Optimization methods
Lecture 1: Introduction.
Convex sets. Convex functions

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What is this course about?

Basic theory

- Convex sets and convex functions
- Optimality conditions
- Introduction to duality

Numerical methods

- First order methods and their accelerated versions
- Quasi-Newton methods
- Introduction to stochastic gradient methods
- Introduction to combinatorial optimization and convex relaxations

The place of this course in the program

- When you train some neural network, you solve some optimization problem
- Possible issues in this process will be discussed in the course
- How to solve these issues we will also discuss

Schedule and deadlines

- Lectures and webinars are once a week

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- Lecture slides are here:
  https://github.com/amkatrutsa/opt_modern_ai_ms

References

- S. Boyd and L. Vandenberghe *Convex Optimization* https://web.stanford.edu/~boyd/cvxbook/
- J. Nocedal, S. J. Wright *Numerical Optimization*
- I. Goodfellow et al *Deep learning book*

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  - many-many others

General methodology

Main steps for exploiting optimization methods in solving real-world problems:

1. Define objective function

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Main steps for exploiting optimization methods in solving real-world problems:

1. Define objective function
2. Define feasible set
3. Optimization problem statement and its analysis
4. Selection of the best algorithm for the stated problem
5. Algorithm implementation and verification its correctness

General problem statement

$$\begin{aligned} &\min_{\mathbf{x}\in\mathcal{X}} f_0(\mathbf{x}) \\ \text{s.t. } & f_i(\mathbf{x}) = 0,\ i = 1, \ldots, p \\ & f_j(\mathbf{x}) \leq 0,\ j = p+1, \ldots, m, \end{aligned}$$

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- $f_0(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ — objective function

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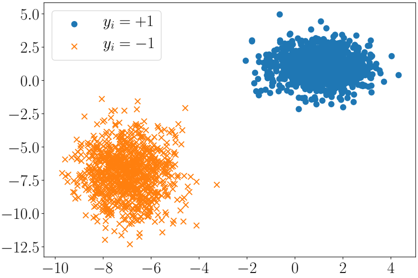
- $f_0(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ — objective function
- $f_k(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ — constraint functions

Linear classification problem

- Given dataset: $(\mathbf{x}_i, y_i)$, $\mathbf{x}_i \in \mathbb{R}^n,\ y_i = \{+1, -1\},\ i = 1, \dots, m$



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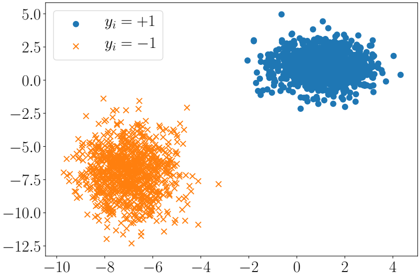

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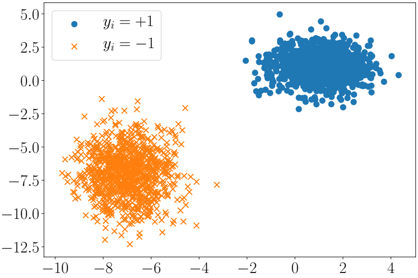

- Linear classifier $\hat{y} = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$
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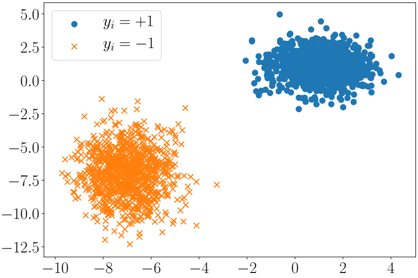

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- $y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 1$

Possible separating hypelplanes

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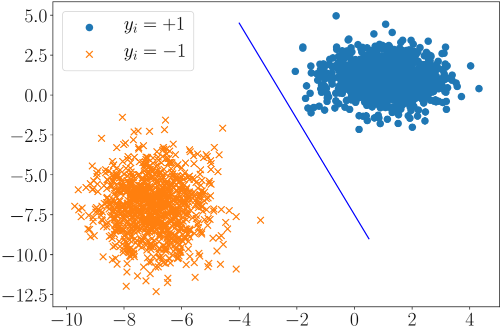

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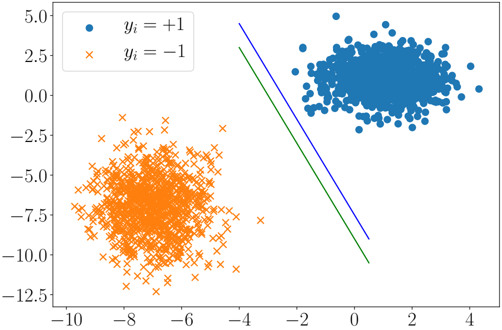

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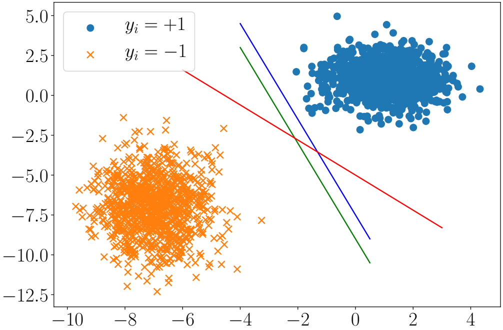

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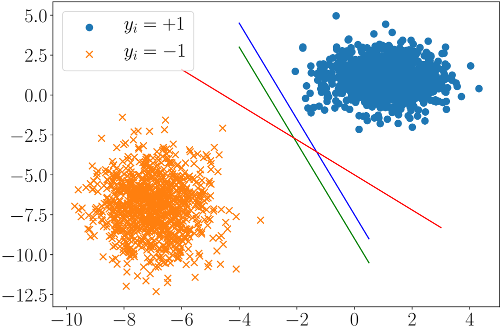

Q: How to define the separating hyperplane uniquely?

Margin maximization

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- For the support samples of every class the following holds

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- Distance between parallel hyperplanes $\mathbf{w}^\top \mathbf{x} + b = c_1$ and $\mathbf{w}^\top \mathbf{x} + b = c_2$:

$$d = \frac{|c_1 - c_2|}{\|\mathbf{w}\|_2} = \frac{2}{\|\mathbf{w}\|_2}$$

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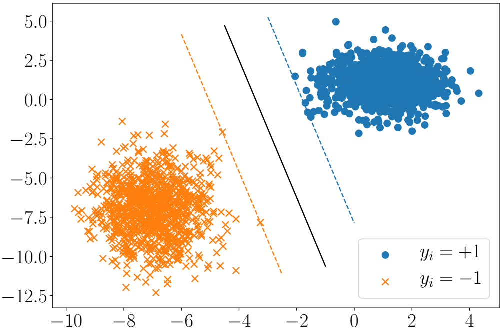
The final optimization problem

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$

$$\text{s.t. } y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 1, \; i = 1, \ldots, m$$

Optimal separating hyperplane



What solutions are possible?

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Definition

A point $\mathbf{x}^*$ *is called a point of* ***global*** *minimum, if* $f(\mathbf{x}) \geq f(\mathbf{x}^*)$ *for all* $\mathbf{x}$ *from the feasible set.*

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*A point $\mathbf{x}^*$ is called a point of **local** minimum, if $f(\mathbf{x}) \geq f(\mathbf{x}^*)$ for all $\mathbf{x}$ from some neighborhood of point $\mathbf{x}^*$ and from feasible set.*

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Another form of problem statement

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How to solve such problems?

In general case:

- NP-complete, i.e. very hard to solve
- randomized algorithms give a trade-off between running time and robustness of approximate solution

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However, some classes of optimization problems can be solved very efficiently

- Linear programming
- Linear least-squares problems
- Low-rank approximation problem
- Convex optimization

Main stages in optimization theory development

- 1940s — linear programming
- 1950s — quadratic programming
- 1960s — geometric programming
- 1990s — polynomial interior point methods for convex conic optimization problems

Modern topics

- Huge-scale optimization problems ($\sim 10^8 - 10^{12}$)

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- Applications of convex optimization

Convex optimization problem

$$\begin{aligned}
&\min_{\mathbf{x}\in\mathbb{R}^n} f_0(\mathbf{x}) \\
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- f_0, f_i — convex functions:

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  where $\alpha, \beta \ge 0$ and $\alpha + \beta = 1$.

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- no analytical solution
- efficient algorithms
- special modeling helps to convert such problems to some standard form

Why convexity is so important?

Ralph Tyrrell Rockafellar (born 1935)

The great watershed in optimization is not between linearity and non-linearity, but convexity and non-convexity.

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Questions:

- Can any convex optimization problem be efficiently solved?
- Is it possible to solve non-convex optimization problems efficiently?

Convex sets

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A set $\mathcal{X} \subseteq \mathbb{R}^n$ *is convex if for all* $\alpha \in [0,1]$ *and for any* $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ *the following holds*

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- Balls in *any proper* norm and ellipsoids
- Set of symmetric and non-negative definite matrices

Intersection of convex sets

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Intersection of finite or infinite number of convex sets $\mathcal{X}_i$ is a convex set:

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- Consider point $\mathbf{z} = \alpha \mathbf{x} + (1 - \alpha)\mathbf{y}$, $\alpha \in [0, 1]$
- Since $\mathcal{X}_i$ is convex for all $i \in \mathcal{I}$, $\mathbf{z} \in \mathcal{X}_i, \ \forall i \in \mathcal{I}$
- Therefore, $\mathbf{z} \in \mathcal{X}$ and $\mathcal{X}$ is convex set

Linear map of convex set

Theorem

If the domain of any linear map is convex, then the image of this map is also convex.

Proof

- Let $\mathcal{X}$ be a convex set and $\mathbf{x}, \mathbf{y} \in \mathcal{X}$

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- Show that $\alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{y}) \in f(\mathcal{X})$, where $\alpha \in [0, 1]$
- Indeed,

$$\alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{y}) = \alpha(\mathbf{A}\mathbf{x} + \mathbf{b}) + (1-\alpha)(\mathbf{A}\mathbf{y} + \mathbf{b}) =$$
$$\mathbf{A}(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) + \mathbf{b} = \mathbf{A}\mathbf{z} + \mathbf{b} = f(\mathbf{z}),$$

where $\mathbf{z} = \alpha\mathbf{x} + (1-\alpha)\mathbf{y} \in \mathcal{X}$

Arithmetic operations under convex sets

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Exercise

Proof that Cartesian product of convex sets is convex

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*A set $\mathcal{K}$ is called **convex** cone if for any points $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{K}$ and any numbers $\theta_1 \geq 0,\ \theta_2 \geq 0$ we have $\theta_1 \mathbf{x}_1 + \theta_2 \mathbf{x}_2 \in \mathcal{K}$.*

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- Symmetric positive semi-definite matrices $\mathbf{S}^n_+ \to$ Semidefinite programming (SDP)

Convex hull

Definition

Convex hull of the set $\mathcal{G}$ is called such set $\mathrm{conv}(\mathcal{G})$ that

- *it is an intersection of all convex sets containing $\mathcal{G}$*
- *it is a set of all convex combinations of points from $\mathcal{G}$*

$$\mathrm{conv}(\mathcal{G}) = \left\{ \sum_{i=1}^{k} \theta_i \mathbf{x}_i \mid \mathbf{x}_i \in \mathcal{G}, \sum_{i=1}^{k} \theta_i = 1, \theta_i \geq 0 \right\}$$

- *it is a minimal convex set containing $\mathcal{G}$*

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- Recover approximate solution of the original problem from the solution of the problem with convex feasible set

Separation of convex sets

Definition

Sets $\mathcal{A}, \mathcal{B}$ are called separated if there exists vector $\mathbf{a} \neq 0$ and a number b such that

- $\mathbf{a}^\top \mathbf{x} + b \geq 0$ *for all* $\mathbf{x} \in \mathcal{A}$
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- Let $\mathbf{c} \in A$ and $\mathbf{d} \in B$ are points where infimum is attained
- Consider $f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x} + b$, where $\mathbf{a} = \mathbf{d} - \mathbf{c}$ and $b = \frac{\|\mathbf{d}\|_2^2 - \|\mathbf{c}\|_2^2}{2}$

- Show that $f(\mathbf{y}) \geq 0$ for all $\mathbf{y} \in B$
- Assume we have $\mathbf{u} \in B$ such that $f(\mathbf{u}) < 0$
- $f(\mathbf{u}) = (\mathbf{d}-\mathbf{c})^\top(\mathbf{u}-\frac{1}{2}(\mathbf{d}+\mathbf{c})) = (\mathbf{d}-\mathbf{c})^\top(\mathbf{u}-\mathbf{d})+\frac{1}{2}\|\mathbf{d}-\mathbf{c}\|_2^2$
- $(\mathbf{d}-\mathbf{c})^\top(\mathbf{u}-\mathbf{d}) < 0$
- Note that

  $$\frac{d}{dt}\|\mathbf{d}-\mathbf{c}+t(\mathbf{u}-\mathbf{d})\|_2^2\Big|_{t=0} = 2(\mathbf{d}-\mathbf{c})^\top(\mathbf{u}-\mathbf{d}) < 0$$

  therefore, for $t \in (0, 1]$

  $$\|\mathbf{d}-\mathbf{c}+t(\mathbf{u}-\mathbf{d})\|_2 \leq \|\mathbf{d}-\mathbf{c}\|_2.$$

- A point $\mathbf{d}+t(\mathbf{u}-\mathbf{d}) \in B$ is closer to $\mathbf{c}$, than to$\mathbf{d}$, we have a contradiction.

Q: does the existence of separating hyperplane imply the non-intersection of convex sets?

Summary on the convex sets

- Definition and geometric interpretation of convex set
- Three main cones
- Operations that preserve convexity
- Separating hyperplane theorem

Definition

Function $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ *is called convex (strictly convex), if* $\mathcal{X}$ *is convex set and* $\forall \mathbf{x}_1, \mathbf{x}_2 \in X$ *and* $\alpha \in [0, 1]$ $(\alpha \in (0, 1))$ *we have:*

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Examples of convex functions

- x^p for $x \geq 0$ and $p \geq 1$
- $x \log x$, where $x > 0$
- $\max\{x_1, \dots, x_n\}$
- $\|\mathbf{x}\|$
- $\log \left(\sum_{i=1}^{n} e^{x_i} \right)$
- $-\log \det \mathbf{X}$ for $\mathbf{X} \in \mathbf{S}^n_{++}$

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Strongly convex function

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Function $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ *is called* ***strongly*** *convex with constant* $m > 0$, *if* $\mathcal{X}$ *is convex set and* $\forall \mathbf{x}_1, \mathbf{x}_2 \in X$ *и* $\alpha \in [0,1]$ *we have:*

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- Convexity $\supset$ strict convexity $\supset$ strong convexity
- Theoretical analysis of methods in the case of strongly convex functions significantly differs from the one for convex functions

Gradient and hessian: preliminaries

Consider $f : \mathbb{R}^n \to \mathbb{R}$

- Directional derivative

$$f'_{\mathbf{d}}(\mathbf{x}) = \lim_{\alpha \to 0} \frac{f(\mathbf{x} + \alpha \mathbf{d}) - f(\mathbf{x})}{\alpha}$$

- Gradient $f'(\mathbf{x})$ is a vector such that $[f'(\mathbf{x})]_i = \frac{\partial f}{\partial x_i}$
- Hessian is a square matrix $f''(\mathbf{x})$ such that $[f''(\mathbf{x})]_{ij} = \frac{\partial f}{\partial x_i x_j}$

Differential criteria of convexity

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Theorem (First order criterion)

Let function $f(\mathbf{x})$ is differentiable and its domain is a convex set $\mathcal{X} \subseteq \mathbb{R}^n$. Then $f(\mathbf{x})$ is strongly convex with $m \geq 0$ iff

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Proof: if f is convex

- By definition: $f(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \alpha f(\mathbf{x}_1) + (1-\alpha) f(\mathbf{x}_2)$

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$$f(\mathbf{x}) - f(\mathbf{x}^*) \geq \langle f'(\mathbf{x}^*), \mathbf{x} - \mathbf{x}^* \rangle + \frac{m}{2} \|\mathbf{x} - \mathbf{x}^*\|_2^2, \quad \forall \mathbf{x}, \mathbf{x}^* \in X.$$

Proof: if f is convex

- By definition: $f(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \alpha f(\mathbf{x}_1) + (1-\alpha) f(\mathbf{x}_2)$
- Re-write in the form $f(\mathbf{x}_2 + \alpha(\mathbf{x}_1 - \mathbf{x}_2)) \leq f(\mathbf{x}_2) + \alpha(f(\mathbf{x}_1) - f(\mathbf{x}_2))$ or
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Differential criteria of convexity

We consider convex function as strongly convex function with $m = 0$.

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- If $\alpha \to 0$, then
  $$\langle f'(\mathbf{x}_2), \mathbf{x}_1 - \mathbf{x}_2 \rangle \leq f(\mathbf{x}_1) - f(\mathbf{x}_2)$$

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f(\mathbf{x}_1) &\geq f(\mathbf{z}) + \langle f'(\mathbf{z}), \mathbf{z} - \mathbf{x}_1 \rangle \mid \cdot\, \alpha \\
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To prove the claim for the strongly convex case, the same arguments can be provided for function $f(\mathbf{x}) - \frac{m}{2}\|\mathbf{x}\|_2^2$.

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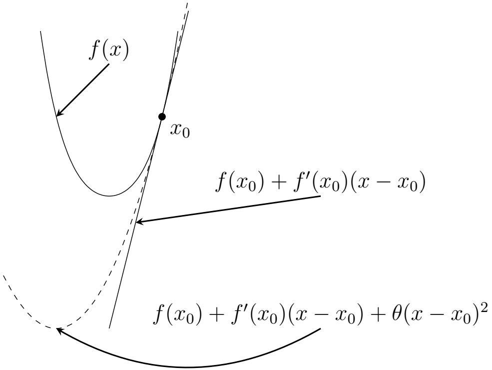
Exercise

Prove that f is strongly convex $\Leftrightarrow f(\mathbf{x}) - \frac{m}{2}\|\mathbf{x}\|_2^2$ is convex.

Illustration for the first order criterion



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Twice continuously differentiable function f is convex $\Leftrightarrow$
$f''(\mathbf{x}) \succeq m\mathbf{I}$

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Reminder

If you want to check the definiteness of a square symmetric matrix, you should use definition or Sylvester criterion

What function compositions preserve convexity?

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- We get a contradiction, therefore assumption is incorrect and $\mathbf{x}^*$ is a point of global minimum

Example of the difficult convex optimization problem

Definition

A set $\mathcal{C}^n = \{\mathbf{A} \in \mathbf{S}^n \mid \mathbf{x}^\top \mathbf{A}\mathbf{x} \geq 0,\ \mathbf{x} \geq 0\}$ *is called copositive cone.*

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Example

The problem of search the maximum independence set of vertices in graph reduces to the convex optimization problem with feasible set $\mathcal{C}^n$. More details see here

Example of the easy to solve non-convex optimization problem

Given the matrix $\mathbf{Q} \in \mathbf{S}^n_{++}$.

$$\begin{aligned} &\min_{\mathbf{x} \in \mathbb{R}^n} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \\ \text{s.t. } &\|\mathbf{x}\|_2 = 1 \end{aligned}$$

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Q: what meaning of $\mathbf{x}^*$ and $f(\mathbf{x}^*)$?

Jensen's inequality

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If function f is convex, then $f\left(\sum_{i=1}^{k}\alpha\mathbf{x}_i\right) \leq \sum_{i=1}^{k}\alpha_i f(\mathbf{x}_i)$, *where* $\sum_{i=1}^{k}\alpha_i = 1,\ \alpha_i \geq 0.$

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- Base $k = 2$ holds according to the definition

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- Consider $k = m$: $f\left(\sum_{i=1}^{m} \hat{\alpha}_i \mathbf{x}_i\right) = f\left(\sum_{i=1}^{m-1} \hat{\alpha} \mathbf{x}_i + \hat{\alpha}_m \mathbf{x}_m\right) =$
  $f\left((1-\hat{\alpha}_m)\sum_{i=1}^{m-1} \frac{\hat{\alpha}_i}{1-\hat{\alpha}_m} \mathbf{x}_i + \hat{\alpha}_m \mathbf{x}_m\right) \leq$
  $(1-\hat{\alpha}_m) f\left(\sum_{i=1}^{m-1} \frac{\hat{\alpha}_i}{1-\hat{\alpha}_m} \mathbf{x}_i\right) + \hat{\alpha}_m f(\mathbf{x}_m) \leq \sum_{i=1}^{k} \alpha_i f(\mathbf{x}_i)$

Corollaries and generalizations

- If we write Jensen's inequality for the function $-\log x$, we get inequality for geometric and arithmetic means

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- The generalization of Jensen's inequality gives the inequality for the convex function of the expected value

$$f(\mathbb{E}(\mathbf{x})) \leq \mathbb{E}(f(\mathbf{x}))$$

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