Optimization for Data Science

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What is Optimization

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

Relevant Notions

$$\min_{x \in C \subseteq \mathbb{R}^d} f(x)$$

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

Applications of optimization

Economics

- Microeconomics: Agents maximizing utility
- Porfolioopimization
- Finance: Option pricing
- Stats: maximum likelyhood

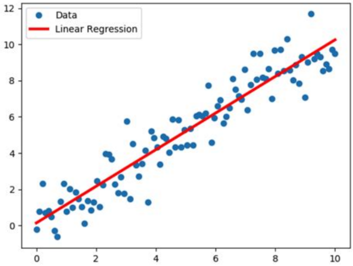
Physics

- soap bubble is a sphere because it minimizes surface tension

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

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 $\lambda \in [0, 1]$.

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

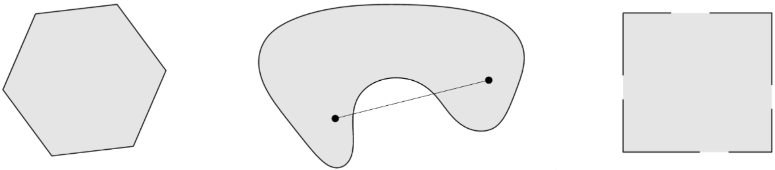


*Figure 2.2 from S. Boyd, L. Vandenberghe

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

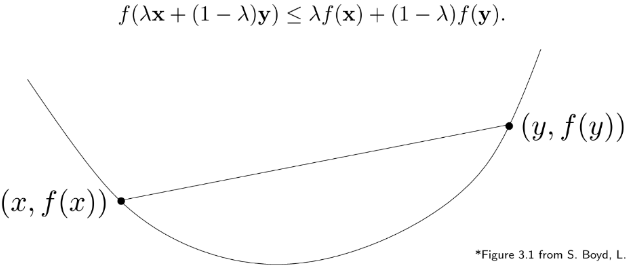


*Figure 3.1 from S. Boyd, L. Vandenberghe

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?

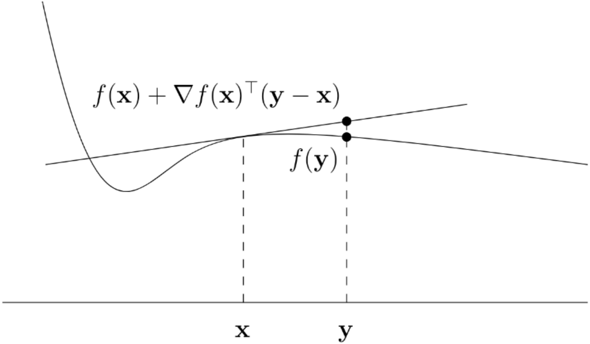
- Every local minimum is a global minimum
- Not all problems are convex but can be used as approximate model

Examples of convex functions

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

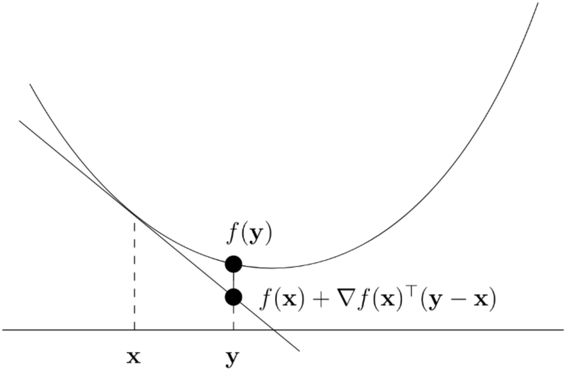
Differentiable function

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



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

First-order characterization of convexity



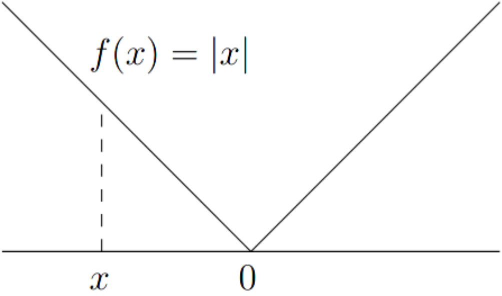
If f is differentiable, then

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

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: $f(x) = \frac{1}{2}x^TQx + c^Tx$, then

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

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

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

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

  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

Constrained minimization

Definition

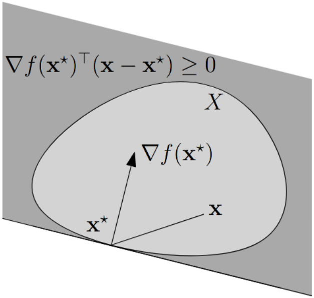
x^* is a minimizer of f over C if

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

Lemma

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

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



Prove this.