Applied Numerical Optimization

Prof. Alexander Mitsos, Ph.D.

What is optimization and how do we use it?

Definition: Numerical (Mathematical) Optimization

Optimization (in everyday language):

Improvement of a good solution by intuitive, brute-force or heuristics-based decision-making

Numerical (Mathematical) Optimization:

Finding the best possible solution using a mathematical problem formulation and a rigorous/ heuristic numerical solution method

Often the term **mathematical programming** is used as an alternative to numerical optimization. This term dates back to the times before computers. The term *programming* referred to the solution of *planning problems*.

For those interested in the history of optimization: *Documenta Mathematica, Journal der Deutschen Mathematiker-Vereinigung, Extra Volume - Optimization Stories, 21st International Symposium on Mathematical Programming, Berlin, August 19–24, 2012*

Formulation of Optimization Problems (1)

The general formulation of an optimization problem consists of:

- The **variables** (also called decision variables, degrees of freedom, parameters, …)
- An **objective function**
- A **mathematical model** for the description of the system to be optimized
- **Additional restrictions** on the optimal solution, including bounds of the variables.

The mathematical model of the system under consideration and the additional restrictions are also referred to as **constraints**.

The objective function can either be **minimized** or **maximized**.

Formulation of Optimization Problems (2)

- The **objective function** describes an economical measure (operating costs, investment costs, profit, etc.), or technological, or ...

- The mathematical modeling of the system results in models to be added to the optimization problem as **equality constraints**.

- The **additional constraints** (mostly linear inequalities) result, for instance, from:
  – plant- or equipment-specific limitations (capacity, pressure, etc.)
  – material limitations (explosion limit, boiling point, corrosivity, etc.)
  – product requirements (quality, etc.)
  – resources (availability, quality, etc.)

[1] Edgar T. F., Himmelblau D. M., Optimization of Chemical Processes, 2nd Edition, McGraw-Hill, 2001.

Solution of Optimization Problems

What defines the solution of an optimization problem?

- Those **values** of the **influencing variables** (decision variables or degrees of freedom) are sought, which maximize or minimize the objective function.
- The values of the degrees of freedom must **satisfy** the **mathematical model** and **all additional constraints** like, for instance, physical or resource limitations at the optimum.
- The solution is, typically, a **compromise** between **opposing effects**. In process design, for instance, the investment costs can be reduced while increasing the operating costs (and vice versa).

Applications of Optimization

Optimization is widely used in science and engineering, and in particular in process and energy systems engineering, e.g.,

- **Business decisions** (determination of product portfolio, choice of location of production sites, analysis of competing investments, etc.)
- **Design decisions: Process, plant and equipment** (structure of a process or energy conversion plant, favorable operating point, selection and dimensions of major equipment, modes of process operation, etc.)
- **Operational decisions** (adjustment of the operating point to changing environmental conditions, production planning, control for disturbance mitigation and set-point tracking, etc.)
- **Model identification** (parameter estimation, design of experiments, model structure discrimination, etc.)

Short Examples

- Engineering: **design** and **operation**

- Operations research, e.g., **airlines**
  - How to **schedule routes**: results in **huge linear programs (LPs)**
  - How to price airline tickets?
    - Should the airline aim at always having full airplanes?
  - Must consider uncertainty, typically as **stochastic formulation**

- **Navigation systems**: how to go from A to B in shortest time (or shortest distance, lowest fuel consumption or ...)

- LaTeX varies **spacing and arrangement of figures** to maximize visual appeal of documents

- Successful **natural processes** not using numerical methods
  - Evolution of species
  - Behavior of animals
  - Equilibrium processes in nature maximize entropy generation

Check Yourself

- What constitutes an optimization problem?
- What types of problems are typically found?
- Why do we typically seek a compromise in optimization?
- What is the difference between a nonlinear program, an optimal control problem and a stochastic program?

Bilevel Optimization in Grad School

max great papers

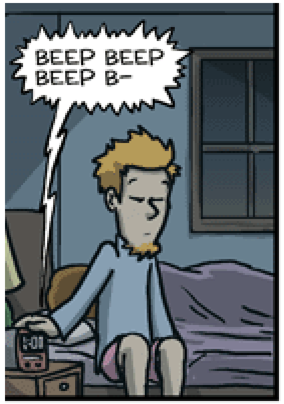
Constraints:

- # nervous breakdowns < OSHA limit
- sponsors happy

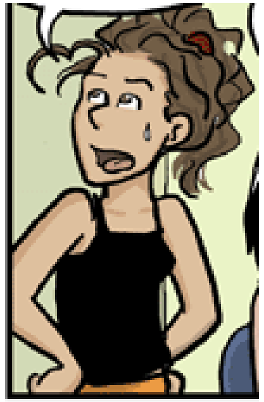
Variables:

- Pressure
Where are my paperz?
- Encouragement
Occasional free beer and food

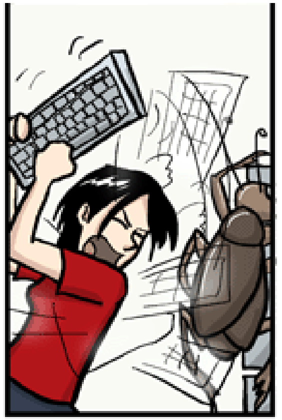
max slack



max social impact



min graduation time



max papers

Constraints:

- sleep > 4hrs
- pay rent
- keep funding

Variables:

- work load
- free lunch schemes
- seem busy schemes

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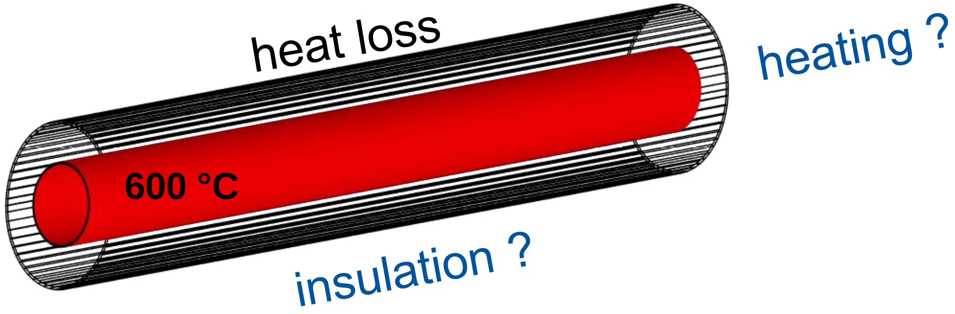
Examples of optimization problems – basic examples

Example: Design of a Pipeline (1)

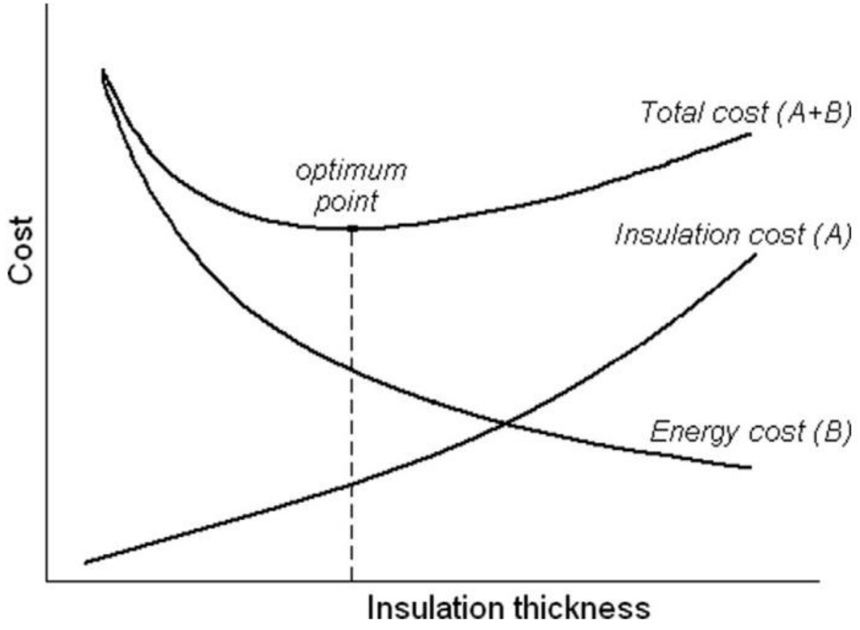
- A fluid at temperature 600°C flows through a pipeline.
- Surface heat losses must be balanced by additional heating.
- The heating costs (**operational costs**) are proportional to the heat loss, which can be reduced by the installation of an insulation (**investment costs**).



Example: Design of a Pipeline (2)

- The aim is to find the best compromise between the cost of additional heating and cost of additional insulation. The **objective function** corresponds thus to the **total (annualized) cost**.

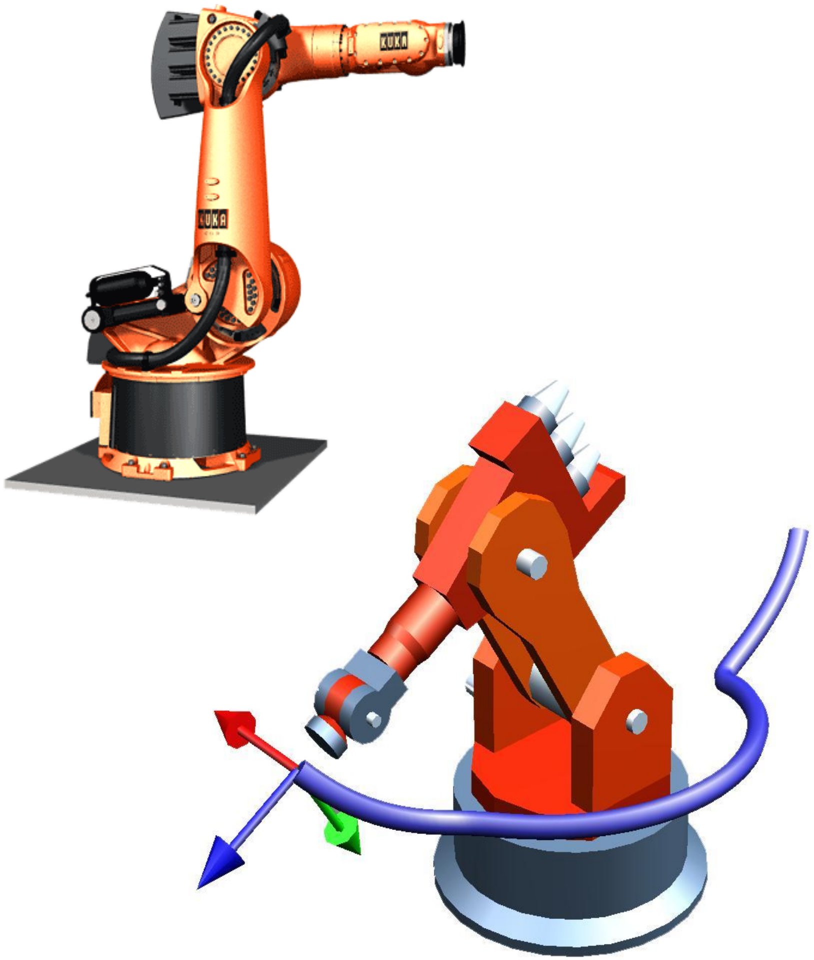
- The **degree of freedom** is the **insulation thickness**.



[1]

[1] Kaynakli, Economic thermal insulation thickness for pipes and ducts: A review study, 2014

Example: Optimal Motion Planning of Robots



Task:

- Transportation and accurate positioning of a part, e.g., during the assembly of an automobile windscreen.

Aims:

- Short cycle time for production, e.g., minimization of transportation time through optimal motion planning
- Correct positioning of the part during assembly
- No collisions during movement

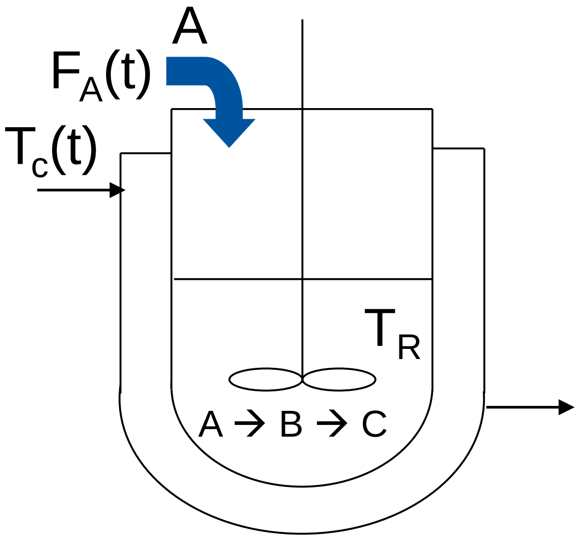
Source: FG Simulation und Systemoptimierung, TU Darmstadt; Kuka Roboter GmbH

Example: Optimization of Semi-batch Reactor Operation

In a semi-batch reactor, a product B should be manufactured according to the reaction scheme

$$A \rightarrow B \rightarrow C$$

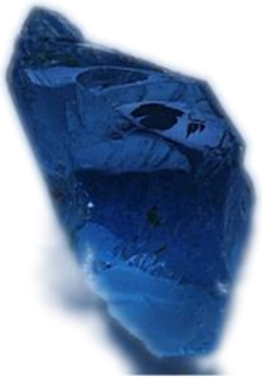
where C is an undesirable by-product.

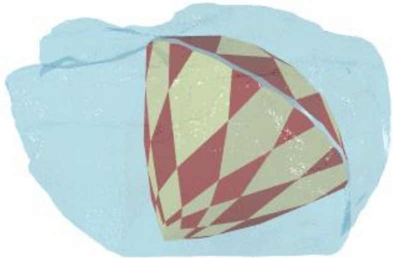


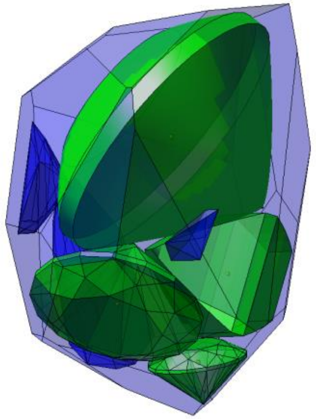
Optimization problem:

- The selectivity of the reaction can be maximized over the batch by manipulating the **dosage of reactant A** and the **reaction temperature**.
- The degrees of freedom are **functions of time.**
- Like in robot motion planning, this problem is an **optimal trajectory planning** problem.

Example: Gemstone Cutting as (Multi-Body) Design Centering Problem

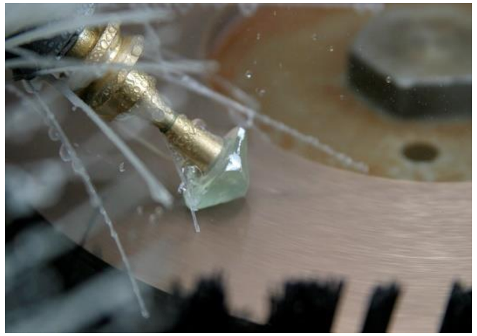






Optimal Cut?

maximize gemstone volume
minimize waste



Fraunhofer ITWM

Pictures from Fraunhofer ITWM
Algorithm by Oliver Stein, solver by ITWM

Check Yourself

- For each of the considered examples, state: variables, objective function, model, additional constraints
- Formulate the application of your interest as an optimization problem
- What are some limits of optimization?

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Examples of optimization problems – solar thermal

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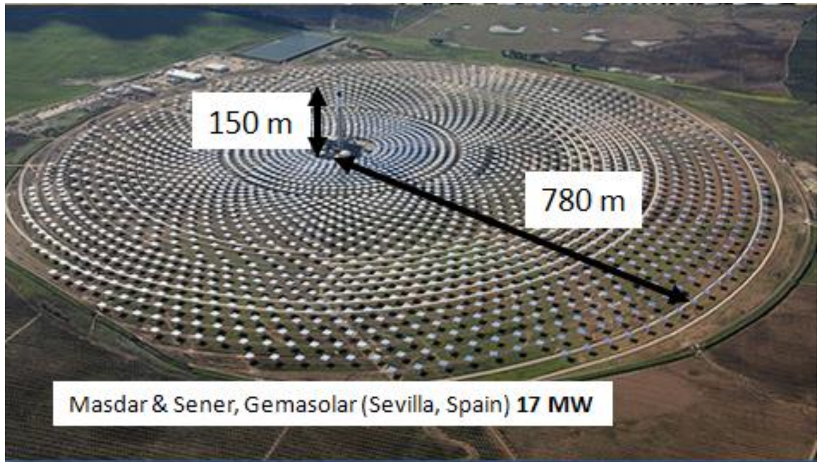
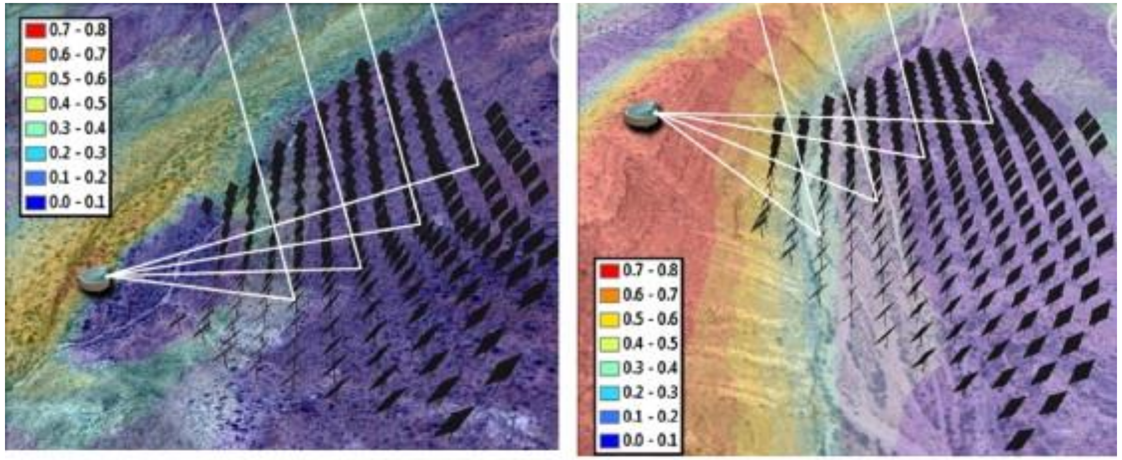
Example: Heliostat Fields – Construct on Plane or Hill?



Masdar & Sener, Collage: D. Codd

eSolar, Collage: D. Codd

- **Renewable energy** requires huge land areas and is expensive
- **Central receiver plants** - a promising scalable technology
- Can use hills in beam-down (CSPonD) or beam-up (“natural-tower")



(A) Beam-down (B) Beam-up

Noone, et int. Mitsos*, Solar Energy

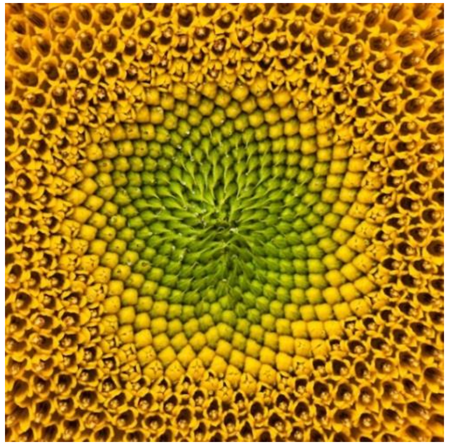
CSPonD: Slocum*, Codd, et int. Mitsos, Solar Energy

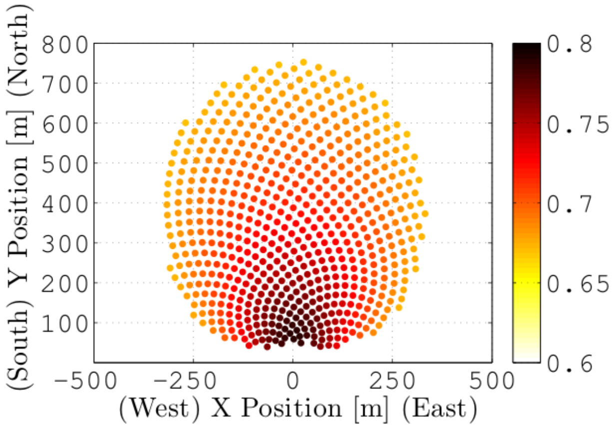
Example: Heliostat Fields – Optimization Applicable?

- Objective: Maximize field efficiency and minimize land area usage
  - Minimize economical & ecological costs
  - Factorial number of local minima
- Noone (with guidance by Mitsos) developed and validated a model suitable for optimization (fast yet accurate, compatible with reverse mode algorithmic differentiation)
- Heuristic global methods (genetic algorithm, multistart) prohibitive for realistic number of heliostats
- Local optimization from arbitrary initial guess not suitable as results are very sensitive to initial guess
- Heuristic solution tried: Start with existing designs and optimize locally
- Result obtained: Spiral pattern recognized by Prof. Manuel Torrilhon
- Long-term goal: Deterministic global optimization using Relaxation of Algorithms [1]

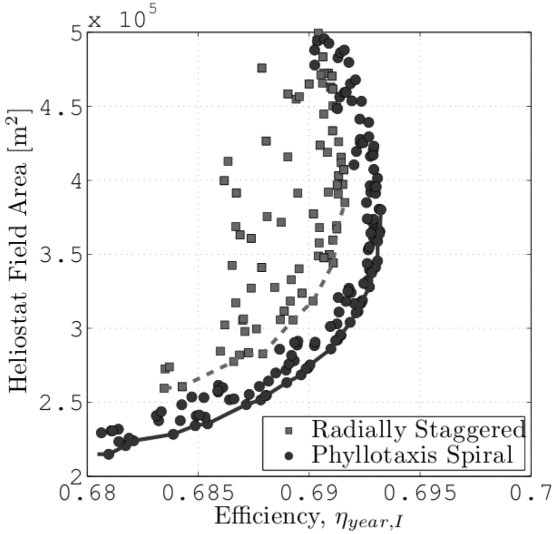
[1] Mitsos A., Chachuat B. and Barton P., McCormick-based relaxations of algorithms. SIAM Journal on Optimization, 2009

Example: Heliostat Field Optimization – Some Results





- Identified **spiral pattern** from **local optimization** of radially staggered pattern [1]
  - Abengoa concurrently proposed spiral
- Optimized biomimetic spiral → appreciable improvement in efficiency, substantial savings in land area.



http://www.bbc.co.uk/mundo/noticias/2012/01/120123_girasol_energia_solar_am.shtml, https://www.popsci.com/technology/article/2012-01/sunflower-design-inspires-more-efficient-solar-power-plants/ and picked up by many more…

[1] Noone C. J., Torrilhon M., Mitsos A., Heliostat field optimization: A new computationally efficient model and biomimetic layout, Solar Energy, 2012

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Examples of optimization problems - wind

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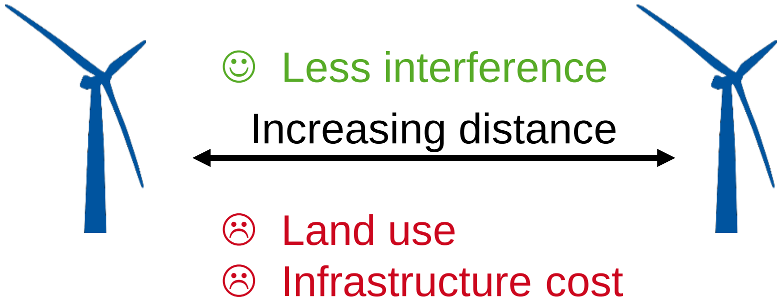
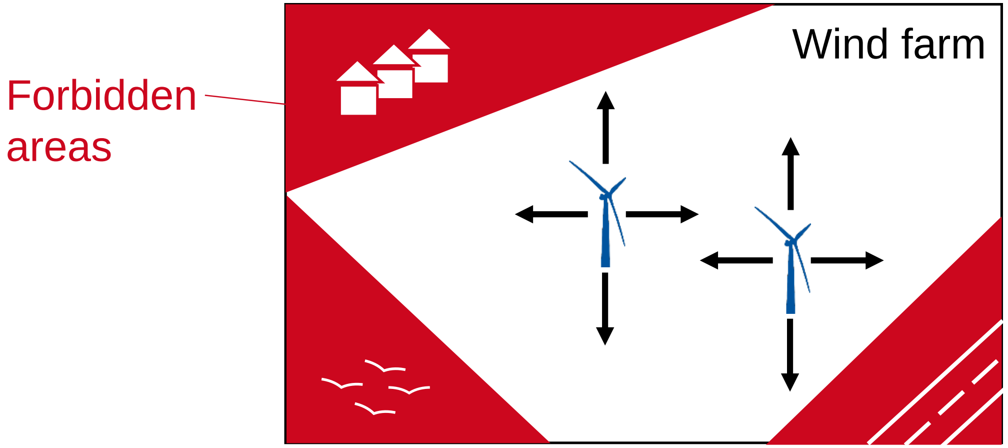
Example: Wind Farm Layout Optimization

- **Wind turbines** are built in groups (=wind farms)
  to produce more electricity in a given limited area
- **Wind farm layout:** Where to position turbines within farm limits?
  Potentially also: How many turbines?
- **Typical objectives:**
  - Maximize annual electricity production
  - Minimize levelized cost of electricity (=cost per unit of electrical energy)

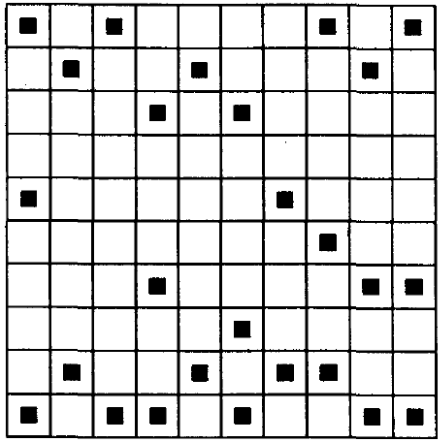
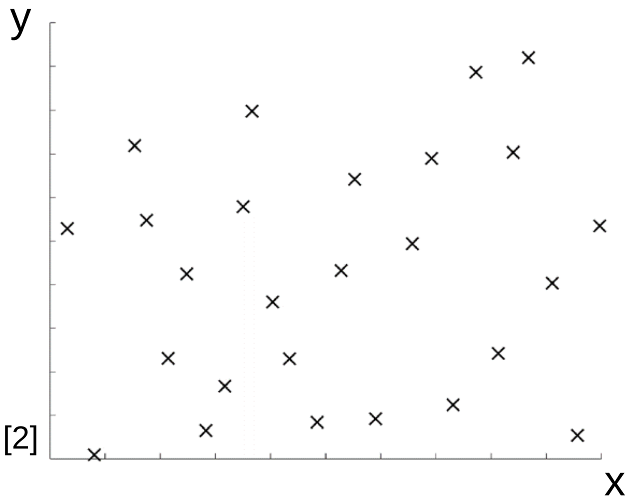
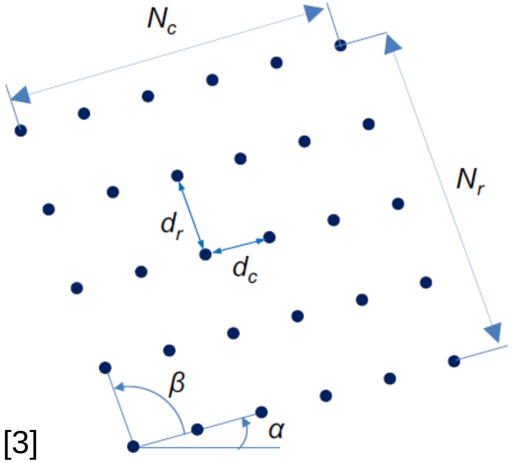
- **Key Factor:** Distance between turbines





[1] https://commons.wikimedia.org/wiki/File:Wind_farm_near_North_Sea_coast.jpg (CC BY-SA 4.0)

Example: Wind Farm Layout Optimization – How to Describe Layout?

Fixed cells	Continuous positions	Patterns
 [1]	 [2]	 [3]
☺ easy to optimize #turbines ☹ less freedom ☹ many discrete variables	☺ most freedom ☹ difficult to optimize #turbines ☹ many continuous variables	☺ few variables ☹ less freedom ☹ complex areas difficult

→ Has implications on applicable optimization algorithms & quality of solution

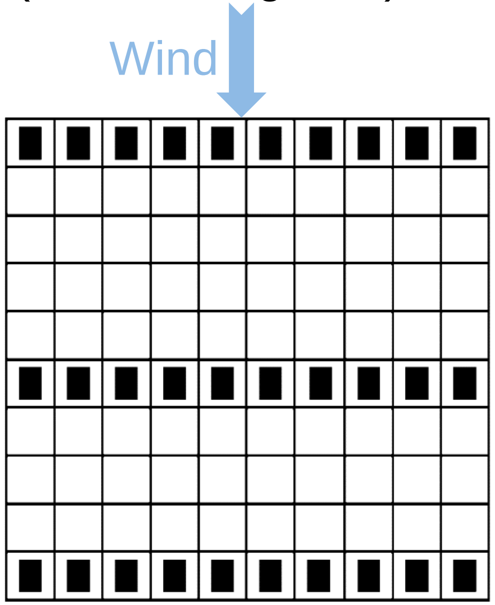
[1] Mosetti et al. (1994). J. Wind Eng. Ind. Aerod., 51, 105.
[2] DuPont & Cagan (2012). J. Mech. Des., 134, 081002. Mod.
[3] González et al. (2017). Appl. Energ., 200, 28.

Example: Wind Farm Layout Optimization – Global Optimization

- **Most basic case:** constant wind from one direction, minimize levelized cost of electricity

Benchmark solution

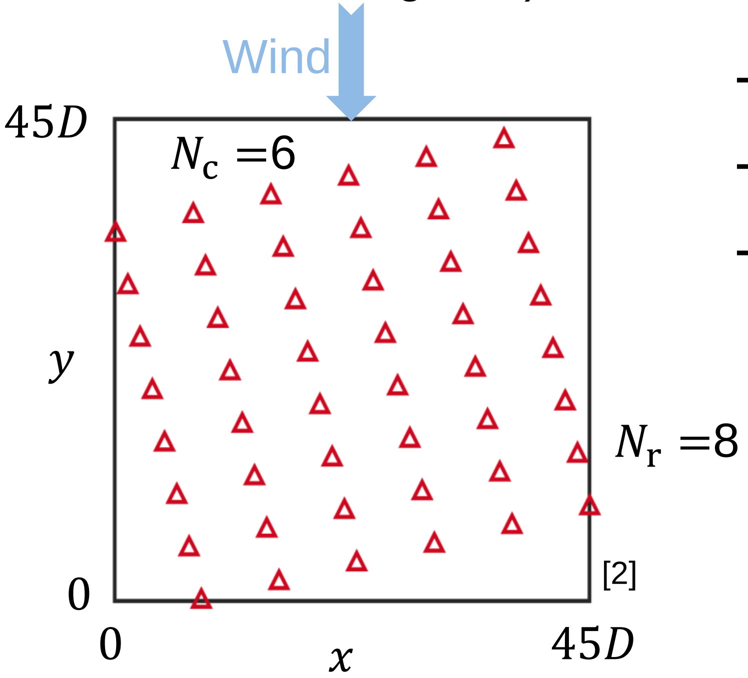
- Fixed cells approach
- Genetic algorithm (stochastic global)



[1]

Improved solution

- Pattern approach
- MAiNGO (open source, deterministic global)



[2]

→ Levelized cost of electricity - 13 %

→ Annual electricity production +68 %

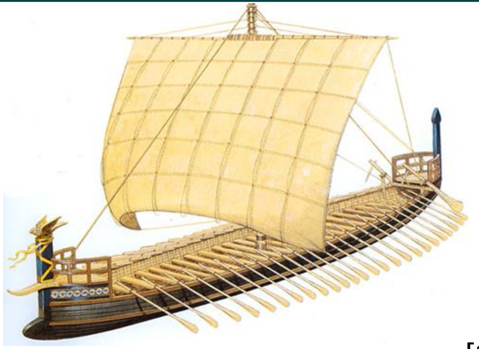
→ Efficiency +4.4 %-pt

→ Both are optimized layouts

→ Problem formulation and algorithm make a difference

[1] Grady et al. (2005), Renew. Energ., 30, 259.
[2] Bongartz (2020), in preparation.

Example: Sailing – Technology Choice



[1]

Ancient sailing: Fixed mast; no boom → mostly downwind

[2]

[3]

Classic sailing: Fixed mast; boom → can go upwind

[4]

Novel hulls (catamaran)
Novel sails (wing, …)

Typically, inventions by human creativity, not by mathematical optimization.

[5]

Windsurfing: Mast moves

[6]

Kite-surfing: No mast

[7]

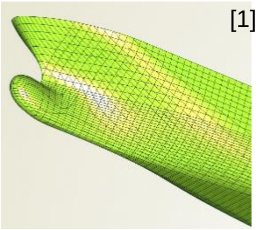
Hydrofoiling: wing in water.
From planning to flying!

[8]

Wing instead of sail or kite.
No mast, no boom, no ropes

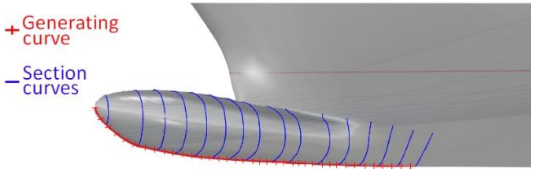
[1] via http://www.salimbeti.com/micenei/ships.htm [2] Photo credit Eva Lambidoni
[3] Photo credit Jörn Viell [4] Alexander Mitsos & Daniel Fouquet (skipper), (photo credit Eva Lambidoni)
[5] Alexander Mitsos (photo credit Stephanie Mitsos) [6] Verena Niem & Dimitris Chatzigeorgiou
[7] Sotiris Kontolios [8] Robby Naish

Example: Sailing – Optimization



CAD model of a ship‘s hull

Infinite degrees of freedom



Geometric parametrization of bulbous bow [2]

Complex physics! Coupled hydro-, aero- and structural-dynamics problem

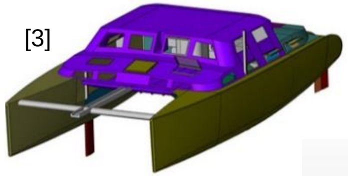
CAD model → Parametric modeler → Shape parameters → Mathematical modeling

Objective function

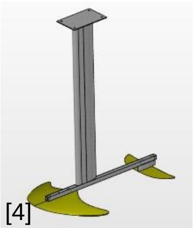
Constraints

Mathematical modeling → Optimization algorithm → Optimal shape

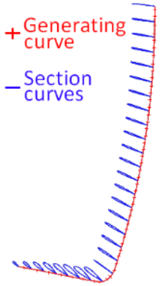
[3]



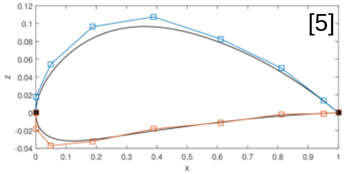
CAD model of a Catamaran



CAD model of a hydrofoil



Geometric parametrization of hydrofoil [2]



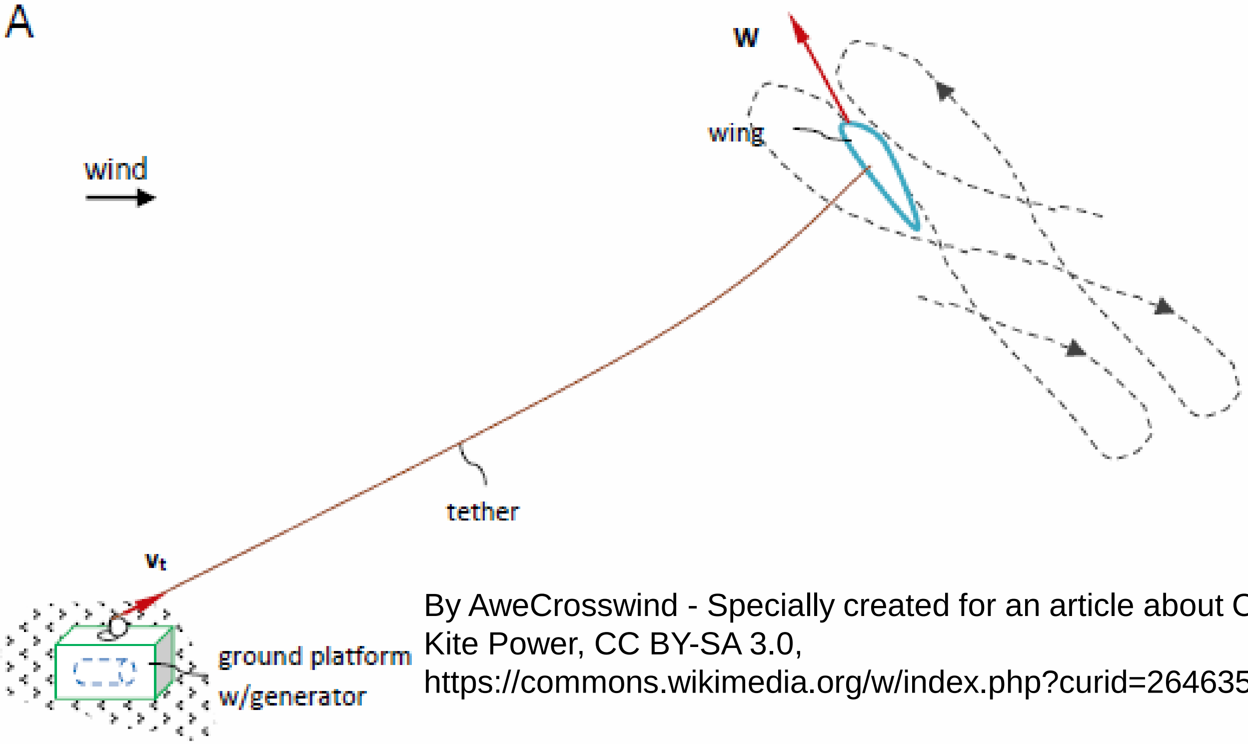
Exemplary geometry approximation using B-splines

Choice of parametrization decides the degrees of freedom

[1] via https://www.friendship-systems.com/solutions/for-ship-design (copyright free)
[2] Berrini et al., Geometric Modelling and Deformation for Shape Optimization of Ship Hulls and Appendages
[3] via http://www.wavescalpel.com/development-first-solidworks-cad-model-for-wavescalpel/ (copyright free)
[4] via https://grabcad.com/ (copyright free)
[5] Masters et al., A Geometric Comparison of Aerofoil Shape Parameterisation Methods, 2016

Renewable Electricity Generation by Kite: Optimization of Operation

- Wind power generation by kite



By AweCrosswind - Specially created for an article about Crosswind Kite Power, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=26463531

- Kite has to be moved to generate power, $\int F(t)v(t)dt > 0$
- Hard optimal control under uncertainty problem

- Optimization over finite control

$$\begin{aligned} &\underset{u(t)}{\text{maximize}} \quad \bar{T}(t_\mathrm{f}) := \frac{1}{t_\mathrm{f}} \int_0^{t_\mathrm{f}} T(t)dt, \\ &\text{subject to} \quad |u(t)| \leq u_\mathrm{max}, \\ &r \sin(\theta(t)) \cos(\phi(t)) \geq z_\mathrm{min}, \\ &|\psi(t)| \leq 2\pi. \end{aligned}$$

- Noisy data, uncertain wind prediction
- Inaccurate control model
- Path found by ad-hoc schemes or based on nonlinear model-predictive control

Costello, Francois & Bonvin European Journal of Control 2017

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Classification and issues of optimization

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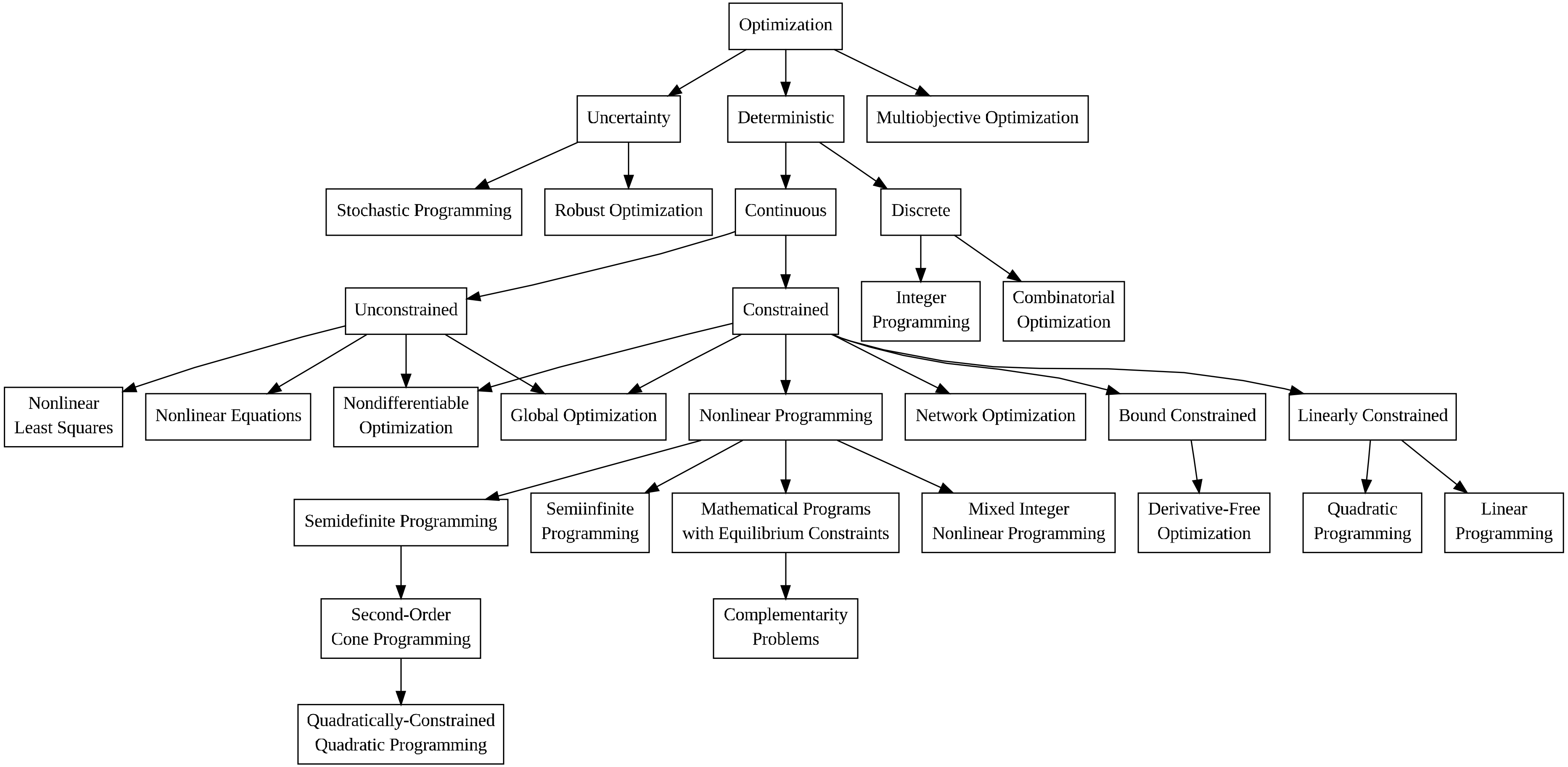
Classification of Optimization Problems

Optimization problems are classified with respect to the type of the objective function, constraints and variables, in particular

- **Linearity of objective function and constraints:**
  - Linear (LP) versus nonlinear programs (NLP)
  - NLPs can be convex or nonconvex, smooth or nonsmooth
- **Discrete and/or continuous variables:**
  - Integer programs (IP) and mixed-integer programs (MIP or MILP and MINLP, respectively)
- **Time-dependence:**
  - Dynamic optimization or optimal control programs (DO or OCP)
- **Stochastic or deterministic models and variables:**
  - Stochastic programs, semi-infinite optimization, …
- **Single objective vs multi-objective, single-level vs multi-level, ...**

NEOS Classification of Stationary Optimization Problems

http://neos-guide.org/content/optimization-taxonomy



Common Terminology Used in Numerical Optimization

- An **optimization problem:** mathematical formulation to find the best possible solution out of all feasible solutions. Typically comprising one or multiple objective function(s), decision variables, equality constraints and/or inequality constraints.

- An **algorithm** is a procedure for solving a problem based on conducting a sequence of specified actions. The terms ‘algorithm’ and ‘solution method’ are commonly used interchangeably.

- A **solver** is the implementation of an algorithm in a computer using a programming language. Often, the terms ‘solver’ and ‘software’ are used interchangeably.

Formulation and Solution of Optimization Problems

1. Determine variables and phenomena of interest through **systems analysis**
2. Define optimality criteria: **objective function(s)** and (additional) **constraints**
3. Formulate a **mathematical model** of the system and determination of **degrees of freedom** (number and nature)
4. Identify of the **problem class** (LP, QP, NLP, MINLP, OCP etc.)
5. Select (or develop) a suitable **algorithm**
6. Solve the problem using a numerical **solve**r
7. **Verify the solution** through sensitivity analysis, understand results, …

Some Issues with Optimization

- Not a button-press technology
  - Need expertise for model formulation, algorithm selection and tuning, checking results, …
- “Optimizer's curse”: solution using good algorithm and bad model will look better than what it is
  - Random error: if the model has a random error and we optimize, the true objective value of the solution found will be worse than the calculated one
  - If model allows for nonphysical solution with good objective value, good optimizer will pick such
    - On the other hand, model has to just lead in correct direction, not be correct
- Many engineering (design) problems are nonconvex, but global algorithms are inherently very expensive
- Often optimal solution at constraint, thus tradeoff good vs. robust solution

Check Yourself

- What is the difference between a nonlinear program, an optimal control problem and a stochastic program?
- What are the steps in formulating and solving an optimization problem?
- What are some issues in optimization?
- Formulate the application of your interest as an optimization problem

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Formal definition of optimization

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Some Simple Optimization Problems and Their Solutions

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$ objective function

$$\text{s.t.} \quad c_i(\boldsymbol{x}) = 0, \forall i \in E$$ equality constraints (EC)

$$c_i(\boldsymbol{x}) \leq 0, \forall i \in I$$ inequality constraints (IC)

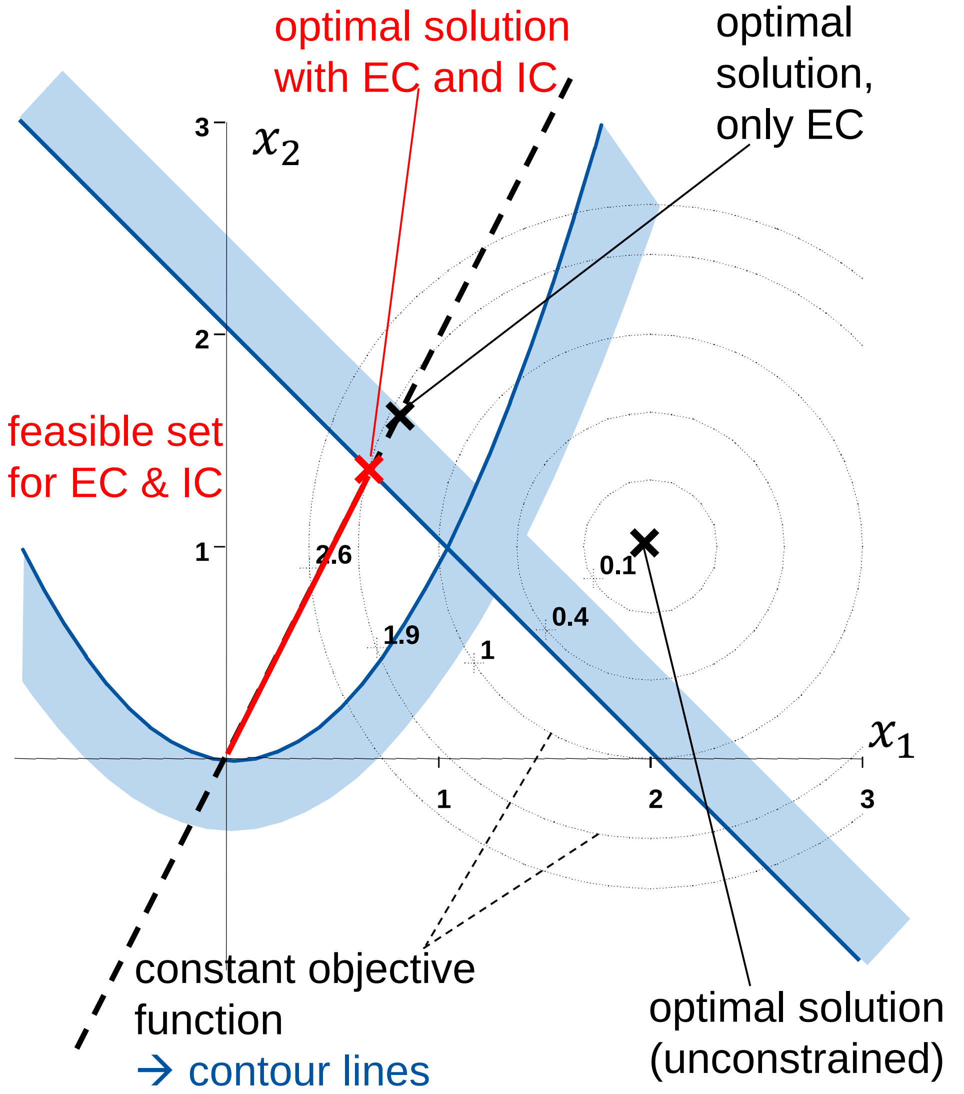
Example:

$$\min_{\boldsymbol{x}} (x_1 - 2)^2 + (x_2 - 1)^2$$

$$\text{s.t.} \quad x_2 - 2x_1 = 0$$

$$x_1^2 - x_2 \leq 0$$

$$x_1 + x_2 \leq 2$$



Nonlinear Optimization Problem (Nonlinear Program, NLP)

General formulation:

$$\min_{\boldsymbol{x}\in D} f(\boldsymbol{x})$$

$$\text{s.t.} \quad c_i(\boldsymbol{x}) = 0, i \in E$$

$$c_i(\boldsymbol{x}) \leq 0, i \in I$$

$\boldsymbol{x} = [x_1, x_2, \ldots, x_n]^T \in D \subseteq R^n$ a vector (point in *n*-dimensional space)

D **host set**

$f : D \to R$ **objective function**

$c_i : D \to R$ constraint functions $\forall\, i \in E \cup I$

E the index set of **equality constraints**

I the index sets of **inequality constraints**

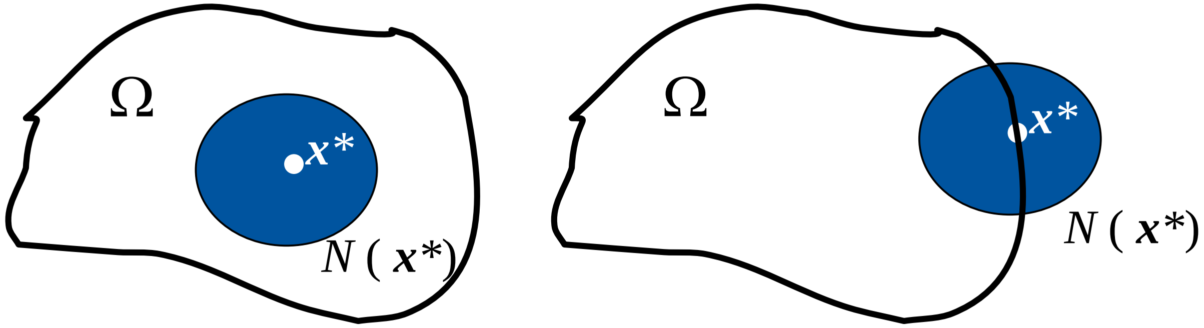
The **constraints** and the host set define **the feasible set**, i.e., the set of all feasible solutions:

$$\Omega = \{\boldsymbol{x} \in D \mid c_i(\boldsymbol{x}) \leq 0\ \forall\, i \in I, c_i(\boldsymbol{x}) = 0\ \forall\, i \in E\}$$

Equivalent formulation: $\boxed{\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x})}$

Definition (optimal solution, minimum):

$$\boxed{\min_{x \in \Omega} f(\boldsymbol{x})}$$



Solution in interior of feasible set

Solution on boundary of feasible set

a) $\boldsymbol{x}^*$ is a local solution if $\boldsymbol{x}^* \in \Omega$ and a neighborhood $N(\boldsymbol{x}^*)$ of $\boldsymbol{x}^*$ exists: $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})\ \forall \boldsymbol{x} \in N(\boldsymbol{x}^*) \cap \Omega$

b) $\boldsymbol{x}^*$ is a strict local solution if $\boldsymbol{x}^* \in \Omega$ and a neighborhood $N(\boldsymbol{x}^*)$ of $\boldsymbol{x}^*$ exists: $f(\boldsymbol{x}^*) < f(\boldsymbol{x})\ \forall \boldsymbol{x} \in N(\boldsymbol{x}^*) \cap \Omega, \boldsymbol{x} \neq \boldsymbol{x}^*$

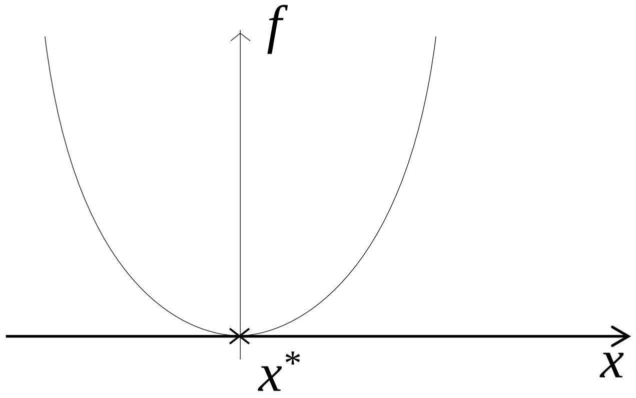
c) $\boldsymbol{x}^*$ is a global solution if $\boldsymbol{x}^* \in \Omega$ and $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})\ \forall \boldsymbol{x} \in \Omega$

More formally, these are solution points

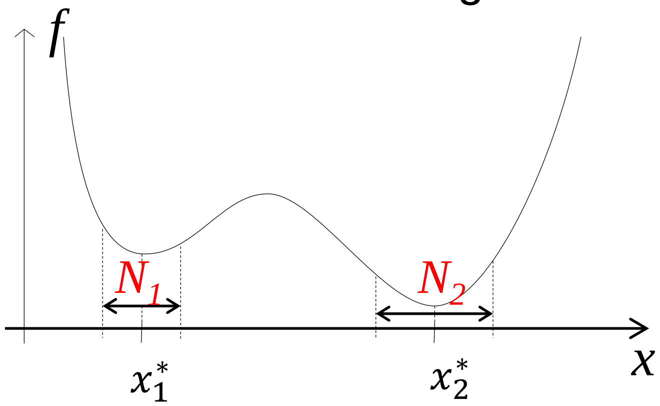
Optimal Solution – Some Examples

$$\min_{x \in R} f(x)$$

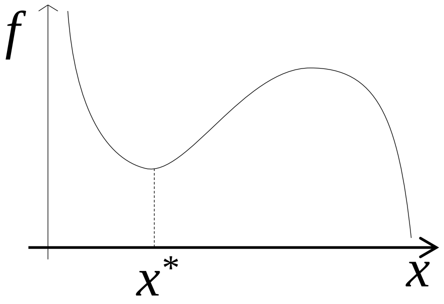
a) strict global minimum



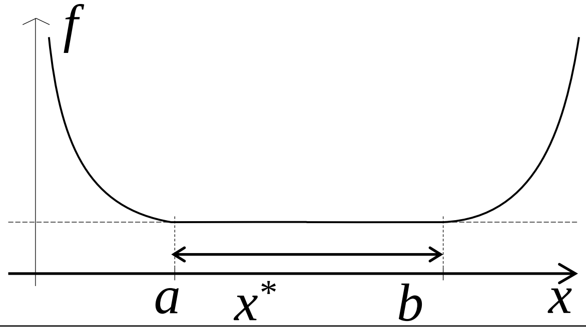
b) Two strict local minima,
out of which one is strict global minimum



c) a strict local minimum,
no global minimum



d) each $x^* \in [a, b]$ is a local and global minimum
no strict minima



Check Yourself

- Write down the general definition of optimization problem
- Definition of local and global solution of an optimization problem?
- Is every local solution also a global solution? Is every global solution also a local solution?
- What is the feasible set of an optimization problem?
- Can a solution be in the interior of the feasible set? On its boundary? Outside the feasible set?
  - Draw the corresponding picture
- For given problem recognize the (local or global) optimal solution points