Optimization for Machine Learning

November 3, 2022

TC2 - Optimisation

Université Paris-Saclay, Orsay, France

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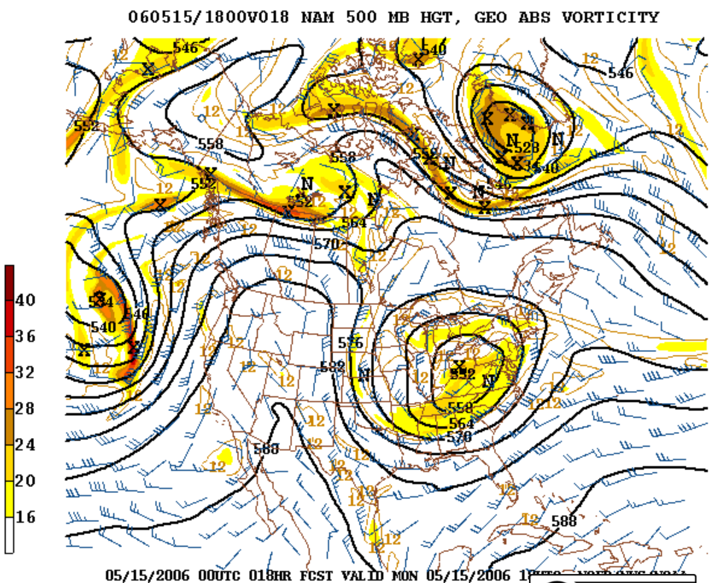
What is Optimization?



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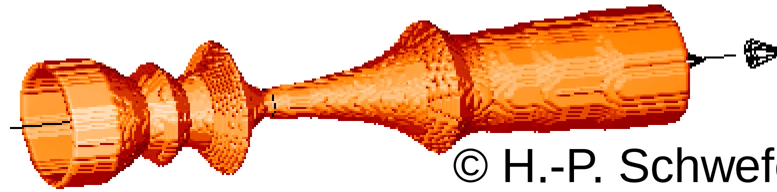

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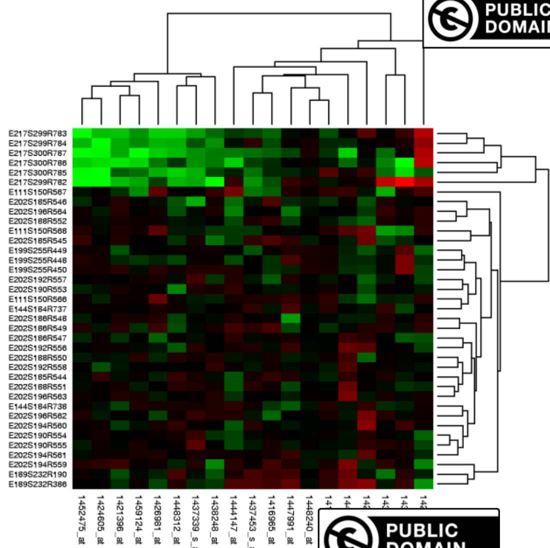

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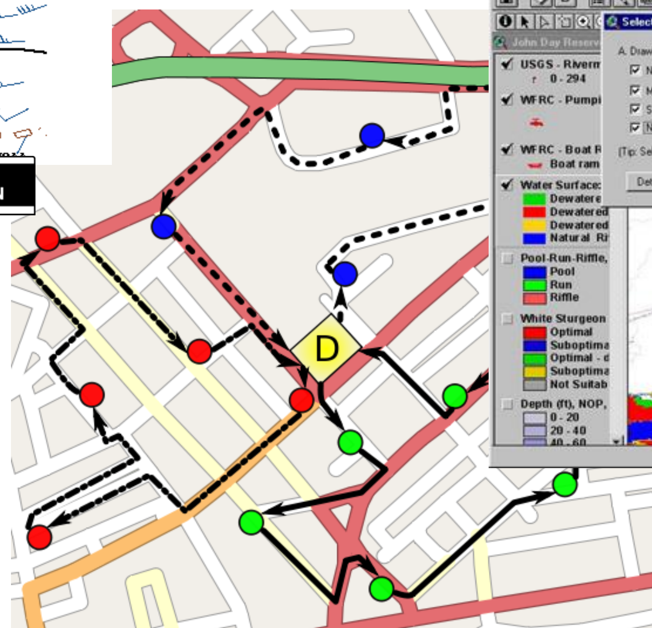

Maly LOLek
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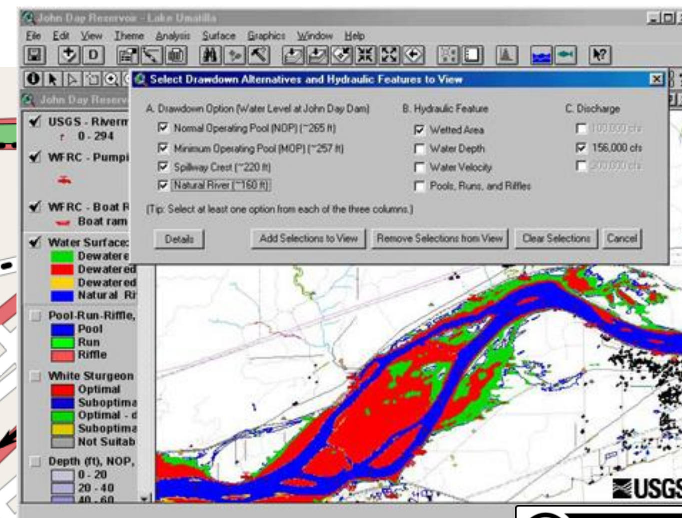

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What is Optimization?

Typically, we aim at

- finding solutions x which minimize f(x) in the shortest time possible
  (maximization is reformulated as minimization)

- or finding solutions x with as small f(x) in the shortest time possible
  (if finding the exact optimum is not possible)

Course Overview

Date		Topic
Thu, 3.11.2022	DB	Introduction
Thu, 10.11.2022	AA	Continuous Optimization I: differentiability, gradients, convexity, optimality conditions
Thu, 17.11.2022	AA	Continuous Optimization II: constrained optimization, gradient-based algorithms, stochastic gradient
Thu, 24.11.2022	AA	Continuous Optimization III: stochastic algorithms, derivative-free optimization written test / « contrôle continue »
Thu, 1.12.2022	DB	Discrete Optimization I: graph theory, greedy algorithms
Thu, 8.12.2022	DB	Discrete Optimization II: dynamic programming, branch&bound
Thu 15.12.2022	DB	Written exam

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Thu 15.12.2022	DB	Written exam
		classes from 13h30 – 16h45 (2nd break at end)

Remarks

- possibly not clear yet what the lecture is about in detail

- but there will be always examples and small exercises to learn "on-the-fly" the concepts and fundamentals

Overall goals:

❶ give a broad overview of where and how optimization is used

❷ understand the fundamental concepts of optimization algorithms

The Final Exam

- will be a written multiple choice exam
- open book
- 2 hours, starting from 13h30
- counts 60% of overall grade

- please prepare pen&paper

Intermediate Written Exam ("contrôle continu")

- instead of a group project
- one smaller written exam/test of about 20min
  - November 24 (4^{th} lecture)
- goal: spread learning of lecture content over the course
- accounts 40% to overall grade
- might be in part multiple choice

All information also available at

`http://www.cmap.polytechnique.fr/~dimo.brockhoff/optimizationSaclay/2022/`

(in particular the lecture slides)

Overview of Today's Lecture

- More examples of optimization problems
  - introduce some basic concepts of optimization problems such as domain, constraint, ...
- Beginning of continuous optimization part
  - typical difficulties in continuous optimization
  - differentiability
  - … [we'll see how far we get]

General Context Optimization

Given:

set of possible solutions *Search space*

quality criterion *Objective function*

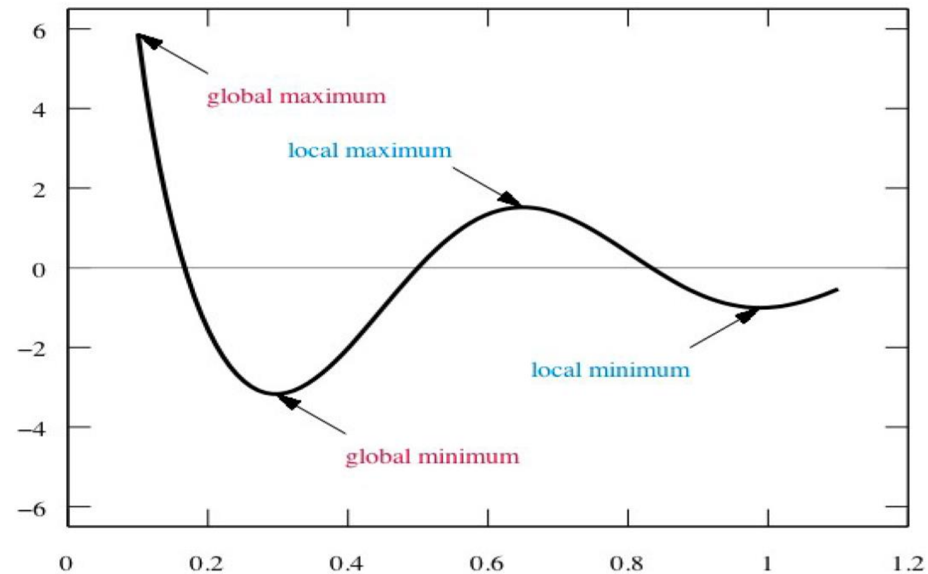
Objective:

Find the best possible solution for the given criterion

Formally:

Maximize or minimize

$$\mathcal{F}: \Omega \longmapsto \mathbb{R},$$
$$x \longmapsto \mathcal{F}(x)$$



Constraints

Maximize or minimize

$$\mathcal{F}: \Omega \longmapsto \mathbb{R},$$
$$x \longmapsto \mathcal{F}(x)$$

unconstrained Ω

Maximize or minimize

$$\mathcal{F}: \Omega \longmapsto \mathbb{R},$$
$$x \longmapsto \mathcal{F}(x)$$

where $g_i(x) \leq 0$
$$h_i(x) = 0$$

example of a constrained Ω

Constraints explicitly or implicitly define the feasible solution set

[e.g. ||x|| - 7 ≤ 0 vs. every solution should have at least 5 zero entries]

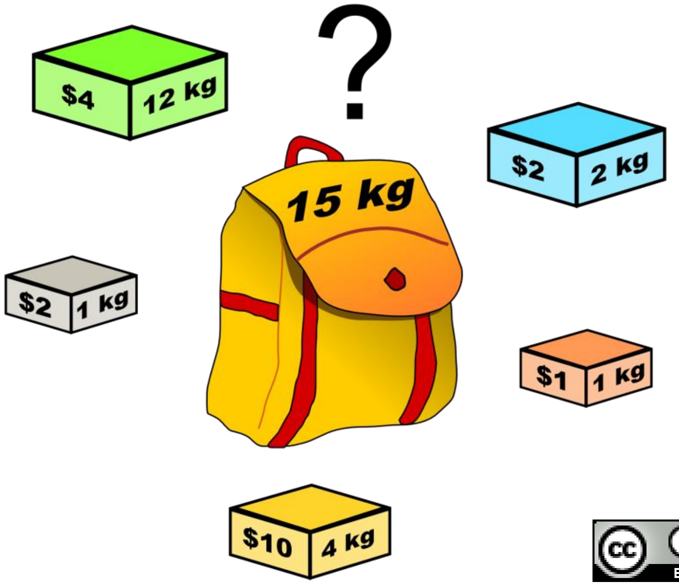
Hard constraints *must* be satisfied while soft constraints are preferred to hold but are not required to be satisfied

[e.g. constraints related to manufacturing precisions vs. cost constraints]

Example 1: Combinatorial Optimization

Knapsack Problem

- Given a set of objects with a given weight and value (profit)
- Find a subset of objects whose overall mass is below a certain limit and maximizing the total value of the objects



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Dake

[Problem of resource allocation with financial constraints]

$$\max \sum_{j=1}^{n} p_j x_j \quad \text{with } x_j \in \{0,1\}$$

$$\text{s.t.} \sum_{j=1}^{n} w_j x_j \leq W$$

$$\Omega = \{0,1\}^n$$

Example 2: Combinatorial Optimization

Traveling Salesperson Problem (TSP)

- Given a set of cities and their distances
- Find the shortest path going through all cities

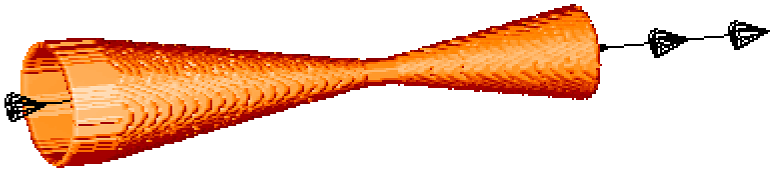
$$\Omega = S_n \text{ (set of all permutations)}$$

Example 3: A "Manual" Engineering Problem

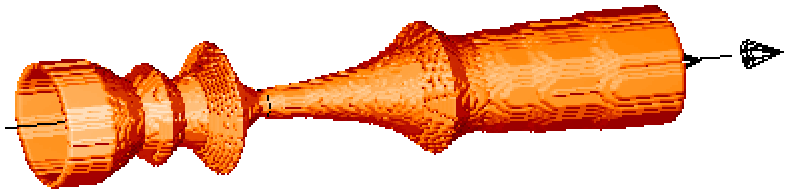
Optimizing a Two-Phase Nozzle [Schwefel 1968+]

- maximize thrust under constant starting conditions
- one of the first examples of Evolution Strategies

initial design:



final design:



$\Omega =$ all possible nozzles of given number of slices

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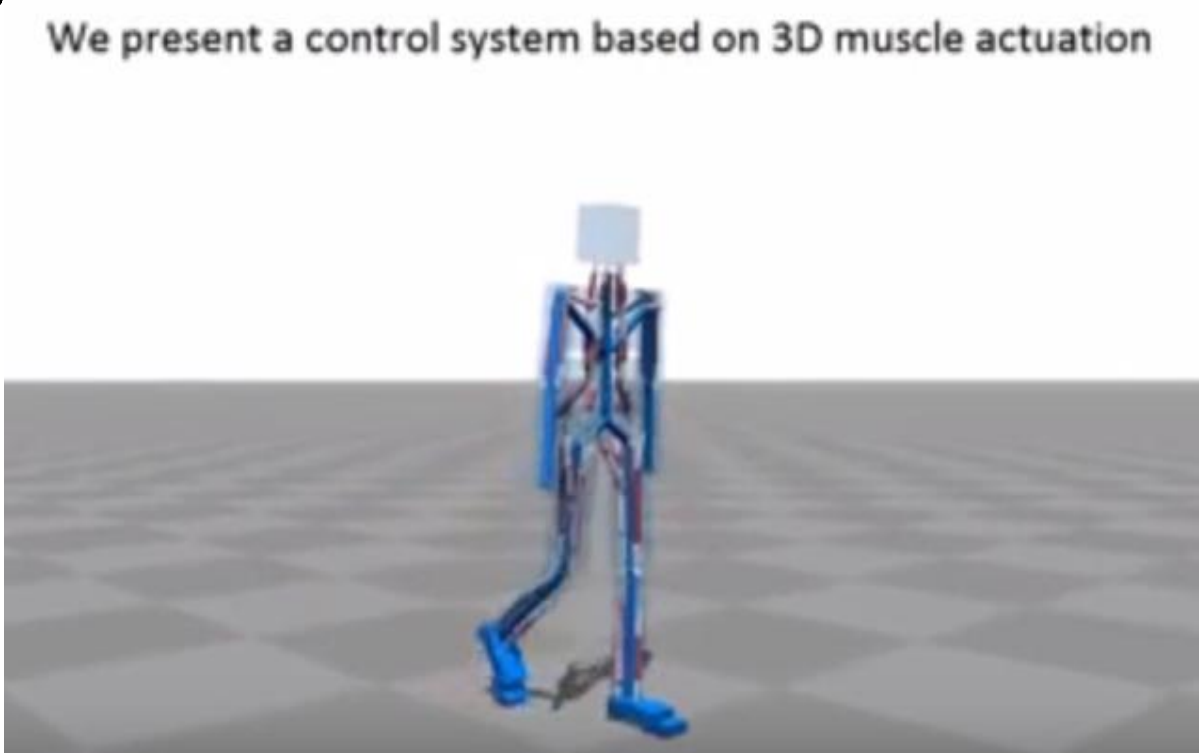
[http://ls11-www.cs.uni-dortmund.de/people/schwefel/EADemos/]

Example 4: Continuous Optimization Problem

Computer simulation teaches itself to walk upright (virtual robots (of different shapes) learning to walk, through stochastic optimization (CMA-ES)), by Utrecht University:

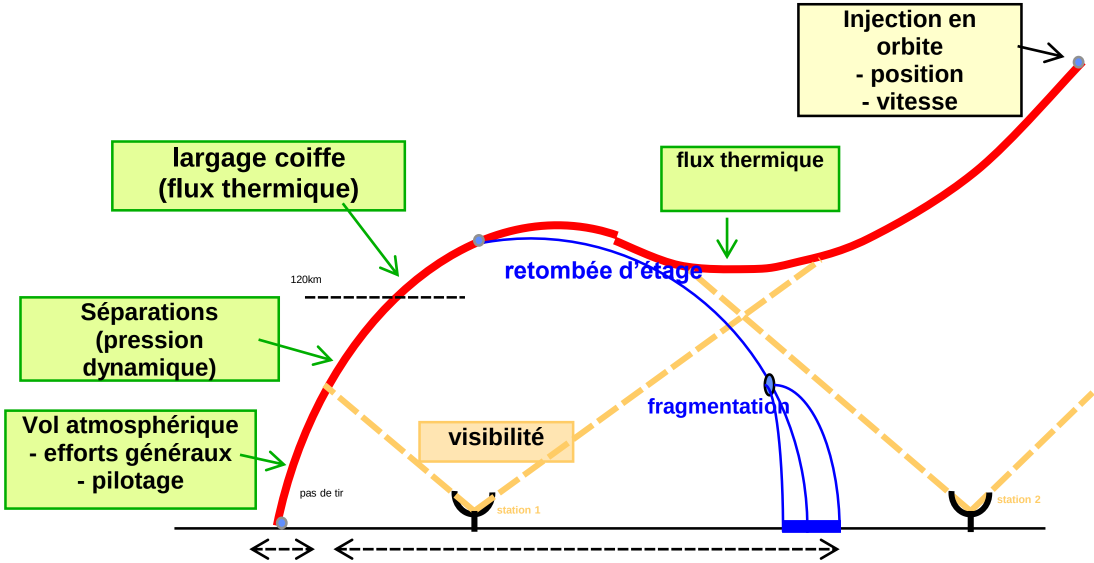


https://www.youtube.com/watch?v=pgaEE27nsQw

T. Geitjtenbeek, M. Van de Panne, F. Van der Stappen: "Flexible Muscle-Based Locomotion for Bipedal Creatures", SIGGRAPH Asia, 2013.

Design of a Launcher

Poppy



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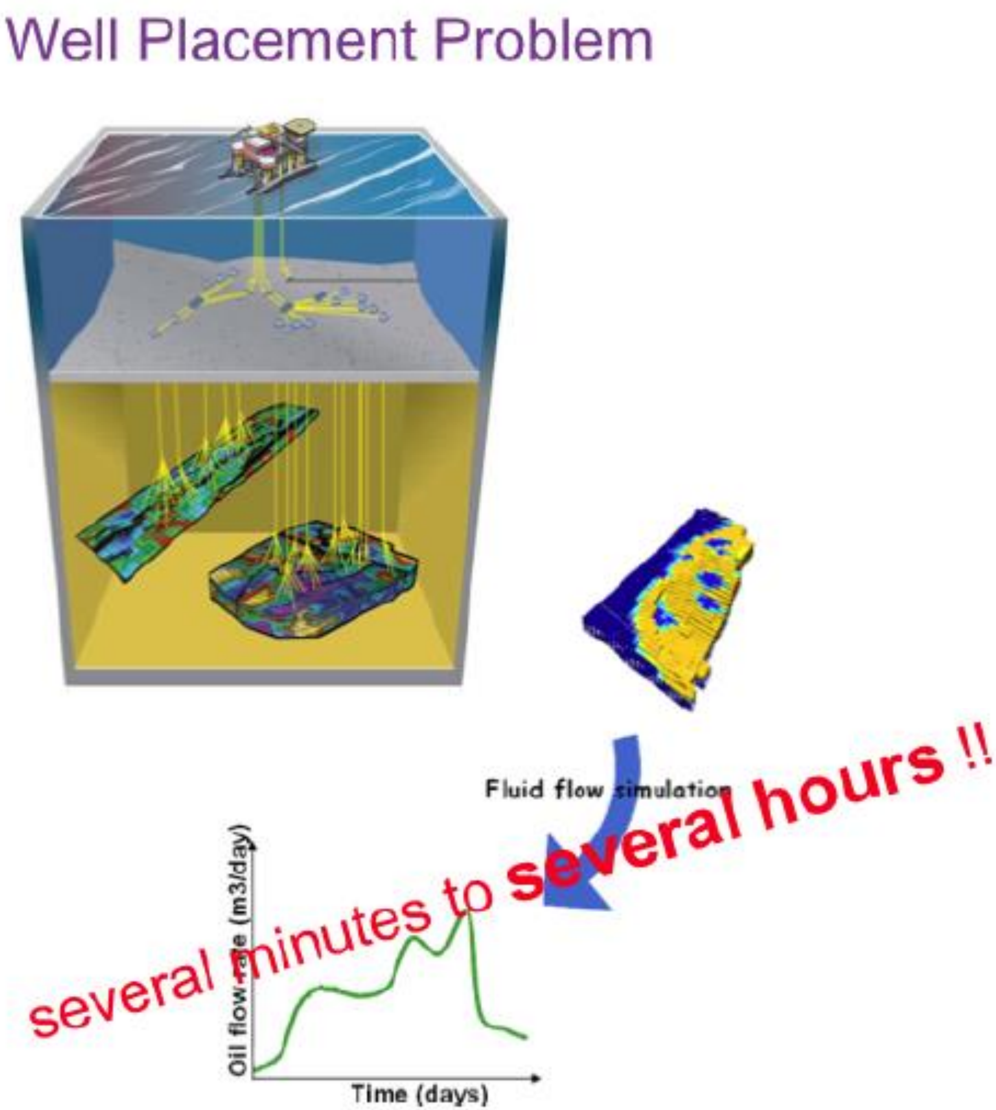
$$\Omega = \mathbb{R}^{23}$$

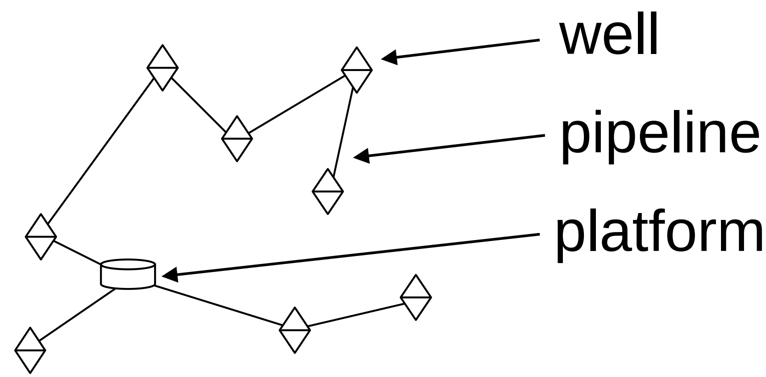
- Scenario: multi-stage launcher brings a satellite into orbit
- Minimize the overall cost of a launch
- Parameters: propellant mass of each stage / diameter of each stage / flux of each engine / parameters of the command law

23 continuous parameters to optimize

+ constraints

Example 6: An Expensive Real-World Problem





for a given structure, per well:

- angle & distance to previous well
- well depth

structure + $\mathbb{R}_+^3 \cdot \#\text{wells}$

$\sigma \in \Omega$: variable length!

Example 7: Data Fitting – Data Calibration

Objective

- Given a sequence of data points $(\boldsymbol{x}_i, y_i) \in \mathbb{R}^p \times \mathbb{R}, i = 1, \dots, N$, find a model "$y = f(\boldsymbol{x})$" that *"explains"* the data

experimental measurements in biology, chemistry, ...

- In general, choice of a parametric model or family of functions $(f_\theta)_{\theta \in \mathbb{R}^n}$

use of expertise for choosing model

or only a simple model is affordable (e.g. linear, quadratic)

- Try to find the parameter $\theta \in \mathbb{R}^n$ fitting best to the data

Fitting best to the data

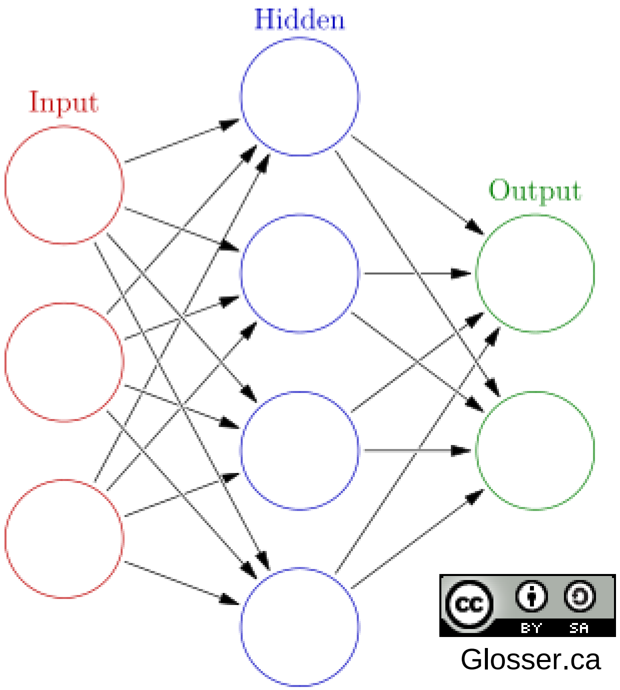
Minimize the quadratic error:

$$\min_{\theta \in \mathbb{R}^n} \sum_{i=1}^{N} |f_\theta(\boldsymbol{x}_i) - y_i|^2$$

Example 8: Deep Learning

Actually the same idea:

match model best to given data



Glosser.ca

Model here:

artificial neural nets
with many hidden layers
(aka deep neural networks)

Parameters to tune:

- weights of the connections (continuous parameter)
- topology of the network (discrete)
- firing function (less common)

Specificity:

- large amount of training data, hence often batch learning

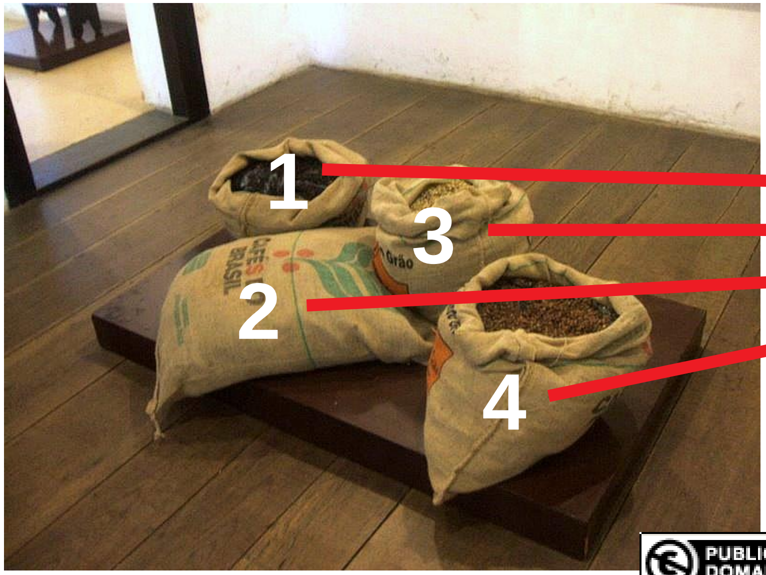
Example 9: Hyperparameter Tuning

Scenario:

- many existing algorithms (in ML and elsewhere) have internal parameters
  - "In machine learning, a hyperparameter is a parameter whose value is set before the learning process begins." --- Wikipedia
  - can be model parameters
    - #trees in random forest
    - #nodes in neural net
    - …
  - or other generic parameters such as learning rates, …
- choice has typically a big impact and is not always obvious
- search space often mixed discrete-continuous or even categorical

Coffee Tasting Problem

- Find a mixture of coffee in order to keep the coffee taste from one year to another
- Objective function = opinion of one expert



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Quasipalm

M. Herdy: "Evolution Strategies with subjective selection", 1996

Many Problems, Many Algorithms?

Observation:

- Many problems with different properties
- For each, it seems a different algorithm?

In Practice:

- often most important to categorize your problem first in order to find / develop the right method
- → problem types

Problem Types

- discrete vs. continuous
  - discrete: integer (linear) programming vs. combinatorial problems
  - continuous: linear, quadratic, smooth/nonsmooth, blackbox/DFO, ...
  - both discrete&continuous variables: mixed integer problem
  - categorical variables (“no order”)
- unconstrained vs. constrained (and then which type of constraint)

Not covered in this introductory lecture:

- deterministic vs. stochastic outcome of objective function(s)
- one or multiple objective functions

Example: Numerical Blackbox Optimization

Typical scenario in the continuous, unconstrained case:

Optimize $f: \Omega \subset \mathbb{R}^n \mapsto \mathbb{R}^k$

derivatives not available or not useful

General Concepts in Optimization

- search domain
  - discrete or continuous or mixed integer or even categorical
  - finite vs. infinite dimension
- constraints
  - bound constraints (on the variables only)
  - linear/quadratic/non-linear constraints
  - blackbox constraints
  - many more

(see e.g. Le Digabel and Wild (2015), https://arxiv.org/abs/1505.07881)

Further important aspects (in practice):

- deterministic vs. stochastic algorithms
- exact vs. approximation algorithms vs. heuristics
- anytime algorithms
- simulation-based optimization problem / expensive problem

continuous optimization

Continuous Optimization

- Optimize f: $\begin{cases} \Omega \subset \mathbb{R}^n \to \mathbb{R} \\ x = (x_1, \ldots, x_n) \to f(x_1, \ldots, x_n) \end{cases}$

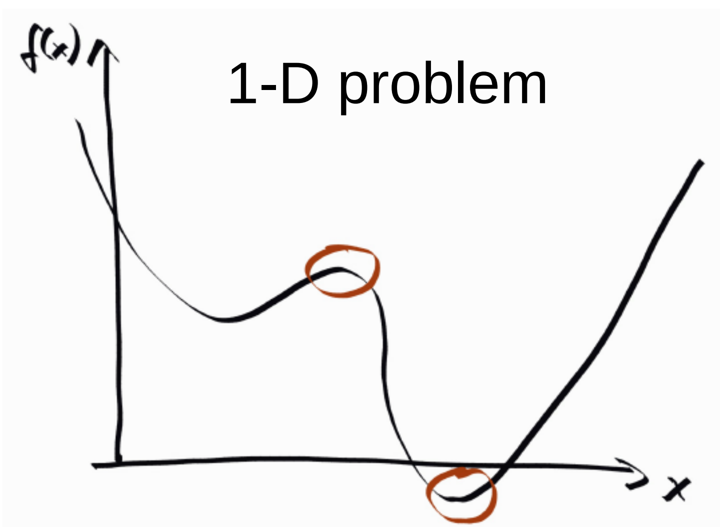
  $\in \mathbb{R}$

  unconstrained optimization

- Search space is continuous, i.e. composed of real vectors $x \in \mathbb{R}^n$

- $n = \begin{cases} \text{dimension of the problem} \\ \text{dimension of the search space } \mathbb{R}^n \text{ (as vector space)} \end{cases}$

1-D problem



2-D level sets

Unconstrained vs. Constrained Optimization

Unconstrained optimization

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

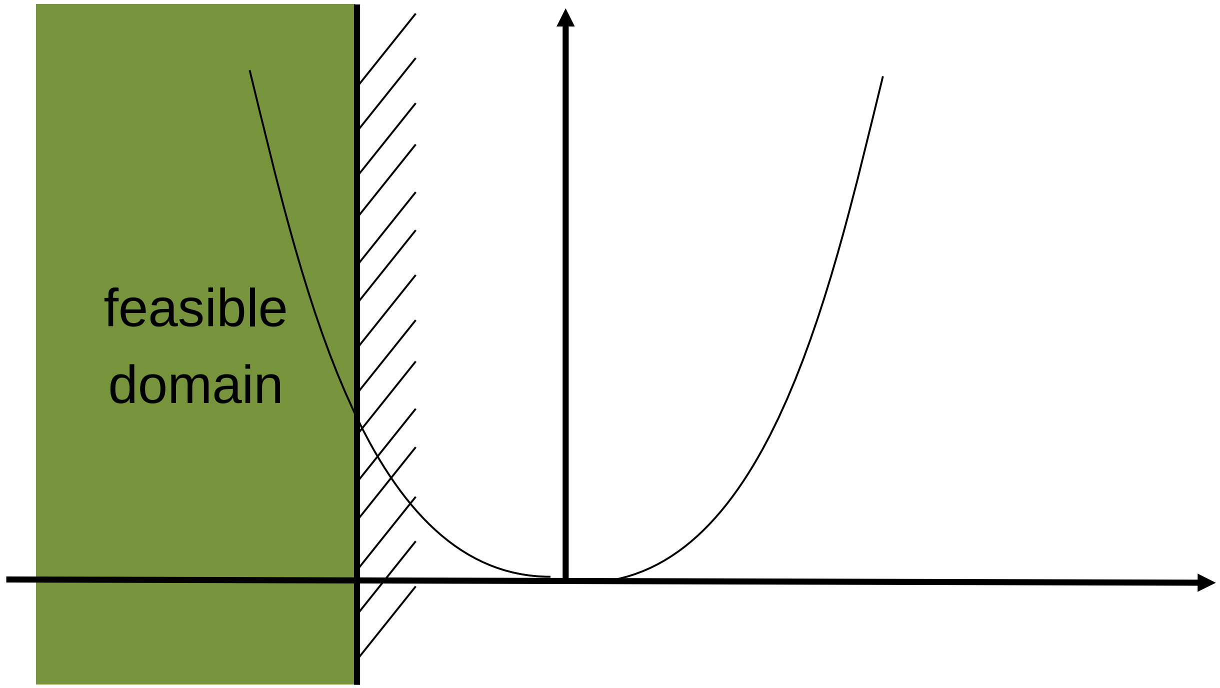
Constrained optimization

- Equality constraints: $\inf \{f(x) \mid x \in \mathbb{R}^n, g_k(x) = 0, 1 \leq k \leq p\}$
- Inequality constraints: $\inf \{f(x) \mid x \in \mathbb{R}^n, g_k(x) \leq 0, 1 \leq k \leq p\}$

where always $g_k\colon \mathbb{R}^n \to \mathbb{R}$

Example of a Constraint

$$\min_{x \in \mathbb{R}} f(x) = x^2 \text{ such that } x \leq -1$$



Analytical Functions

Example: 1-D

$$f_1(x) = a(x - x_0)^2 + b$$

where $x, x_0, b \in \mathbb{R}, a \in \mathbb{R}$

Generalization:

convex quadratic function

$$f_2(x) = (x - x_0)^T A \, (x - x_0) + b$$

where $x, x_0 \in \mathbb{R}^n, b \in \mathbb{R} \;\; , A \in \mathbb{R}^{\{\mathrm{n} \times n\}}$

and A symmetric positive definite (SPD)

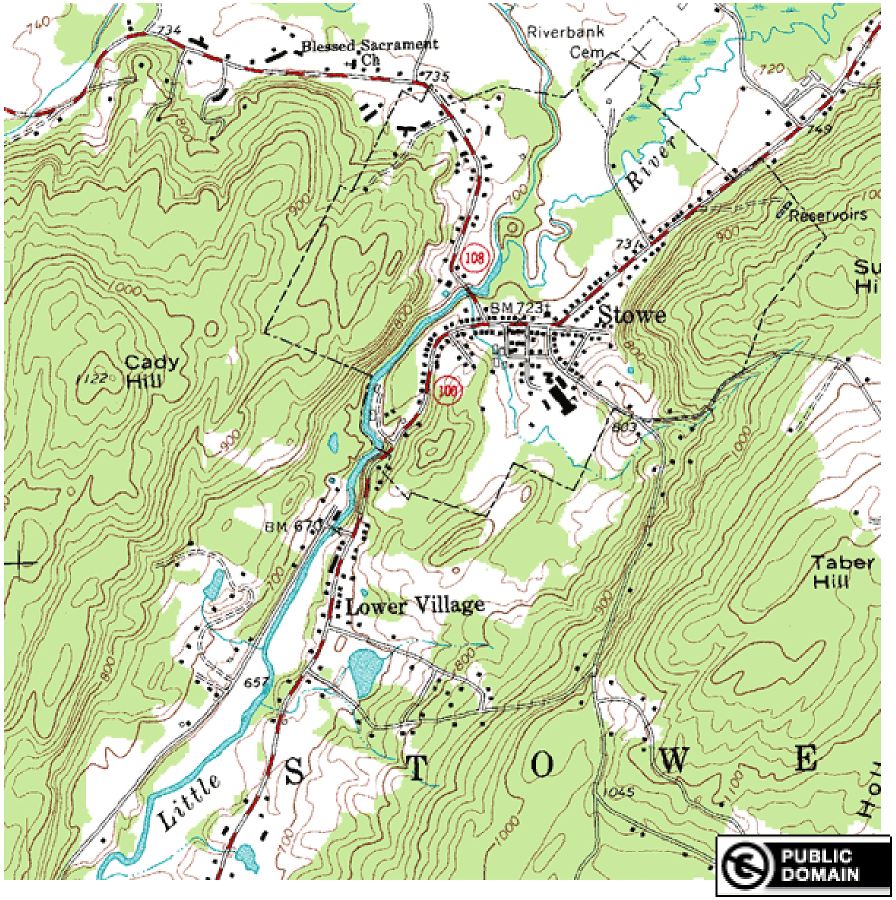
Exercise:
What is the minimum of $f_2(x)$?

Continuation of exercise:
What are the level sets of f_2?

Reminder: level sets of a function

$$L_c = \{x \in \mathbb{R}^n \mid f(x) = c\}$$

(similar to topography lines / level sets on a map)



Levels Sets of Convex Quadratic Functions

Continuation of exercise:
What are the level sets of f_2?

- Probably too complicated in general, thus an example here
- Consider $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}, b = 0, n = 2$
  a) Compute $f_2(x)$.
  b) Plot the level sets of $f_2(x)$.
  c) More generally, for $n = 2$, if A is SPD with eigenvalues $\lambda_1 = 9$ and $\lambda_2 = 1$, what are the level sets of $f_2(x)$?

What Makes a Function Difficult to Solve?

- dimensionality

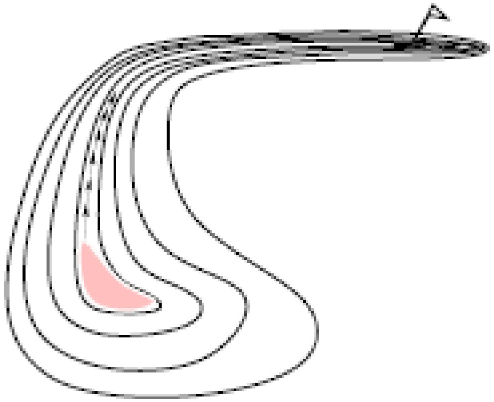
  (considerably) larger than three

- non-separability

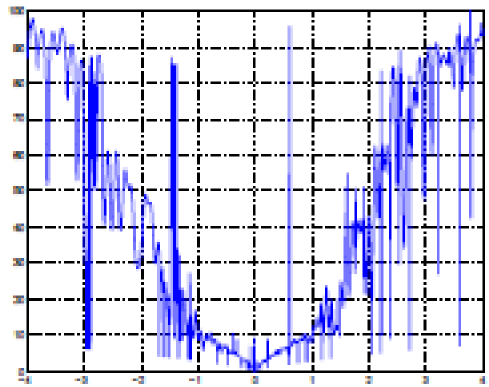
  dependencies between the objective variables

- ill-conditioning
- ruggedness

  non-smooth, discontinuous, multimodal, and/or noisy function



a narrow ridge



cut from 3D example, solvable with an evolution strategy

Curse of Dimensionality

- The term *Curse of dimensionality* (Richard Bellman) refers to problems caused by the rapid increase in volume associated with adding extra dimensions to a (mathematical) space.

- Example: Consider placing 100 points onto a real interval, say $[0,1]$. To get similar coverage, in terms of distance between adjacent points, of the 10-dimensional space $[0,1]^{10}$ would require $100^{10} = 10^{20}$ points. The original 100 points appear now as isolated points in a vast empty space.

- Consequently, a search policy (e.g. exhaustive search) that is valuable in small dimensions might be useless in moderate or large dimensional search spaces.

Separable Problems

Definition (Separable Problem)

A function f is separable if

$$\underset{(x_1,\dots,x_n)}{\operatorname{argmin}} f(x_1,\dots,x_n) = \left(\underset{x_1}{\operatorname{argmin}} f(x_1,\dots),\dots,\underset{x_n}{\operatorname{argmin}} f(\dots,x_n)\right)$$

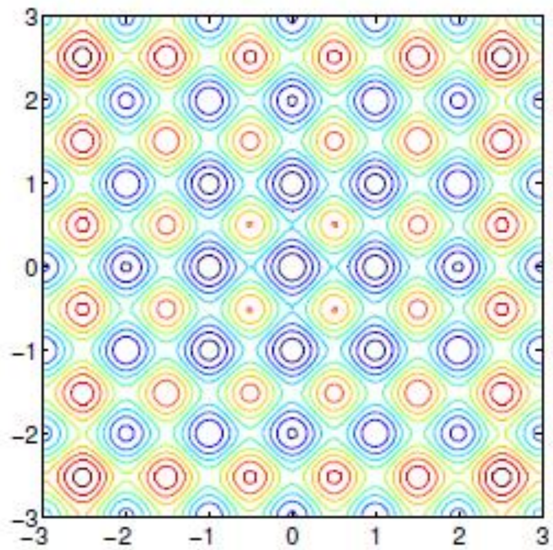
$\Longrightarrow$ it follows that f can be optimized in a sequence of n independent 1-D optimization processes

Example:

Additively decomposable functions

$$f(x_1,\dots,x_n) = \sum_{i=1}^{n} f_i(x_i)$$

Rastrigin function



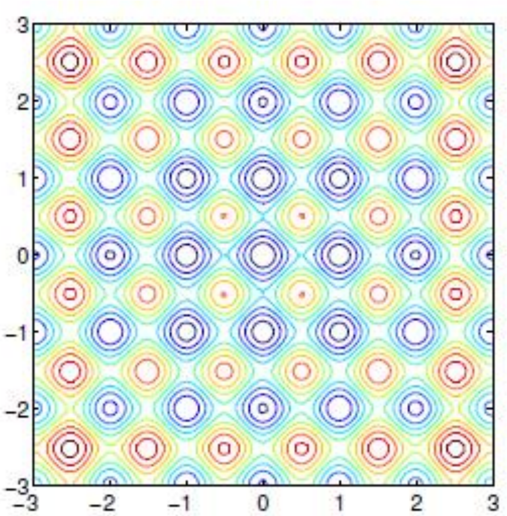
Non-Separable Problems

Building a non-separable problem from a separable one [1,2]

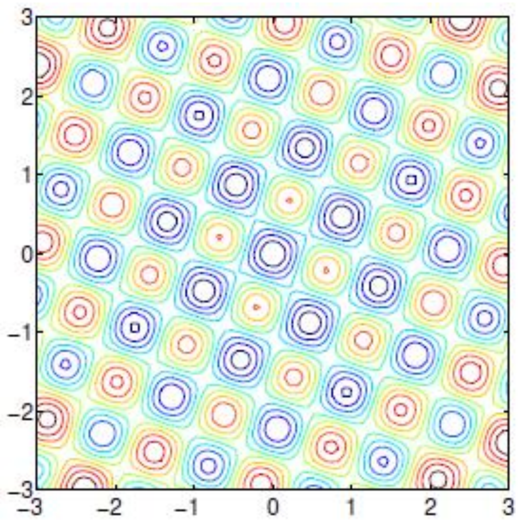
Rotating the coordinate system

- $f: \boldsymbol{x} \mapsto f(\boldsymbol{x})$ separable
- $f: \boldsymbol{x} \mapsto f(R\boldsymbol{x})$ non-separable

R rotation matrix



$\xrightarrow{R}$



[1] N. Hansen, A. Ostermeier, A. Gawelczyk (1995). "On the adaptation of arbitrary normal mutation distributions in evolution strategies: The generating set adaptation". Sixth ICGA, pp. 57-64, Morgan Kaufmann

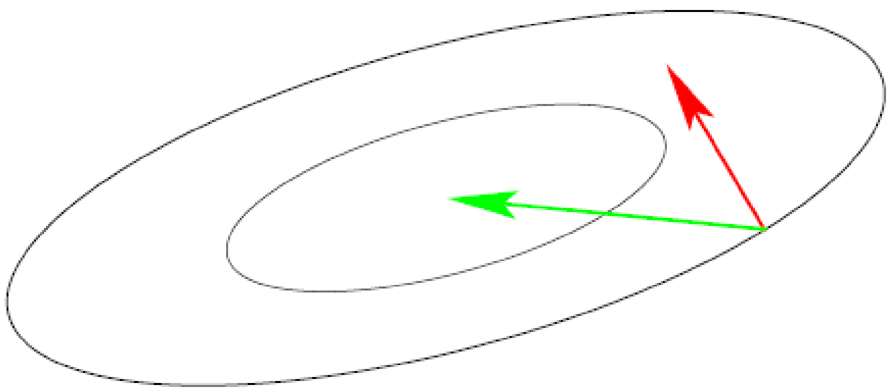
[2] R. Salomon (1996). "Reevaluating Genetic Algorithm Performance under Coordinate Rotation of Benchmark Functions; A survey of some theoretical and practical aspects of genetic algorithms." BioSystems, 39(3):263-278

Ill-Conditioned Problems: Curvature of Level Sets

Consider the convex-quadratic function

$$f(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^*)^T H(\boldsymbol{x} - \boldsymbol{x}^*) = \frac{1}{2}\sum_i h_{i,i} x_i^2 + \frac{1}{2}\sum_{i,j} h_{i,j} x_i x_j$$

H is Hessian matrix of f and symmetric positive definite



gradient direction $-f'(x)^T$

Newton direction $-H^{-1}f'(x)^T$

Ill-conditioning means squeezed level sets (high curvature). Condition number equals nine here. Condition numbers up to 10^{10} are not unusual in real-world problems.

If $H \approx I$ (small condition number of H) first order information (e.g. the gradient) is sufficient. Otherwise second order information (estimation of H^{-1}) information necessary.

Different Notions of Optimum

Unconstrained case

- local vs. global
  - local minimum $\boldsymbol{x}^*$: $\exists$ a neighborhood V of $\boldsymbol{x}^*$ such that $\forall \boldsymbol{x} \in \mathrm{V}: f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$
  - global minimum: $\forall \boldsymbol{x} \in \Omega: f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$
- strict local minimum if the inequality is strict

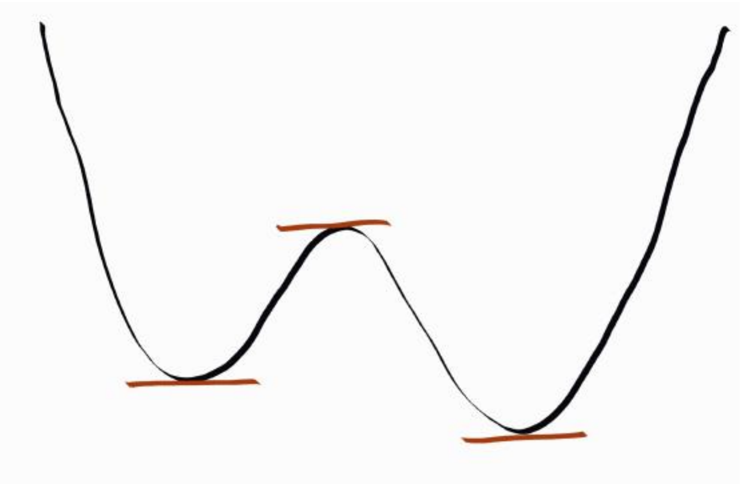
Constrained case

- a bit more involved
- hence, later in the lecture ☺

Mathematical Characterization of Optima

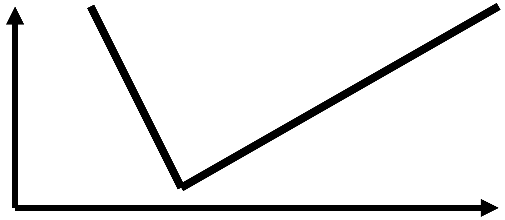
Objective: Derive general characterization of optima

Example: if $f: \mathbb{R} \to \mathbb{R}$ differentiable,
$f'(x) = 0$ at optimal points



- generalization to $f: \mathbb{R}^n \to \mathbb{R}$?
- generalization to constrained problems?

Remark: notion of optimum independent of notion of derivability

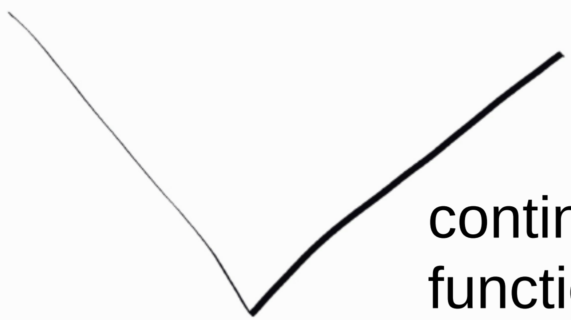


optima of such function can be easily approached by certain type of methods

Reminder: Continuity of a Function

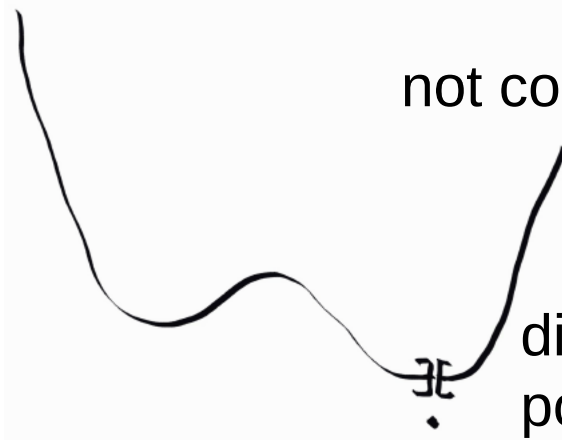
$f : (V, || \, ||_V) \longrightarrow (W, || \, ||_W)$ is continuous in $x \in V$ if

$\forall \epsilon > 0, \exists \eta > 0$ such that $\forall y \in V$: $||x - y||_V \leq \eta$; $||f(x) - f(y)||_W \leq \epsilon$



continuous
function

not continuous



discontinuity
point

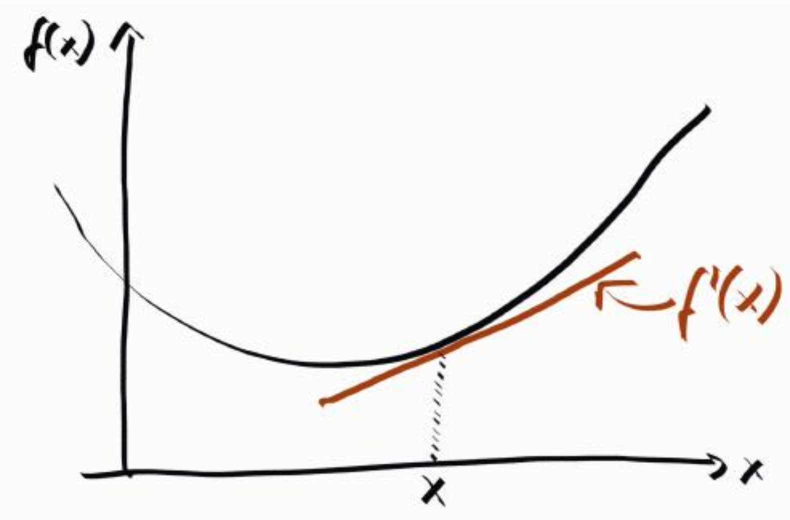
Reminder: Differentiability in 1D (n=1)

$f: \mathbb{R} \to \mathbb{R}$ is differentiable in $x \in \mathbb{R}$ if

$$\lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \text{ exists, } h \in \mathbb{R}$$

Notation:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



The derivative corresponds to the slope of the tangent in x.

Reminder: Differentiability in 1D (n=1)

Taylor Formula (Order 1)

If f is differentiable in x then

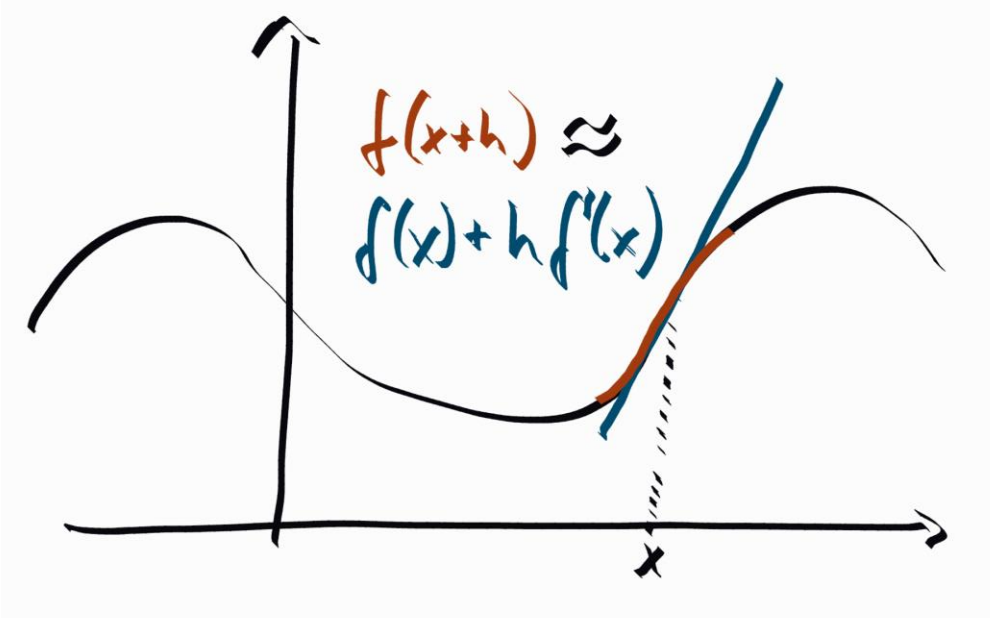
$$f(x+h) = f(x) + f'(x)h + o(||h||)$$

i.e. for h small enough, $h \longmapsto f(x+h)$ is approximated by $h \longmapsto f(x) + f'(x)h$

$h \longmapsto f(x) + f'(x)h$ is called a first order approximation of $f(x+h)$

Reminder: Differentiability in 1D (n=1)

Geometrically:



The notion of derivative of a function defined on $\mathbb{R}^n$ is generalized via this idea of a linear approximation of $f(x+h)$ for h small enough.

How to generalize this to arbitrary dimension?

Gradient Definition Via Partial Derivatives

- In $(\mathbb{R}^n, \|\ \ \|_2)$ where $\|\boldsymbol{x}\|_2 = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$ is the Euclidean norm deriving from the scalar product $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^T \boldsymbol{y}$

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

- Reminder: partial derivative in x_0

$$\mathrm{f_i}\colon\ y \to f\left(x_0^1, \dots, x_0^{i-1}, y, x_0^{i+1}, \dots, x_0^n\right)$$

$$\frac{\partial f}{\partial x_i}(x_0) = f_i{}'(x_0)$$

Exercise: Gradients

Exercise:

Compute the gradients of

a) $f(x) = x_1$ with $x \in \mathbb{R}^n$
b) $f(x) = a^T x$ with $\mathrm{a}, x \in \mathbb{R}^n$
c) $f(x) = x^T x$ $(= ||\mathrm{x}||^2)$ with $x \in \mathbb{R}^n$

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Some more examples:

- in $\mathbb{R}^n$, if $f(\boldsymbol{x}) = \boldsymbol{x}^T A \boldsymbol{x}$, then $\nabla f(\boldsymbol{x}) = (A + A^T)\boldsymbol{x}$
- in $\mathbb{R}$, $\nabla f(\boldsymbol{x}) = f'(\boldsymbol{x})$

Gradient: Geometrical Interpretation

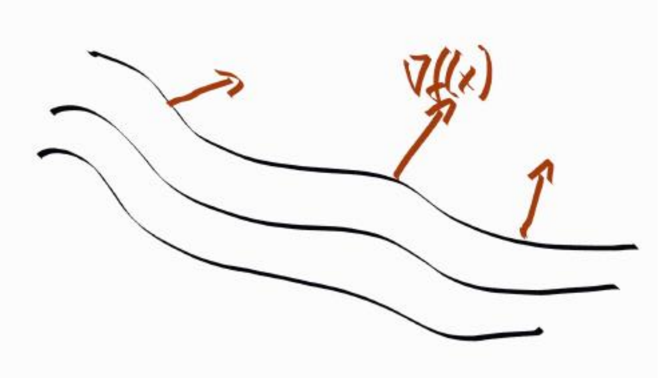
Exercise:

Let $L_c = \{\boldsymbol{x} \in \mathbb{R}^n \mid f(\boldsymbol{x}) = c\}$ be again a level set of a function $f(\boldsymbol{x})$. Let $\boldsymbol{x}_0 \in L_c \neq \emptyset$.

Compute the level sets for $f_1(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x}$ and $f_2(\boldsymbol{x}) = ||\boldsymbol{x}||^2$ and the gradient in a chosen point x_0 and observe that $\nabla f(\boldsymbol{x_0})$ is ***orthogonal*** to the level set in x_0.

Again: if this seems too difficult, do it for two variables (and a concrete $\boldsymbol{a} \in \mathbb{R}^2$) and draw the level sets and the gradients.

More generally, the gradient of a differentiable function is orthogonal to its level sets.



Taylor Formula – Order One

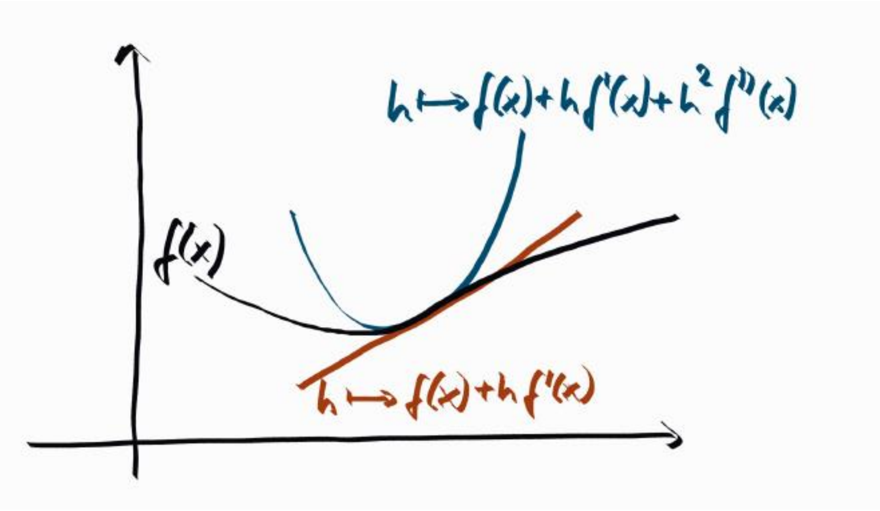
$$f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) + \left(\nabla f(\boldsymbol{x})\right)^T \boldsymbol{h} + o(||\boldsymbol{h}||)$$

Reminder: Second Order Differentiability in 1D

- Let $f: \mathbb{R} \to \mathbb{R}$ be a differentiable function and let $f': x \to f'(x)$ be its derivative.
- If f' is differentiable in x, then we denote its derivative as $f''(x)$
- $f''(x)$ is called the *second order derivative* of f.

Taylor Formula: Second Order Derivative

- If $f: \mathbb{R} \to \mathbb{R}$ is two times differentiable then
$$f(x+h) = f(x) + f'(x)h + f''(x)h^2 + o(||h||^2)$$
i.e. for h small enough, $h \to f(x) + hf'(x) + h^2 f''(x)$ approximates $h + f(x+h)$
- $h \to f(x) + hf'(x) + h^2 f''(x)$ is a quadratic approximation (or order 2) of f in a neighborhood of x



- The second derivative of $f: \mathbb{R} \to \mathbb{R}$ generalizes naturally to larger dimension.

Hessian Matrix

In $(\mathbb{R}^n, \langle x, y\rangle = x^T y)$, $\nabla^2 f(x)$ is represented by a matrix called the Hessian matrix. It can be computed as

$$\nabla^2(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Exercise on Hessian Matrix

Exercise:

Let $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A\,\boldsymbol{x}$, $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$.

Compute the Hessian matrix of f.

If it is too complex, consider $f: \begin{cases} \mathbb{R}^2 \to \mathbb{R} \\ \boldsymbol{x} \to \frac{1}{2}\boldsymbol{x}^T A\,\boldsymbol{x} \end{cases}$ with $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}$

Second Order Differentiability in $\mathbb{R}^n$

Taylor Formula – Order Two

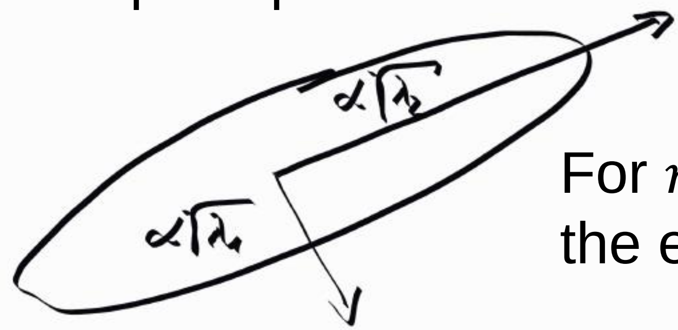
$$f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) + \left(\nabla f(\boldsymbol{x})\right)^T \boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T\left(\nabla^2 f(\boldsymbol{x})\right) \boldsymbol{h} + o(||\boldsymbol{h}||^2)$$

Back to Ill-Conditioned Problems

We have seen that for a convex quadratic function

$f(x) = \frac{1}{2}(x - x_0)^T A(x - x_0) + b$ of $x \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$, A SPD, $b \in \mathbb{R}^n$:

1) The level sets are ellipsoids. The eigenvalues of A determine the lengths of the principle axes of the ellipsoid.



For $n = 2$, let λ_1, λ_2 be the eigenvalues of A.

2) The Hessian matrix of f equals to A.

Ill-conditioned convex quadratic problems are problems with large ratio between largest and smallest eigenvalue of A which means large ratio between longest and shortest axis of ellipsoid.

This corresponds to having an ill-conditioned Hessian matrix.

Gradient Direction Vs. Newton Direction

Gradient direction: $-\nabla f(\boldsymbol{x})$

Newton direction: $-\left(H(\boldsymbol{x})\right)^{-1} \cdot \nabla f(\boldsymbol{x})$

with $H(\boldsymbol{x}) = \nabla^2 f(\boldsymbol{x})$ being the Hessian at $\boldsymbol{x}$

Exercise:

Let again $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A\, \boldsymbol{x}$, $\boldsymbol{x} \in \mathbb{R}^2$, $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix} \in \mathbb{R}^{2\times 2}$.

Plot the gradient and Newton direction of f in a point $x \in \mathbb{R}^n$ of your choice (which should not be on a coordinate axis) into the same plot with the level sets, we created before.

Gradient Direction Vs. Newton Direction

Gradient direction: $-\nabla f(\boldsymbol{x})$

Newton direction: $-\left(H(\boldsymbol{x})\right)^{-1} \cdot \nabla f(\boldsymbol{x})$

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Exercise:

Let again $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A\, \boldsymbol{x}$, $\boldsymbol{x} \in \mathbb{R}^2$, $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix} \in \mathbb{R}^{2\times 2}$.

Plot the gradient and Newton direction of f in a point $x \in \mathbb{R}^n$ of your choice (which should not be on a coordinate axis) into the same plot with the level sets, we created before.

- remind level sets: axis-parallel ellipsoids, axis-ratio=3
- remind gradient: $A\boldsymbol{x}$
- remind Hessian: A

Conclusions

I hope it became clear...

…what kind of optimization problems we are interested in

…what are level sets and how to plot them

…what difficulties a problem can have

…what the gradient is
(and that it is generally orthogonal to the level sets)

…what the Hessian is and

…what's the difference between gradient and Newton direction.