactly what he/she wants AND you may misunderstand him/her...

Which is the best velocity x with which I should throw a stone (in an $\alpha = 15^\circ$ angle) so that it lands exactly 100m away?



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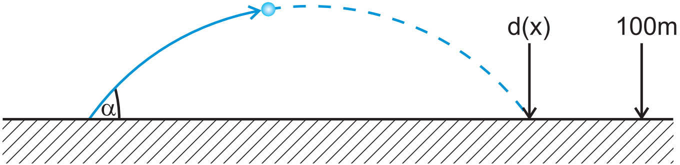

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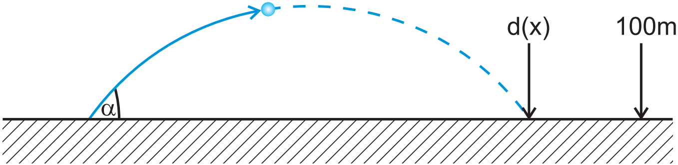

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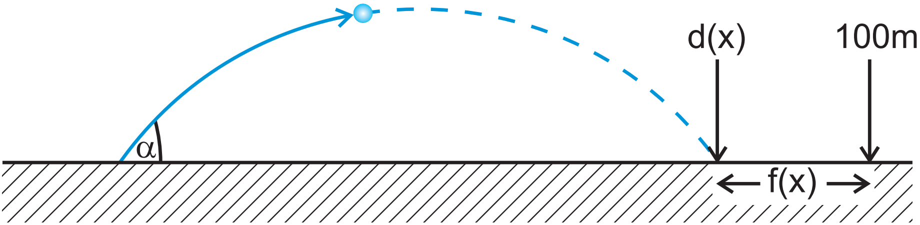

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Listing: Blueprint of Objective Function for Stone's Throw Probleml

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public final class StoneThrowObjective implements IObjectiveFunction<Number> {

  public final double compute(final Number x) {
    final double v = x.doubleValue();
    final double d = (((v * v) / 9.80665d) * Math.sin(((2.0d * 15.0d) / 180.0d) *
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    return Math.abs(100d - d);
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- But what if the stone is an irregularly shaped object (like a chair) and we also include air drag, gravitation, wind, limit forces on the stone-throwing arm, costs for electricity of moving the joints, wear of joins, imprecision of movements, make α variable, ...?

Example: Traveling Salesman Problem

A salesman wants to visit n cities in the shortest possible time. No city should be visited twice and he wants arrive back at the origin by the end of the tour [1–3].

w(a,b)	Shanghai	Hefei	Guangzhou	Chengdu
Beijing	1244 km	1044 km	2174 km	1854 km
Chengdu	2095 km	1615 km	1954 km	
Guangzhou	1529 km	1257 km		
Hefei	472 km			

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Definition (Traveling Salesman Problem)

The goal of the Traveling Salesman Problem (TSP) is to find a cyclic path of minimum total weight which visits all vertices of a weighted graph. [1, 2, 4, 5]

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- Solution Space:

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  $\mathbf{\Pi}(Z) =$ set of all permutations of the elements of the given set Z

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  Example: $\mathbf{\Pi}(\{123\}) = \{(1,2,3);(1,3,2);(2,1,3);(2,3,1);(3,1,2);(3,2,1)\}$

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- Objective Function: Minimize $f(x) = dist(\text{Hefei}, x[0]) + \sum_{i=0}^{2} dist(x[i], x[i+1]) + dist(x[3], \text{Hefei})$

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  This formula is not so nice: we cannot simply "solve" it for a minimum $x \in \mathbb{X}$.

Listing: Solution space $\mathbb{X}$

```java
public final class ChinaTSPObjective implements IObjectiveFunction<int[]> {

  public final double compute(final int[] x) {
    double dist;

    dist = ChinaTSPObjective.distance(ChinaTSPObjective.HEFEI, x[0]);

    for (int i = 1; i < x.length; i++) {
      dist += ChinaTSPObjective.distance(x[i - 1], x[i]);
    }

    return (dist + ChinaTSPObjective.distance(x[x.length - 1], ChinaTSPObjective.HEFEI));
  }
}
```

Example: Traveling Salesman Problem

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- Simply test all possible solutions...

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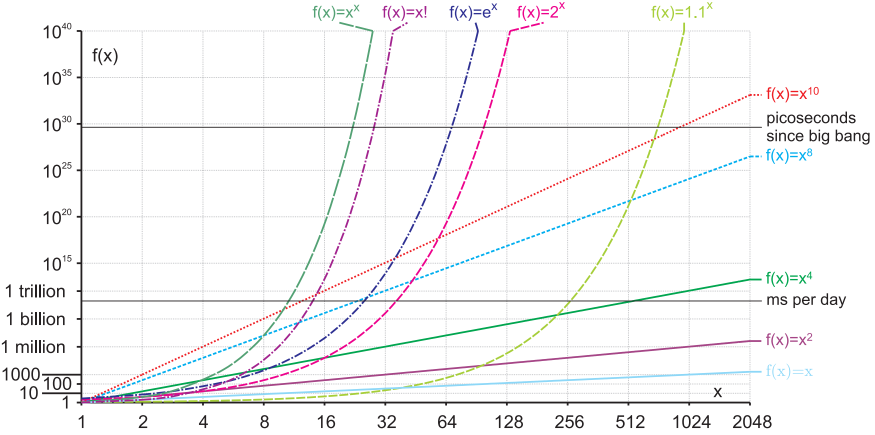
x_1	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Chengdu	$\rightarrow$	Guangzhou	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	7425km
x_2	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Chengdu	$\rightarrow$	Shanghai	$\rightarrow$	Guangzhou	$\rightarrow$	Hefei	7566km
x_3	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Guangzhou	$\rightarrow$	Chengdu	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	8311km
x_4	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Guangzhou	$\rightarrow$	Shanghai	$\rightarrow$	Chengdu	$\rightarrow$	Hefei	7886km
x_5	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Shanghai	$\rightarrow$	Chengdu	$\rightarrow$	Guangzhou	$\rightarrow$	Hefei	7381km
x_6	Hefei	$\rightarrow$	Beijing	$\rightarrow$	Shanghai	$\rightarrow$	Guangzhou	$\rightarrow$	Chengdu	$\rightarrow$	Hefei	6815km
x_7	Hefei	$\rightarrow$	Chengdu	$\rightarrow$	Beijing	$\rightarrow$	Guangzhou	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	8787km
x_8	Hefei	$\rightarrow$	Chengdu	$\rightarrow$	Beijing	$\rightarrow$	Shanghai	$\rightarrow$	Guangzhou	$\rightarrow$	Hefei	7857km
x_9	Hefei	$\rightarrow$	Chengdu	$\rightarrow$	Guangzhou	$\rightarrow$	Beijing	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	8602km
x_{10}	Hefei	$\rightarrow$	Chengdu	$\rightarrow$	Shanghai	$\rightarrow$	Beijing	$\rightarrow$	Guangzhou	$\rightarrow$	Hefei	8743km
x_{11}	Hefei	$\rightarrow$	Guangzhou	$\rightarrow$	Beijing	$\rightarrow$	Chengdu	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	8637km
x_{12}	Hefei	$\rightarrow$	Guangzhou	$\rightarrow$	Chengdu	$\rightarrow$	Beijing	$\rightarrow$	Shanghai	$\rightarrow$	Hefei	7566km

Example: Traveling Salesman Problem

- Simply test all possible solutions. . . ??
- Size of solution space: $|\mathbb{X}| = \frac{1}{2}(n-1)!$ ⇐ factorial, not exclamation mark



(Figure inspired by [6])

- Simply test all possible solutions. . . ??
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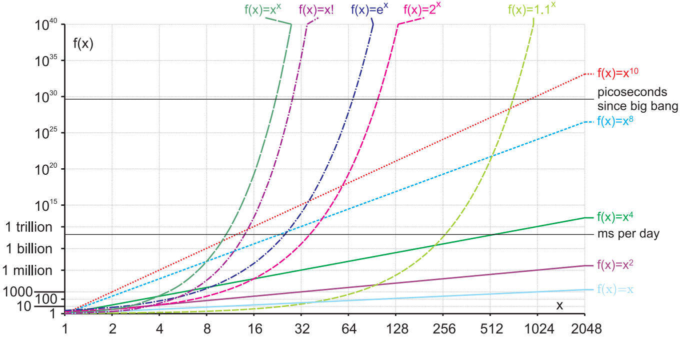

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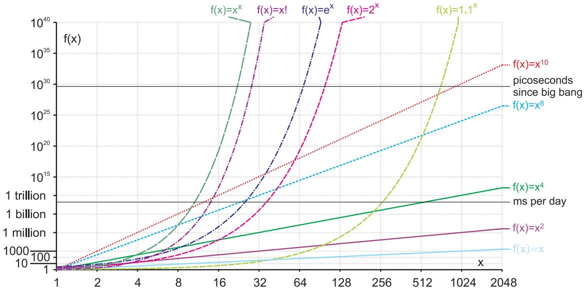
Example: Traveling Salesman Problem

- Simply test all possible solutions. . . ??
- Size of solution space: $|\mathbb{X}| = \frac{1}{2}(n-1)!$
- Algorithm which is better than this *exhaustive enumeration* needed
- You will learn quite a lot of these in this lecture!



(Figure inspired by [6])

- What could be suitable solution spaces and objectives for
  1. Bin Packing [7]
  2. Circuit Layout [8, 9]
  3. Find the roots of a function $g(x)$ [10–13]
  4. Shortest Path / Routing [14–16]
  5. Find mathematical formula fitting to given data [17–19]
  6. Job Shop Scheduling [18, 20]
  7. Stock Prediction [21–24]
  8. Truss Optimization [25–27]
  9. Medical Classification [28]
  10. Airplane Wing Design [29–32]

Further Examples

- Antenna design [33–41]
- Analog Electrical Circuit Design [42–45]
- Interactive Optimization [46–51]

Section Outline

1. Introduction
2. Optimization Problem
3. What is Good?
4. Metaheuristics
5. Putting it Together
6. Summary

What does "good" mean?

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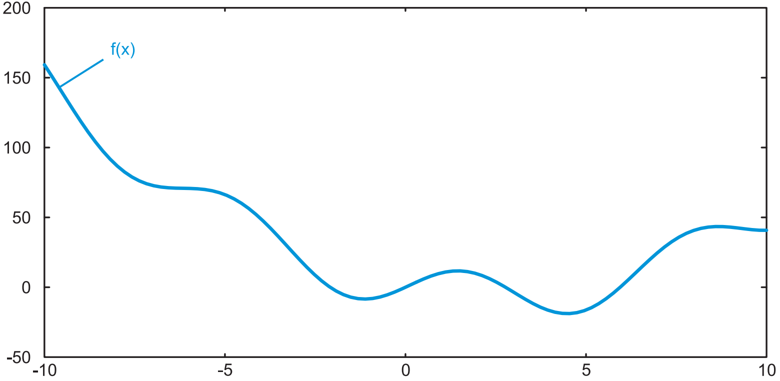
- But what does "good" mean?

- Assume that the objective function f is a steady, continuous, and differentiable function $f : \mathbb{R} \mapsto \mathbb{R}$ with a single real-valued parameter x.



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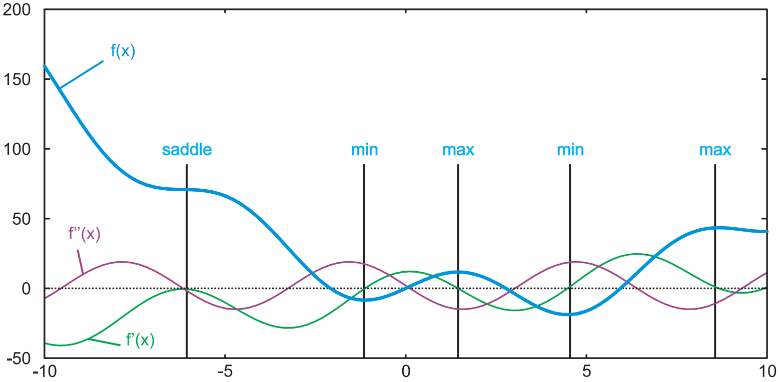

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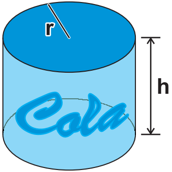
$$V(r,h) \quad = \quad \pi r^2 h \text{...... volume of cylinder} \tag{11}$$



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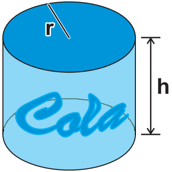

(11)

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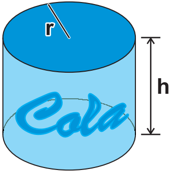

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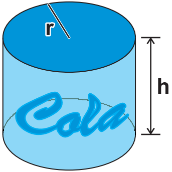
$$\mathbb{X} = (r,h) : r,h \in \mathbb{R}^+ \text{ ...... solution space: } r \text{ and } h \text{ define a cylinder}$$



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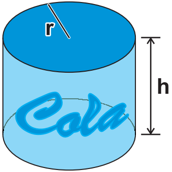

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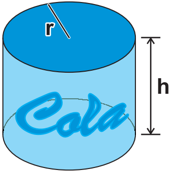

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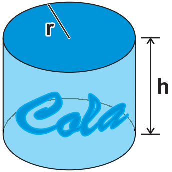

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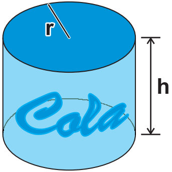
$$



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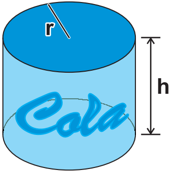

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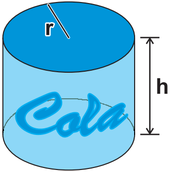
$$f'(r) = 4\pi r + 2V_d * -r^{-2} \text{......first derivative of } f \text{ for } r \quad (7)$$

$$0 = 4\pi r - \frac{2V_d}{r^2} \text{......solve for extrema}$$



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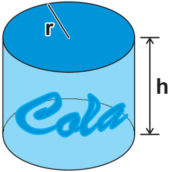
$$2V_d = 4\pi r^3 \text{......still solving...}$$



(12)

Example: Cheap Cola Can

Task: Construct a cylindrical cola can capable of holding 355mL with the minimum material costs.

$$\begin{aligned}
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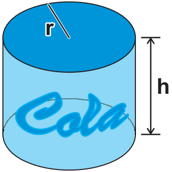
r^\star &\approx \sqrt[3]{\frac{2 * 0.003\,55\text{m}^3}{4\pi}} \approx 0.038\text{m} \approx 3.8\text{cm} \text{......OK, } r \text{ is found}
\end{aligned}$$



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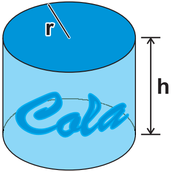

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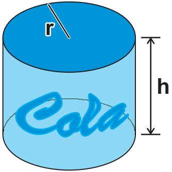

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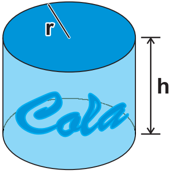

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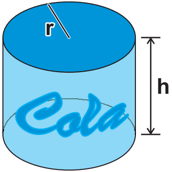

Problem solved with high school maths – no optimization algorithm needed.

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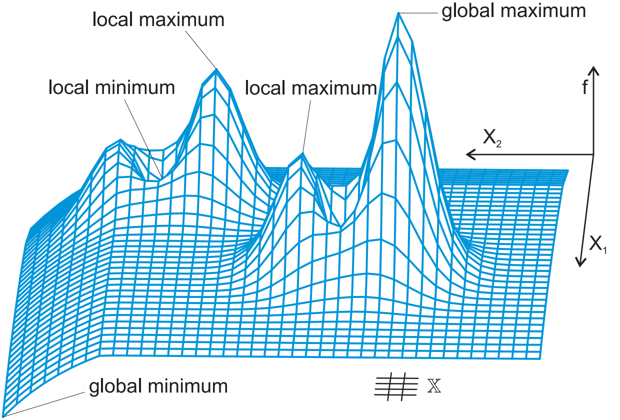

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- Other example: Genetic Programming [17], where the solutions are tree data structures, e.g., representing mathematical formulas

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Definition (Global Optimum of a Single Objective Function)

Depending on whether the objective function is subject to minimization or maximization, a global optimum is either a global minimum or a global maximum.

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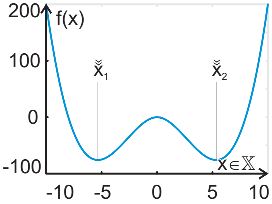

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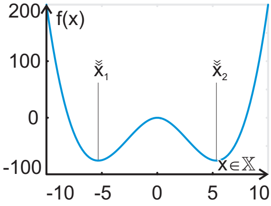

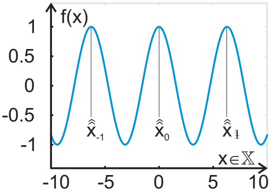

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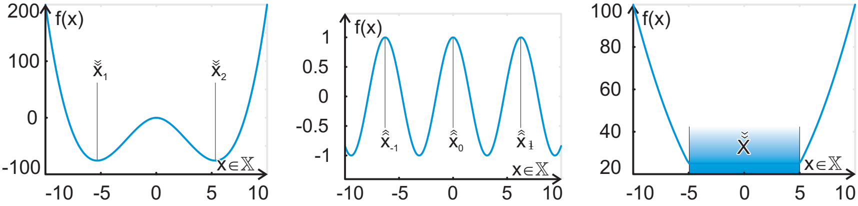

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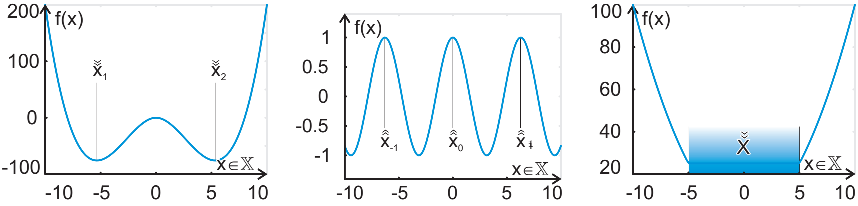

Definition (Global Optimal Set)

The optimal set $X^{\star} \subseteq \mathbb{X}$ of an optimization problem is the set that contains all its globally optimal solutions.

Examples for “good”

1. Bin Packing
2. Circuit Layout
3. Find the roots of a function $g(x)$
4. Shortest Path / Routing
5. Find mathematical formula fitting to given data
6. Job Shop Scheduling
7. Stock Prediction
8. Truss Optimization
9. Medical Classification
10. Airplane Wing Design
11. Antenna design
12. Analog Electrical Circuit Design
13. Interactive Optimization

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Definition (Optimization Result $\tilde{X}$)

The set $\tilde{X} \subseteq \mathbb{X}$ contains output elements $\tilde{x} \in \mathbb{X}$ of an optimization process.

- usually we only return one single solution $\tilde{x}$, i.e., $\tilde{X} \equiv \{\tilde{x}\}$

Components of a Optimization Problem

Now we have discussed the basic components of an optimization problem from a more mathematical point of view.

1. the solution space $\mathbb{X}$,
2. the objective function(s) $f : \mathbb{X} \mapsto \mathbb{R}$, and
3. the concept of "good" (minimize? maximize? multi-objective?).

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  - If we do this well or can learn how to do this best, we can win!

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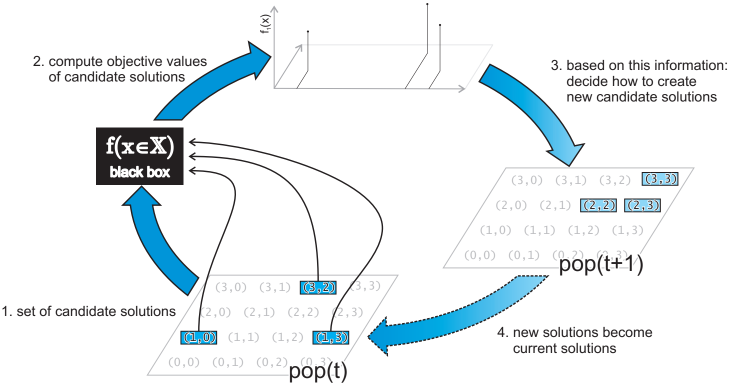
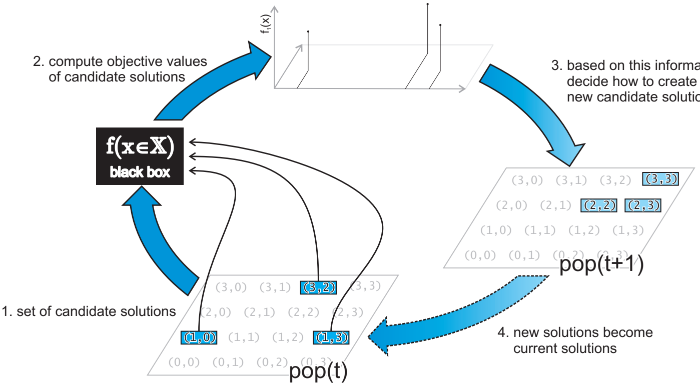
  1. We have a potentially extremely large set $\mathbb{X}$ of solutions.
  2. Do we know exactly what features good (or the best) solutions have? NO
  3. Can we "directly" solve f for the optima (e.g., by differentiating it)? NO
  4. Can we simply test all candidate solution $x \in \mathbb{X}$? NO
- So what can we do?
  - We know the data structure for elements of $\mathbb{X}$.
  - So we can randomly create instances x!
  - And we can modify some existing (previously created) instances x!
  - And we can maybe even combine existing instances x_1 and x_2!
  - If we do this well or can learn how to do this best, we can win!
  - This is the idea behind all *metaheuristics*

- Start with one (or multiple) initially generated candidate solutions (we call this set of solutions "population" pop)



How a Metaheuristic Works

- Start with one (or multiple) initially generated candidate solutions (we call this set of solutions "population" pop)
- Iteratively refine the solution(s) in a loop (e.g., by making small random changes)



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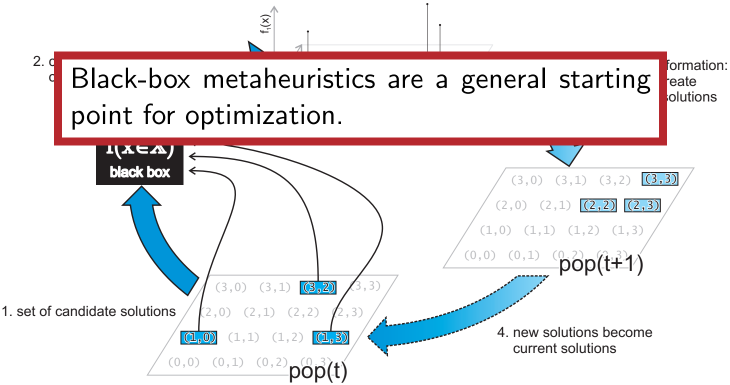

Black-box metaheuristics are a general starting point for optimization.

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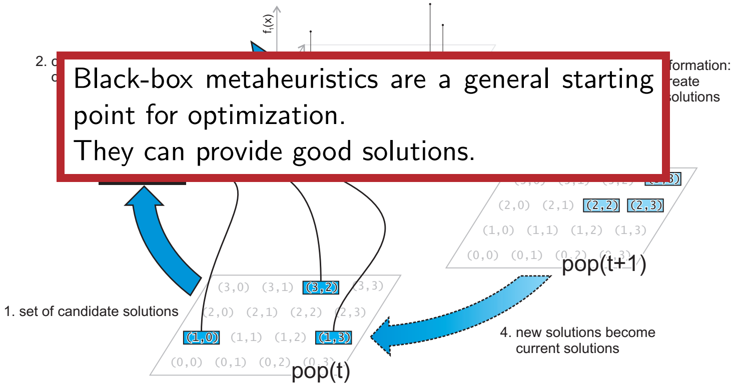

Black-box metaheuristics are a general starting point for optimization.
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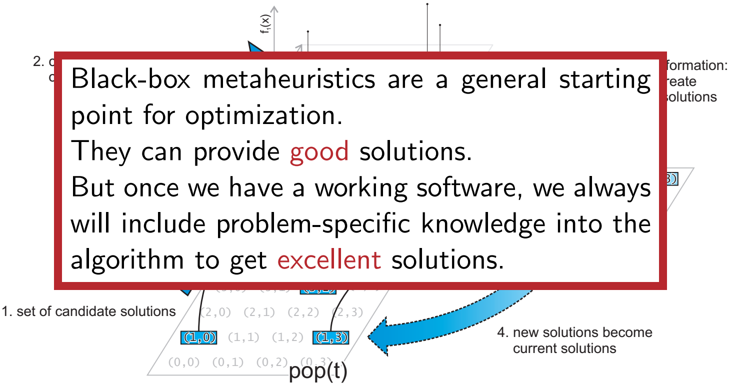

Black-box metaheuristics are a general starting point for optimization.
They can provide good solutions.
But once we have a working software, we always will include problem-specific knowledge into the algorithm to get excellent solutions.

Search Space

- OK, we have a data structure $\mathbb{X}$ for the candidate solutions and an objective function $f : \mathbb{X} \mapsto \mathbb{R}$ telling us how good they are

Search Space

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- Idea: Sometimes, we can use well-known data structures for $\mathbb{X}$, e.g., $\mathbb{R}^n \equiv$ `double[]`

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  Example: Finding the roots of a real function $g(x)$ (use real vector)

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- Besides the solution space $\mathbb{X}$ we can use a search space $\mathbb{G}$ an *internal* data structure for representing the possible solutions from $\mathbb{X}$

Search Space

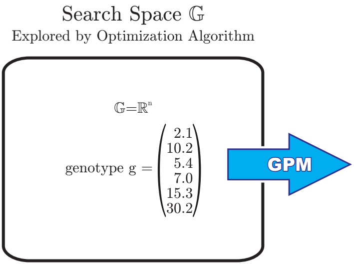
Search Space $\mathbb{G}$

Explored by Optimization Algorithm

$\mathbb{G}=\mathbb{R}^n$

$$\text{genotype } g = \begin{pmatrix} 2.1 \\ 10.2 \\ 5.4 \\ 7.0 \\ 15.3 \\ 30.2 \end{pmatrix}$$

As a metaphor based on biological genetics, the search space is often called *genome*, points in the search space are called *genotypes*, the solution space (solution space) is called *phenome*, its elements are called *phenotypes*, and the translation between phenotypes and genotypes is called *genotype-phenotype-mapping*.



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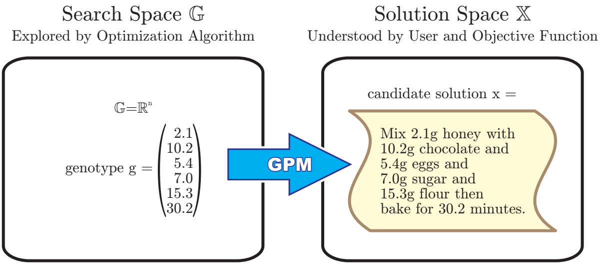

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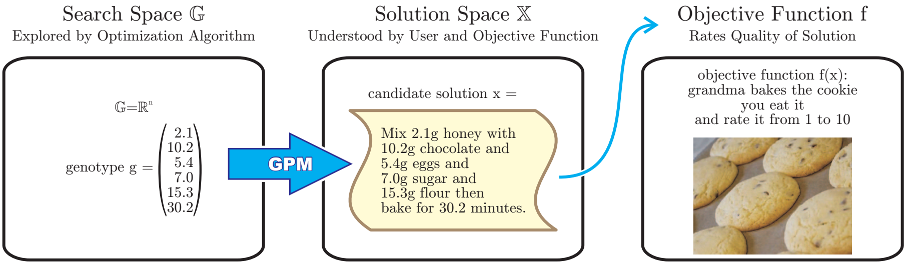

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Search Space

From the programmer's perspective, we can say:

Listing: Search space $\mathbb{G}$

```
public class MySearchSpace extends Object {
  ...
  }

//or, instead, maybe a simple or primitive type
//or an array...
```

Definition (Genotype-Phenotype Mapping)

The genotype-phenotype mapping (GPM) $\mathrm{gpm} : \mathbb{G} \mapsto \mathbb{X}$ is a left-total binary relation which maps the elements of the search space $\mathbb{G}$ to elements in the solution space $\mathbb{X}$.

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- if $\mathbb{G} = \mathbb{X}$, the genotype-phenotype mapping is (usually) the identity mapping
- this is often the case, but not always [25, 52]

From the programmer's perspective, we can say:

Listing: Mapping from search- to solution space: $\mathrm{gpm} : \mathbb{G} \mapsto \mathbb{X}$

```
public interface IGPM<G, X> {
  public abstract X gpm(final G genotype);
}
```

Search Space + GPM

Search Space $\mathbb{G}$

Explored by Optimization Algorithm

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GPM

Solution Space $\mathbb{X}$

Understood by User and Objective Function

candidate solution x =

Mix 2.1g honey with
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Objective Function f

Rates Quality of Solution

objective function f(x):
grandma bakes the cookie
you eat it
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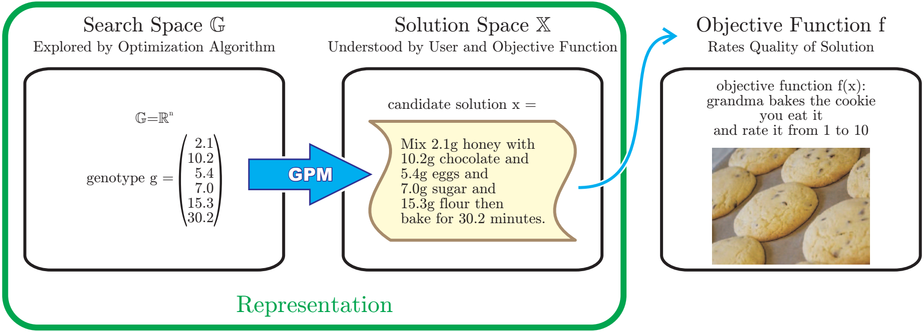
Search Space + GPM



- $\mathbb{G}$, $\mathbb{X}$, and gpm together are called Representation

Search Space + GPM

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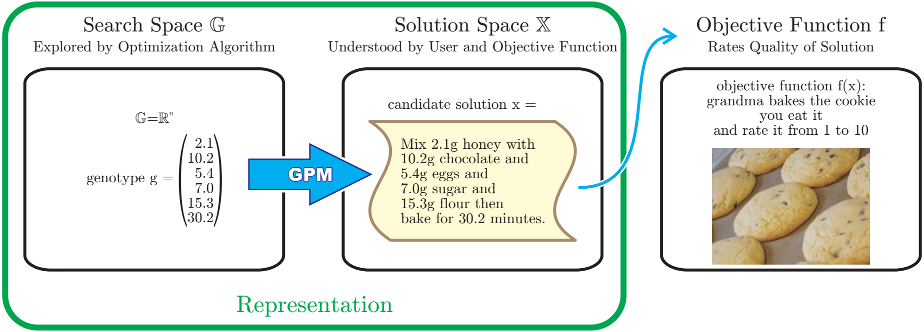
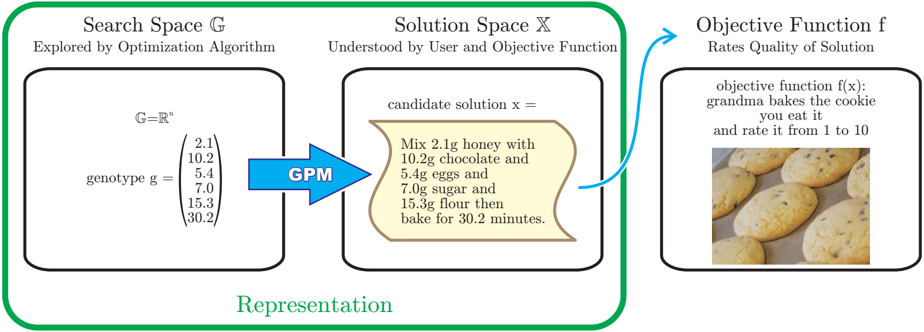


- The choice of the representation has tremendous impact on the results!

Search Space + GPM



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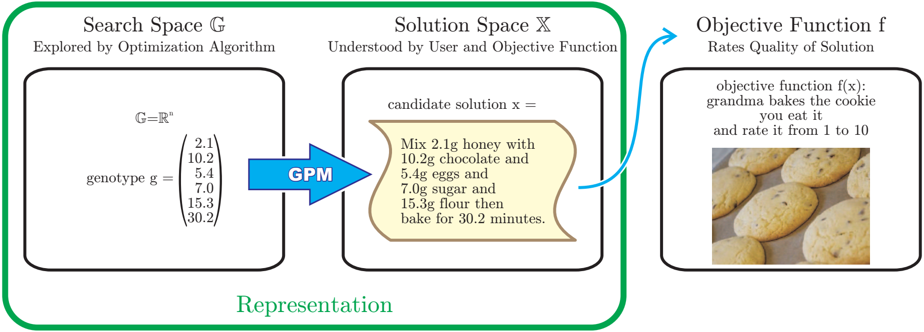

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  - It determines the number of potential solutions.

Search Operations

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Definition (Search Operation)

A search operation receives 0 or more elements from the search space $\mathbb{G}$ as parameter and returns a new genotype.

Search Operations

From the programmer's perspective, we can say:

Listing: Nullary search operation $\text{searchOp} : \emptyset \mapsto \mathbb{G}$

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public interface INullarySearchOperation<G> {
  public abstract G create(final Random r);
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- this could be a random instance or an instance constructed using some particular algorithm

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- it then returns a modified copy of that instance.
- the modification is usually small and random

Termination Criterion

- So, we have $\mathbb{X}$, f, $\mathbb{G}$, and $\mathrm{gpm}\ldots$ what else do we need?
  - An operation which creates instances of data structure $\mathbb{G}$,
  - Operators which modify or combines such data structures

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  3. stop when no further improvement can be detected
  4. stop when a sufficiently good solution has been detected
  5. ...

Listing: Termination Criterion $\text{shouldTerminate} : \mapsto \{\texttt{true}, \texttt{false}\}$

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- Directly after every time the optimization algorithm has created a new solution x and computed $f(x)$, it must call `shouldTerminate()`
- If `shouldTerminate()` returns `true`, the algorithm must immediately stop and return the best solution candidate it has seen so far
- One could implement `ITerminationCriterion` and `IObjectiveFunction` in the same object to stop once a goal solution quality was reached.

Example Termination Criterion

Listing: A criterion stopping after a given amount of steps.

```
public class MaxSteps implements ITerminationCriterion {
  /** the number of remaining steps */
  private int m_remaining;


  public MaxSteps(final int steps) {
    super();
    this.m_remaining = steps;
  }


  public boolean shouldTerminate() {
    return ((--this.m_remaining) < 0);
  }
}
```

Section Outline

Putting it Together

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Putting it Together

Then a metaheuristic, black-box optimization looks like:

Definition (Individual)

An individual is a record where we can store all information that belongs to a solution, such as the genotype $g \in \mathbb{G}$, the corresponding phenotype $x \in \mathbb{X}$, and the objective value that we get when computing $f(x)$.

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- Objective Functions $f : \mathbb{X} \mapsto \mathbb{R}$

谢谢
Thank you

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Caspar David Friedrich, “Der Wanderer über dem Nebelmeer”, 1818
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