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

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/girafe-ai/msai-optimization`

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*

General methodology

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

1. Define objective function

General methodology

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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

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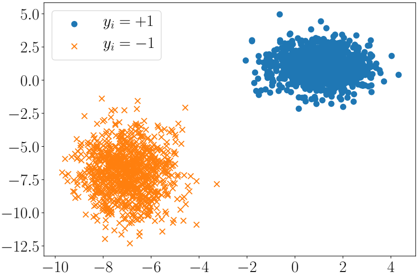
- $f_0(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ — objective function
- $f_k(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ — constraint functions

Linear classification problem

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



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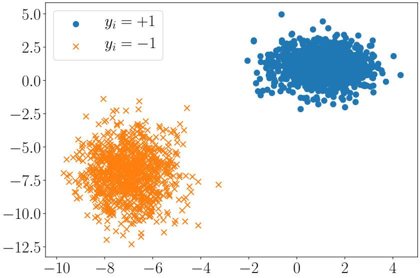

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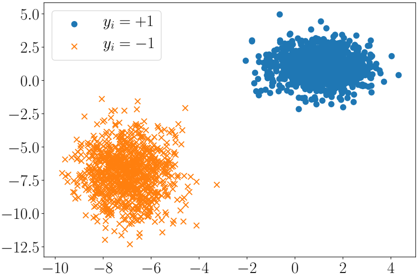

- Linear classifier $\hat{y} = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + b)$
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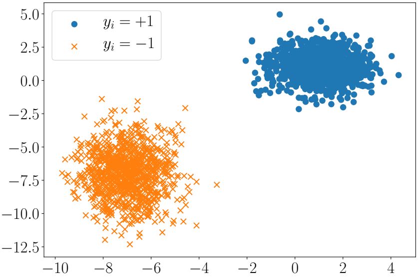

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- $y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 1$

Possible separating hypelplanes

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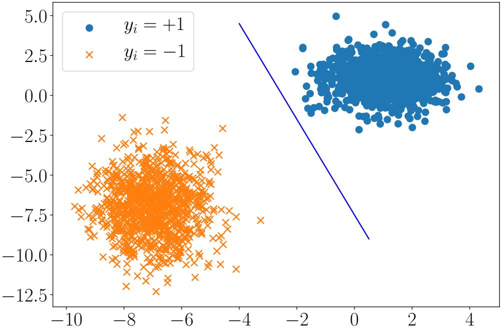

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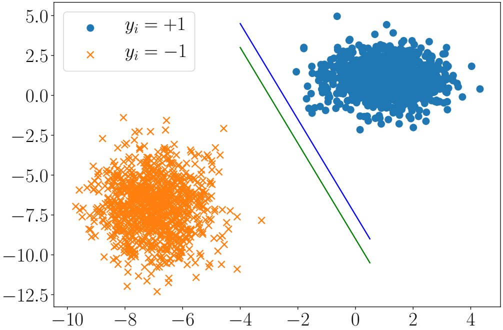

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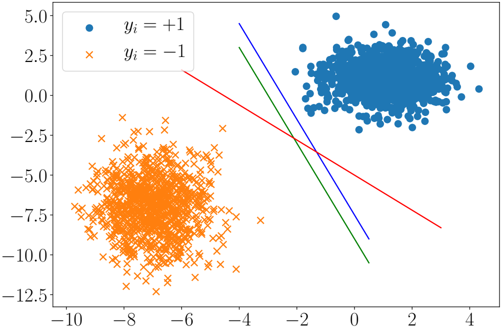

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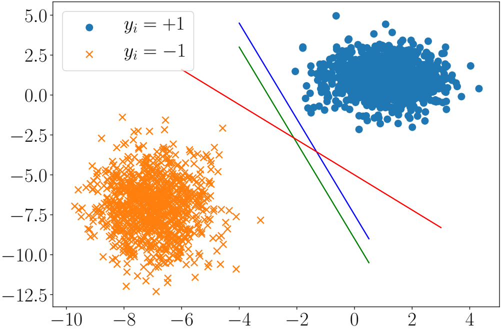

Q: How to define the separating hyperplane uniquely?

Margin maximization

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- 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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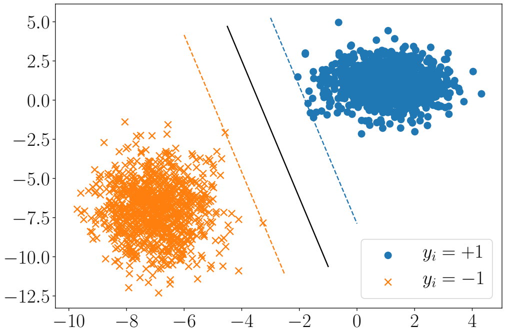
The final optimization problem

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

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

Optimal separating hyperplane



What solutions are possible?

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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:

- 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

Convex optimization problem

$$\begin{aligned} &\min_{\mathbf{x}\in\mathbb{R}^n} f_0(\mathbf{x}) \\ \text{s.t. } &f_i(\mathbf{x}) \le 0,\ i = 1, \ldots, m \\ &\mathbf{A}\mathbf{x} = \mathbf{b} \end{aligned}$$

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- f_0, f_i — convex functions:

$$f(\alpha\mathbf{x}_1 + \beta\mathbf{x}_2) \le \alpha f(\mathbf{x}_1) + \beta f(\mathbf{x}_2),$$

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

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  where $\alpha, \beta \geq 0$ and $\alpha + \beta = 1$.
- 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)

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- Local minimum is also global minimum
- Necessary optimality condition is also sufficient

Convex sets

Definition

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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- 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

Affine map of convex set

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If the domain of any affine 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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- Let f be an affine map: $f(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$
- Show that $\alpha f(\mathbf{x}) + (1 - \alpha) f(\mathbf{y}) \in f(\mathcal{X})$, where $\alpha \in [0, 1]$

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- 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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Minkowski sum of two convex sets is convex set.

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  where $\mathbf{y}_1 \in C_1$ and $\mathbf{y}_2 \in C_2$ since sets C_1, C_2 are convex.

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Corollary

Linear combination of convex sets is convex set

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- Let $\hat{\mathbf{x}} = \hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2$ and $\tilde{\mathbf{x}} = \tilde{\mathbf{x}}_1 + \tilde{\mathbf{x}}_2$ belong to $\mathcal{X}$. Show that $\alpha\hat{\mathbf{x}} + (1-\alpha)\tilde{\mathbf{x}} \in \mathcal{X}$
- Indeed,

  $\alpha\hat{\mathbf{x}}+(1-\alpha)\tilde{\mathbf{x}} = [\alpha\hat{\mathbf{x}}_1+(1-\alpha)\tilde{\mathbf{x}}_1]+[\alpha\hat{\mathbf{x}}_2+(1-\alpha)\tilde{\mathbf{x}}_2] = \mathbf{y}_1+\mathbf{y}_2,$

  where $\mathbf{y}_1 \in C_1$ and $\mathbf{y}_2 \in C_2$ since sets C_1, C_2 are convex.

Corollary

Linear combination of convex sets is convex set

Exercise

Proof that Cartesian product of convex sets is convex

Cones

Definition

A set $\mathcal{K}$ is a cone if for any $\mathbf{x} \in \mathcal{K}$ and arbitrary number $\theta \geq 0$ we have $\theta \mathbf{x} \in \mathcal{K}$.

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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 $\mathbf{S}^n_+ \rightarrow$ 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

Convex function

Definition

Function $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ is called convex (strictly convex), if $\mathcal{X}$ is convex set and $\forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}$ 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 $x > 0$
- $\max\{x_1, \ldots, x_n\}$
- $\|\mathbf{x}\|$
- $\log \left(\sum_{i=1}^{n} e^{x_i} \right)$
- $-\log \det \mathbf{X}$ for $\mathbf{X} \in \mathbf{S}^n_{++}$

Epigraph and convexity

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   - From the convexity of f follows $\alpha t_1 + (1-\alpha)t_2 \geq \alpha f(\mathbf{x}_1) + (1-\alpha) f(\mathbf{x}_2) \geq f(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2)$.

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   - From the definition of epigraph follows convexity of f

Strongly convex function

Definition

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* $\forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}$ *и* $\alpha \in [0, 1]$ *we have:*
$$f(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \alpha f(\mathbf{x}_1) + (1-\alpha) f(\mathbf{x}_2) - \frac{m}{2}\alpha(1-\alpha)\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2$$

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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

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

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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

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

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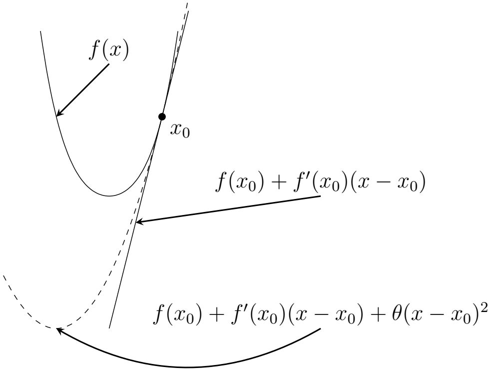
Illustration for the first order criterion



Theorem (Second order criterion)

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

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- Scalar composition $h(f(\mathbf{x}))$

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- $f(\mathbf{x}^*) \leq f(\mathbf{z}) \leq \alpha f(\mathbf{y}^*) + (1 - \alpha)f(\mathbf{x}^*) < f(\mathbf{x}^*)$
- We get a contradiction, therefore assumption is incorrect and $\mathbf{x}^*$ is a point of global minimum

Jensen's inequality

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

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

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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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