Lecture 7: Optimization

CSE4130: 기초머신러닝

Junsuk Choe (최준석)

Roadmap

(1) Optimization Using Gradient Descent

(2) Constrained Optimization and Lagrange Multipliers

(3) Convex Sets and Functions

(4) Convex Optimization

(5) Convex Conjugate

Summary

- Training machine learning models = finding a good set of parameters
- A good set of parameters = Solution (or close to solution) to some optimization problem
- Directions: Unconstrained optimization, Constrained optimization, Convex optimization
- High-school math: A necessary condition for the optimal point: $f'(x) = 0$ (stationary point)
    - Gradient will play an important role

Roadmap

(1) Optimization Using Gradient Descent

(2) Constrained Optimization and Lagrange Multipliers

(3) Convex Sets and Functions

(4) Convex Optimization

(5) Convex Conjugate

Unconstrained Optimization and Gradient Algorithms

- Goal

$$\min f(\boldsymbol{x}), \quad f(\boldsymbol{x}) : \mathbb{R}^n \mapsto \mathbb{R}, \quad f \in C^1$$

- Gradient-type algorithms

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \gamma_k \boldsymbol{d}_k, \quad k = 0, 1, 2, \ldots$$

- Lemma. Any direction $\boldsymbol{d} \in \mathbb{R}^{n \times 1}$ that satisfies $\nabla f(\boldsymbol{x}) \cdot \boldsymbol{d} < 0$ is a descent direction of f at $\boldsymbol{x}$. That is, if we let $\boldsymbol{x}_\alpha = \boldsymbol{x} + \alpha \boldsymbol{d}$, $\exists \bar{\alpha} > 0$, such that for all $\alpha \in (0, \bar{\alpha}]$, $f(\boldsymbol{x}_\alpha) < f(\boldsymbol{x})$.
- Steepest gradient descent[1]. $\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)^\mathsf{T}$.
- Finding a local optimum $f(\boldsymbol{x}_\star)$, if the step-size γ_k is suitably chosen.
- Question. How do we choose $\boldsymbol{d}_k$ for a constrained optimization?

[1] In some cases, just gradient descent often means this steepest gradient descent.

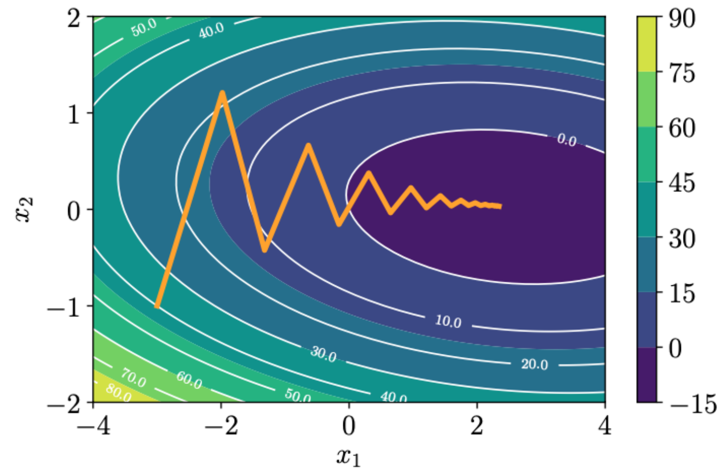
Example

- A quadratic function $f : \mathbb{R}^2 \mapsto \mathbb{R}$.

$$f\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) = \frac{1}{2}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} 2 & 1 \\ 1 & 20 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} 5 \\ 3 \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

whose gradient is $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} 2 & 1 \\ 1 & 20 \end{pmatrix} - \begin{pmatrix} 5 \\ 3 \end{pmatrix}^{\mathsf{T}}$

- $\boldsymbol{x}_0 = (-3 - 1)^{\mathsf{T}}$
- constant step size $\alpha = 0.085$
- Zigzag pattern



Taxonomy

- Goal: $\min L(\boldsymbol{\theta})$ for n training data
- Based on the amount of training data used for each iteration
  - Batch gradient descent (the entire n)
  - Mini-batch gradient descent($k < n$ data)
  - Stochastic gradient descent (one sampled data)
- Based on the adaptive method of update
  - Momentum, NAG, Adagrad, RMSprop, Adam, etc
- `https://ruder.io/optimizing-gradient-descent/`

Stochastic Gradient Descent (SGD)

- Assume $L(\boldsymbol{\theta}) = \sum_{i=1}^{n} L_n(\boldsymbol{\theta})$ (which happens in many cases in machine learning, e.g., negative log-likelihood in regression)
- Gradient update

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \gamma_k \nabla L(\boldsymbol{\theta}_k)^\mathsf{T} = \boldsymbol{\theta}_k - \gamma_k \sum_{n=1}^{N} \nabla L_n(\boldsymbol{\theta}_k)^\mathsf{T}$$

  - Batch gradient: $\sum_{n=1}^{N} \nabla L_n(\boldsymbol{\theta}_k)^\mathsf{T}$
  - Mini-batch gradient: $\sum_{n \in \mathcal{K}} \nabla L_n(\boldsymbol{\theta}_k)^\mathsf{T}$ for a suitable choice of $\mathcal{K}, |\mathcal{K}| < n$
  - Stochastic gradient: $\nabla L_n(\boldsymbol{\theta}_i)^\mathsf{T}$ for some (randomly chosen) i. Noisy approximation to the real gradient.
- Tradeoff: computation burden vs. exactness

Adaptivity for Better Convergence: Momemtum

- Step size.
  - Too small: slow update, Too big: overshoot, zig-zag, often fail to converge
- Adaptive update: smooth out the erratic behavior and dampens oscillations
- Gradient descent with momentum

  $$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \gamma_i \nabla f(\boldsymbol{x}_k)^\mathsf{T} + \alpha \Delta \boldsymbol{x}_k, \quad \alpha \in [0,1]$$

  $$\Delta \boldsymbol{x}_k = \boldsymbol{x}_k - \boldsymbol{x}_{k-1}$$

  - Memory term: $\alpha \Delta \boldsymbol{x}_k$, where α is the degree of how much we remember the past
  - Next update = a linear combination of current and previous updates

Roadmap

Standard Constrained Optimization Problem

- An optimization problem in standard form:

$$
\begin{aligned}
\text{minimize } & f(\boldsymbol{x}) \\
\text{subject to } & g_i(\boldsymbol{x}) \leq 0, \quad i = 1, 2, \ldots, m \quad (\textit{Inequality constraints}) \\
& h_j(\boldsymbol{x}) = 0, \quad j = 1, 2, \ldots, p \quad (\textit{Equality constraints})
\end{aligned}
$$

- Variables: $\boldsymbol{x} \in \mathbb{R}^n$. Assume nonempty feasible set
- Optimal value: p^*. Optimizer: $\boldsymbol{x}^*$

Problem Solving via Langrange Multipliers

- Duality
  - Bound or solve an optimization problem via a different optimization problem!
  - We'll develop the basic Lagrange duality theory for a general optimization problem, then specialize for convex optimization
- Idea: augment the objective with a weighted sum of constraints
  - Lagrangian:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = f(\boldsymbol{x}) + \sum_{i=1}^{m} \lambda_i g_i(\boldsymbol{x}) + \sum_{i=1}^{p} \nu_i h_i(\boldsymbol{x})$$

  - Lagrange multipliers (dual variables): $\boldsymbol{\lambda} = (\lambda_i : i = 1, \cdots, m) \succeq 0$, $\boldsymbol{\nu} = (\nu_1, \cdots, \nu_p)$
  - Lagrange dual function:

$$\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\nu})$$

Lower Bound on the Optimal Value

- The dual function $\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu})$ is the lower bound on the optimal value p^*.
- Theorem. $\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq p^*, \quad \forall \boldsymbol{\lambda} \succeq 0, \ \boldsymbol{\nu}$
- Proof. Consider feasible $\tilde{\boldsymbol{x}}$. Then,

$$\mathcal{L}(\tilde{\boldsymbol{x}}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = f(\tilde{\boldsymbol{x}}) + \sum_{i=1}^{m} \lambda_i g_i(\tilde{\boldsymbol{x}}) + \sum_{i=1}^{p} \nu_i h_i(\tilde{\boldsymbol{x}}) \leq f(\tilde{\boldsymbol{x}})$$

  since $g_i(\tilde{\boldsymbol{x}}) \leq 0$ and $\lambda_i \geq 0$.
  Hence, $\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq \mathcal{L}(\tilde{\boldsymbol{x}}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \leq f(\tilde{\boldsymbol{x}})$ for all feasible $\tilde{\boldsymbol{x}}$. Therefore, $\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq p^*$.

Lagrangian Dual Problem

- Lower bound from Lagrange dual function depends on $(\boldsymbol{\lambda}, \boldsymbol{\nu})$.
- Question. What's the best lower bound?

Langrangian dual problem
$$\begin{array}{ll} \text{maximize} & \mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) \\ \text{subject to} & \boldsymbol{\lambda} \succeq 0 \end{array}$$

- Dual variables: $(\boldsymbol{\lambda}, \boldsymbol{\nu})$
- Always a convex optimization, because $\mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu})$ is always concave over $\boldsymbol{\lambda}, \boldsymbol{\nu}$.
  - Infimum over $\boldsymbol{x}$ of a family of affine functions in $(\boldsymbol{\lambda}, \boldsymbol{\nu})$ (we will see this later)
- Denote the optimal value of Lagrange dual problem by d^*.

Weak Duality

- What's the relationship between d^* and p^*?

Weak Duality

$d^* \leq p^*$

- Weak duality always hold (even if the primal problem is not convex):
- Optimal duality gap: $p^* - d^*$
- Efficient generation of the lower bounds through the dual problem

Roadmap

(1) Optimization Using Gradient Descent

(2) Constrained Optimization and Lagrange Multipliers

(3) Convex Sets and Functions

(4) Convex Optimization

(5) Convex Conjugate

Convex Optimization

- Convex optimization problem

$$\begin{aligned} \text{minimize} \quad & f(\boldsymbol{x}) \\ \text{subject to} \quad & \boldsymbol{x} \in \mathcal{X}, \end{aligned}$$

  where $f(\boldsymbol{x}) : \mathbb{R}^n \mapsto \mathbb{R}$ is a convex function, and $\mathcal{X}$ is a convex set.

- The watershed between easily solvable problem and intractable ones is not 'linearity', but 'convexity'

- Let's overview the background of convex functions, convex sets, and their basic properties.

Convex Set

- Set $\mathcal{C}$ is a convex set if the line segment between any two points in $\mathcal{C}$ lies in $\mathcal{C}$, i.e., if for any $x_1, x_2 \in \mathcal{C}$ and any $\theta \in [0,1]$, we have $\theta x_1 + (1-\theta)x_2 \in \mathcal{C}$
- Convex hull of $\mathcal{C}$ is the set of all convex combinations of points in $\mathcal{C}$:

$$\left\{ \sum_{i=1}^{k} \theta_i x_i \mid x_i \in \mathcal{C}, \theta_i \geq 0, i = 1, 2, \ldots, k, \sum_{i=1}^{k} \theta_i = 1 \right\}$$

- What is k? For all k? For some k?

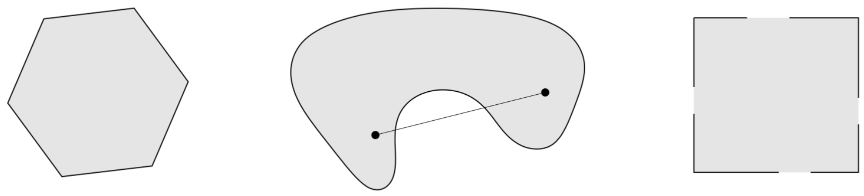
- Generalize to infinite sums and integrals:

$$\sum_{i=1}^{\infty} \theta_i x_i \in \mathcal{C}, \quad \int_{\mathcal{C}} p(x) x dx \in \mathcal{C},$$

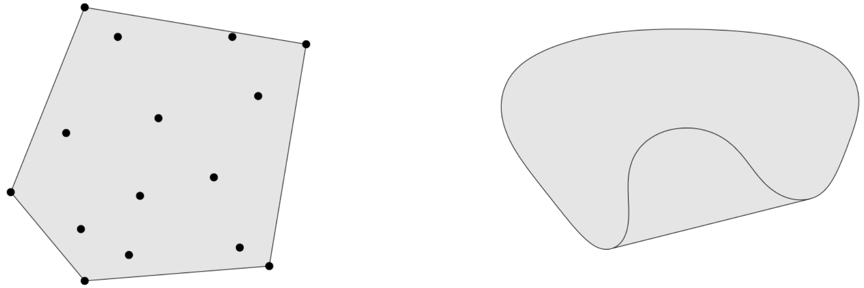
where $\sum_{i=1}^{\infty} \theta_i = 1$ and $p(x)$ is a pdf of some random variable.

Examples

- Convex and Non-convex sets



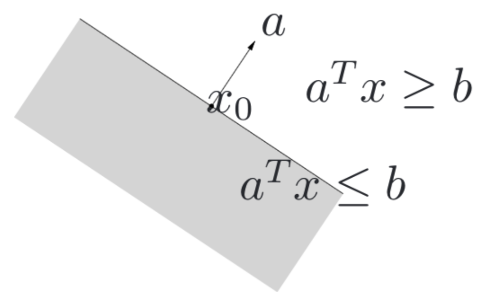
- Convex hulls



Examples of Convex Sets

- Hyperplane in $\mathbb{R}^n$ is a set: $\{x \mid a^\mathsf{T} x = b\}$ where $a \in \mathbb{R}^n, a \neq 0, b \in \mathbb{R}$
  In other words, $\{x \mid a^\mathsf{T}(x - x_0) = 0\}$, where x_0 is any point in the hyperplane, i.e., $a^\mathsf{T} x_0 = b$.

- Divides $\mathbb{R}^n$ into two halfspaces:
  $\{x | a^\mathsf{T} x \leq b\}$ and $\{x | a^\mathsf{T} x > b\}$

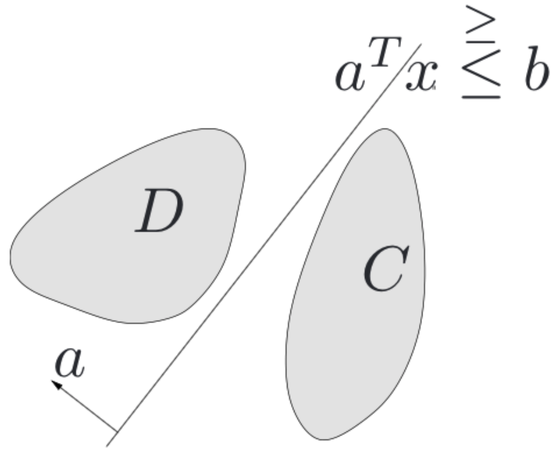


- Polyhedron is the solution set of a finite number of linear equalities and inequalities (intersection of finite number of halfspaces and hyperplanes)

  $$\mathcal{P} = \{x \mid a_j^\mathsf{T} x \leq b_j, j = 1, \ldots, m, c_j^\mathsf{T} x = d_j, j = 1, \ldots, p\} = \{x \mid Ax \leq b, Cx = d\}$$

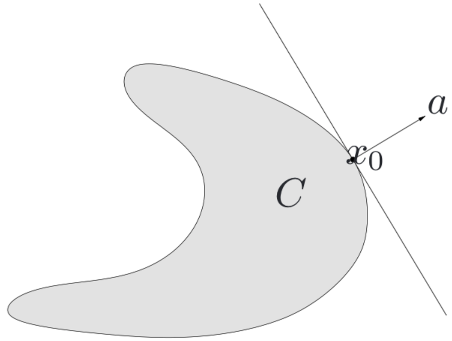
- Polytope: a bounded polyhedron

Separating Hyperplane Theorem



- $\mathcal{C}$ and $\mathcal{D}$: non-intersecting convex sets, i.e., $\mathcal{C} \bigcap \mathcal{D} = \phi$.
- Then, there exist $a \neq 0$ and b such that $a^\mathsf{T} x \leq b$ for all $x \in \mathcal{C}$ and $a^\mathsf{T} x \geq b$ for all $x \in \mathcal{D}$.

Supporting Hyperplane Theorem



- Given a set $\mathcal{C} \in \mathbb{R}^n$ and a point x_0 on its boundary, if $a \neq 0$ satisfies $a^\mathsf{T} x \le a^\mathsf{T} x_0$ for all $x \in \mathcal{C}$, then $\{x | a^\mathsf{T} x = a^\mathsf{T} x_0\}$ is called a supporting hyperplane to $\mathcal{C}$ at x_0
- For any nonempty convex set $\mathcal{C}$ and any x_0 on boundary of $\mathcal{C}$, there exists a supporting hyperplane to $\mathcal{C}$ at x_0
- What happens if $\mathcal{C}$ is non-convex?

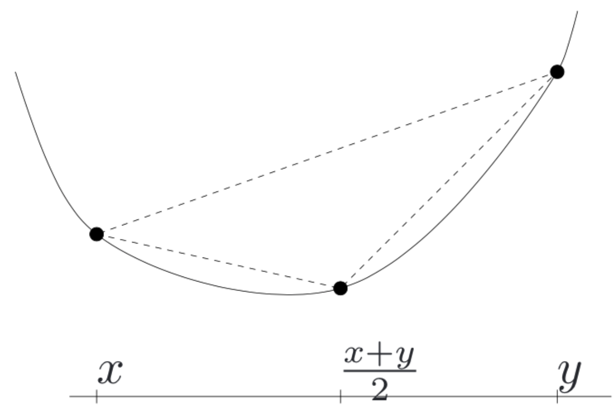
Convex Functions

- $f : \mathbb{R}^n \mapsto \mathbb{R}$ is a convex function if dom f is a convex set and for all $x, y \in$ dom f and $\theta \in [0, 1]$, we have

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

- f is strictly convex if the strict inequality in the above holds for all $x \neq y$ and $0 < \theta < 1$.

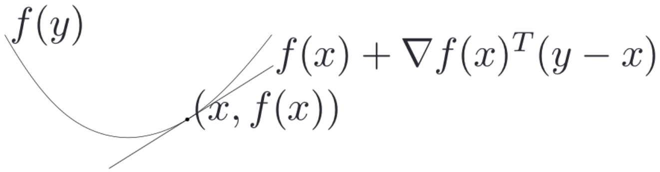
- f is concave if $-f$ is convex
- Affine functions preserve convexity.
- Jensen's inequality. For a rv X, $f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$.



Conditions of Convex Functions (1)

- First-order condition. For differentiable functions, f is convex iff

  $$f(y) - f(x) \geq \nabla f(x)^{\mathsf{T}}(y - x), \quad \forall x, y \in \text{dom } f, \text{and dom } f \text{ is convex}$$



- Example. $f(y) = y^2$.
- $f(y) \geq \tilde{f}_x(y)$ where $\tilde{f}_x(y)$ is the first order Taylor expansion of $f(y)$ at x.
- Local information (first order Taylor approximation) about a convex function provides global information (global underestimator).
- If $\nabla f(x) = 0$, then $f(y) \geq f(x)$, $\forall y$. Thus, x is a global minimizer of f

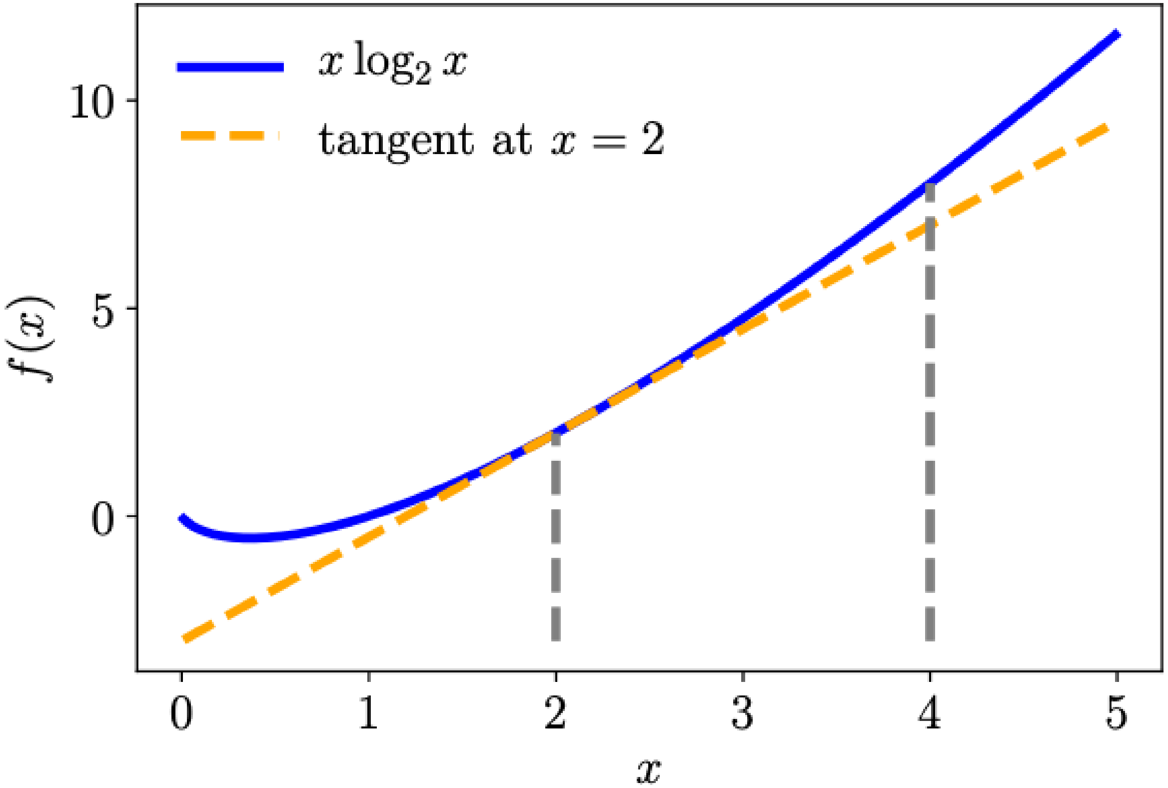
Conditions of Convex Functions (2)

- Second-order condition. For twice differentiable functions, f is convex iff

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

  for all $x \in \mathrm{dom}\, f$ (upward slope) and $\mathrm{dom}\, f$ is convex
- Example: $f(x) = x^2$.
- Meaning: The graph of the function have positive (upward) curvature at x.

Example 7.3



Examples of Convex or Concave Functions

- e^{ax} is convex on $\mathbb{R}$, for any $a \in \mathbb{R}$
- x^a is convex on $\mathbb{R}_{++}$ when $a \geq 1$ or $a \leq 0$, and concave for $0 \leq a \leq 1$
- $|x|^p$ is convex on $\mathbb{R}$ for $p \geq 1$
- $\log x$ is concave on $\mathbb{R}_{++}$
- $x \log x$ is strictly convex on $\mathbb{R}_{++}$
- Every norm on $\mathbb{R}^n$ is convex
- $f(x) = \max\{x_1, \ldots, x_n\}$ is convex on $\mathbb{R}^n$
- $f(x) = \log \sum_{i=1}^n e^{x_i}$ is convex on $\mathbb{R}^n$
- $f(x) = (\prod_{i=1}^n x_i)^{\frac{1}{n}}$ is concave on $\mathbb{R}^n_{++}$

Convexity-Preserving Operations

- $f = \sum_{i=1}^{n} w_i f_i$ convex if f_i are all convex and $w_i \geq 0$
- $g(x) = f(Ax + b)$ is convex iff $f(x)$ is convex
- $f(x) = \max\{f_1(x), f_2(x)\}$ convex if f_i convex.
- $g(x) = \inf_{y \in \mathcal{C}} f(x, y)$ is convex if f is convex in (x, y) and $\mathcal{C}$ is convex

Example 7.4

Roadmap

(1) Optimization Using Gradient Descent

(2) Constrained Optimization and Lagrange Multipliers

(3) Convex Sets and Functions

(4) Convex Optimization

(5) Convex Conjugate

Standard Convex Optimization

- A standard convex optimization problem with variables $\boldsymbol{x}$:

$$\begin{array}{ll} \text{minimize} & f(\boldsymbol{x}) \\ \text{subject to} & g_i(\boldsymbol{x}) \leq 0, \quad i = 1, 2, \ldots, m \\ & {a_i}^\mathsf{T} \boldsymbol{x} = b_i, \quad i = 1, 2, \ldots, p \end{array}$$

  where $f, f_1, \ldots, f_m$ are convex functions.

- Minimize convex objective function (or maximize concave objective function)
- Upper bound inequality constraints on convex functions ($\Rightarrow$ Constraint set is convex)
- Equality constraints must be affine (Only affine functions leads to a convex set for the equality constraints)

Useful Tips

- Minimization problem
  - Problem: min $f(x)$ s.t. $f_i(x) \leq 0, \quad g_i(x) = 0, \quad x$
  - $f(x)$: convex, $f_i(x)$: convex, $g_i(x)$: affine
  - $L(x, \lambda, \mu) = f(x) + \sum_i \lambda_i f_i(x) + \sum_i \mu_i g_i(x)$
  - $\inf_x L(x, \lambda, \mu) = \mathcal{D}(\lambda, \mu)$
  - $\max_{\lambda \geq 0} \mathcal{D}(\lambda, \mu)$
- Maximization problem
  - Problem: max $f(x)$ s.t. $f_i(x) \geq 0, \quad g_i(x) = 0, \quad x$
  - $f(x)$: concave, $f_i(x)$: concave, $g_i(x)$: affine
  - $L(x, \lambda, \mu) = f(x) + \sum_i \lambda_i f_i(x) + \sum_i \mu_i g_i(x)$
  - $\sup_x L(x, \lambda, \mu) = \mathcal{D}(\lambda, \mu)$
  - $\min_{\lambda \geq 0} \mathcal{D}(\lambda, \mu)$

Linear Programming

- Primal problem

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^d} \quad & \boldsymbol{c}^\mathsf{T}\boldsymbol{x} \\ \text{subject to} \quad & \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b}, \end{aligned}$$

where $\boldsymbol{A} \in \mathbb{R}^{m\times d}$ and $\boldsymbol{b} \in \mathbb{R}^m$.

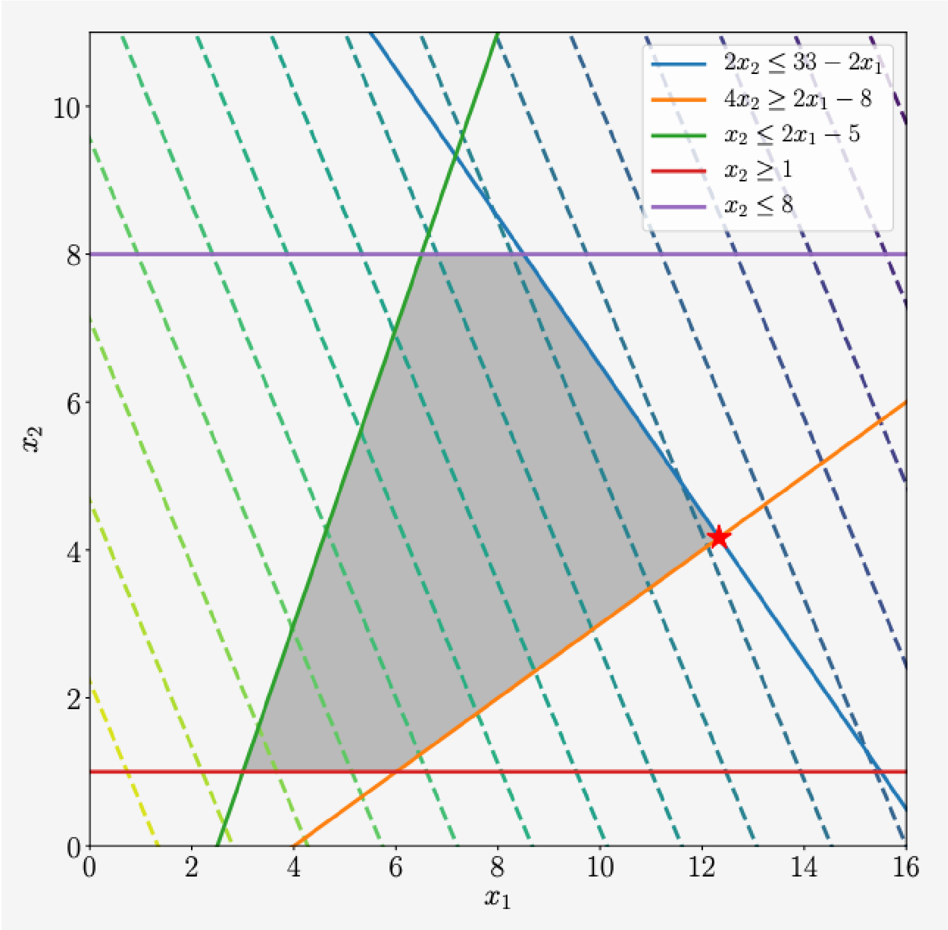
- Dual problem

$$\begin{aligned} \max_{\boldsymbol{\lambda}\in\mathbb{R}^m} \quad & -\boldsymbol{b}^\mathsf{T}\boldsymbol{\lambda} \\ \text{subject to} \quad & \boldsymbol{c} + \boldsymbol{A}^\mathsf{T}\boldsymbol{\lambda} = \boldsymbol{0}, \ \boldsymbol{\lambda} \succeq \boldsymbol{0}, \end{aligned}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^m$.

- The Lagrangian: $\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda}) = (\boldsymbol{c} + \boldsymbol{A}^\mathsf{T}\boldsymbol{\lambda})^\mathsf{T}\boldsymbol{x} - \boldsymbol{\lambda}^\mathsf{T}\boldsymbol{b}$, whose derivative w.r.t. $\boldsymbol{x}$ becomes zero, when $\boldsymbol{c} + \boldsymbol{A}^\mathsf{T}\boldsymbol{\lambda} = \boldsymbol{0}$.
- The dual function: $\mathcal{D}(\boldsymbol{\lambda}) = -\boldsymbol{\lambda}^\mathsf{T}\boldsymbol{b}$

Example 7.5



$2x_2 \leq 33 - 2x_1$
$4x_2 \geq 2x_1 - 8$
$x_2 \leq 2x_1 - 5$
$x_2 \geq 1$
$x_2 \leq 8$
x_1
x_2
0
2
4
6
8
10
12
14
16

Quadratic Programming

- Primal problem

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^d} \quad & \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} + c^\top \boldsymbol{x} \\ \text{subject to} \quad & \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b}, \end{aligned}$$

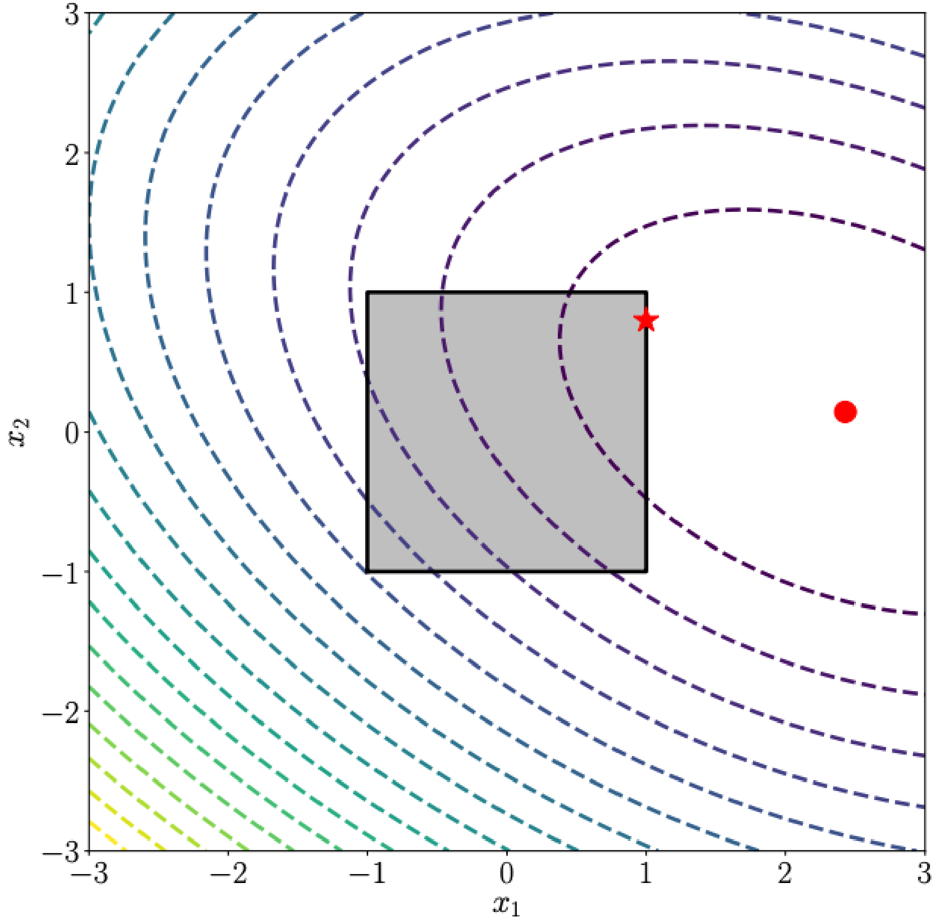
where $\boldsymbol{A} \in \mathbb{R}^{m\times d}$, $\boldsymbol{b} \in \mathbb{R}^m$, $\boldsymbol{c} \in \mathbb{R}^d$, the square matrix $\boldsymbol{Q}$ is symmetric, positive definite.

- Dual problem

$$\begin{aligned} \max_{\boldsymbol{\lambda}\in\mathbb{R}^m} \quad & \left(-\frac{1}{2}(\boldsymbol{c} + \boldsymbol{A}^\top\boldsymbol{\lambda})^\top \boldsymbol{A}\boldsymbol{Q}^{-1}(\boldsymbol{c} + \boldsymbol{A}^\top\boldsymbol{\lambda}) - \boldsymbol{\lambda}^\top \boldsymbol{b} \right) \\ \text{subject to} \quad & \boldsymbol{\lambda} \succeq \boldsymbol{0}, \end{aligned}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^m$.

Example 7.6



Roadmap

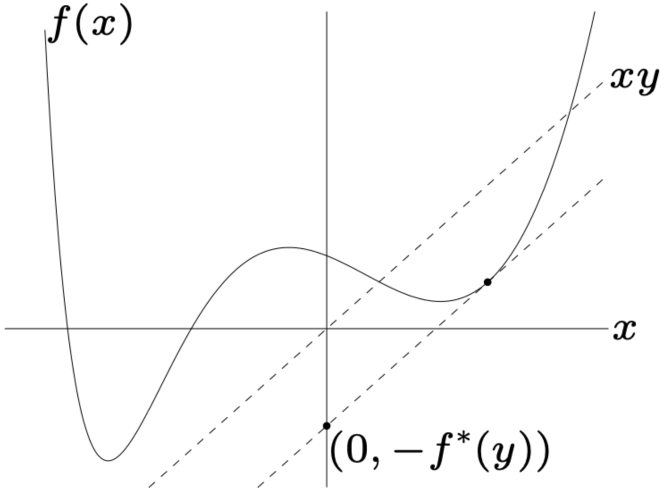
Conjugate Function: Definition and Meaning

- Given $f : \mathbb{R}^n \mapsto \mathbb{R}$, the conjugate function $f^* : \mathbb{R}^n \mapsto \mathbb{R}$ defined as:

$$f^*(\boldsymbol{y}) = \sup_{\boldsymbol{x} \in \mathrm{dom}\ f} (\boldsymbol{y}^\mathsf{T} \boldsymbol{x} - f(\boldsymbol{x}))$$

with domain consisting of $\boldsymbol{y} \in \mathbb{R}^n$ for which the supremum is finite

- Assume $\mathbb{R}^1$.
- For a given slope of y, $yx - f(x)$ is the vertical distance between the line yx and $f(x)$.
- Thus, $f^*(y)$ is the maximum distance



Conjugate Function: Properties

- Given $f : \mathbb{R}^n \mapsto \mathbb{R}$, the conjugate function $f^* : \mathbb{R}^n \mapsto \mathbb{R}$ defined as:

  $$f^*(\boldsymbol{y}) = \sup_{\boldsymbol{x} \in \text{dom } f} (\boldsymbol{y}^\top \boldsymbol{x} - f(\boldsymbol{x}))$$

  with domain consisting of $\boldsymbol{y} \in \mathbb{R}^n$ for which the supremum is finite

- $f^*(\boldsymbol{y})$: always convex (the pointwise supremum of a family of affine functions of $\boldsymbol{y}$)

- $f^{**} = f$ if f is convex and closed

- Fenchel's inequality: $f(\boldsymbol{x}) + f^*(\boldsymbol{y}) \geq \boldsymbol{y}^\top \boldsymbol{x}$ for all $\boldsymbol{x}, \boldsymbol{y}$ (by definition)
  - Example. $f(x) = |x|^2/2$. Then, $f^*(y) = |y|^2/2$. Thus, F-inequality tells us:

$$\frac{1}{2}(|x|^2 + |y|^2) \geq xy$$

Examples of Conjugate Functions

- $f(x) = ax + b$, $f^*(a) = -b$
- $f(x) = -\log x$, $f^*(y) = -\log(-y) - 1$ for $y < 0$
- $f(x) = e^x$, $f^*(y) = y \log y - y$
- $f(x) = x \log x$, $f^*(y) = e^{y-1}$
- $f(x) = \frac{1}{2} x^\mathsf{T} Q x$, $f^*(y) = \frac{1}{2} y^\mathsf{T} Q^{-1} y$ (Q is positive definite)
- $f(x) = \log \sum_{i=1}^n e^{x_i}$,

  $$f^*(y) = \begin{cases} \sum_{i=1}^n y_i \log y_i & \text{if } y \succeq 0 \text{ and } \sum_{i=1}^n y_i = 1, \\ \infty & \text{otherwise} \end{cases}$$

Conjugate Function and Lagrangian Dual Function

- They are closely related. Consider the following problem:

$$\begin{array}{ll} \text{minimize} & f(\boldsymbol{x}) \\ \text{subject to} & \boldsymbol{Ax} \preceq \boldsymbol{b}, \\ & \boldsymbol{Cx} = \boldsymbol{d} \end{array}$$

- Using the conjugate of f, we can write the dual function as:

$$\begin{aligned} \mathcal{D}(\boldsymbol{\lambda}, \boldsymbol{\nu}) &= \inf_{\boldsymbol{x}} \left(f(\boldsymbol{x}) + \boldsymbol{\lambda}^\top (\boldsymbol{Ax} - \boldsymbol{b}) + \boldsymbol{\nu}^\top (\boldsymbol{Cx} - \boldsymbol{d}) \right) \\ &= -\boldsymbol{b}^\top \boldsymbol{\lambda} - \boldsymbol{d}^\top \boldsymbol{\nu} + \inf_{\boldsymbol{x}} \left(f(\boldsymbol{x}) + (\boldsymbol{A}^\top \boldsymbol{\lambda} + \boldsymbol{C}^\top \boldsymbol{\nu})^\top \boldsymbol{x} \right) \\ &= -\boldsymbol{b}^\top \boldsymbol{\lambda} - \boldsymbol{d}^\top \boldsymbol{\nu} - f^* \left(-\boldsymbol{A}^\top \boldsymbol{\lambda} - \boldsymbol{C}^\top \boldsymbol{\nu} \right) \end{aligned}$$

References

[1] This lecture slide is mainly based upon
https://yung-web.github.io/home/courses/mathml.html (made by Prof. Yung Yi, KAIST EE)

[2] Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong. Mathematics for machine learning. Cambridge University Press, 2020.