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Stochastic optimization

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Content

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Title

Global Optimization Algorithms
– Theory and Application –

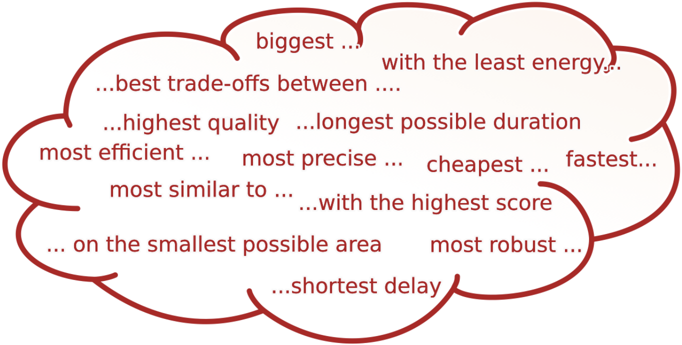
Web sources

Newest Version: https://thomasweise.github.io/aitoa/aitoa.html
Sources/CVS-Repository: goa-taa.cvs.sourceforge.net

The search for optimal states

Nature

- Minimize the energy of electrons
- Molecules combine during freezing
- biological principle of survival of the fittest



Definition — Economical View

Is a situation which requires deciding for one choice from a set of possible alternatives in order to reach a predefined/required benefit at minimal costs.

Definition — Mathematical View

An optimization problem requires finding an input value $x^* \in \mathbb{X}$ from a set of $\mathbb{X}$ that mathematical function $f : \mathbb{X} \to \mathbb{R}$ takes on the smallest possible value.

Route Planning for a Logistics Company

Example

Goal

Build a system which tells a logistics company what it needs to do to fulfill all transportation orders at minimum costs.

Goal

The goal of optimization then would be to find the assignment of containers to delivery orders and vehicles and of vehicles to routes, which maximizes the profit. And it should do so within a limited, feasible time.

Route Planning for a Logistics Company

Example

A customer:

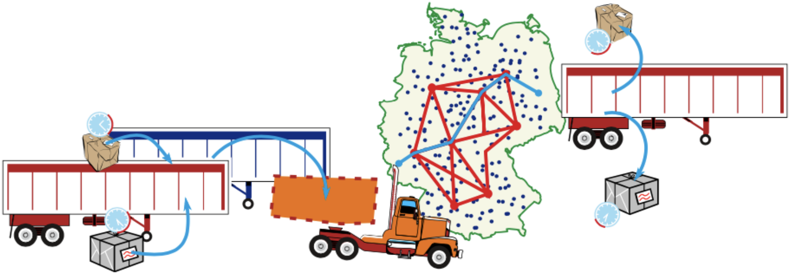
1. A customer orders one or more containers to be delivered to a specified location within a certain time window.
2. The customer fills the containers with goods.
3. Goods are transported to a specified destination in a time window.

A logistics company:

1. Have to deal with many customers.
2. Have many depots with tracks.
3. May use trains for transportation.
4. Tracks have different capacities.
5. Trains differ in capacities.
6. Trains travel on specified schedule.
7. Possibility to change the means of transportation.
8. The cost vary from different means of transportation.

Route Planning for a Logistics Company

Example



A simple example of logistics task.

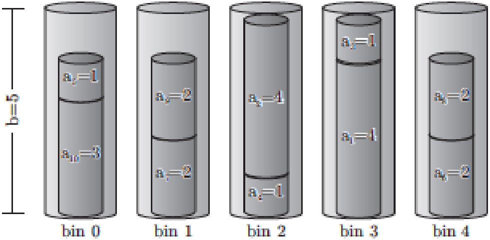
Goal

Is to find the shortest round-trip tour visiting n cities,

Robot example

A robot arm needs to drill several holes into a circuit board. Finding the shortest tour means solving a TSP.

`https://en.wikipedia.org/wiki/Travelling_salesman_problem`



distribution of n=10 objects of size a_1 to a_{10} in k=5 bins of size b=5

A $k \in \mathbb{N}$ bins is known and given. Each bin is defined with the size $b \in \mathbb{N}$. The $n \in \mathbb{N}$ objects with the specified weights $a_1, a_2, \ldots, a_n$ are given.

Goal

Can the n objects be distributed over the k bins in a way that none of the bins flows over?

The bin packing problem can be formalized as ”whether a mapping x from the numbers $1..n$ to $1..k$ exists so that the following equation holds:

$$\exists x : \forall i \in 0..k-1 : \left(\sum_{\forall j \in x[i]} a_j \right) \leq b$$

The question could be transformed into an optimization problem to find the smallest number k of bins of size b which can contain all the objects listed in a.

$$f_{bp}(x) = \sum_{i=0}^{k-1} \max \left\{ 0, \left(\sum_{\forall j \in x[i]} a_j \right) - b \right\}$$

Goal

Is to distribute a set of tasks to machines in a way that all deadlines are met or in other words to minimize the makespan — the total length of the schedule (that is, when all the jobs have finished processing).

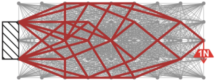
In a JSS or (Job Shop Problem JSP), a set T of jobs $t_i \in T$ is given, where each job t_i consists of a number of sub-tasks $t_{i,j}$. A partial order is defined on the sub-tasks $t_{i,j}$ in each job t_i which describes the order in sub-tasks (precedence constraints). Jobs need to be scheduled on m machines with varying processing power.

Goal

To construct a truss which can hold a certain weight with at most a certain amount of iron.

truss structure: fixed points (left), possible beam locations (gray), applied force (right, F)

possible optimization result: beam thicknesses (dark gray), unused beams (thin light gray)



Goal

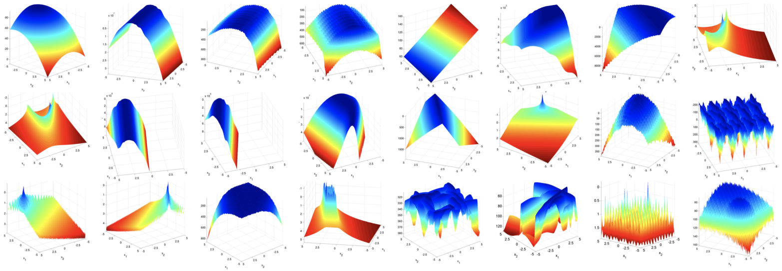
To construct a logic circuit to satisfy Boolean formula.

$$(x_1 \vee \neg x_2 \vee x_3) \wedge (\neg x_2 \vee \neg x_3 \vee x_4) \wedge (\neg x_1 \vee \neg x_3 \vee \neg x_4)$$

Logic optimization is a process of finding an equivalent representation of the specified logic circuit under one or more specified constraints. This process is a part of a logic synthesis applied in digital electronics and Integrated circuit design.

Goal

Find the minima of complex, multi-dimensional mathematical formulas



Combinatorial optimization problems are defined over a finite (or numerable infinite) discrete problem space $\mathbb{X}$ when candidate solutions can be:

1. set of elements from finite sets, $x \in \mathbb{X} \Rightarrow x = \{x1, x2, ...\}$,
2. finite sequence or permutation of elements x_i chosen from finite sets, i. e., $x \in \mathbb{X} \Rightarrow x = (x_1, x_2, ...)$
3. tree or graph structures with node or edge
4. any form of nesting, combination, partitions, or subsets of the above.

Combinatorial problems
Examples

- Traveling Salesman Problem
- Vehicle Routing Problems
- graph coloring
- graph partitioning
- scheduling
- packing
- satisfiability problems.

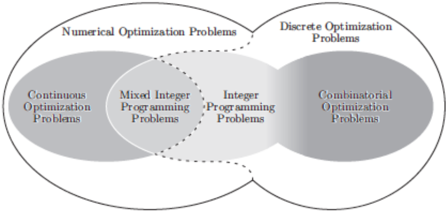
Numerical Optimization Problem
Taxonomy

Numerical optimization problems are problems that are defined over problem spaces which are subspaces of (uncountable infinite) numerical spaces, such as the real or complex vectors ($\mathbb{X} \in \mathbb{R}^n$ or $\mathbb{X} \in \mathbb{C}^n$).

- Function optimization
- engineering design optimization tasks
- classification
- data mining tasks.

The candidate solutions of combinatorial problems stem from finite sets and are discrete. They can be expressed as discrete numerical vectors and thus could be solved with methods for numerical optimization, such as integer programming techniques.

Every discrete numerical problem can also be expressed as continuous numerical problem because any vector from the $\mathbb{R}^n$ can be transformed to $\mathbb{Z}^n$ by simply rounding each of its elements. Hence, the techniques for continuous optimization can theoretically be used for discrete numerical problems (integer programming).



Optimization definition

Optimization is the process of solving an optimization problem, i. e., finding suitable solutions for it.

Definition — Global optimization

Global optimization is the optimization to find solution/s x^* for a given optimization problem which have the property that no other, better solutions exist.

Optimization Algorithm

Is an algorithm suitable to solve optimization problems.

Dedicated algorithms

are specialized to exactly solve a given class of problems in the shortest possible time. They are most often deterministic and apply exact theoretical knowledge about the problem. For example the shortest paths from a source node to the other nodes in a network can best be found with Dijkstra's algorithm.

Optimization algorithms

Is used if the dedicated algorithm is not known. In general in two cases:

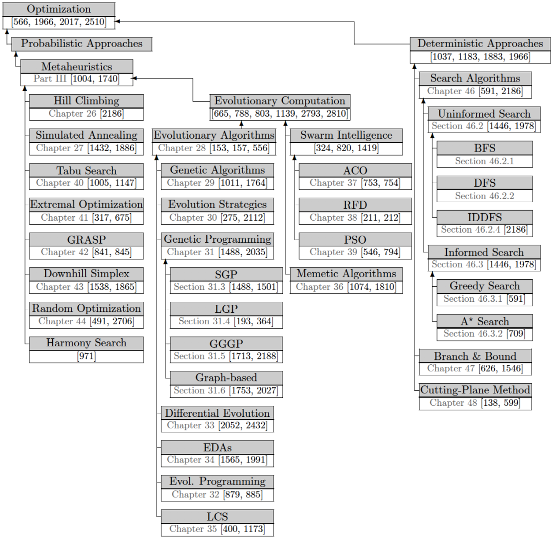
- the problem is too specific
- problems are "general"

They require

- a data structure for a possible (candidate) solution
- a function f which measures the quality of a candidate solution

They search for a candidate for which f has the best value(s).

Algorithms
Overview



Deterministic algorithm

There exists at most one way to proceed in every step. If there is no way to proceed, the algorithm terminates. Features:

- For the same input data always returns the same results.
- If the algorithm deal with two candidate solutions x_1 and x_2 then it uses a basic rule which calculates the objective function f: If $f(x_1) < f(x_2)$, then x_1 is chosen and x_2 otherwise.
- Deterministically chooses the candidate solution with the better f value.

Probabilistic Algorithms
When to use?

- If the relation between a candidate solution and its “fitness” is not obvious,
- If the relation between a candidate solution and its “fitness” dynamically changing,
- If the relation between a candidate solution and its “fitness” too complex,
- the size of the search space is enormous,

Definition

A randomized (or probabilistic or stochastic) algorithm includes at least one instruction based on random numbers.

- It may produce different results for the same input.
- Basic rule is Probabilistic Decision Making: If $f(x_1) < f(x_2)$, then choose x_1 with some probability p, but in $1 - p$ cases continue with x_2.
- Most probabilistic algorithms used for optimization are Monte Carlo-based approaches. They trade guaranteed global optimum for a shorter runtime.

The term heuristic stems from the Greek *heuriskein* which translates to ”to find” or to ”to discover”.

Definition

A heuristic function Φ is a part of an optimization algorithm that uses the information currently gathered by the algorithm to help to decide which candidate solution should be tested next or how the next individual can be produced.

Heuristic values $\Phi(p)$ often represent indirect criteria such as the approximate distance or cost needed from p to get to the global optimum.

Definition

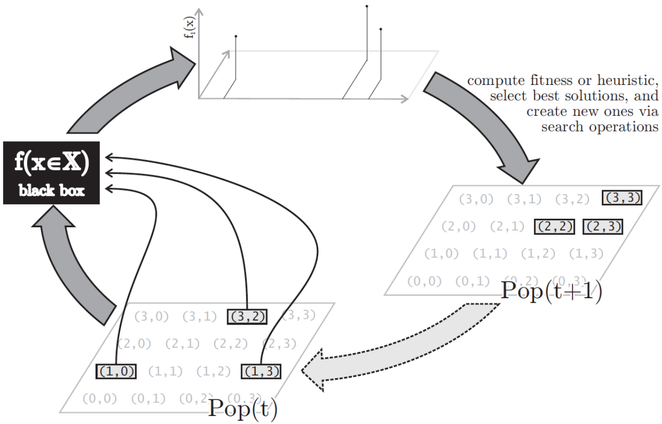
A metaheuristic is a method for solving general classes of problems. It combines objective functions or heuristics in an abstract and hopefully efficient way, usually without deep optimization problem analysis, i. e., by treating them as black box-procedures.

They obtain knowledge on the structure of the problem space and the objective functions by applying statistics from stochastically sampling the search space.

Many metaheuristics are inspired by a model of some natural phenomenon or physical process.

Metaheuristics are not necessarily probabilistic methods.

Black box in metaheuristics
Overview



Speed and precision are often conflicting objectives, at least in terms of probabilistic algorithms.

Rule

A general rule of thumb is that you can gain improvements in accuracy of optimization only by investing more time.

Definition

Online optimization need to be solved in a short time usually ranging between ten milliseconds to a few minutes.

Online optimization is often carried out repetitively – for example, new commands continuously arrive in an engine. Therefore, they need to be scheduled to minimize the delay.
Examples

- robot localization,
- load balancing,
- services composition for business processes
- updating a factory's machine job schedule after new orders came in.

Definition

In offline optimization, time is not so important and a user is willing to wait maybe up to days or weeks in order to get the optimal or close-to-optimal result.

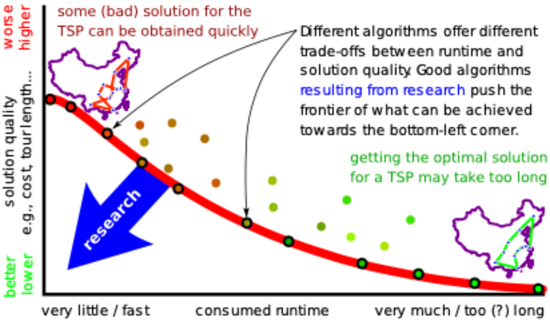
For example

- design,
- some data mining tasks,
- or creating long-term schedules for transportation crews.

These optimization usually perform only once in a long time.

Solution quality and runtime
continue

We can use algorithms we hope that they find a good approximation of the optimum, i.e., a solution which is very good with respect to the objective function, but which do not guarantee that their result will be the best possible solution.



Exercises

1. Name an optimization problem from daily life. Describe the criteria which are subject to optimization, whether they should be maximized or minimized, and how the investigated space of possible solutions looks like.
2. Name an optimization problem which is either engineering, business, or science. Describe it the same way as requested above.

Thank you for your attention