Introduction to optimization

Julia Wrobel

Overview

Today, we cover:

- Intro to optimization
- Rates of convergence
- Beginning of gradient methods
    - Steepest descent
    - Newton's Method

Announcements

- HW2 posted and due 2/11 at 10:00AM
- No class Thursday, 2/12

Readings:

- Peng Chapter 2 (rates of convergence)
- Peng Chapter 3 (general optimization)

Optimization terminology

We will consider the following general optimization problem:

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

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

Optimization terminology

We will consider the following general optimization problem:

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

- A point $\mathbf{x} \in \mathbf{R}^\mathbf{p}$ 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
- 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 $R > 0$, $f(x^*) \leq f(x)$.

Least squares linear regression

Given 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 $f^* = \|Y - X(X^TX)^{-1}X^TY\|_2^2$
- the globally optimal $\beta^* = (X^TX)^{-1}X^TY$
  - also locally optimal, the only locally optimal point

Unconstrained optimization problem

Consider minimizing differentiable function f

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

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

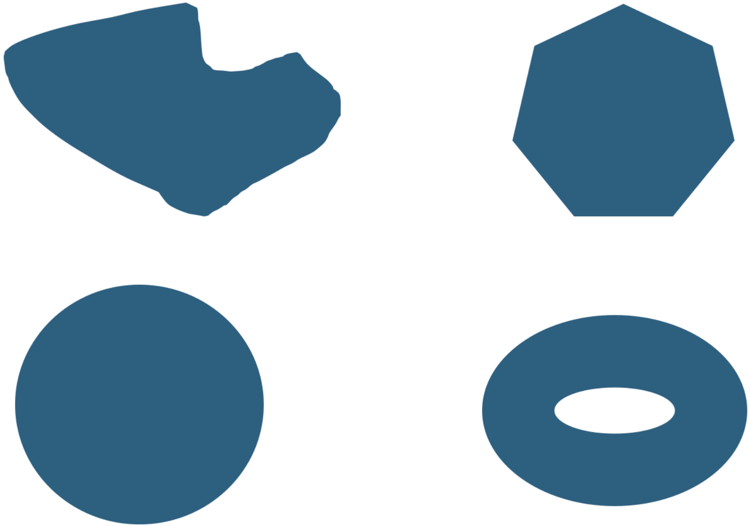
$$\nabla f(x^*) = 0.$$

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 sets



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

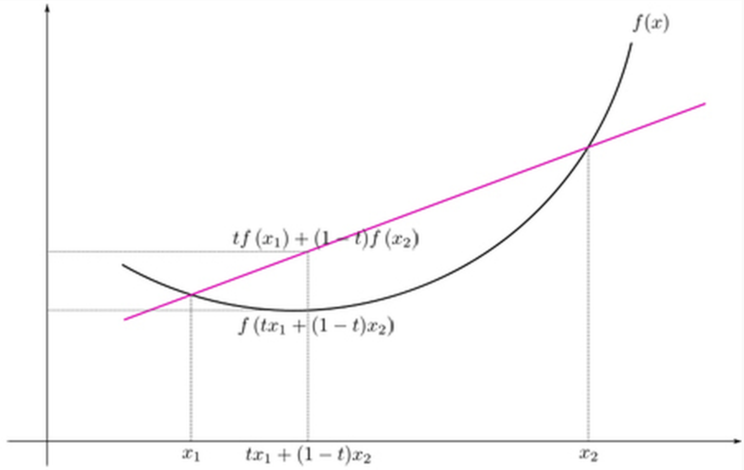


Figure 1: Convex function, basic definition

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

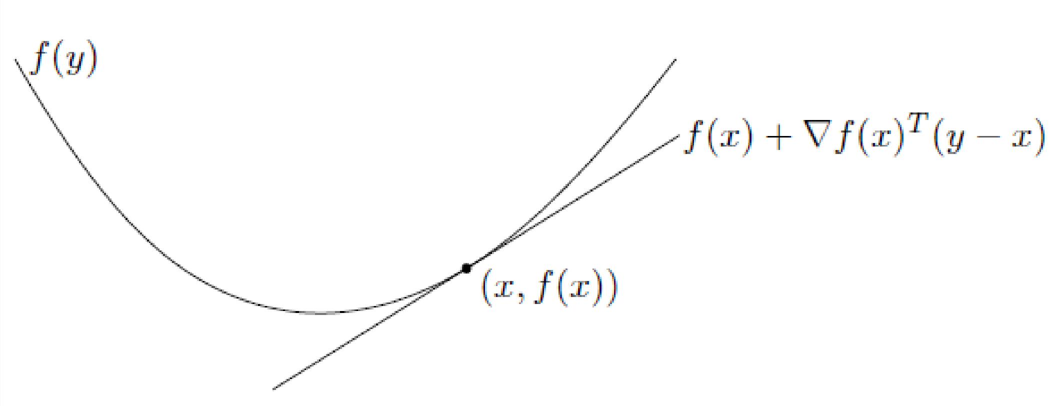


Figure 2: Convex function, first order condition

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.

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

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

Examples of convex functions

- $-\log(x)$
- e^x
- $|x|^p$, $p \geq 1$
- Any norm on $\mathbb{R}^p$
- $-\log(\text{det}(\Sigma))$, 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

Example

Least squares loss function is convex

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

Why?

- The hessian is $\nabla^2 f(\beta) = 2X^T X \succeq 0$ (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 $f(x^*) = 0$, 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

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

Example: Least Squares

This is equivalent to

$$X^T X\beta = X^T Y$$

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

- If $X^T X$ 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)

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

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

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

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

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

MLE example

MLE optimization problem

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

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

The optimality conditions

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

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

Summary

Unconstrained optimization problem with differentiable f:

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

To find global optimum, need to solve optimality conditions

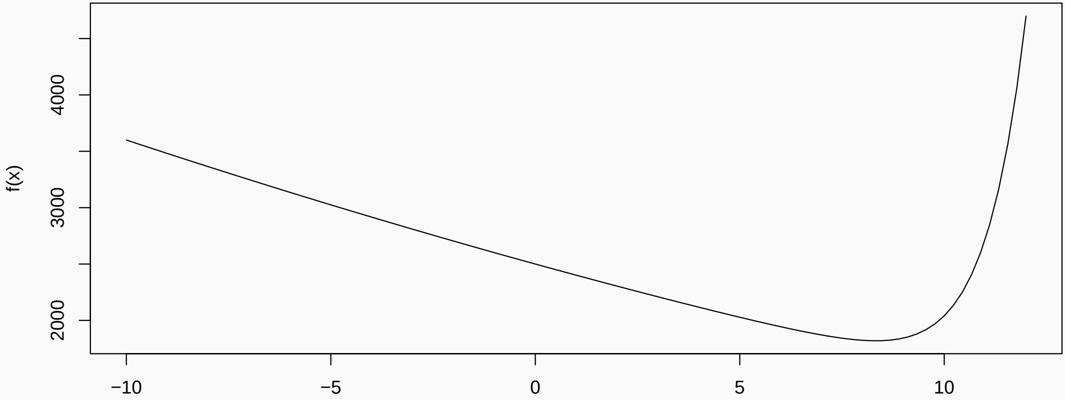
$$\nabla f(x) = 0.$$

For **convex** f, any solution to above is **globally optimal**.

- Least squares problem has closed form solution.
- What if exact solution is not tractable? Need **numerical methods**

Example 1

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



Rates of convergence

One of the ways algorithms can be compared is via their rates of convergence to some limiting value.

- Typically we have an iterative algorithm that is trying to find the max/min of an objective function f
  - Want to estimate how long it will take to reach that optimal value
- Three rates of convergence we will focus on:
  - **linear** (slowest)
  - **superlinear** (faster)
  - **quadratic** (fastest)

Algorithms that require more information about f (such as its derivative) tend to converge more quickly.

Linear convergence

Suppose we have a sequence $\{x_n\}$ such that $x_n \to x_\infty \in \mathcal{R}^k$.
Convergence is **linear** if there exists $r \in (0, 1)$ such that:

$$\frac{\|x_{n+1} - x_\infty\|}{\|x_n - x_\infty\|} \leq r$$

for all sufficiently large n.

Linear convergence

Example: the sequence $x_n = 1 + \frac{1}{2}^n$ converges linearly to $x_\infty = 1$.

Superlinear convergence

We say a sequence $\{x_n\}$ converges to x_∞ **superlinearly** if we have

$$\lim_{n\to\infty} \frac{\|x_{n+1} - x_\infty\|}{\|x_n - x_\infty\|} = 0$$

for all sufficiently large n.

Superlinear convergence

Example: $x_n = 1 + (\frac{1}{n})^n$ converges superlinearly to 1.

Quadratic convergence

Quadratic convergence is the fastest form of convergence discussed here. We say a sequence $\{x_n\}$ converges to x_∞ at a **quadratic** rate if there exists some constant $0 < M < \infty$ such that

$$\frac{\|x_{n+1} - x_\infty\|}{\|x_n - x_\infty\|^2} \leq M$$

for all sufficiently large n.

Quadratic convergence

Example: $x_n = 1 + (\frac{1}{n})^{2n}$ converges quadratically to 1.

Gradient methods: steepest (gradient) descent

- Choose a step size $\alpha > 0$
  - Sometimes called **learning rate** or **learning step**
- Start with an initial guess x_0
- At each iteration t, compute $x_{t+1} = x_t - \alpha \nabla f(x_t)$
- Continue until some **convergence criterion** is met
  i.e. $f(x_{t+1}) \approx f(x_t)$

Idea: Move α units in the direction of *steepest descent*, which is the direction that is orthogonal to the contours of f at the point x_n

- This attempts to find solution to $\nabla f(x) = 0$

Steepest descent

In practice, can require many steps (iterations) to reach the minimum when parameters are highly correlated.

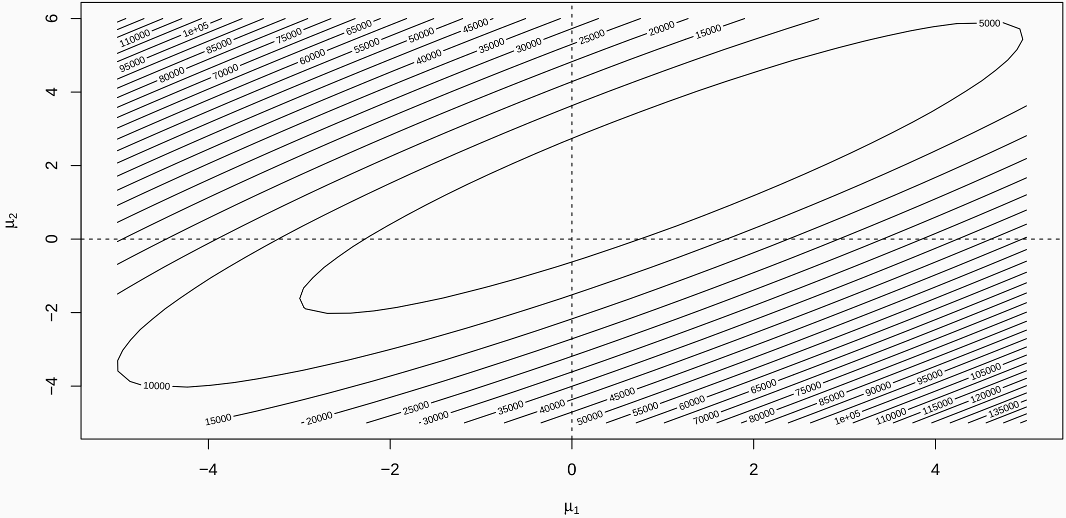
Example: Bivariate Normal.

- Can use steepest descent to estimate the MLE of the mean
- True $\mu = (1, 2)$
- True $\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$

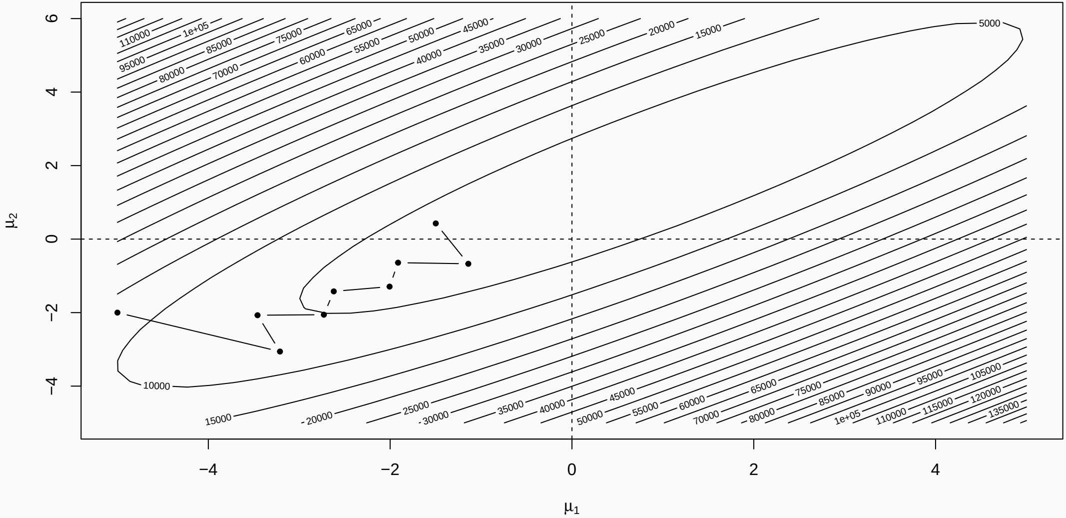
Parameters are highly correlated!

- Try starting value $\mu_0 = (-5, -2)$

Steepest descent



Steepest descent



Steepest descent - example

- For simplicity, focus on one-dimensional case first

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

The choice of step size is very important!!

- **Too small** α - very small difference between updates, larger number of iterations
- **Too large** α - oscillations, may not converge

Lab exercise

Use **Exercise 1** in lab to check different values of α on the given function.

How did we monitor convergence in this code? Why?

Steepest descent in practice

- Very simple
- Only requires the first derivative
- Used in many machine learning methods, i.e. in neural nets (with additional stochastic updates)

Newton's method

Goal is to find solution x^* to

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

By Taylor expansion, can approximate $\nabla f(x^*)$ around a given point x:

$$\nabla f(x^*) = \nabla f(x) + \nabla^2 f(x)(x^* - x) + \text{higher order terms.}$$

Newton's method

Since $\nabla f(x^*) = 0$, must have $\nabla f(x) + \nabla^2 f(x)(x^* - x) \approx 0$, leading to

$$x^* \approx x - \{\nabla^2 f(x)\}^{-1} \nabla f(x).$$

One dimensional case update, Newton's method

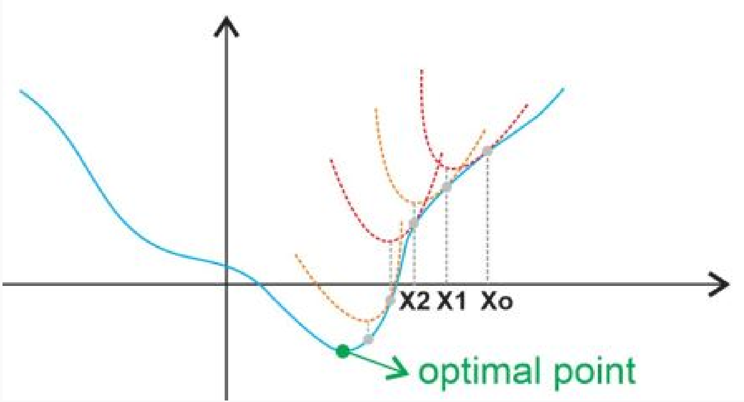
$$x_{t+1} = x_t - \frac{f'(x_t)}{f''(x_t)}$$

Steepest descent (one dimensional)

$$x_{t+1} = x_t - \alpha f'(x_t)$$

Newton's method - illustration

- The closer is x_0 to the optimal value x^*, the faster the convergence



Newton's method - example

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

$$\nabla f'(x) = 2 + e^x/50$$

See **Exercise 2** in lab to implement this example.

- How does it compare to the steepest descent approach in number of iterations?
- Computation time?

Recall

Convex optimization problem:

$$\text{minimize}_x\, f(x), \quad f - \text{convex function.}$$

To find global optimum, need to solve optimality conditions

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

Steepest descent algorithm and Newton's method aim to find any solution to the above, so may be applied with nonconvex problems as well **but**

- only guaranteed to converge to a **global** optimum if convex
- solution may be a local min, local max, or saddle point

Resources

- old paper on convexity in GLMs
- Peng, Advanced Statistical Computing, chapters 2 and 3