Introduction to Optimization

Approximation Algorithms and Heuristics

November 9, 2015

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Course Overview

Date		Topic
Mon, 21.9.2015		Introduction
Mon, 28.9.2015	D	Basic Flavors of Complexity Theory
Mon, 5.10.2015	D	Greedy algorithms
Mon, 12.10.2015	D	Branch and bound (switched w/ dynamic programming)
Mon, 2.11.2015	D	Dynamic programming *[salle Proto]*
Fri, 6.11.2015	D	Approximation algorithms and heuristics *[S205/S207]*
Mon, 9.11.2015	**C**	**Introduction to Continuous Optimization I *[S118]***
Fri, 13.11.2015	C	Introduction to Continuous Optimization II *[from here onwards always: S205/S207]*
Fri, 20.11.2015	C	Gradient-based Algorithms
Fri, 27.11.2015	C	~~End of Gradient-based Algorithms + Linear Programming~~ *Stochastic Optimization and Derivative Free Optimization I*
Fri, 4.12.2015	C	Stochastic Optimization and Derivative Free Optimization II
Tue, 15.12.2015		Exam

Overview of Today's Lecture

Introduction to Continuous Optimizaation

- examples (from ML / black-box problems)
- typical difficulties in optimization (e.g. constraints)

Mathematical Tools to Characterize Optima

- reminders about differentiability, gradient, Hessian matrix

Further Details on Remaining Lectures

Introduction to Continuous Optimization

- examples (from ML / black-box problems)
- typical difficulties in optimization (e.g. constraints)

Mathematical Tools to Characterize Optima

- reminders about differentiability, gradient, Hessian matrix
- unconstraint optimization
  - first and second order conditions
  - convexity
- constrained optimization

Gradient-based Algorithms

- quasi-Newton method (BFGS)

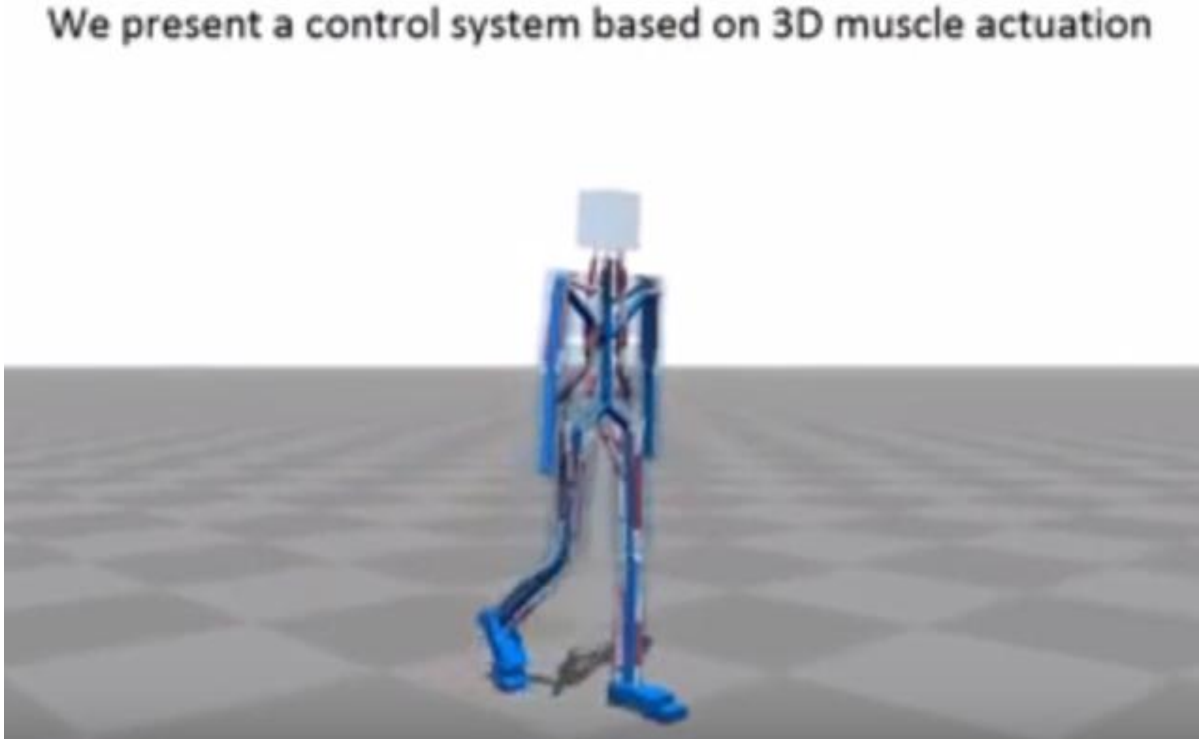
Learning in Optimization / Stochastic Optimization

- CMA-ES (adaptive algorithms / Information Geometry)
- PhD thesis possible on this topic

strongly related to ML, new promising research area, interesting open questions

First Example of a 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=yci5FuI1ovk

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

Continuous Optimization

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

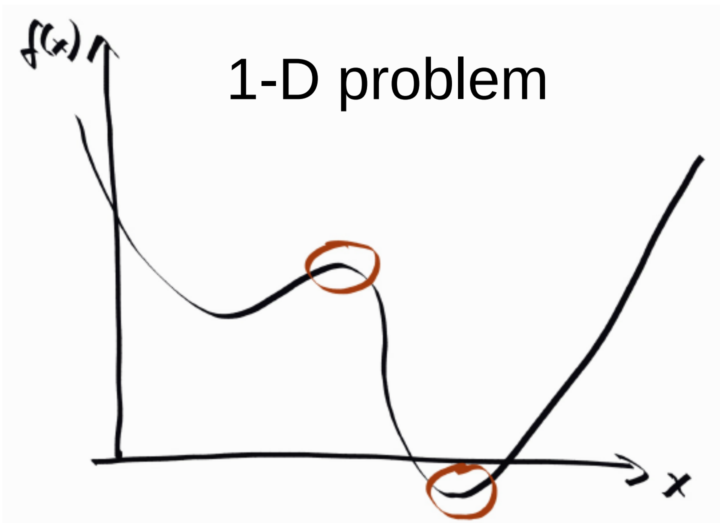
  $\in \mathbb{R}$

  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

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

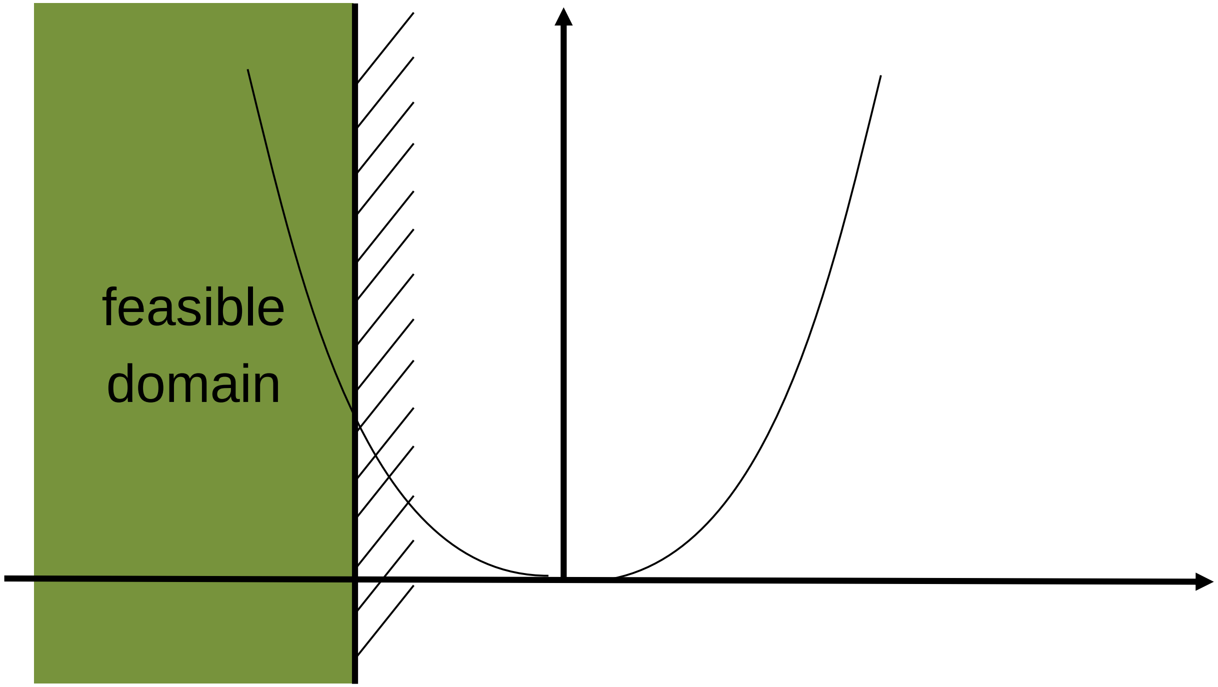
Constrained optimization

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

and A symmetric positive definite (SPD)

Exercise:

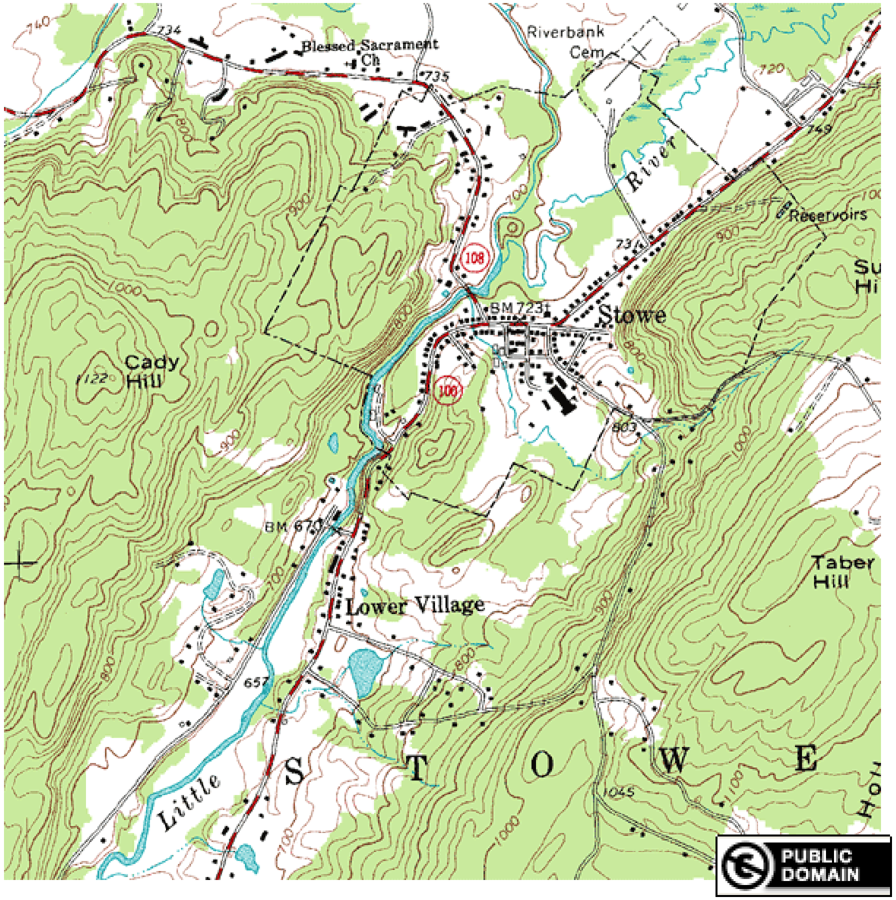
What is the minimum of $f_2(x)$?

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) Optional: More generally, for $n = 2$, if A is SPD with eigenvalues $\lambda_1 = 9$ and $\lambda_2 = 1$, what are the level sets of $f_2(x)$?

Example Problems

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 simple models only affordable (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:

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

Supervised Learning:

Predict $y \in \mathcal{Y}$ from $\boldsymbol{x} \in \mathcal{X}$, given a set of observations (examples) $\{y_i, \boldsymbol{x}_i\}_{i=1,\ldots,N}$

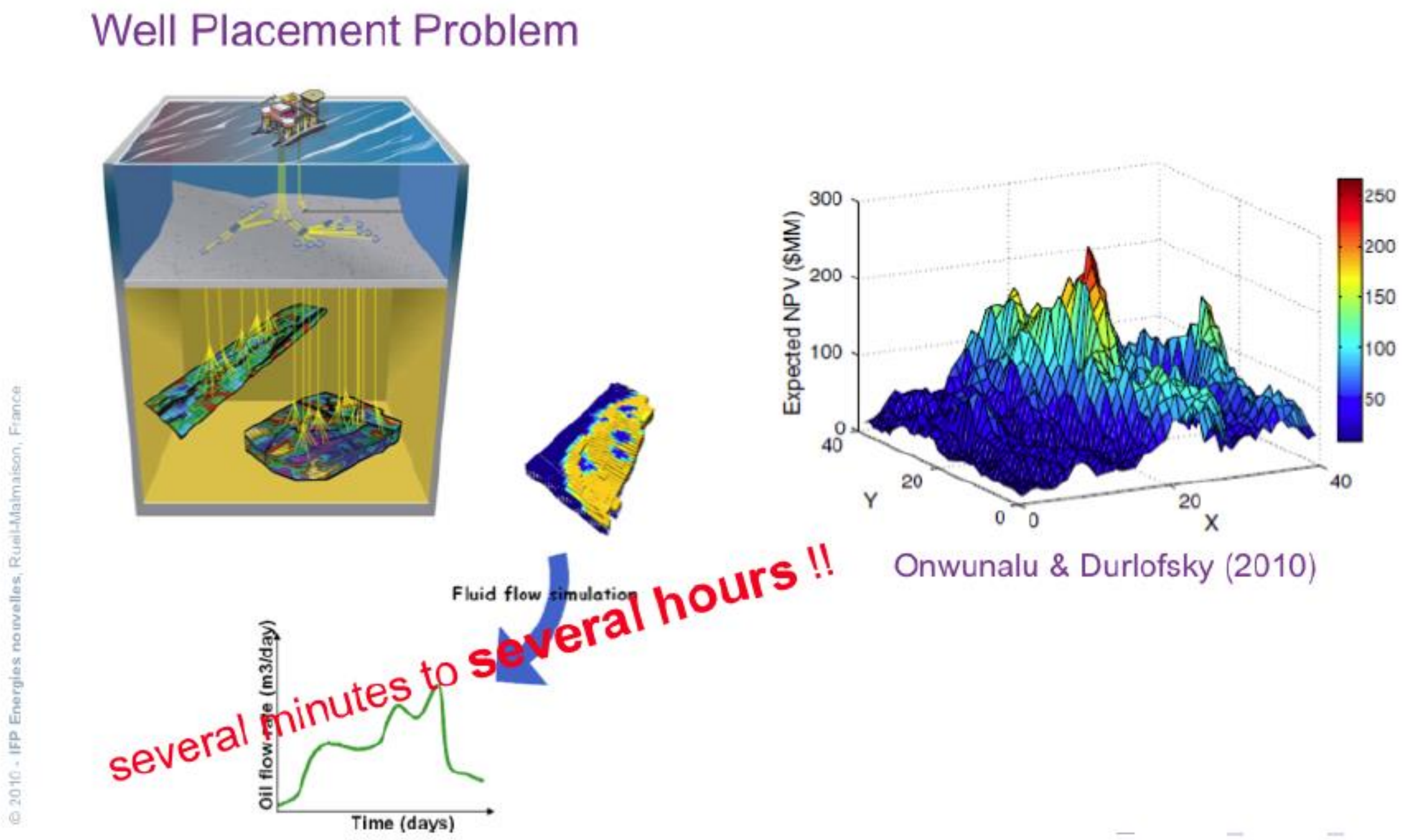
(Simple) Linear regression

Given a set of data: $\{y_i, \underbrace{x_i^1, \ldots, x_i^p}_{\boldsymbol{x}_i^T}\}_{i=1\ldots N}$

$$\min_{\boldsymbol{w}\in\mathbb{R}^p,\beta\in\mathbb{R}} \underbrace{\sum_{i=1}^{N} |\boldsymbol{w}^T \boldsymbol{x}_i + \beta - y_i|^2}_{||\widetilde{\boldsymbol{X}}\widetilde{\boldsymbol{w}} - \mathbf{y}||^2}$$

$\widetilde{\boldsymbol{X}} \in \mathbb{R}^{N\times(p+1)}$, $\widetilde{\boldsymbol{w}} \in \mathbb{R}^{p+1}$

same as data fitting with linear model, i.e. $f_{(\boldsymbol{w},\beta)}(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + \beta$, $\theta \in \mathbb{R}^{p+1}$


Well Placement Problem
Fluid flow simulation
Oil flow rate (m3/day)
Time (days)
several minutes to several hours !!
Expected NPV ($MM)
300
200
100
0
40
20
Y
0
0
20
40
X
250
200
150
100
50
Onwunalu & Durlofsky (2010)
© 2010 - IFP Energies nouvelles, Rueil-Malmaison, France

Function Difficulties

What Makes a Function Difficult to Solve?

- dimensionality

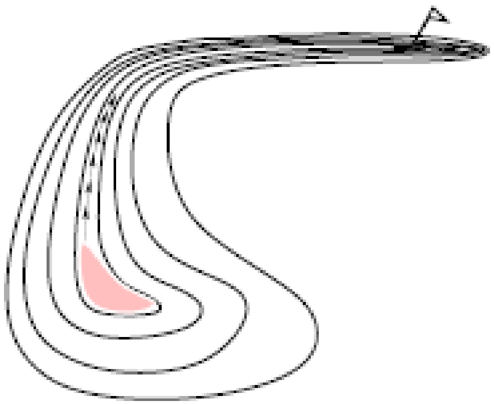
  (considerably) larger than three

- non-separability

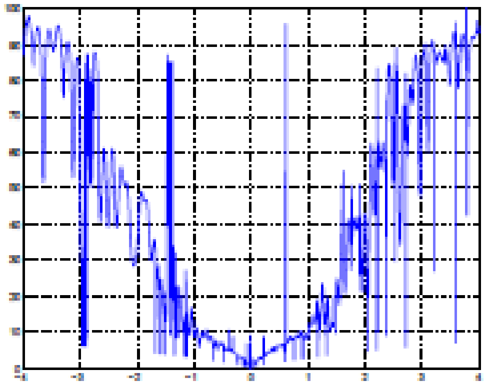
  dependencies between the objective variables

- 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.

Definition (Separable Problem)

A function f is separable if

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

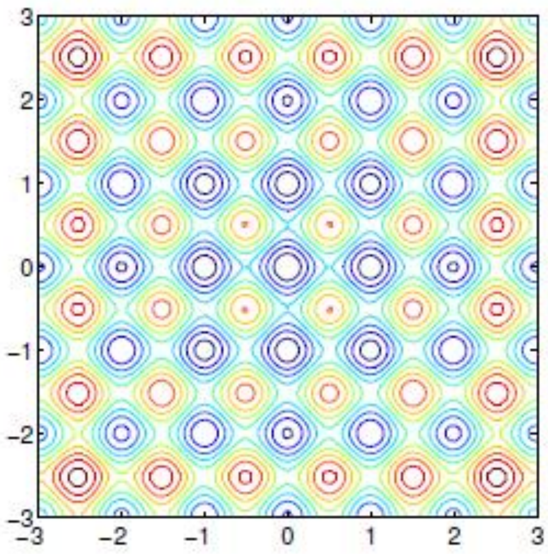
$\Longrightarrow$ it follows that f can be optimized in a sequence of n independent 1-D optimization processes

Example:

Additively decomposable functions

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

Rastrigin function



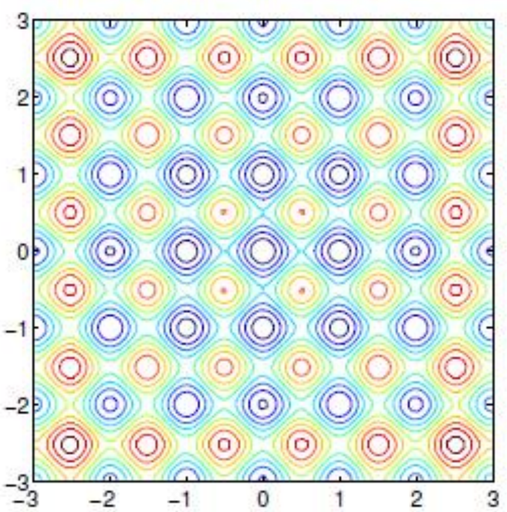
Non-Separable Problems

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

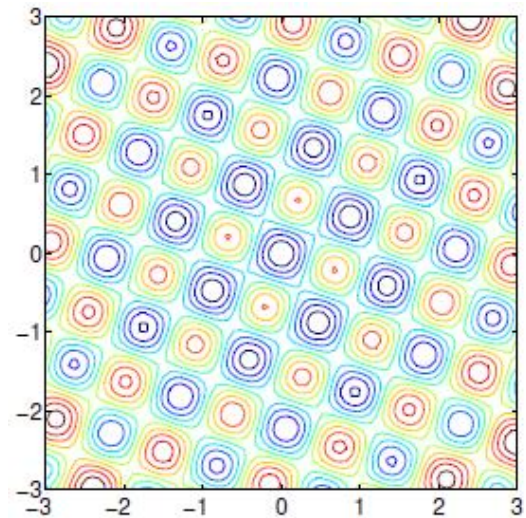
Rotating the coordinate system

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

R rotation matrix



$\xrightarrow{R}$



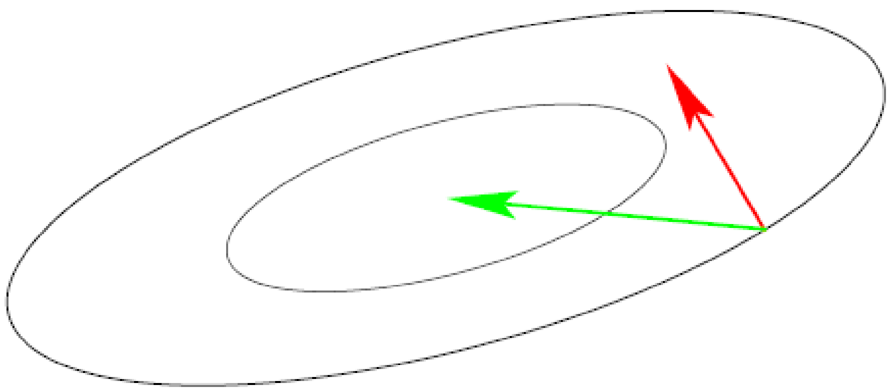
[1] N. Hansen, A. Ostermeier, A. Gawelczyk (1995). "On the adaptation of arbitrary normal mutation distributions in evolution strategies: The generating set adaptation". Sixth ICGA, pp. 57-64, Morgan Kaufmann
[2] R. Salomon (1996). "Reevaluating Genetic Algorithm Performance under Coordinate Rotation 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 of SPD matrix A = ratio between largest and smallest eigenvalue

Condition number equals nine here (kind of well-conditioned). Condition numbers up to 10^{10} are not unusual in real-world problems.

Mathematical Tools to Characterize Optima

Different Notions of Optimum

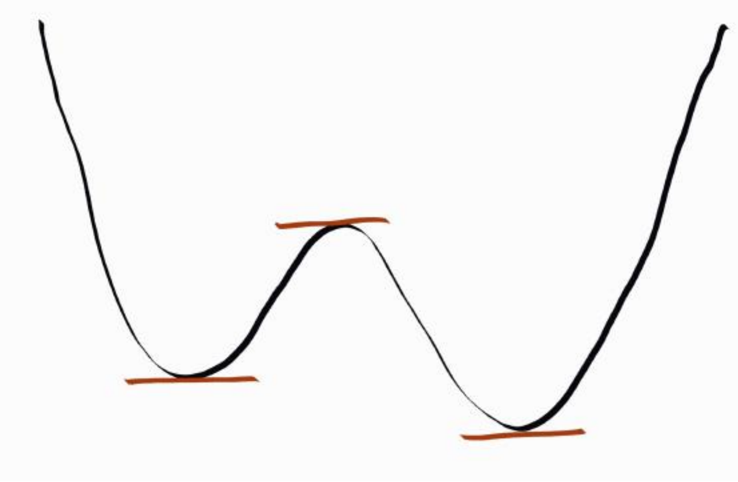
Unconstrained case

- 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

Mathematical Characterization of Optima

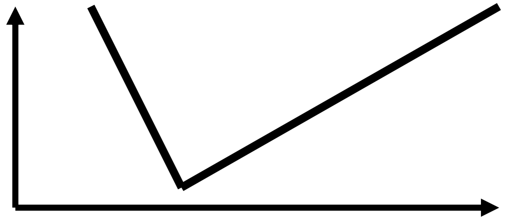
Objective: Derive general characterization of optima

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?

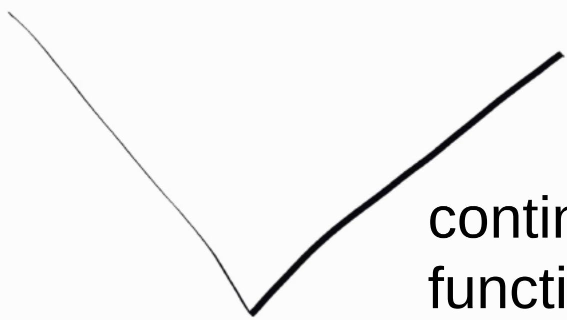
Remark: notion of optimum independent of notion of differentiability



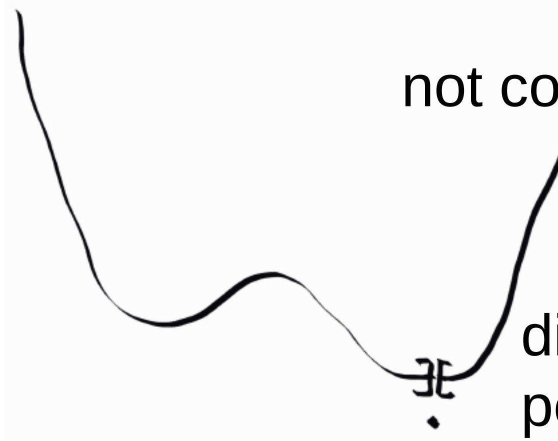
optima of such function can be easily approached by certain type of methods

$f: (V, || \, ||_V) \longrightarrow (W, || \, ||_W)$ 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

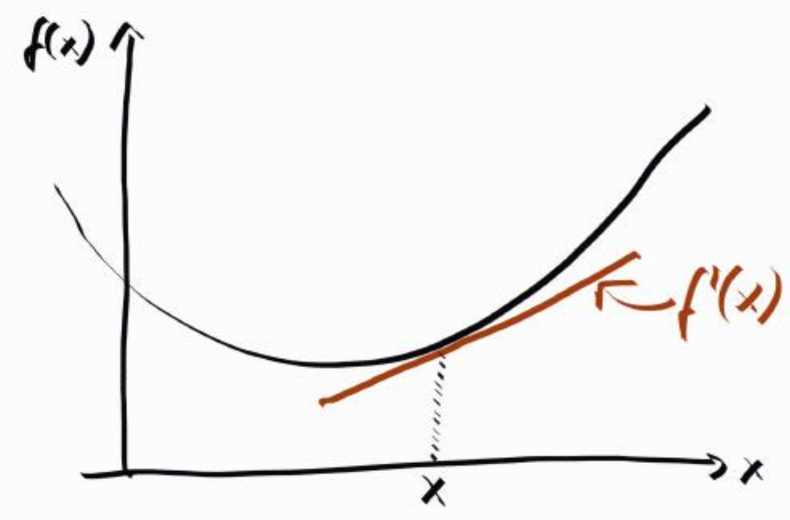
discontinuity
point

$f: \mathbb{R} \to \mathbb{R}$ 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)

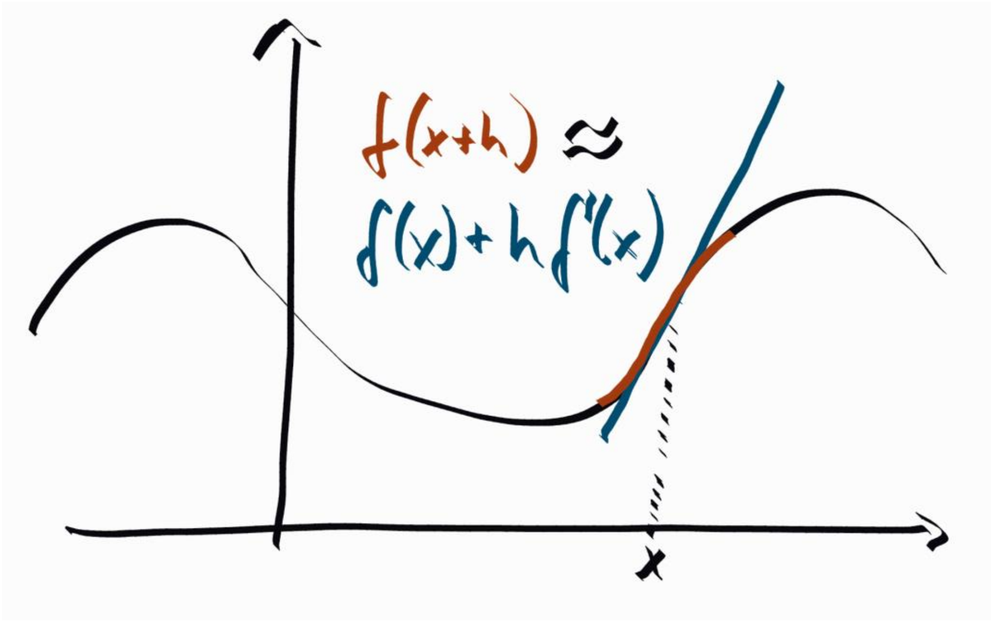
If f is differentiable in x then

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

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

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

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.

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 $x \in \mathbb{R}^n$

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 $x \in \mathbb{R}^n$

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 $\mathbb{R}$, $\nabla f(\boldsymbol{x}) = f'(\boldsymbol{x})$

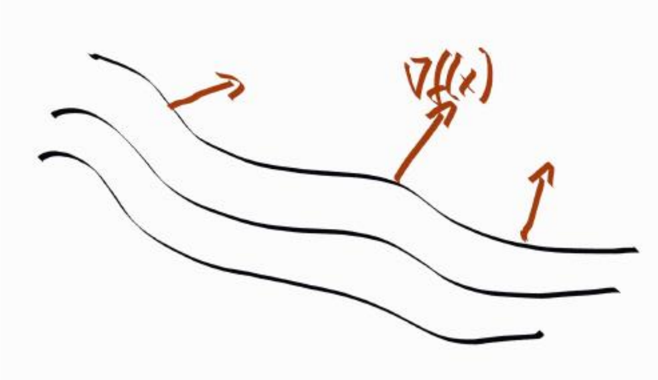
Gradient: Geometrical Interpretation

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 $\boldsymbol{x}_0 \in L_c \neq \emptyset$.

Plot the level sets for $f(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x}$ and $f(\boldsymbol{x}) = ||\boldsymbol{x}||^2$, compute 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.

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



Taylor Formula – Order One

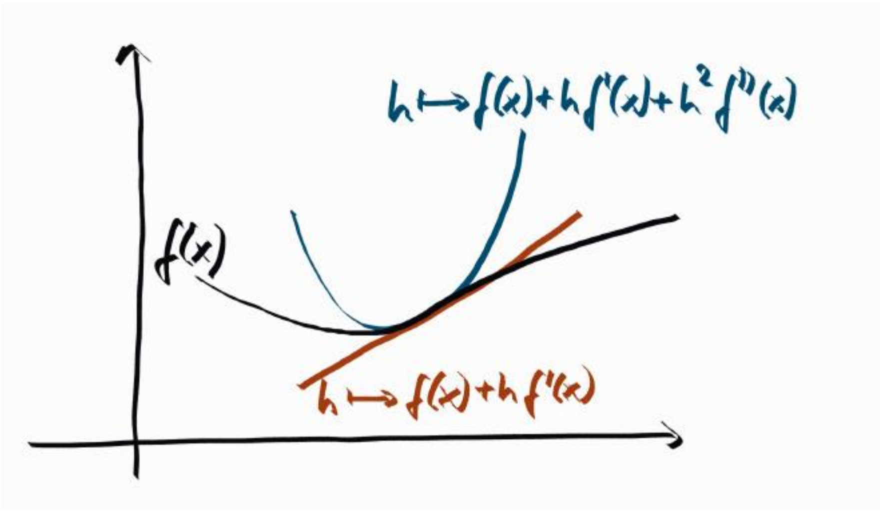
$$f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) + \left(\nabla f(\boldsymbol{x})\right)^T \boldsymbol{h} + o(||\boldsymbol{h}||)$$

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

Compute the Hessian matrix of f.

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

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

Taylor Formula – Order Two

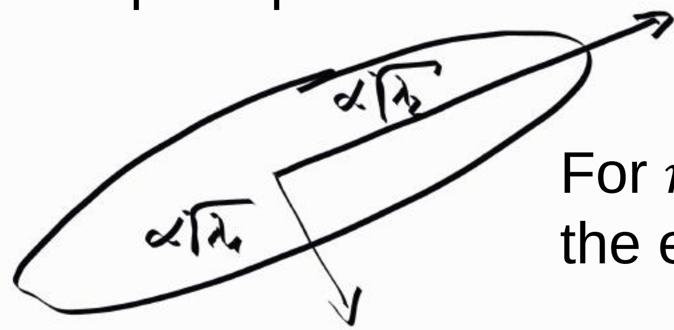
$$f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) + \left(\nabla f(\boldsymbol{x})\right)^T \boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T\left(\nabla^2 f(\boldsymbol{x})\right) \boldsymbol{h} + o(||\boldsymbol{h}||^2)$$

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 $H(\boldsymbol{x}) = \nabla^2(\boldsymbol{x})$ 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.

Conclusions

I hope it became clear...

...what are the difficulties to cope with when solving numerical optimization problems

in particular dimensionality, non-separability and ill-conditioning

...what are gradient and Hessian

...what is the difference between gradient and Newton direction