Topic 4: Introduction to Optimization

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Optimization

Good references (*see syllabus*):

- "Convex Optimization" by Boyd and Vandenberghe
- Chapter 5 in "Statistical Learning with Sparsity" by Hastie et al.

Optimization terminology

We will consider the following general optimization problem:

$$
\begin{aligned}
\text{minimize}_x \quad & f(\mathbf{x}) \\
\text{subject to} \quad & g_j(\mathbf{x}) \leq 0, \quad j = 1, 2, ..., m; \\
& h_k(\mathbf{x}) = 0, \quad k = 1, 2, ..., l.
\end{aligned}
$$

- $\mathbf{x} \in \mathbf{R^p}$: **optimization variable** (in this class, could be a scalar, vector or a matrix)
- $f(\mathbf{x}) : \mathbf{R^p} \rightarrow \mathbf{R}$: **objective function**
- $g_j : R^p \rightarrow R$ and $g_j(\mathbf{x}) \leq 0$: **inequality constraints**
- $h_k : R^p \rightarrow R$ and $h_k(\mathbf{x}) = 0$: **equality constraints**
- If no constraints: **unconstrained problem**

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- A point $\mathbf{x} \in \mathbf{R^p}$ is **feasible** if it satisfies all the constraints. Otherwise, it's **infeasible**.
- The **optimal value** f^* is the minimal value of f over the set of feasible points

Example 1: Least squares linear regression

Given training data $X \in R^{n \times p}$ and $Y \in R^n$ with $rank(X) = p$

$$\text{minimize}_\beta \|Y - X\beta\|_2^2$$

- **unconstrained** optimization problem
- any $\beta \in R^p$ is **feasible**
- the optimal value $f^* = \|Y - X(X^\top X)^{-1} X^\top Y\|_2^2$

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- The **optimal value** f^* is the minimal value of f over the set of feasible points
- x^* is **globally optimal** if x is *feasible* and $f(x^*) = f^*$
- x^* is **locally optimal** if x is *feasible* and for each feasible x in the neighborhood $\|x - x^*\|_2 \leq R$ for some $R > 0$, $f(x^*) \leq f(x)$.

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- any $\beta \in R^p$ is **feasible**
- the optimal value $f^* = \|Y - X(X^\top X)^{-1} X^\top Y\|_2^2$
- the globally optimal $\beta^* = (X^\top X)^{-1} X^\top Y$ (also locally optimal, the only locally optimal point)

Example 2: Principal Component Analysis

Given training data $X \in R^{n \times p}$ that is column-centered, the first principal loading $v \in R^p$ is found as the solution to

$$\text{minimize}_v \{-v^\top X^\top X v\}$$
$$\text{subject to} \quad v^\top v = 1.$$

- optimization problem with one **equality constraint**
- $v = \mathbf{0}$ is **infeasible**
- the optimal value f^* is minus the largest eigenvalue of $X^\top X$
- the globally optimal v^* is the eigenvector of $X^\top X$ corresponding to the largest eigenvalue

Unconstrained optimization problem

Consider minimizing differentiable function f

$$\text{minimize}_x f(x)$$

A point x' is called **stationary** if

$$\nabla f(x') = 0.$$

All local optimal points are **stationary** points.

Globally optimal x^* satisfies $\nabla f(x^*) = 0$, but locally optimal and stationary points also satisfy it.

For **convex** f, any solution to $\nabla f(x^*) = 0$ is globally optimal.

Convex optimization problems

- Very common in statistics, *easier* to solve, genereally have nice algorithms

Definition

A function $f : R^p \to R$ is **convex** if for all $x_1, x_2 \in R^p$ and all $\alpha \in [0, 1]$,

$$f(\alpha x_1 + (1-\alpha)x_2) \leq \alpha f(x_1) + (1-\alpha) f(x_2)$$

and is **strictly convex** if for all $x_1, x_2 \in R^p$, $x_1 \neq x_2$, and all $\alpha \in (0, 1)$

$$f(\alpha x_1 + (1-\alpha)x_2) < \alpha f(x_1) + (1-\alpha) f(x_2)$$

- **Interpretation**: The chord between two points is always above the function

Convex optimization problems

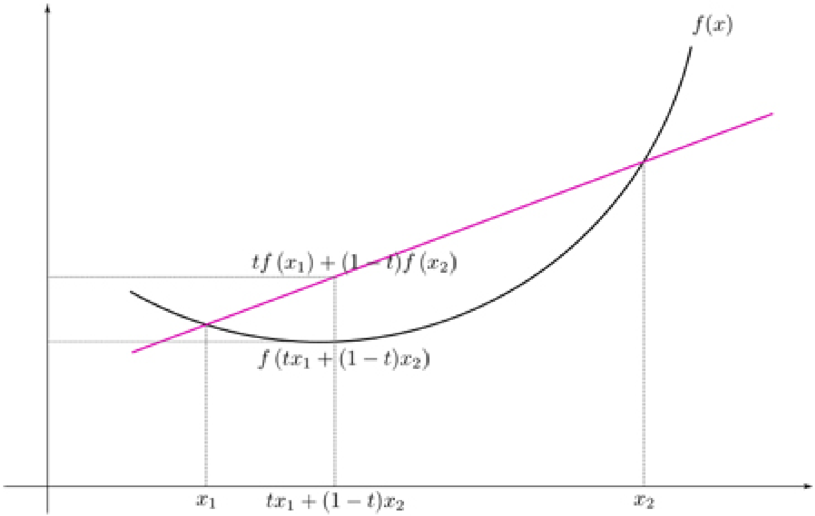

Figure 1: Convex function, basic definition

Convex optimization problems

Theorem

First order conditions (for differentiable f)

- f *is convex* $\iff$ $f(y) \geq f(x) + \nabla f(x)^\top (y-x)$, $\forall x, y \in \mathbb{R}^p$.
- f *is strictly convex* $\iff$ $f(y) > f(x) + \nabla f(x)^\top (y-x)$, $\forall x, y \in \mathbb{R}^p$ *and* $x \neq y$.

- **Interpretation**: function lies above its tangent

Convex optimization problems

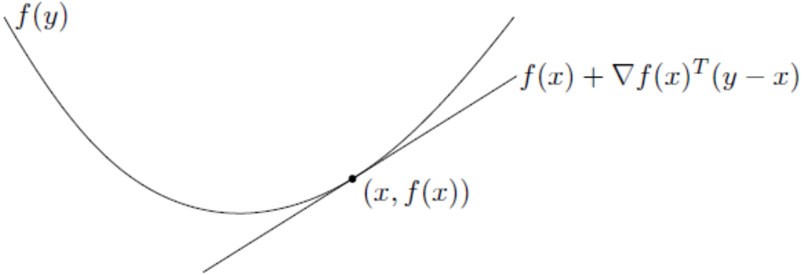

Figure 2: Convex function, first order condition

Convex optimization problems

Theorem

Second order conditions (for twice differentiable f)

- f *is convex* $\iff$ *Hessian* $\nabla^2 f(x) \succeq 0$, $\forall x \in \mathbb{R}^p$. *(pos.semi-def)*
- f *is strictly convex* $\iff$ *Hessian* $\nabla^2 f(x) \succ 0$, $\forall x \in \mathbb{R}^p$ *(strictly pos.semi-def)*

- Often easiest to check in practice, i.e.

$$f(x) = x^2, \quad \nabla^2 f(x) = 2 > 0.$$

$$f(x) = \|x\|_2^2, \quad \nabla f(x) = 2x, \quad \nabla^2 f(x) = 2I \succ 0.$$

Examples of convex functions

- $-\log(x)$
- e^x
- $|x|^p$, $p \geq 1$
- Any norm on $\mathbb{R}^p$
- $-\log(\det(\Sigma))$, where Σ is positive definite

Operations that preserve convexity

- Non-negative weighted sum: $\sum_{i=1}^{k} w_i f_i$, where $w_i \geq 0$ and $f_i, i = 1, ..., k$ are convex functions.
- If f is convex, and $g(x) = f(Ax + b)$, then g is convex.
- If $f_1, ..., f_k$ are convex functions, then $\max(f_1, ..., f_k)$ is also convex.
- ... not exhaustive list

What about convex function applied to another convex function?

If $h(x)$ is convex, and $f(x)$ is convex, then $g(x) = f(h(x))$ is **not necessarily** convex

- $g(x) = -x^2$
- $g(x) = (\|x\|_2^2 - 1)^2$

Special case: if $h(x) = Ax + b$ (linear), then $g(x)$ is convex

- g(x) = (-x)ˆ2
- g(x) = (x - 1)ˆ2

Example

Least squares loss function is convex

$$f(\beta) = \|Y - X\beta\|_2^2$$

Why?

- The hessian is $\nabla^2 f(\beta) = 2X^\top X \succeq 0$ (semi positive definite)
- $f(\beta) = g(Y - X\beta)$, where $g(x) = \|x\|_2^2$ is convex as a norm squared

Recall unconstrained optimization problem

Consider minimizing differentiable function f

$$\text{minimize}_x f(x)$$

A point x' is called **stationary** if

$$\nabla f(x') = 0.$$

All local optimal points are **stationary** points.

Globally optimal x^* satisfies $\nabla f(x^*) = 0$, but locally optimal and stationary points also satisfy it.

Unconstrained convex optimization problem

Consider

$$\text{minimize}_x f(x)$$

This is a **convex** optimization problem if $f(x)$ is **convex**

Important property 1: any locally optimal point of a convex problem is globally optimal

Important property 2: If f is differentiable, x^* is optimal if and only if

$$\nabla f(x)|_{x=x^*} = 0.$$

Example: Least Squares

Least squares solves

$$\text{minimize}_\beta \|Y - X\beta\|_2^2$$

This is a convex unconstrained optimization problem, so the solution must satisfy

$$\begin{aligned}\nabla\|Y - X\beta\|_2^2 &= \nabla(\|Y\|_2^2 - 2Y^\top X\beta + \beta^\top X^\top X\beta)\\ &= -2X^\top Y + 2X^\top X\beta = 0\end{aligned}$$

This is equivalent to

$$X^\top X\beta = X^\top Y$$

If $X^\top X$ is **invertible**, global solution is $\beta^* = (X^\top X)^{-1}X^\top Y$.

Example: Least Squares

Least squares solves

$$\text{minimize}_\beta \|Y - X\beta\|_2^2$$

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This is equivalent to

$$X^\top X\beta = X^\top Y$$

If $X^\top X$ is **not invertible**, **multiple** global solutions (give same f^*)

Example: Maximum Likelihood Estimation

Observations x_i, $i = 1, \ldots, n$, independent samples from distribution with density $f(x;\theta)$ with some parameter $\theta \in \mathbb{R}^d$

Maximum Likelihood Estimator (MLE)

$$\widehat{\theta} = \arg\max_{\theta} \prod_{i=1}^{n} f(x_i;\theta)$$

Typically, we maximize **log-likelihood** which is equivalent to

$$\widehat{\theta} = \arg\min_{\theta} \left\{ -\sum_{i=1}^{n} \log f(x_i;\theta) \right\}$$

This is **convex optimization** if $-log(f)$ is convex or f is -log-convex.

MLE example

Normal likelihood with known variance σ^2

$$f(x;\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\theta)^2}{2\sigma^2}\right)$$

Here θ is the unknown mean.

Log-likelihood

$$\log f(x;\theta) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(x-\theta)^2 = C - \frac{1}{2\sigma^2}(x-\theta)^2$$

MLE optimization problem

$$\widehat{\theta} = \arg\min_{\theta} \left\{ -\sum_{i=1}^{n} -\frac{1}{2\sigma^2}(x_i-\theta)^2 \right\} = \arg\min_{\theta} \sum_{i=1}^{n}(x_i-\theta)^2$$

MLE example

MLE optimization problem

$$\widehat{\theta} = \arg\min_{\theta} \left\{ -\sum_{i=1}^{n} -\frac{1}{2\sigma^2}(x_i - \theta)^2 \right\} = \arg\min_{\theta} \sum_{i=1}^{n}(x_i - \theta)^2$$

This is **convex optimization problem**. Why?

The optimality conditions

$$-2\sum_{i=1}^{n} x_i + 2n\theta = 0.$$

The optimal $\widehat{\theta} = n^{-1}\sum_{i=1}^{n} x_i = \bar{x}$ - sample mean.

Summary

Unconstrained optimization problem with differentiable f:

$$\text{minimize}_x f(x).$$

To find global optimum, need to solve optimality conditions

$$\nabla f(x) = 0.$$

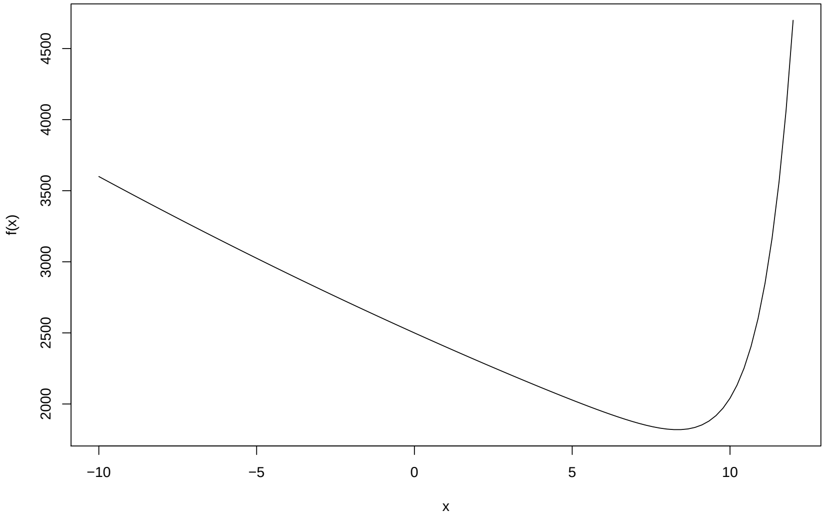
For **convex** f - any solution to above is **globaly optimal**.

Least squares problem has closed form solution.

What if exact solution is not tractable? Need **numerical methods**

Example 1

$$f(x) = (x - 50)^2 + e^x/50$$



General purpose solver

For one-dimensional optimization, one can utilize R function *optimize*

```
  f <- function(x){
    (x - 50)^2 + exp(x)/50
  }
optimize(f, interval = c(-1000, 1000))
```

```
## $minimum
## [1] 8.334841
##
## $objective
## [1] 1819.316
```

General purpose solver

One can also start with optimality conditions and treat it as a root-finding problem

$$f(x) = (x - 50)^2 + e^x/50, \quad f'(x) = 2x - 100 + e^x/50 = 0$$

R function *uniroot*

```
  fprime <- function(x){
    2 * x - 100 + exp(x)/50
  }
uniroot(fprime, interval = c(-1000, 1000))
```

```
## $root
## [1] 8.334836
##
## $f.root
## [1] 9.380346e-06
##
## $iter
## [1] 16
```

General purpose solver

One can also translate root finding problem into optimization problem (the root must exist).

Suppose you want to find the root of

$$g(x) = 0.$$

- Let $f(x) = g(x)^2$, then one can consider

  $$\text{minimize}_x f(x).$$

  You can then use *optimize* function on $f(x)$.

- You can also take an integral of $g(x)$ to find $f(x)$ such that $\nabla f(x) = g(x)$, and then use *optimize* on $f(x)$.