Computational Data Analysis

Machine Learning

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Basic Optimization

Outline

- Concept
- Convex/concave function
- First-order condition
- Second-order condition
- Langragian and dual function
- KKT conditions

Motivation

We have seen quite a few optimization problems in machine learning already

Clustering:

$$\min_{c,\pi} \frac{1}{m} \sum_{i=1}^{m} \left\| x^i - c^{\pi(i)} \right\|^2$$

PCA:

$$\max_{w:\|w\|\leq 1} \frac{1}{m} \sum_{i=1}^{m} \left(w^\top x^i - w^\top \mu \right)^2$$

MLE:

$$\theta = argmax_\theta \log P(\mathcal{D}|\theta) = argmax_\theta \log \prod_{i=1}^{m} P(x^i|\theta)$$

Motivation

Optimization is foundational to ML

- Modeling (together with statistics and geometric models)
  - Clustering, PCA, MLE, regression, support vector machine, deep learning, ….
- Solutions methods
  - Heuristics (e.g., k-means)
  - Special methods (e.g., PCA, EM)
  - General methods (e.g., gradient descent, SGD)

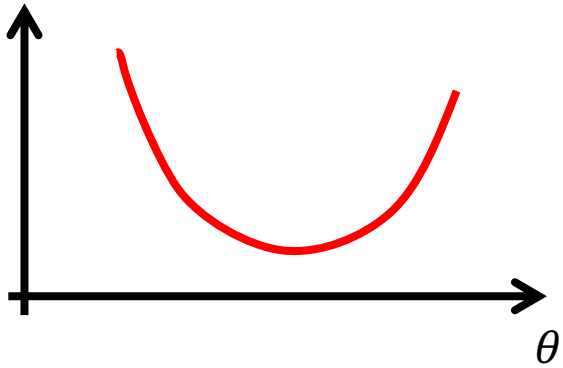
Three components

- Decision variables
- Constraints
- Objective function

Main watershed in optimization

- Convex/Nonconvex optimization (different strategy for solving them)

Convex vs. non-convex



Convex problem

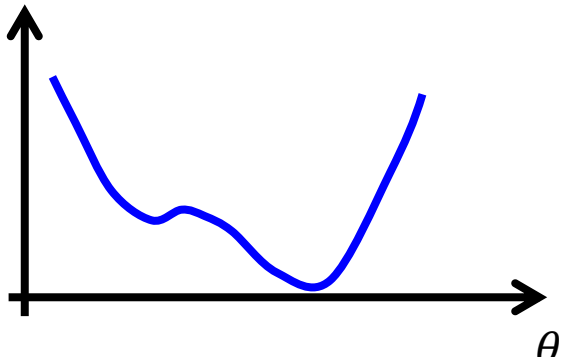
- e.g. linear regression
- Can be solved efficiently (find global optimal solution) in polynomial time
- Gradient descent (or many acceleration methods e.g., Newton method) can converge to global solution

Non-convex problem

- e.g. clustering, maximum likelihood for GMM
- Cannot find global solution in polynomial time

(NP-hard)

- Use heuristics to find local optimal solution



Optimization

- Definition: An optimization problem is specified by

$$\begin{aligned} &\text{minimize} && f_0(x) \\ &\text{subject to} && f_i(x) \leq 0,\ i = 1, \ldots, m \\ &&& h_i(x) = 0,\ i = 1, \ldots, p \end{aligned}$$

- A convex optimization problem has the following requirements
  - The objective function $f_0(x)$ must be convex
  - The inequality constraint functions $f_i(x)$ must be convex
  - The equality constraint functions $h_i(x)$ must be affine

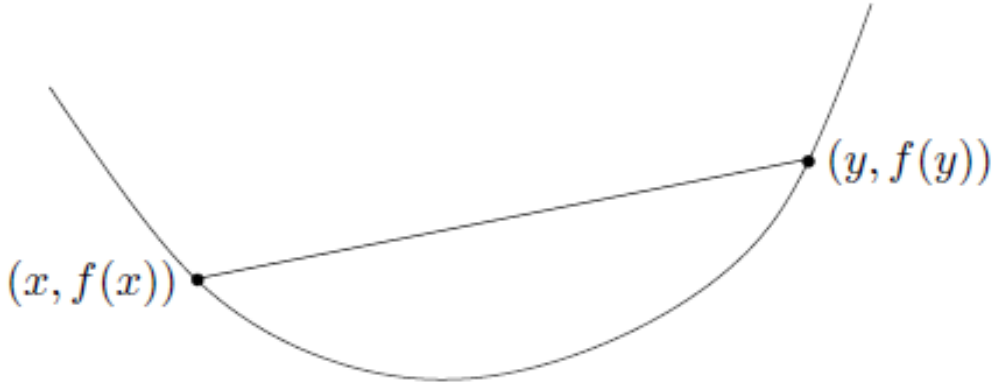
- Eg. support vector machines (SVM), logistic regression, maximum likelihood, ridge regression, …

Convex Functions

- Definition: A function $f: R^n \rightarrow R$ is convex if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$, and $0 \leq \theta \leq 1$, we have

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y)$$

- Geometrically, the line segment between $(x, f(x))$ and $(y, f(y))$ lies above the graph of f

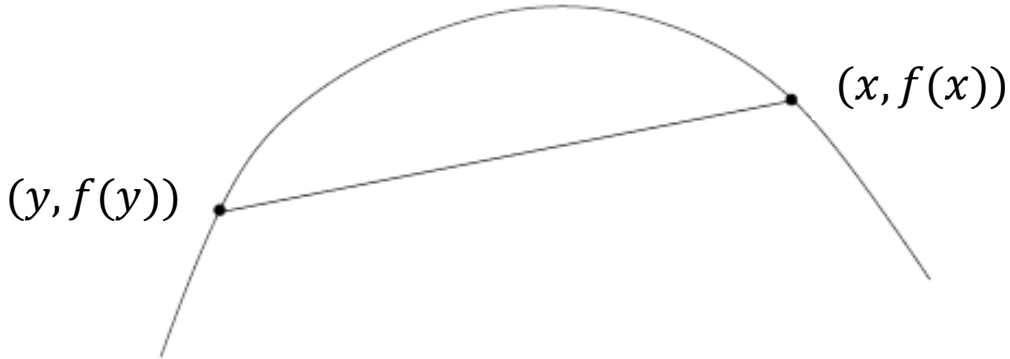


Concave Functions

- Definition: A function $f: R^n \rightarrow R$ is concave if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$, and $0 \leq \theta \leq 1$, we have

$$f(\theta x + (1-\theta)y) \geq \theta f(x) + (1-\theta) f(y)$$

- Geometrically, the line segment between $(x, f(x))$ and $(y, f(y))$ lies below the graph of f



Examples

- Exponential: e^{ax} for every $a \in R$
- Powers: x^a is convex on R_{++} when $a \geq 1$ or $a \leq 0$; concave (i.e., $-f$ is convex) for $0 \leq a \leq 1$
- Powers of absolute vaue: $|x|^p$ for $p \geq 1$
- Logarithm: $\log x$ is concave on R_{++}
- Negative entropy: $x \log x$ is convex
- Norms: All norms are convex (nonnegative; homogeneous; triangular inequality)
- Max function: $f(x) = \max\{x_1, \ldots, x_n\}$ is convex
- Log-determinant: $f(X) = \log \det X$ is convex for all positive definite matrices

Used in EM

Used in multivariate Gaussian fit

Operations that Preserve Convexity

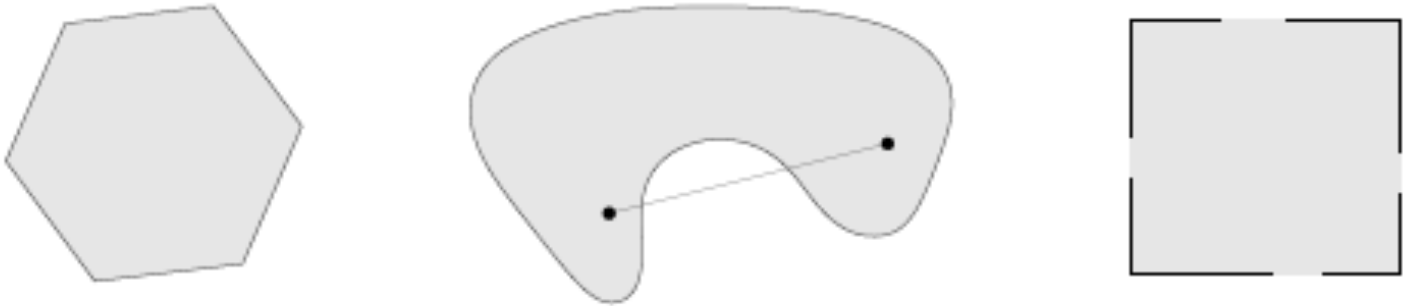
- Nonnegative weighted sums: If $f_1, \dots, f_m$ are convex, and $w_1, \dots, w_m \geq 0$, then
$$f = w_1 f_1 + \cdots + w_m f_m$$
is convex

- Composition with an affine mapping: suppose f is convex, then
$$g(x) = f(Ax + b)$$
with $\mathbf{dom} g = \{x | Ax + b \in \mathbf{dom} f\}$ is convex

- Pointwise maximum and supremum: If f_1 and f_2 are convex, then $f(x) = \max\{f_1, f_2\}$ is also convex. It easily extends to multiple functions.

Convex Set

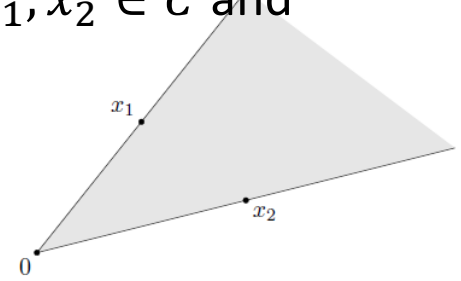
- Definition: A set A is convex, if for every $0 \leq \alpha \leq 1$ it satisfies
  - $\forall x,\ y \in A \rightarrow \alpha x + (1-\alpha)y \in A$
- The line segment between any two points is also in the set.
- Examples of convex and non-convex sets



Common Convex Set

- Cones: A set C is a convex cone, if for any $x_1, x_2 \in C$ and $\theta_1, \theta_2 \geq 0$, we have

$$\theta_1 x_1 + \theta_2 x_2 \in C$$

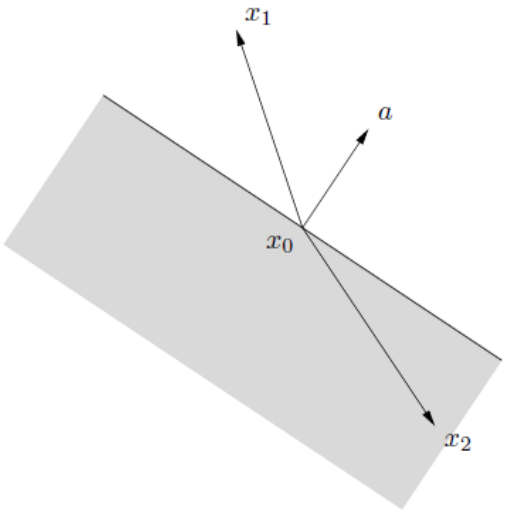


- Hyperplanes and halfspaces:
  A set is hyperplane if

$$\{x | a^\top (x - x_0) = 0, a \neq 0\}$$

  A halfspace is

$$\{x | a^\top (x - x_0) \leq 0, a \neq 0\}$$



Common Convex Set

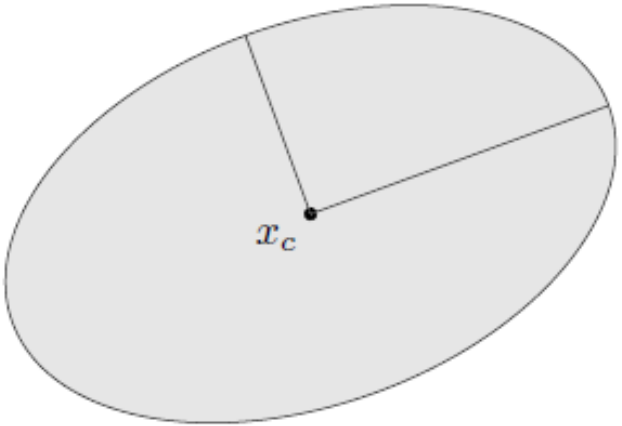
- Euclidean balls: A Euclidean ball has the form

$$B(x_c, r) = \{x | \|x - x_c\|_2 \leq r\}$$

- Ellipsoids:

$$E = \{x | (x - x_c)^\top P^{-1} (x - x_c) \leq 1\}$$

  - The eigen-vectors and eigen-values determine the direction and shape of the semi-axes



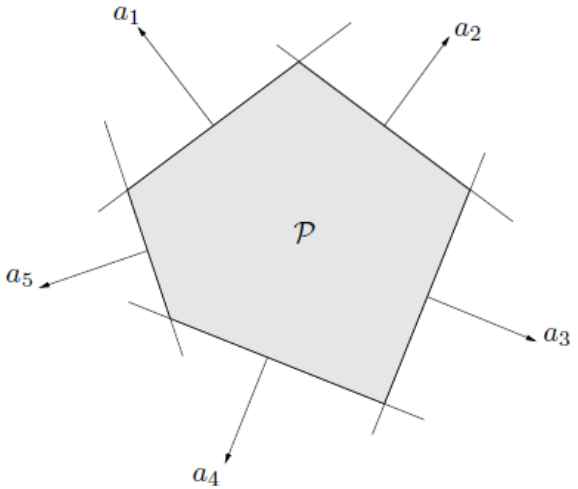
Used in support vector novelty detection

Common Convex Set

- Polyhedra: Intersection of a *finite* set of halfspaces/hyperplanes

$$P = \{x | a_j^\top x \leq b_j, j = 1, \ldots, m, c_j^\top x = d_j, j = 1, \ldots, p\}$$

- It is defined by as the solution set of a finite number of linear equalities and inequalities



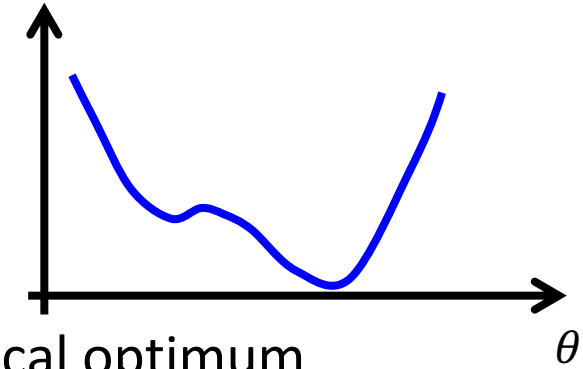
Used in SVM

Global vs. local optimum

- Global optimum: a point x^* in the feasible set is a global optimum iff

$$f_0(x^*) \leq f_0(x)$$

for all x in the feasible set

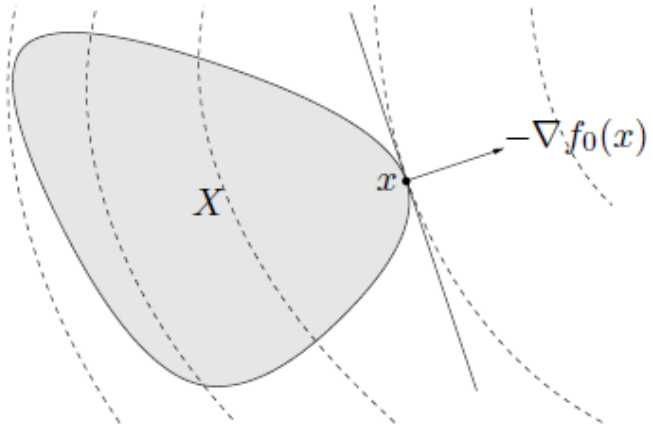


- Local optimum: a point x^* in the feasible set is a local optimum iff there exists $r > 0$, such that for all $x \in \{x | \|x - x^*\| \leq r\}$ and also in the feasible set, we have $f_0(x^*) \leq f_0(x)$

- For convex optimization problem, any local optimum is also a global optimum

First order optimality condition

- Let X denotes the feasible set, then x is optimal iff
$$\nabla f_0(x)^\top (y - x) \geq 0 \text{ for all } y \in X$$
- For an unconstrained problem, the condition becomes
$$\nabla f_0(x) = 0$$
- Geometrically, if $\nabla f_0(x) \neq 0$, it means $-\nabla f_0(x)$ is orthogonal to the feasible set at x



Constrained vs. unconstrained

For an unconstrained problem, the condition becomes

$$\nabla f_0(x) = 0$$

For constrained problem, we need to use the Lagrangian

$$L(x, \mu, \lambda) = f_0(x) + \sum_{i=1}^{p} \mu_i h_i(x) + \sum_{i=1}^{m} \lambda_i f_i(x)$$

$$\text{s.t.} \quad \lambda_i \geq 0$$

to transform it into an unconstrained problem

It is a lower bound of $f_0(x)$ for all $x \in X$, since $h_i(x)=0$, $f_i(x) \leq 0$ and $\lambda_i \geq 0$

$$L(x, \mu, \lambda) \leq f_0(x) \text{ for all } x \in X$$

Lagrange dual function

- The Lagrange dual function is

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda)$$

- It is a lower bound for the optimal value

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda) \leq L(x^*, \mu, \lambda) \leq f_0(x^*)$$

- We want to maximize the lower bound to make it tight

$$g(\mu^*, \lambda^*) = \max g(\mu, \lambda)$$

Primal and Dual problems

- Primal problem

$$\begin{aligned} &\text{minimize} && f_0(x) \\ &\text{subject to} && f_i(x) \leq 0, \ i = 1, \dots, m \\ &&& h_i(x) = 0, \ i = 1, \dots, p \end{aligned}$$

- Dual problem

$$\begin{aligned} &\text{maximize} && g(\mu, \lambda) \\ &\text{subject to} && \lambda_i \geq 0, \ i = 1, \dots, m \end{aligned}$$

- Strong duality (for convex problems, with mild condition)

$$g(\mu^*, \lambda^*) = f_0(x^*)$$

- Slater's condition: There exists an x inside the relative interior of the domain X such that, $f_i(x) < 0, \ i = 1, \dots, m$

KKT Optimality conditions

The following list of conditions for an optimal triplet (x^*, μ^*, λ^*), are called KKT conditions

- $\nabla f_0(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla f_i(x^*) + \sum_{i=1}^{p} \mu_i^* \nabla h_i(x^*) = 0$
- $\lambda_i^* f_i(x^*) = 0$ (complementarity condition)
- $f_i(x^*) \leq 0$
- $h_i(x^*) = 0$
- $\lambda_i^* \geq 0$


SUMMARY