

# Optimization for Data Science

Axel Böhm

September 30, 2021

## 1 Introduction

## 2 Methods

## 3 Convexity

# Course organization

- ◇ Lectures (contribution counts)
- ◇ hands on sessions on some Thursdays
- ◇ a small weekly problem set
- ◇ Project
- ◇ oral exam

Find everything on github.

# What is Optimization

*Given a function  $f$  which represents some cost/regret/loss (or gain/profit/utility) we aim to find the argument/decision associated with the smallest cost (or largest profit).*

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

- ◇ variables, parameters, candidate solutions  $x$
- ◇ objective function  $f$  (typically real-valued)
- ◇ typically: technical assumptions on  $f$
- ◇ constrained set  $C \subset \mathbb{R}^d$
- ◇ convexity / differentiability

# Applications of optimization

## Economics

- ◇ Microeconomics: Agents maximizing utility
- ◇ Game theory and equilibria
- ◇ Stats: maximum likelihood

## Physics

- ◇ soap bubble is a sphere because it minimizes surface tension

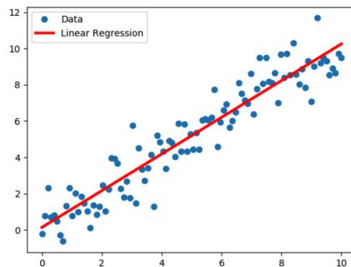
## Chemistry

- ◇ Protein folding

# Optimization for ML

$$\min_{\beta_1, \beta_0} \sum_{i=1}^n (\beta_1 x_i + \beta_0 - y_i)^2$$

For data points  $(x_i, y_i)$ .



# Optimization for ML

- ◇ Mathematical modeling
  - ▶ defining & modeling the problem
  - ▶ finding a good metric / what is success
  - ▶ accuracy vs. solvability trade-off
- ◇ Computational optimization
  - ▶ running an (appropriate) optimization algorithm
- ◇ theory vs. practice
  - ▶ libraries available, but algorithms treated as “black box” by practitioners
  - ▶ we will try and understand why and how they work

# Optimization Algorithms

*Simplicity rules in the large scale setting.*

Main approaches:

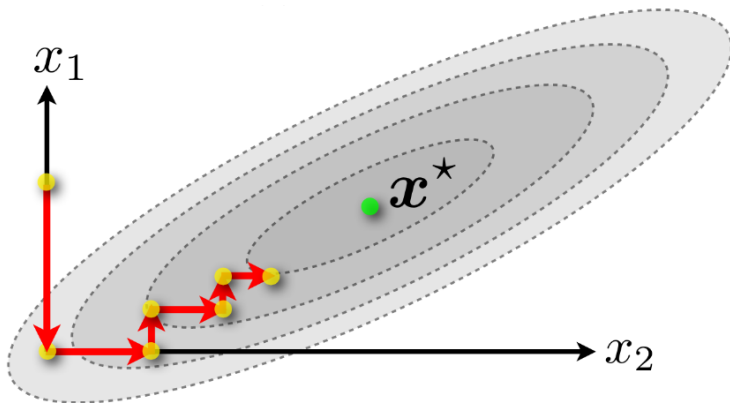
- ◇ First order methods: **gradient descent**
- ◇ Stochastic gradient descent (SGD)
- ◇ Coordinate descent

History

- ◇ 1847: Cauchy proposes gradient descent
- ◇ 1950s: Linear programming, operations research, soon followed by nonlinear
- ◇ 1980s: general convergence theory
- ◇ 2005-today: large scale optimization, SGD, distributed optimization

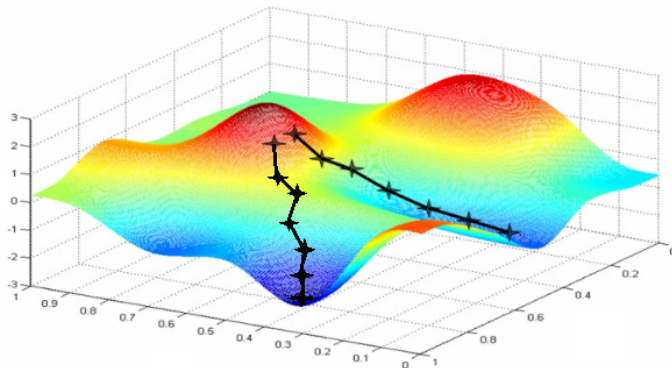


# Example: Coordinate descent

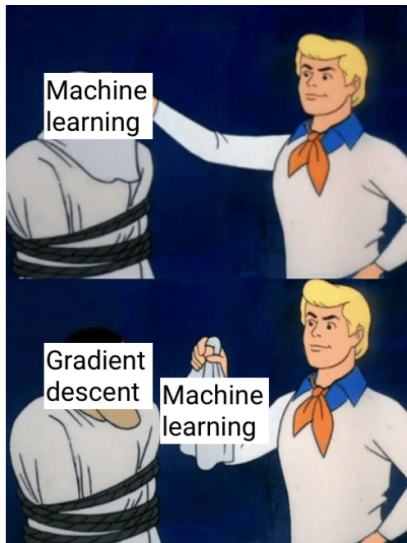


**Strategy:** Minimize along one coordinate at a time, while keeping the others fixed.

# Example: Gradient descent



**Strategy:** Follow the direction of (local) steepest descent.



Machine learning behind the  
scenes

# Optimization in other settings

## ◇ Second order

- ▶ if high precision in solution is required
- ▶ too **expensive** in high dimensions

## ◇ Zeroth order

- ▶ no gradient or functional representation available
- ▶ only function values
- ▶ for simulation, hyperparameters, black box models

## ◇ constrained problems

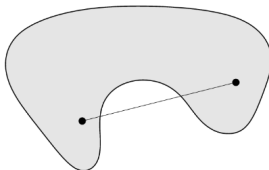
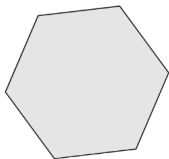
## ◇ discrete optimization

- ▶ involving graphs, traveling salesman
- ▶ scheduling

# Convex sets

A set  $C$  is **convex** if the line segment between any two points remains inside  $C$ , i.e. for any  $x, y \in C$  and  $\lambda \in [0, 1]$ .

$$\lambda x + (1 - \lambda)y \in C.$$



\*Figure 2.2 from S. Boyd, L. Vandenberghe

Which of these sets are convex?

# Properties of convex sets

- ◇ intersection remains convex
- ◇ can separated by a hyperplane
- ◇ projections onto them are unique

# Convex functions

We call a function  $f \rightarrow \mathbb{R} \cup \{+\infty\}$  **convex** if the function values lie below the line segment between  $(x, f(x))$  and  $(y, f(y))$

$$f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1 - \lambda)f(\mathbf{y}).$$



\*Figure 3.1 from S. Boyd, L. Vandenberghe

Sometimes we will call  $\{x : f(x) < +\infty\}$  the domain of  $f$ .

# Convex optimization

Are of the form

$$\min_x f(x) \quad \text{such that } x \in C$$

where **both**

- ◇  $f$  is a convex function
- ◇  $C$  is a convex set

Why?

- ◇ Every local minimum is a global minimum
- ◇ Not all problems are convex but can be used as approximate model



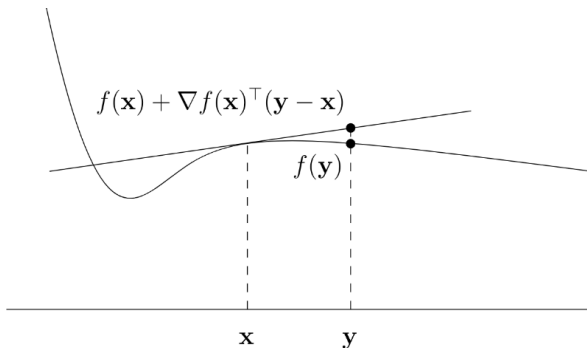
# Examples of convex functions

- ◇ linear:  $f(x) = a^T x$
- ◇ affine:  $f(x) = a^T x + b$
- ◇ exponential:  $f(x) = e^{\alpha x}$
- ◇ norms,  $\|\cdot\|_1, \|\cdot\|_2, \|\cdot\|_\infty$
- ◇ composition of linear and convex:  
for example  $f(x) = \|Ax - b\|^2$

show this

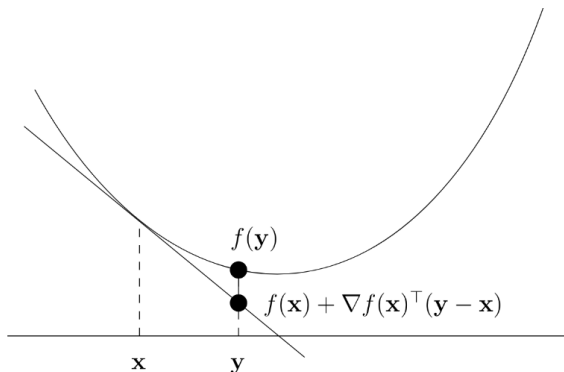
# Differentiable function

Derivative at a point is the **best linear approximation** of the function at this point.



Graph of  $f(x) + \nabla f(x)^\top (y - x)$  is a **tangent hyperplane** to the graph of  $f$  at  $(x, f(x))$

# First-order characterization of convexity



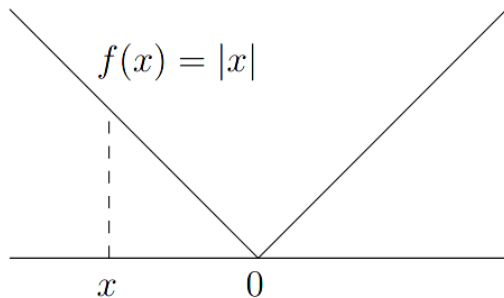
If  $f$  is differentiable, then

$f$  is convex if and only if:  $f(y) \geq f(x) + \nabla f(x)^\top(y - x)$

# Nonsmooth functions

do in fact play a role in practice

- ◇ ReLu, Hinge loss, norms
- ◇ can induce sparsity in the solution
- ◇ appear as the maximum over a family of functions (max pooling, or min-max)



## Second-order characterization of convexity

If  $f$  is **twice differentiable** then it is **convex** if and only if its Hessian  $\nabla^2 f(x) \mathbb{R}^d$ , given by

$$\nabla^2 f(x)_{ij} := \frac{\partial^2 f}{\partial x_i \partial x_j}$$

is **positive semidefinite**, i.e.

$$\nabla^2 f(x) \succcurlyeq 0$$

A matrix  $M$  is *positive semidefinite* if  $x^T M x \geq 0$  for all  $x$ .  
Also used in algorithm like *Newtons* method.

# Examples

- ◇ **quadratic function:**  $f(x) = \frac{1}{2}x^T Qx + c^T x$ , then

$$\nabla^2 f(x) = Q$$

and  $f$  is convex iff  $Q \succcurlyeq 0$ .

- ◇ **least squares objective:**  $f(x) = \|Ax - b\|^2$ , then

$$\nabla^2 f(x) = A^T A$$

is always convex for any  $A$ .

# Local minima are global

## Definition

A **local minimum** of  $f$  is a point  $\bar{x}$  such that there exists  $\epsilon > 0$

$$f(\bar{x}) \leq f(y) \quad \forall y : \text{s.t. } \|\bar{x} - y\| \leq \epsilon$$

## Lemma

*Let  $x^*$  be local minimum of a convex function  $f$  then  $x^*$  is a global minimum.*

Prove this!

# Critical points are global minima

## Definition

We call a point  $\bar{x}$  **critical** or **stationary** if  $\nabla f(\bar{x}) = 0$ .

## Lemma

*If  $\bar{x}$  is a stationary point of the **convex** function  $f$ , then  $\bar{x}$  is a **global minimizer** of  $f$ .*

Prove this and give a geometric intuition in words using the first order characterization of convexity



# Strong convexity

## Definition

We call  $f$  **strongly convex** if there exist  $\mu > 0$  such that

$$f - \frac{\mu}{2} \|\cdot\|^2 \text{ is convex.}$$

Equivalently:

- ◇ can be lower bounded by a quadratic

$$f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|y - x\|^2 \leq f(y)$$

- ◇ Hessian is pos. def. everywhere

$$\nabla^2 f(x) \succ 0.$$

# Constrained minimization

## Definition

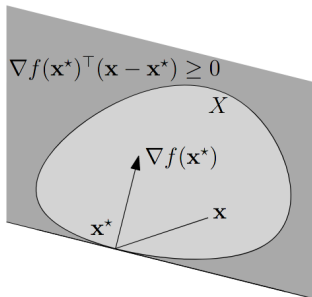
$x^*$  is a minimizer of  $f$  over  $C$  if

$$f(x^*) \leq f(x), \forall x \in C$$

## Lemma

$x^*$  is a minimizer of  $f$  over  $C$  if and only if

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0 \quad \forall x \in C$$



# Proof

$x^*$  is a minimizer of  $f$  over  $C$  if and only if

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0 \quad \forall x \in C$$

Assume that  $f(x^*) \leq f(x)$  for all  $x \in C$  then  $\forall t \in [0, 1]$

$$\begin{aligned} 0 &\leq f(x^* + t(x - x^*)) - f(x^*) \\ 0 &\leq \lim_{t \rightarrow 0} \frac{f(x^* + t(x - x^*)) - f(x^*)}{t} \\ &= \langle \nabla f(x^*), x - x^* \rangle. \end{aligned}$$

where the last equality follows from the chain rule.