Mathematics for Machine Learning

— Continuous Optimization: Preliminary Convex Optimization

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Credits for the resource

- The slides are based on the textbooks:
 - Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.
 - Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.
- We could partially refer to the monograph: Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

Outline

- Convex Programming
- 2 Linear Programming
- Quadratic Programming

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Our Focus & Motivation

Convex Optimization.

- A class of optimization problems where we can guarantee global optimality.
 - $f(\cdot)$ is a convex function.

The constraints $g(\cdot)$ and $h(\cdot)$ form convex sets.

Convex Sets & Functions

Convex set

A set C is convex if for any $\mathbf{x}, \mathbf{y} \in C$, we have

$$\forall \alpha \in [0,1], \alpha \mathbf{x} + (1-\alpha)\mathbf{y} \in \mathcal{C}.$$

Convex function

A function $f: \mathcal{C} \subseteq \mathbb{R}^D \mapsto \mathbb{R}$ is convex if for any $\mathbf{x}, \mathbf{y} \in \mathcal{C}$,

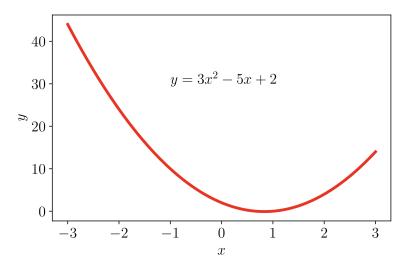
$$\forall \alpha \in [0,1], f((1-\alpha)\mathbf{x} + \alpha\mathbf{y}) \leq (1-\alpha)f(\mathbf{x}) + \alpha f(\mathbf{y}).$$

Equivalently, if f is differentiable (i.e., $\nabla f(\mathbf{x})$ exists for all $\mathbf{x} \in \mathcal{C}$), then f is convex if and only if for all $\mathbf{x}, \mathbf{y} \in \mathcal{C}$,

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla_{\mathbf{x}} f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}).$$

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An Example of Convex Functions



Remark

• If f(x) is twice differentiable (i.e., the Hessian exists for all $x \in C$), then

 $f(\mathbf{x})$ is convex $\iff \nabla_{\mathbf{x}}^2 f(\mathbf{x})$ is positive semidefinite.

Example

Show that $f(x) = x \lg x$ is convex for x > 0.

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• Note: $\lg x := \log_2 x$ and $\ln x := \log_e x$.

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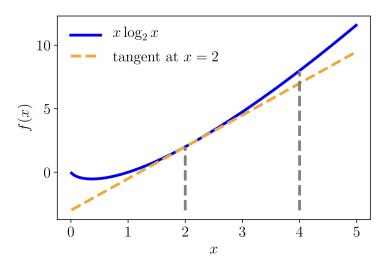
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- Compute $\nabla_x f(x)$.

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- Note: $\lg x := \log_2 x$ and $\ln x := \log_e x$.
- Compute $\nabla_x f(x)$.
- Say given x = 2, y = 4, compute $f(x) + \nabla_x f(x)^\top (y x)$.



Example (Theorem)

Theorem

Given a nonnegative real $\alpha \geq 0$ and two convex functions f_1 and f_2 , then $\alpha \cdot f_1 + (1 - \alpha)f_2$ is still convex.

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By definition,

$$f_1(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \leq \alpha f_1(\mathbf{x}) + (1 - \alpha)f_1(\mathbf{y})$$

$$f_2(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \leq \alpha f_2(\mathbf{x}) + (1 - \alpha)f_2(\mathbf{y}).$$

Summing up:

$$f_1(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) + f_2(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y})$$

$$\leq \alpha f_1(\mathbf{x}) + (1 - \alpha)f_1(\mathbf{y}) + \alpha f_2(\mathbf{x}) + (1 - \alpha)f_2(\mathbf{y})$$

$$\alpha (f_1(\mathbf{x}) + f_2(\mathbf{x})) + (1 - \alpha)(f_1(\mathbf{y}) + f_2(\mathbf{y})).$$

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Linear Programming

• Consider the special case that all the preceding functions are linear.

$$\label{eq:continuity} \begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad \mathbf{c}^\top \mathbf{x} \\ \text{subject to} \quad \mathbf{A} \mathbf{x} \leq \mathbf{b}. \end{aligned}$$

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

• The Lagrangian:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{c}^{\top} \mathbf{x} + \boldsymbol{\lambda}^{\top} (\boldsymbol{A} \mathbf{x} - \mathbf{b})$$

where $\lambda \in \mathbb{R}^m$ is the vector of non-negative Lagrange multipliers.

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Rearranging the terms:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = (\mathbf{c} + \boldsymbol{A}^{\top} \boldsymbol{\lambda})^{\top} \mathbf{x} - \boldsymbol{\lambda}^{\top} \mathbf{b}.$$

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ullet Thus, the dual Lagrangian is $\mathcal{D}(oldsymbol{\lambda}) = - oldsymbol{\lambda}^{ op} oldsymbol{b}.$

- Recall that we would like to maximize $\mathcal{D}(\lambda)$ and the constraint that $\lambda \geq \mathbf{0}$.
- The dual optimization problem is

$$\max_{\pmb{\lambda} \in \mathbb{R}^m} \qquad -\pmb{b}^{\top} \pmb{\lambda}$$
 subject to
$$\pmb{c} + \pmb{A}^{\top} \pmb{\lambda} = \pmb{0}$$

$$\pmb{\lambda} \geq \pmb{0}$$

which is also a linear program but with m variables.

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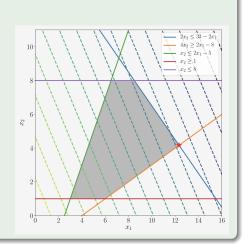
* Solve the primal or the dual program depending on whether m (i.e., # constraints) or d (i.e., # variables) is larger.

Consider the linear program

$$\min_{\mathbf{x} \in \mathbb{R}^2} - \begin{bmatrix} 5 \\ 3 \end{bmatrix}^\top \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

subject to

$$\begin{bmatrix} 2 & 2 \\ 2 & -4 \\ -2 & 1 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} 33 \\ 8 \\ 5 \\ -1 \\ 8 \end{bmatrix}$$



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Quadratic Programming

Consider the case of a convex quadratic objective function, where the constraints are affine:

$$\min_{\mathbf{x} \in \mathbb{R}^d} \qquad \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} + \mathbf{c}^\top \mathbf{x}$$
 subject to
$$\mathbf{A} \mathbf{x} \leq \mathbf{b},$$

where

- $\mathbf{A} \in \mathbb{R}^{m \times d}, \mathbf{b} \in \mathbb{R}^m$ and $\mathbf{c} \in \mathbb{R}^d$.
- $Q \in \mathbb{R}^{d \times d}$: a positive definite matrix. d variables and m linear constraints.

ML Math - Vector Calculus Quadratic Programming

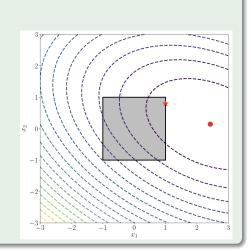
Example

Consider the quadratic program

$$\min_{\mathbf{x} \in \mathbb{R}^2} \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{\top} \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix}^{\top} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 5 \\ 3 \end{bmatrix}^{\top} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

subject to

$$\left[egin{array}{ccc} 1 & 0 \ -1 & 0 \ 0 & 1 \ 0 & -1 \end{array}
ight] \left[egin{array}{c} x_1 \ x_2 \end{array}
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The Lagrangian is given by

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \frac{1}{2} \mathbf{x}^{\top} \boldsymbol{Q} \mathbf{x} + \mathbf{c}^{\top} \mathbf{x} + \boldsymbol{\lambda}^{\top} (\boldsymbol{A} \mathbf{x} - \mathbf{b})$$
$$= \frac{1}{2} \mathbf{x}^{\top} \boldsymbol{Q} \mathbf{x} + (\mathbf{c} + \boldsymbol{A}^{\top} \boldsymbol{\lambda})^{\top} \mathbf{x} - \boldsymbol{\lambda}^{\top} \mathbf{b}.$$

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Taking the derivative w.r.t. \mathbf{x} and setting it to zero:

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Note that ${m Q}$ is invertible (: positive definite \Rightarrow nonzero eigenvalues \Rightarrow nonzero determinant), then

$$\mathbf{x} = -\mathbf{Q}^{-1}(\mathbf{c} + \mathbf{A}^{\top} \boldsymbol{\lambda}).$$

(Thanks to Yo-Cheng Chang)

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Taking the derivative w.r.t. \mathbf{x} and setting it to zero:

$$Qx + (c + A^{T}\lambda) = 0.$$

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Substituting it back to $\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$, we get the dual Lagrangian

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$$\mathcal{D}(\lambda) = -rac{1}{2}(\mathbf{c} + \mathbf{A}^{ op}\lambda)^{ op} \mathbf{\mathit{Q}}^{-1}(\mathbf{c} + \mathbf{A}^{ op}\lambda) - \lambda^{ op}\mathbf{b}.$$

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Therefore, the dual optimization problem is given by

$$\max_{m{\lambda} \in \mathbb{R}^m} \quad -rac{1}{2}(\mathbf{c} + m{A}^ op m{\lambda})^ op m{Q}^{-1}(\mathbf{c} + m{A}^ op m{\lambda}) - m{\lambda}^ op \mathbf{b}$$
 subject to $m{\lambda} \geq \mathbf{0}$

Heads up: Application in Support Vector Machine (SVM).

Discussions