Georgia Tech College of Computing

CX4240 Spring 2026

Brief Intro to Optimization

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Basic / Prerequisites

- Probability
  - Distributions, densities, marginalization, conditioning
- Statistics
  - Mean, variance, maximum likelihood estimation
- Linear Algebra and Optimization
  - Vector, matrix, multiplication, inversion, eigen-value decomposition
- Coding Skills
  - Pytorch and/or JAX

Machine Learning for Apartment Hunting

- Suppose you are to move to Atlanta
- And you want to find the most reasonably priced apartment satisfying your needs:

Living area (ft^2)	# bedroom	Monthly rent ($)
230	1	900
506	2	1800
433	2	1500
190	1	800
…		
150	1	?
270	1.5	?

Linear Regression Model

- Assume y is a linear function of x (features) plus noise ϵ

$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n + \epsilon$$

where ϵ is an error model as Gaussian $N(0, \sigma^2)$ Probability

- Let $\theta = (\theta_0, \theta_1, \dots, \theta_n)^\top$, and augment data by one dimension

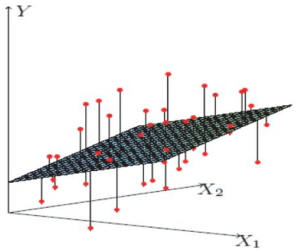
$$x \leftarrow (1, x)^\top$$

Linear algebra

Then $y = \theta^\top x + \epsilon$

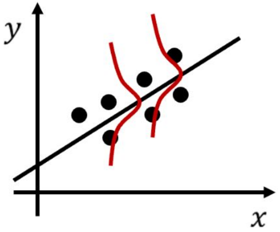
Linear algebra

Gaussian Likelihood



- Assume y is a linear in x plus noise ϵ

$$y = \theta^\top x + \epsilon$$



- Assume ϵ follows a Gaussian $N(0, \sigma)$

$$p(y^i \mid x^i; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

- By independence assumption, likelihood is

$$L(\theta) = \prod_i^m p(y^i \mid x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

Probability

MLE

$$L(\theta) = \prod_{i}^{m} p\left(y^i \middle| x^i; \theta\right) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

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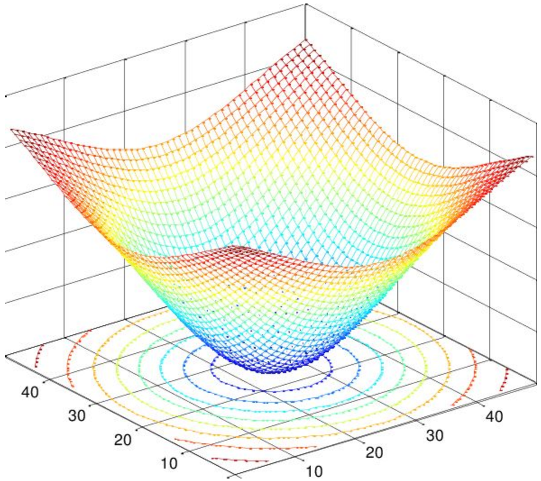
$$\max_{\theta} \; \log L(\theta) = -\frac{1}{2\sigma^2}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2 - m\log(\sqrt{2\pi}\sigma)$$

Optimization

Least Mean Square for Linear Regression

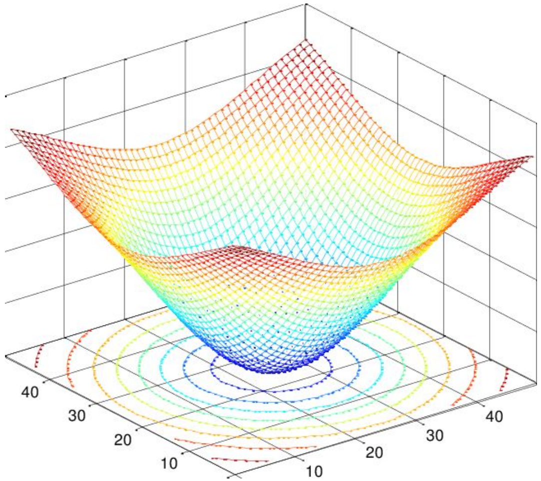
Optimization Problem



$$\text{minimize } f(\theta)$$

- $\theta \in \mathbf{R}^d$ is the variable or decision variable
- $f: \mathbf{R}^d \to \mathbf{R}$ is the objective function
- goal is to choose θ to minimize f

Optimization Problem



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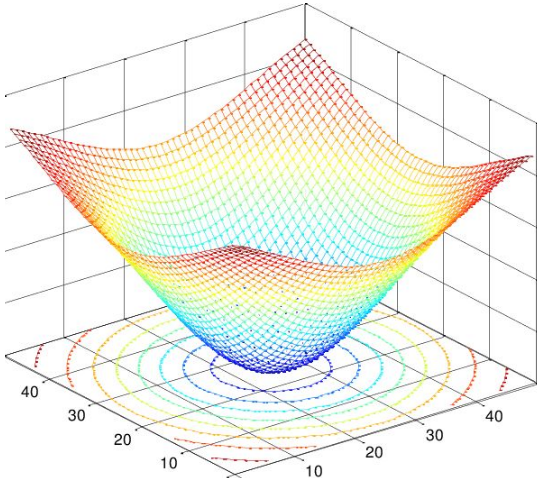

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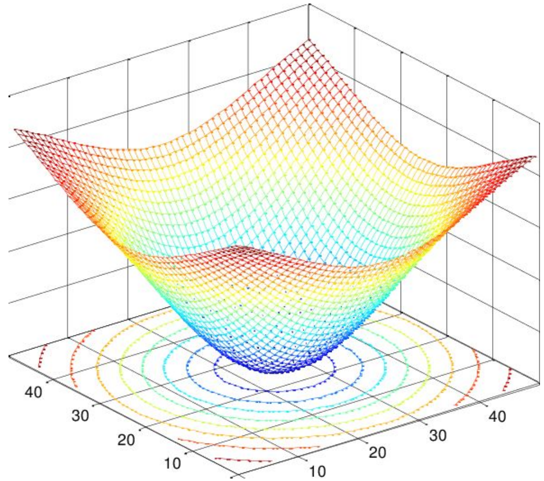

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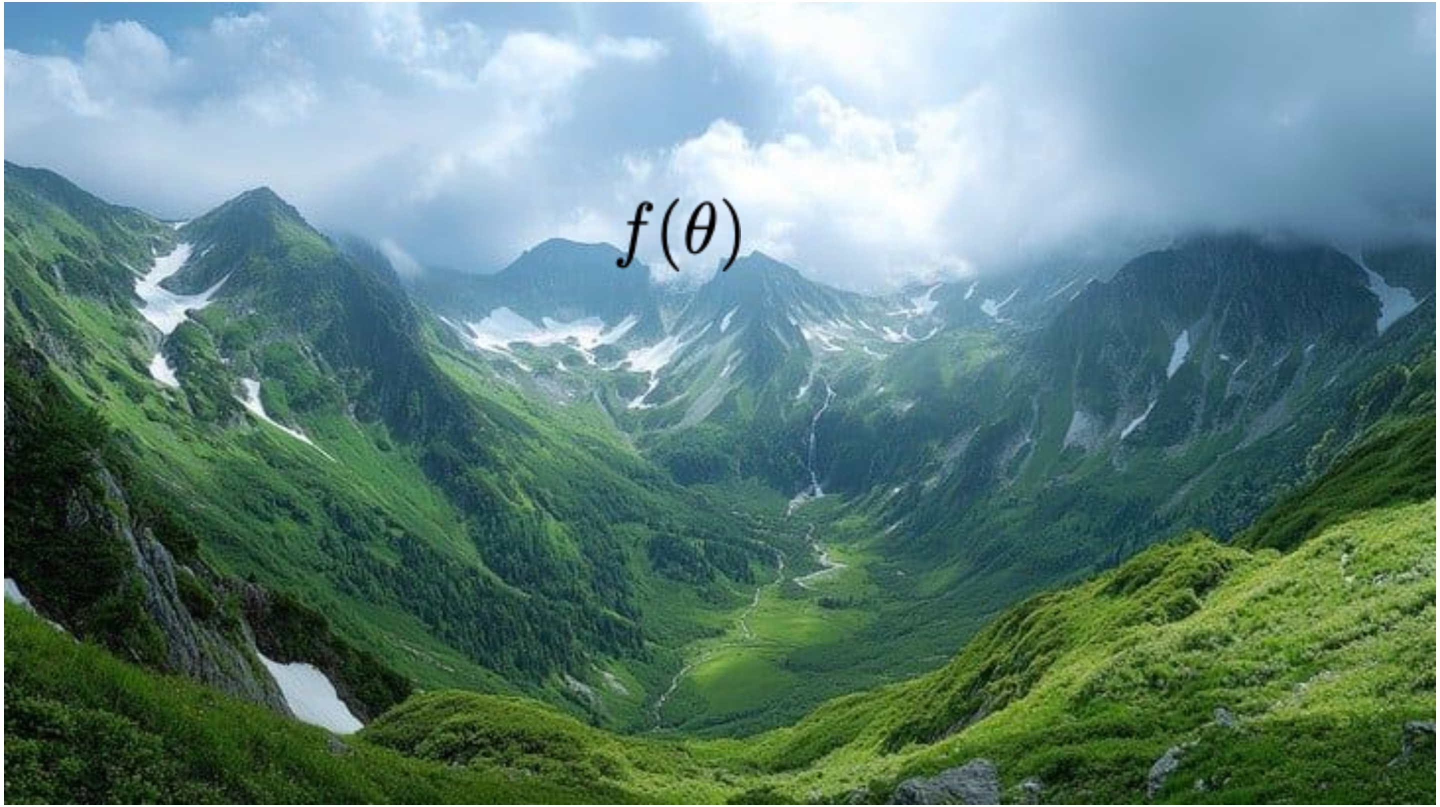
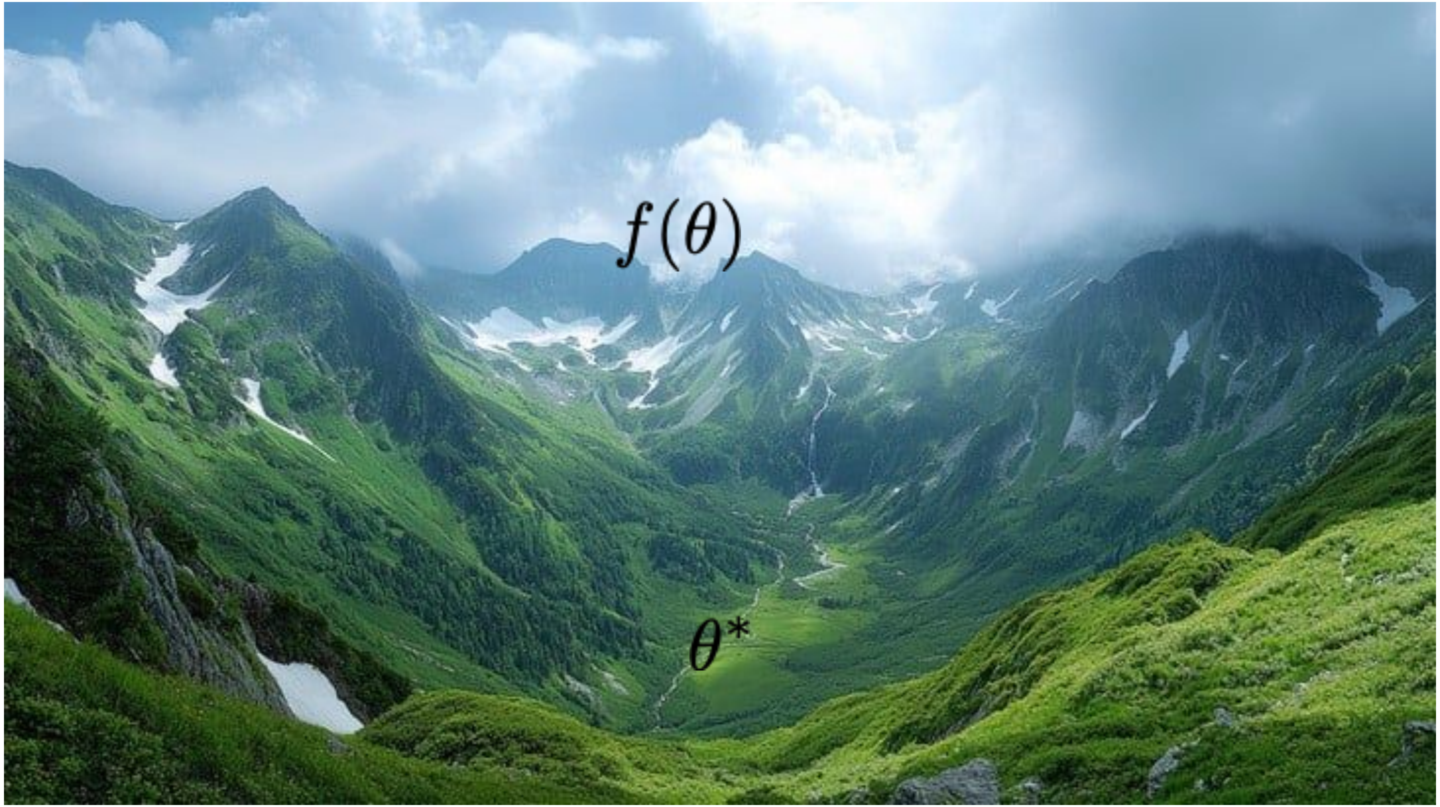
- $\theta \in \mathbf{R}^d$ is the variable or decision variable
- $f: \mathbf{R}^d \to \mathbf{R}$ is the objective function
- goal is to choose θ to minimize f
- θ^* is optimal means that for all $\theta, f(\theta) \geq f(\theta^\star)$
- $f^\star = f(\theta^\star)$ is the optimal value of the problem

$$\theta^* = \arg\min_\theta \; f(\theta)$$

$$f^* = \min_\theta \; f(\theta)$$


$f(\theta)$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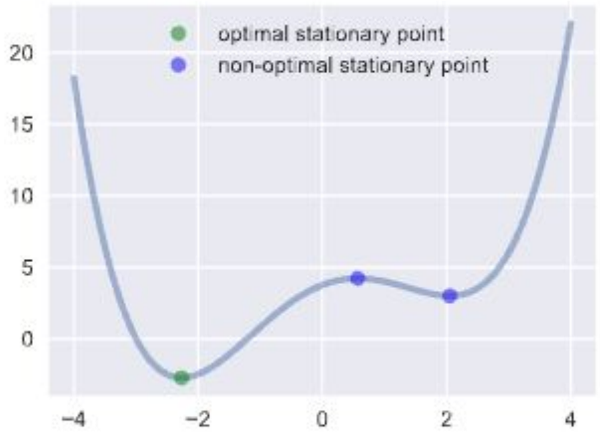
Optimality Condition



- let's assume that f is differentiable, i.e., partial derivatives $\frac{\partial f(\theta)}{\partial \theta_i}$ exist
- if $\theta^\star$ is optimal, then $\nabla f(\theta^\star) = 0$
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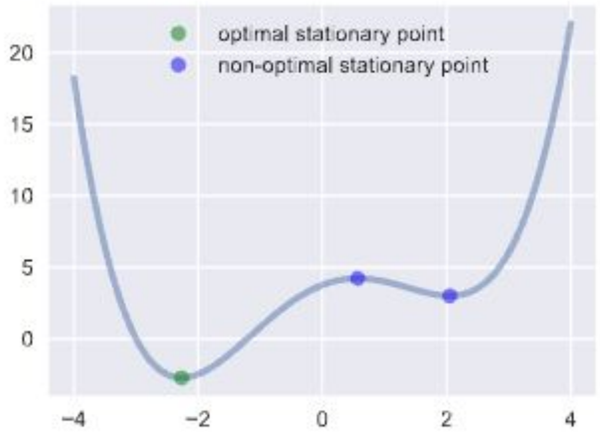

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- we call points that satisfy $\nabla f(\theta) = 0$ stationary points
- not all stationary points are optimal

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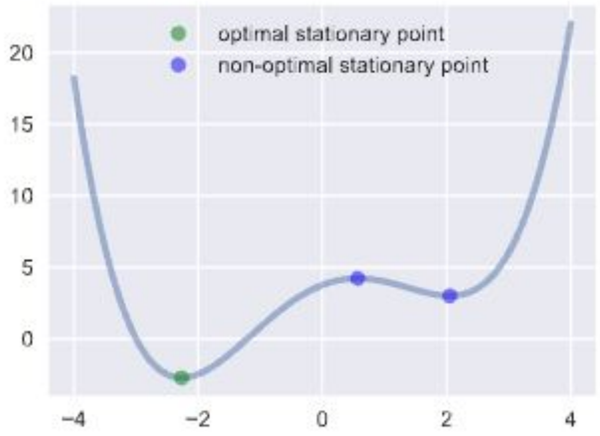

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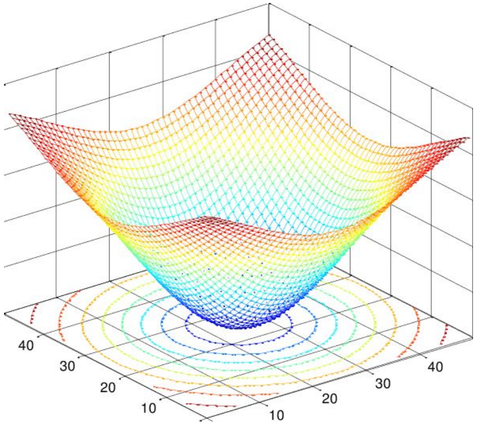

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What if optimality condition is difficult to be solved?

Local Search

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Iterative Algorithm

- iterative algorithm computes a sequence $\theta^1, \theta^2, \ldots$
- θ^k is called the k th iterate
- θ^1 is called the starting point

$$f(\theta^{k+1}) < f(\theta^k), k = 1,2, \ldots$$

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Gradient Descent

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Gradient Descent

Gradient Descent

Gradient Method Summary

choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0, h^1 = 1$)
for $k = 1,2, \dots, k^{\text{max}}$

1. compute $\nabla f(\theta^k)$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
2. form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
3. if $f(\theta^{\text{tent}}) < f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}, h^{k+1} = 1.2h^k$
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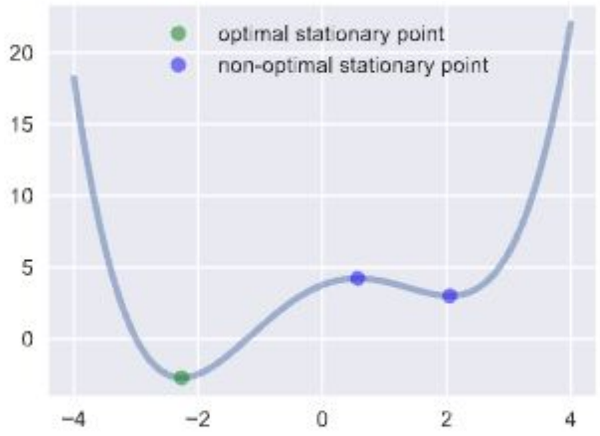

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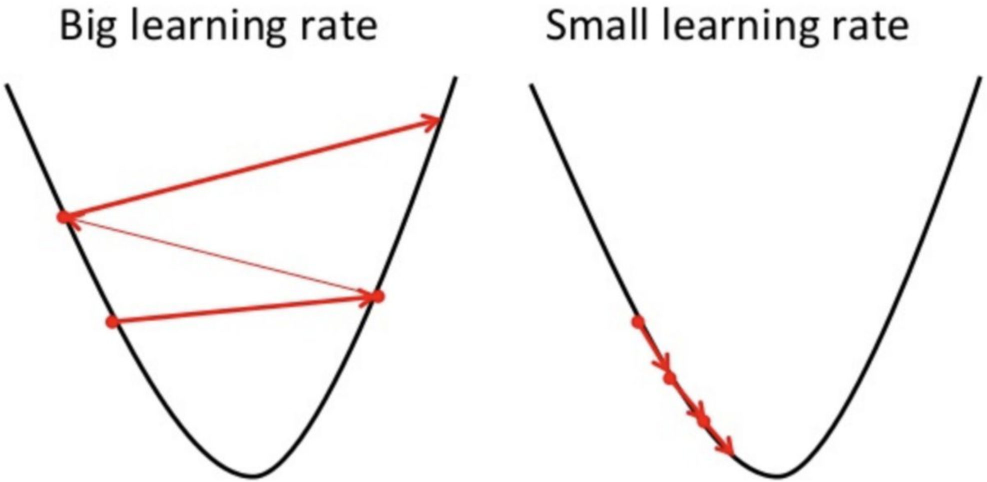
Step-size Matters



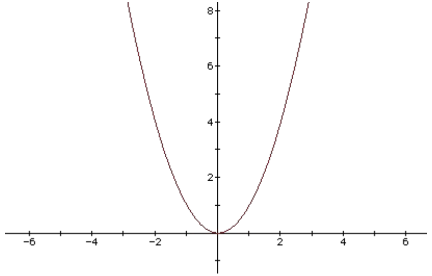
Stopping Criterion

- in practice, we stop after a finite number K of steps
- typical stopping criterion: stop if $\left\|\nabla f(\theta^k)\right\|_2 \leq \epsilon$ or $k = k^{\max}$
- ϵ is a small positive number, the stopping tolerance
- $k^{\max}$ is the maximum number of iterations

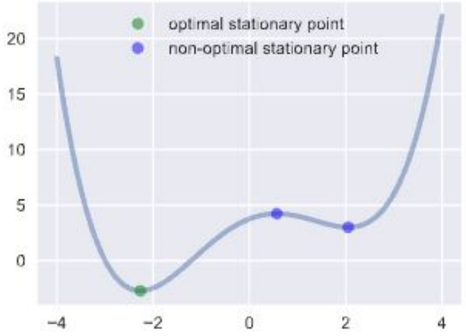
Gradient Method Convergence

- (assuming some technical conditions hold) we have

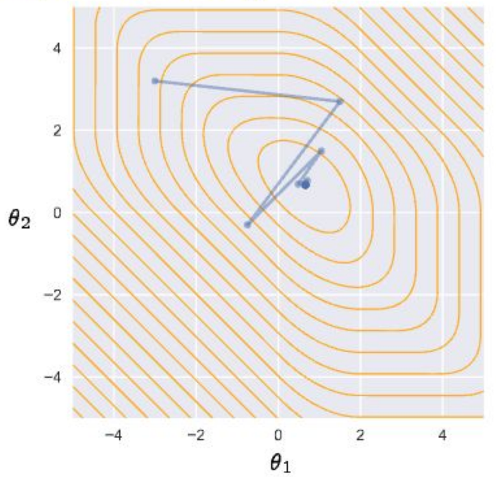
$$\left\|\nabla f\left(\theta^k\right)\right\|_2 \to 0 \text{ as } k \to \infty$$

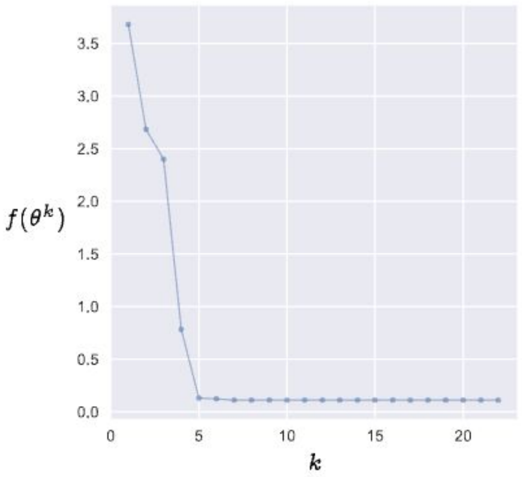


- i.e., the gradient method always finds a stationary point
- for convex problems
  - ➢ gradient method is non-heuristic
  - ➢ for any starting point $\theta^1, f\left(\theta^k\right) \to f^\star$ as $k \to \infty$
- for non-convex problems
  - ➢ gradient method is heuristic
  - ➢ we can (and often do) have $f\left(\theta^k\right) \nrightarrow f^\star$

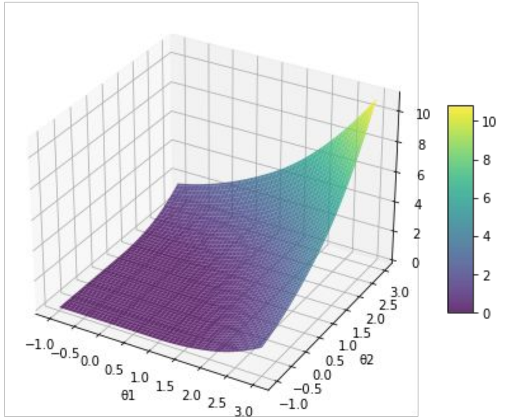


Example: Convex Objective





- $f(\theta) = \frac{1}{3}\left(p^{\text{hub}}(\theta_1 - 1) + p^{\text{hub}}(\theta_2 - 1) + p^{\text{hub}}(\theta_1 + \theta_2 - 1)\right)$
- f is convex
- optimal point is $\theta^\star = (2/3, 2/3)$, with $f^\star = 1/9$



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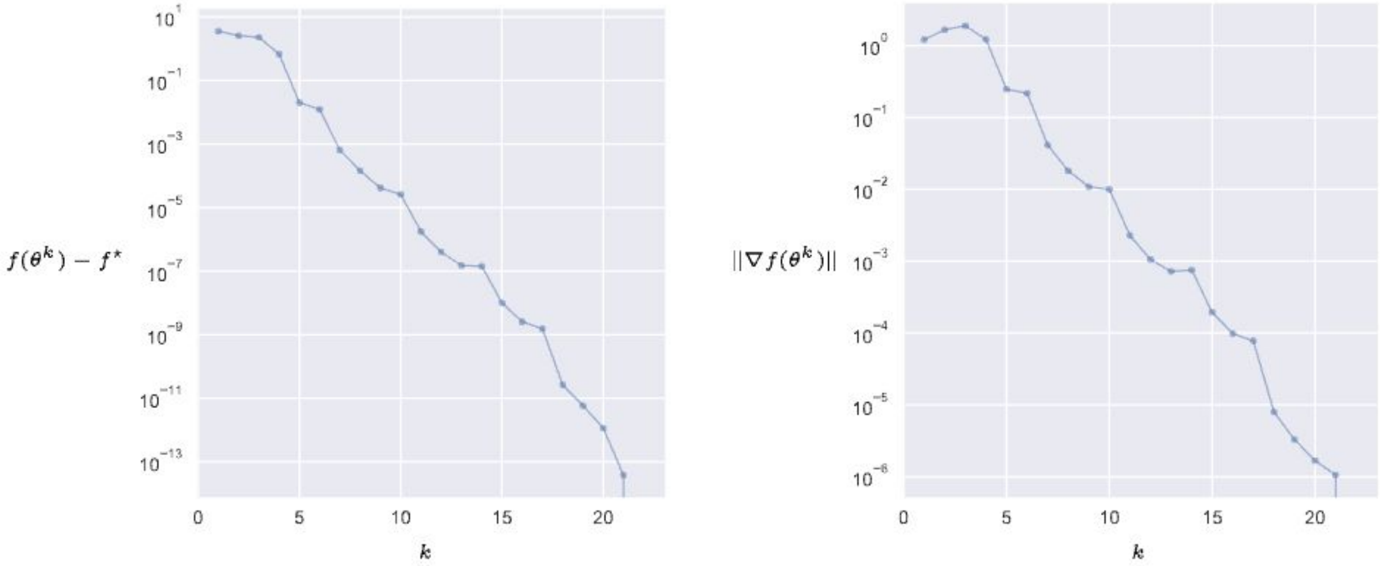
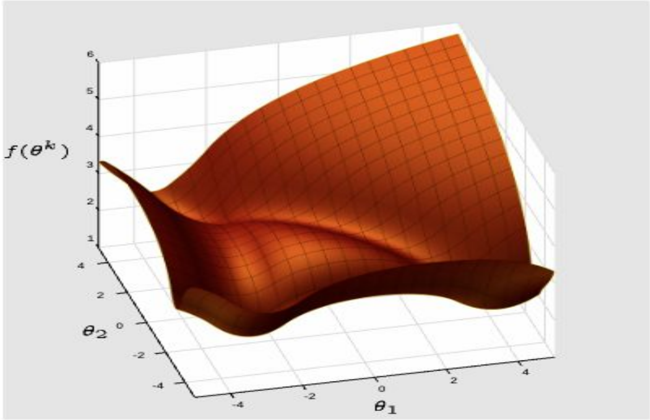


- $f(\theta^k)$ is a decreasing function of k, (roughly) exponentially
- $\|\nabla f(\theta^k)\| \to 0$ as $k \to \infty$

Example: Non-Convex Objective



- gradient algorithm converges, but limit depends on initial guess

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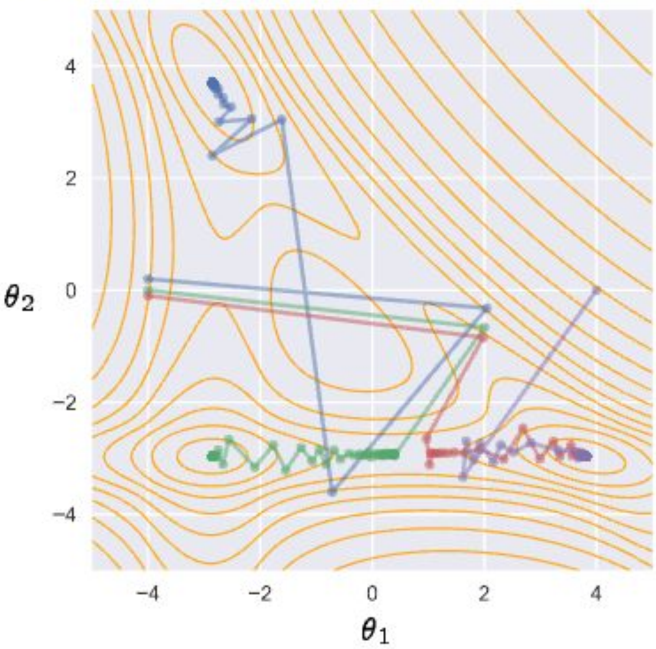

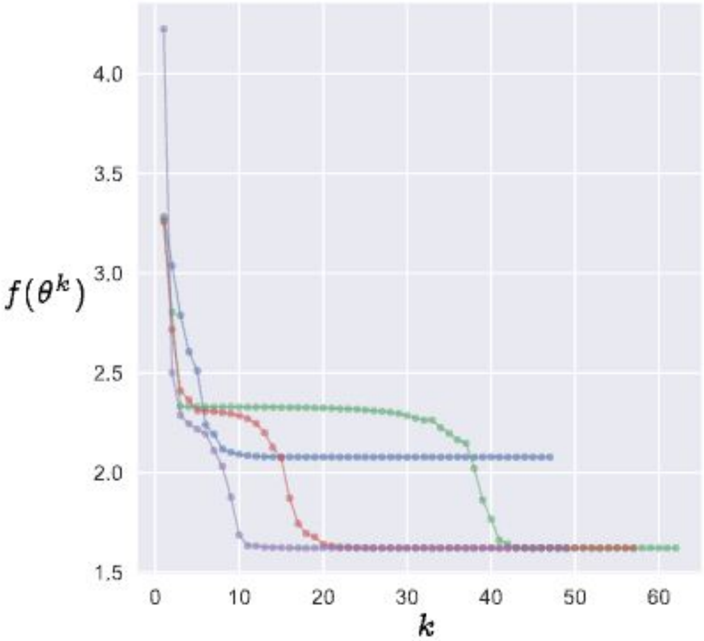

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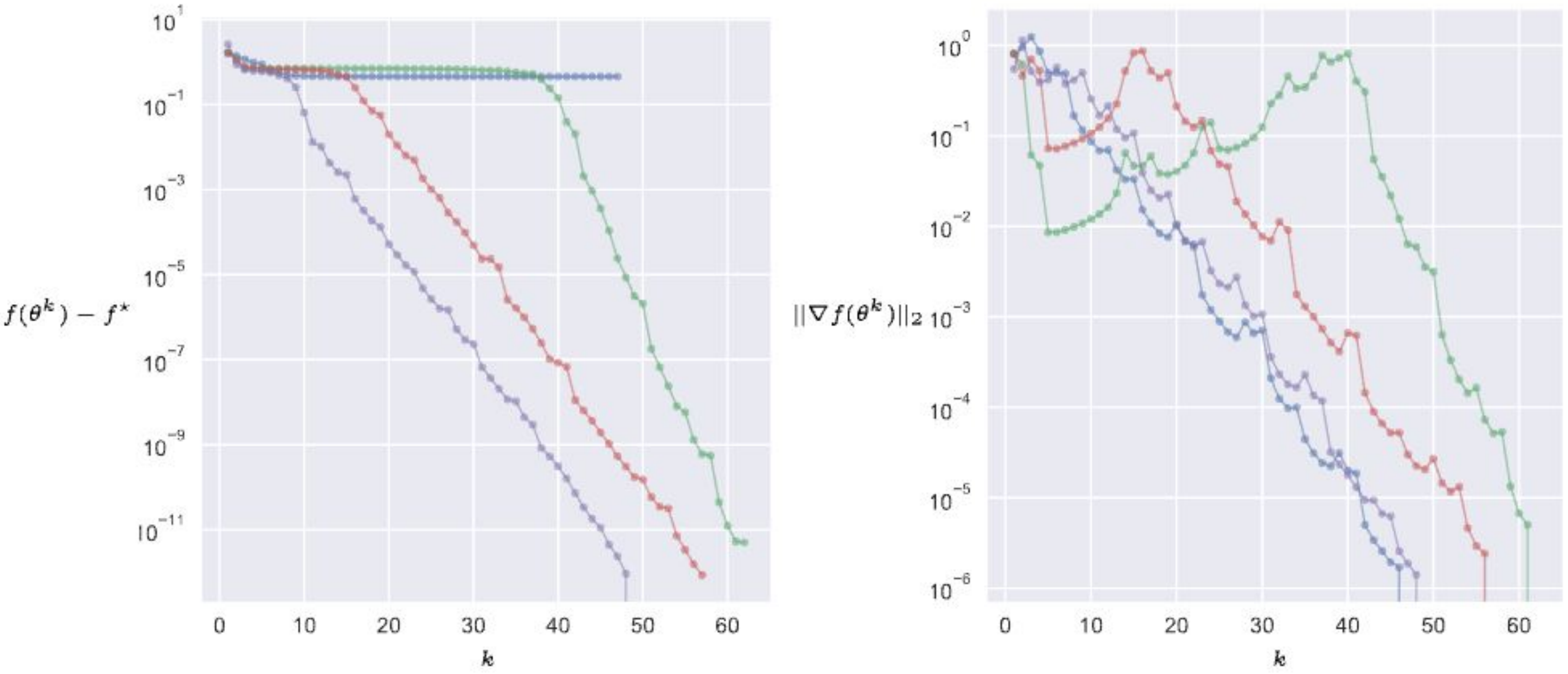

Stochastic Gradient Descent

Goal: minimize $f(\theta) = \frac{1}{n}\sum_{i=1} f(x_i, y_i; \theta)$

Initialize $\theta^0 \in \mathbb{R}^d$ randomly
Iterate until convergence:

- $\nabla f(\theta)|_{\theta=\theta^t} = \frac{1}{n}\sum_{i=1}^{n} \nabla f(x_i, y_i, \theta)|_{\theta=\theta^t}$
- $\theta^{t+1} = \theta^t - \eta \nabla f(\theta)|_{\theta=\theta^t}$

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Initialize $\theta^0 \in \mathbb{R}^d$ randomly
Iterate until convergence:

- Randomly sample a point (x_i, y_i) from the n data points
- Compute noisy gradient $\tilde{g}^t = \nabla f(x_i, y_i; \theta)|_{\theta=\theta^t}$
- Update $\theta^{t+1} = \theta^t - \eta\tilde{g}^t$

Intuition of why Stochastic GD can work

Claim: the random noisy gradient is an unbiased estimate of the true gradient

Note the point (x_i, y_i) is uniformly random sampled from n data points, we have:

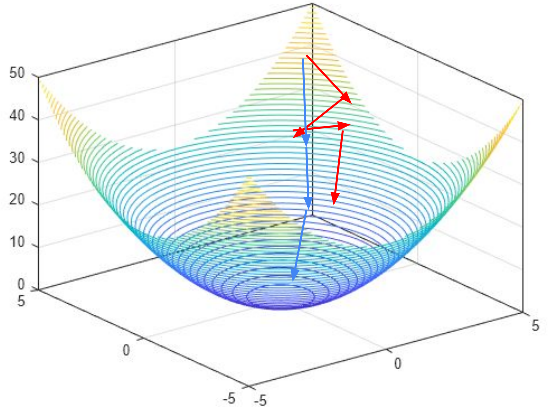
$$\mathbb{E}[\nabla f(x_i, y_i; \theta)]$$

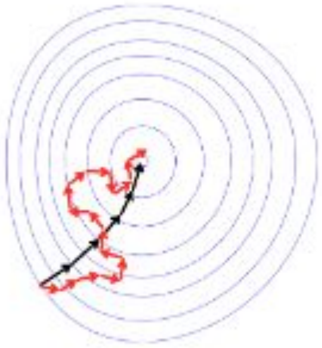
$$= \frac{1}{n}\sum_{i=1}^{n} \nabla f(x_i, y_i; \theta) = \nabla \left[\frac{1}{n}\sum_{i=1}^{n} f(x_i, y_i; \theta)\right] = \nabla f(\theta)$$

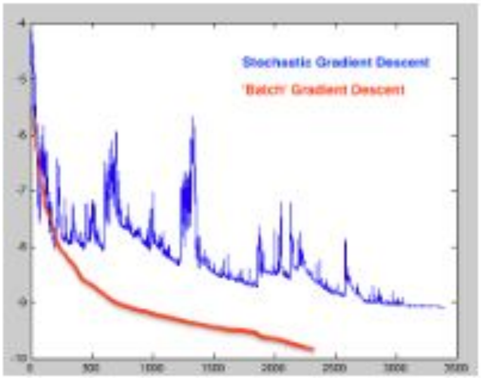
Stochastic gradient descent generally makes more iterations than gradient descent.

Each iteration is much cheaper (by a factor of n).

$$\vec{\nabla} f(\vec{\theta}) = \vec{\nabla} \sum_{j=1}^{n} f_j(\vec{\theta}) \text{ vs. } \vec{\nabla} f_j(\vec{\theta})$$







Apply GD and SGD to LMS

$$\max_{\theta} \; \log L(\theta) = -\frac{1}{2\sigma^2}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2 - m\log(\sqrt{2\pi}\sigma)$$

- The gradient of LMS is

$$\frac{1}{m}\nabla_\theta \log L(\theta) = \frac{1}{m\sigma^2}\sum_{i=1}^{m}(y^i - \theta^\top x^i)\, x^i$$

- The stochastic gradient of LMS is

$$\nabla_\theta \log L(\theta)\Big|_{\text{sample } i} = \frac{1}{\sigma^2}\left(y^i - \theta^\top x^i\right) x^i$$

Summary

- Random Search
- Closed-form
- Iterative methods:
  - Local Search
  - Gradient Descent
  - Stochastic Gradient Descent

- Homework 1 is released
- Due: 11:59PM EST, 02/04/2026

Q&A