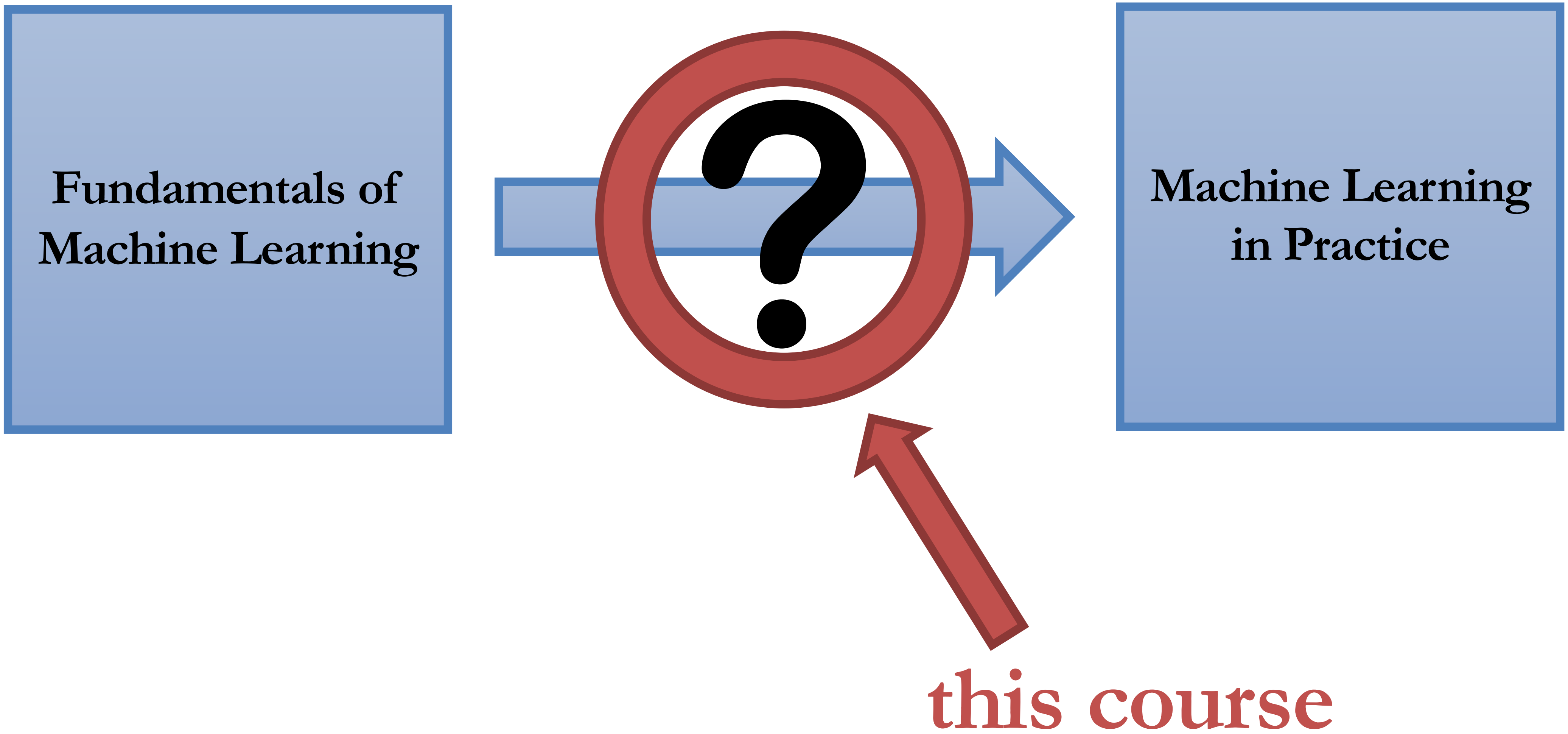
CS6787: Advanced Machine Learning Systems

CS6787 Lecture 1 — Fall 2018


Fundamentals of Machine Learning
?
Machine Learning in Practice
this course

What’s missing in the basic stuff?

Efficiency!

Motivation:

Machine learning applications involve large amounts of data

More data → Better services

Better systems → More data

How do practitioners make their systems better?

How do we improve our systems?

Course outline

- The use methods for accelerating convergence
  - Make ML algorithms converge in fewer iterations

Part 1

- They use metaparameter optimization
  - How to set parameters of these techniques automatically

Part 2

- They use techniques for improving runtime
  - Making each iteration of the algorithm run faster

Part 3

- They use machine learning hardware and frameworks
  - Using specialized tools to get more performance from less effort

Part 4

Course Format

One half

Traditional lectures

Broad description of techniques

One half

Important papers

Presentations by **you**

In-class discussions

Reviews of each paper

Prerequisites

- Basic ML knowledge (CS 4780)
- Math/statistics knowledge
  - At the level of the entrance exam for CS 4780

Grading

- Paper presentations
- Discussion participation
- Paper reviews
- Final project

Paper presentations

- Presenting in groups of two-to-three
- Papers listed on the website
- 25-minute presentation slot for each paper
- **Signups on Wednesday**

Discussion and Paper Reviews

- Each paper presentation will be followed by questions and breakout discussion
- Please **read at least one of the papers** before coming to class
  - And at least skim the other paper, so you know what to expect
- For each class period, **submit a review** of one of the two papers
  - Detailed instructions are on the course webpage

Final Project

- **Open-ended**: work on what you think is interesting!
- Groups of up to three
- Your proposed project must include:
  - The **implementation** of a machine learning system for some task
  - Exploring one or more of the **techniques discussed in the course**
  - To **empirically evaluate performance** and compare with a baseline.

Late Policy

- This is a graduate level course
- Two free late days for each of the paper reviews
- No late days on the final project
  - To make things easy on the graders

Questions?

Stochastic Gradient Descent: The Workhorse of Machine Learning

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Optimization

- Much of machine learning can be written as an optimization problem

$$\min_{x} \sum_{i=1}^{N} f(x; y_i)$$

model

loss function

training examples

- Example loss functions: logistic regression, linear regression, principle component analysis, neural network loss, empirical risk minimization

Types of Optimization

- Convex optimization
  - The **easy case**
  - Includes logistic regression, linear regression, SVM
- Non-convex optimization
  - **NP-hard in general**
  - Includes deep learning

~~A good strategy~~:

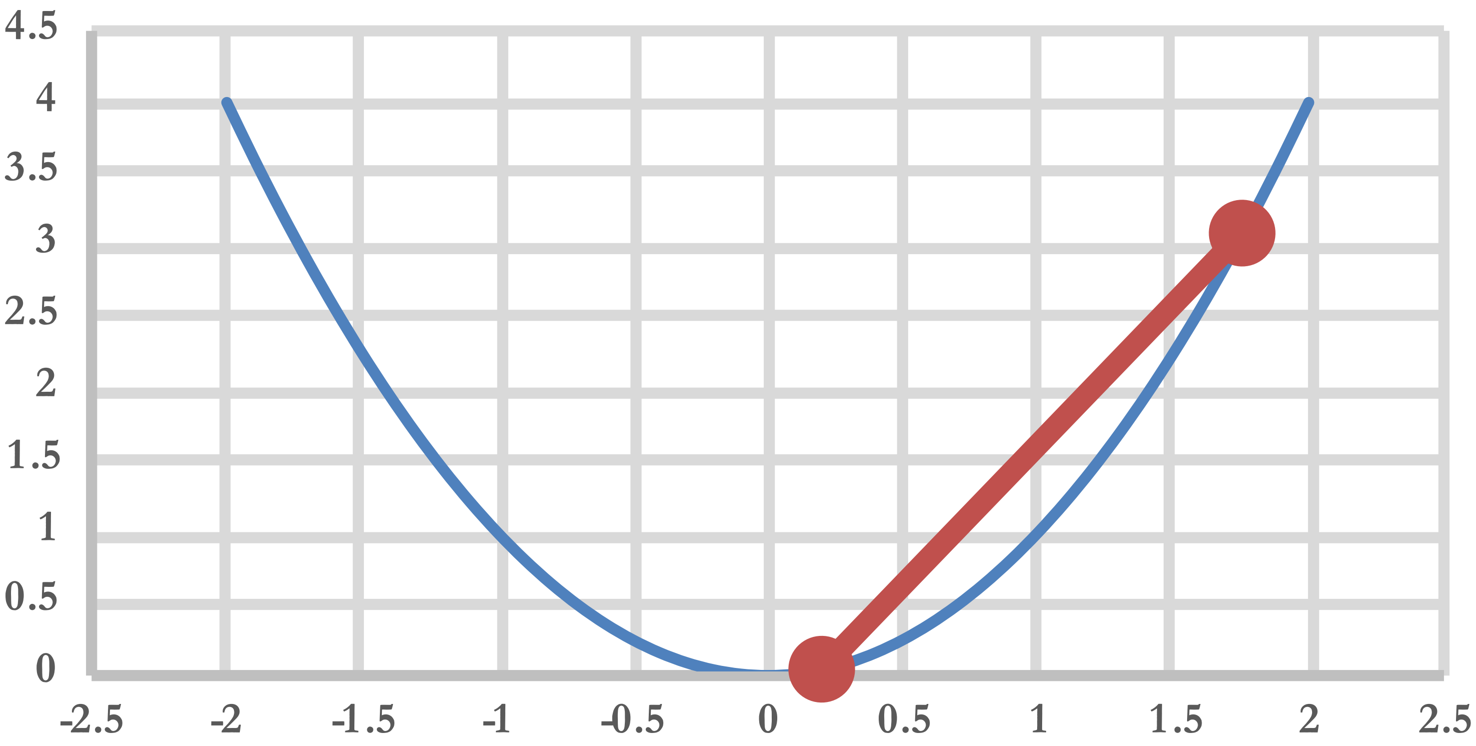
Build intuition about techniques from the convex case where we can prove things…

…and apply it to better understand more complicated systems.

An Abridged Introduction to Convex Functions

Convex Functions

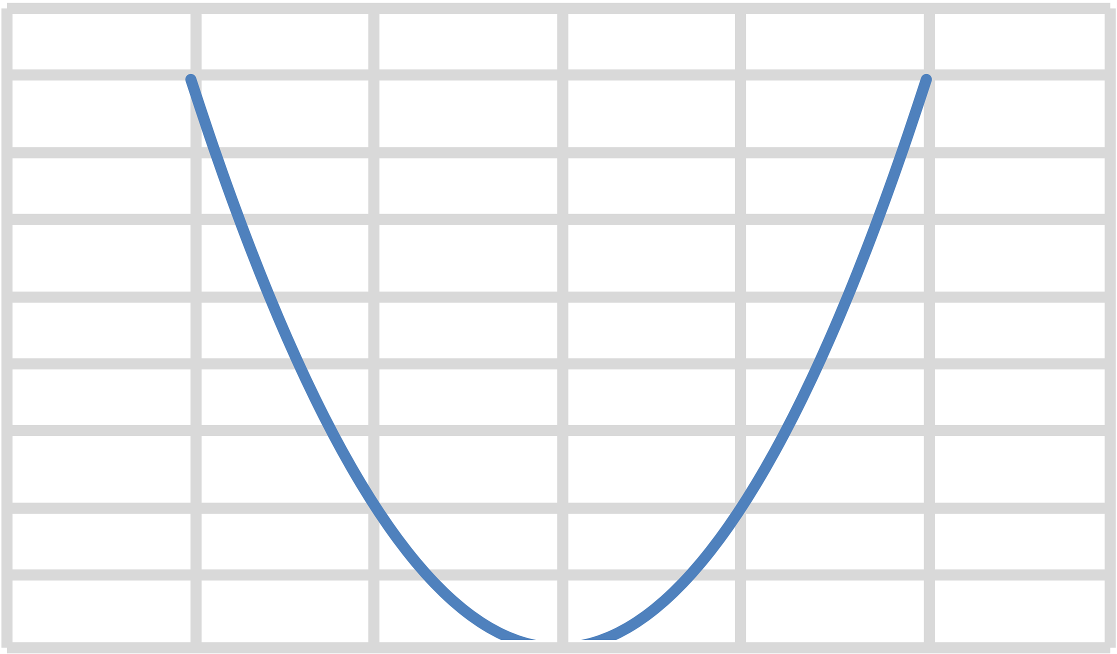
$$\forall \alpha \in [0,1],\ f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y)$$



$f(x) = x^2$

Example: Quadratic

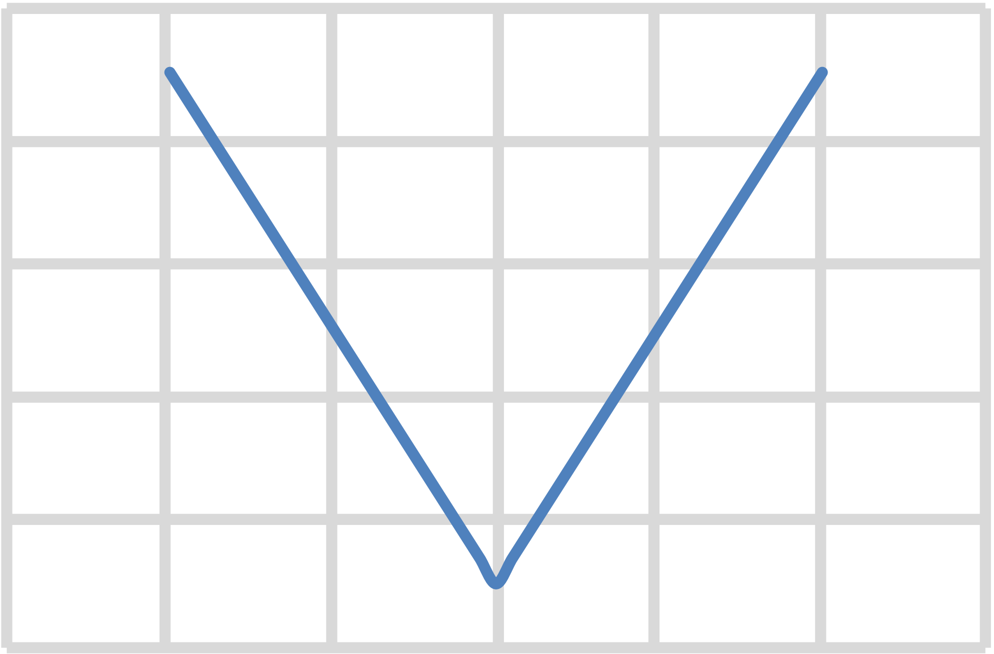
$$f(x) = x^2$$



$$\begin{aligned}(\alpha x + (1-\alpha)y)^2 &= \alpha^2 x^2 + 2\alpha(1-\alpha)xy + (1-\alpha)^2 y^2 \\ &= \alpha x^2 + (1-\alpha)y^2 - \alpha(1-\alpha)(x^2 + 2xy + y^2) \\ &\leq \alpha x^2 + (1-\alpha)y^2\end{aligned}$$

Example: Abs

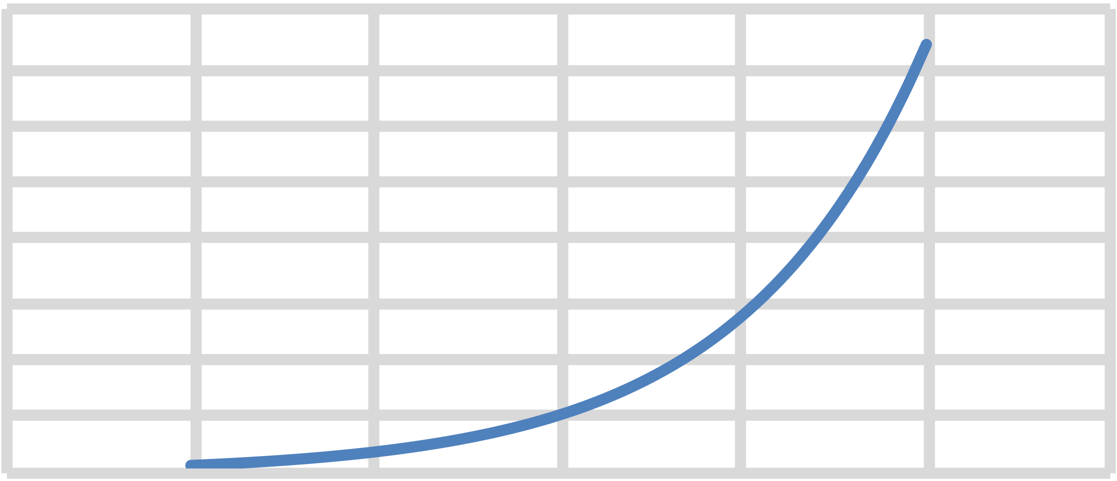
$$f(x) = |x|$$



$$\begin{aligned} |\alpha x + (1-\alpha)y| &\leq |\alpha x| + |(1-\alpha)y| \\ &= \alpha|x| + (1-\alpha)|y| \end{aligned}$$

Example: Exponential

$$f(x) = e^x$$



$$
\begin{aligned}
e^{\alpha x+(1-\alpha)y} = e^y e^{\alpha(x-y)} &= e^y \sum_{n=0}^{\infty} \frac{1}{n!}\alpha^n (x-y)^n \\
&\leq e^y \left(1 + \alpha \sum_{n=1}^{\infty} \frac{1}{n!}(x-y)^n\right) \qquad \text{(if } x > y\text{)} \\
&= e^y \left((1-\alpha) + \alpha e^{x-y}\right) \\
&= (1-\alpha)e^y + \alpha e^x
\end{aligned}
$$

Properties of convex functions

- Any line segment we draw between two points lies above the curve

- Corollary: every local minimum is a global minimum
  - Why?

- This is what makes convex optimization easy
  - It suffices to find a local minimum, because we know it will be global

Properties of convex functions (continued)

- Non-negative combinations of convex functions are convex

$$h(x) = af(x) + bg(x)$$

- Affine scalings of convex functions are convex

$$h(x) = f(Ax + b)$$

- Compositions of convex functions are **NOT** generally convex
  - Neural nets are like this

$$h(x) = f(g(x))$$

Convex Functions: Alternative Definitions

- First-order condition

$$\langle x - y, \nabla f(x) - \nabla f(y) \rangle \geq 0$$

- Second-order condition

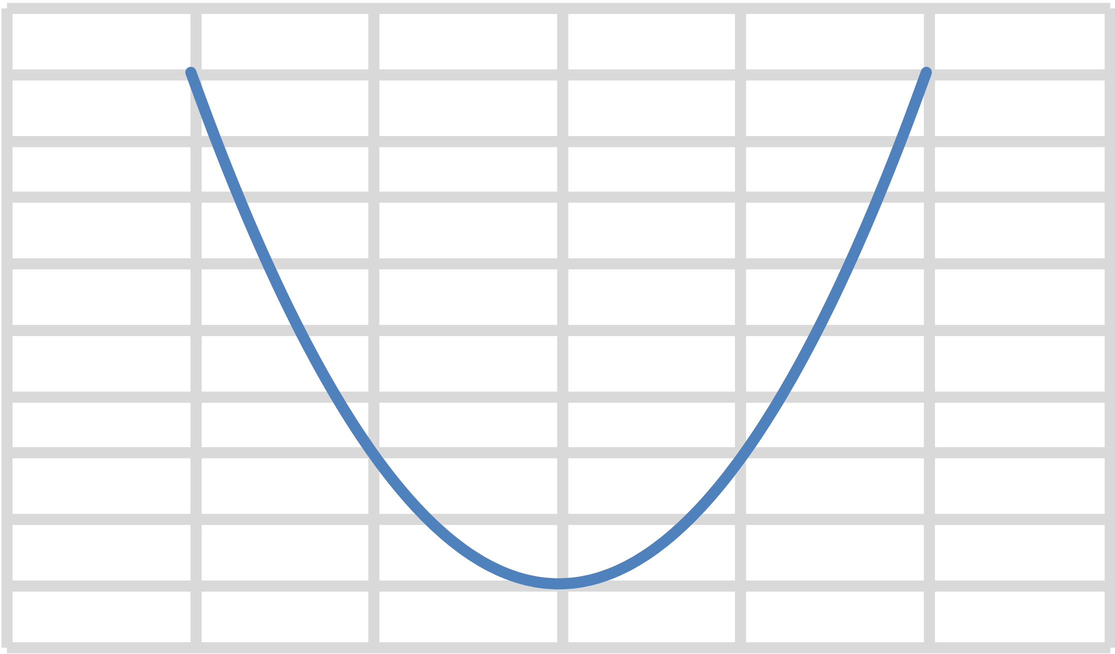
$$\nabla^2 f(x) \succeq 0$$

  - This means that the matrix of second derivatives is positive semidefinite

$$A \succeq 0 \Leftrightarrow \forall x,\ \langle x, Ax \rangle \geq 0$$

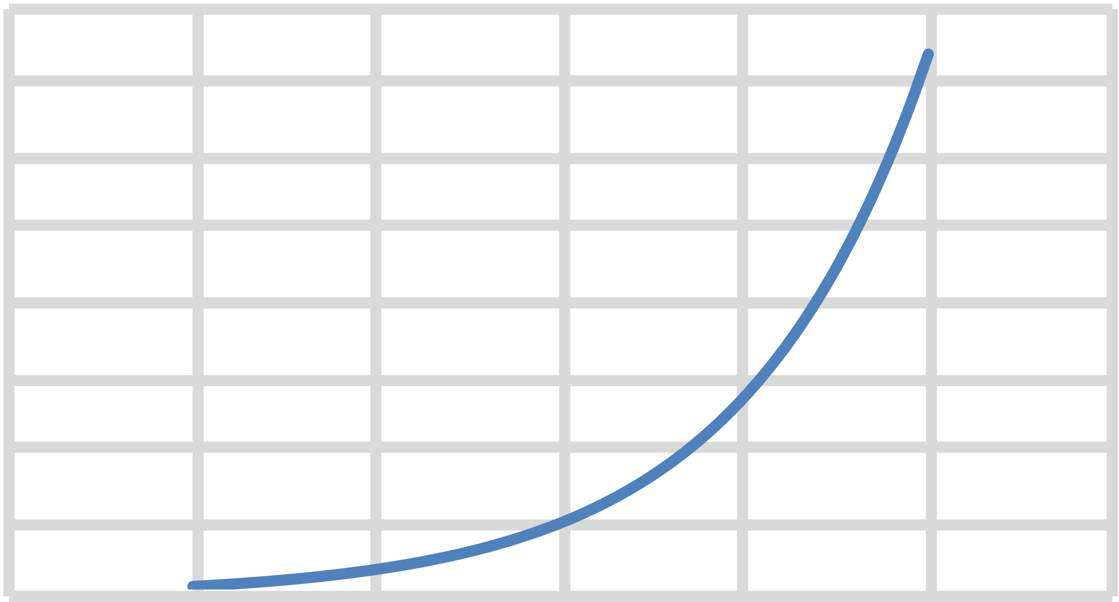
Example: Quadratic

$$f(x) = x^2$$



$$f''(x) = 2 \geq 0$$

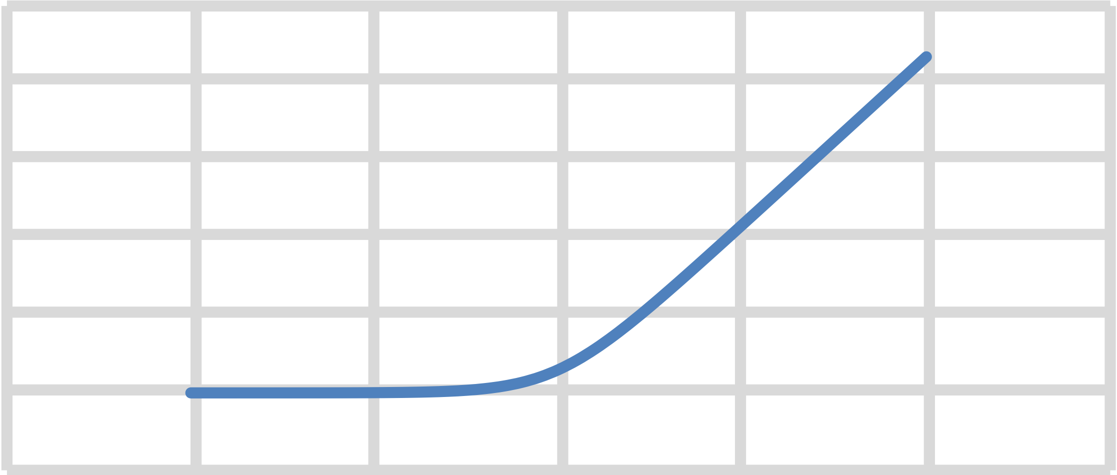
Example: Exponential



$$f(x) = e^x$$

$$f''(x) = e^x \geq 0$$

Example: Logistic Loss



$$f(x) = \log(1 + e^x)$$

$$f'(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$$

$$f''(x) = -\frac{-e^{-x}}{(1 + e^{-x})^2} = \frac{1}{(1 + e^x)(1 + e^{-x})} \geq 0.$$

Strongly Convex Functions

- Basically the easiest class of functions for optimization
  - First-order condition:

$$\langle x - y, \nabla f(x) - \nabla f(y) \rangle \geq \mu \|x - y\|^2$$

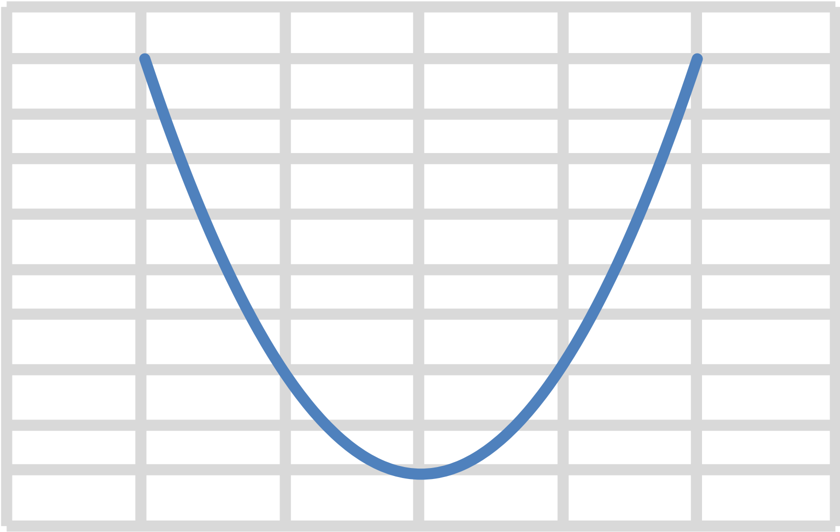
  - Second-order condition:

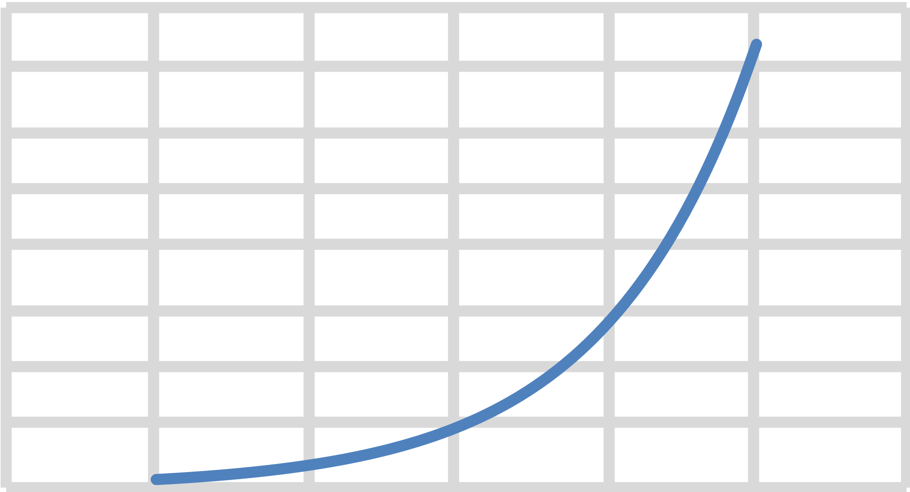
$$\nabla^2 f(x) \succeq \mu I$$

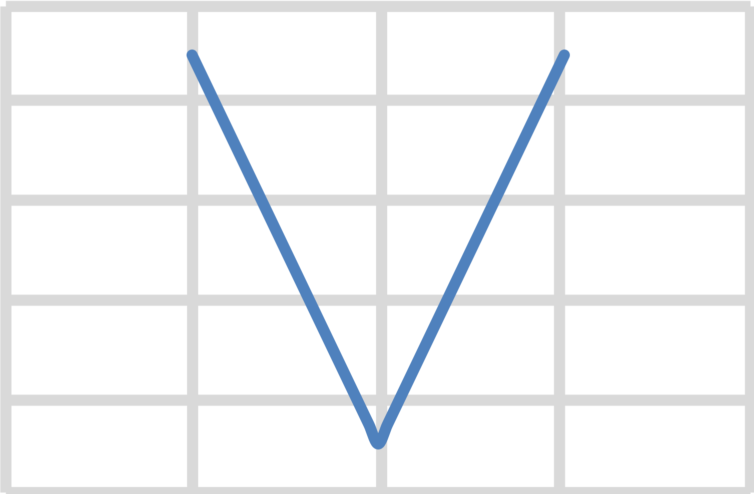
  - Equivalently:

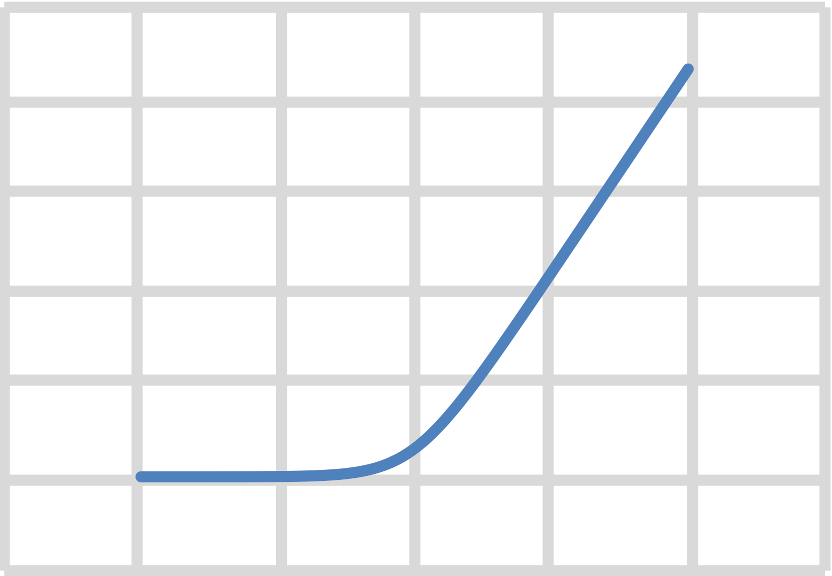
$$h(x) = f(x) - \frac{\mu}{2}\|x\|^2 \text{ is convex}$$

Which of the functions we've looked at are strongly convex?

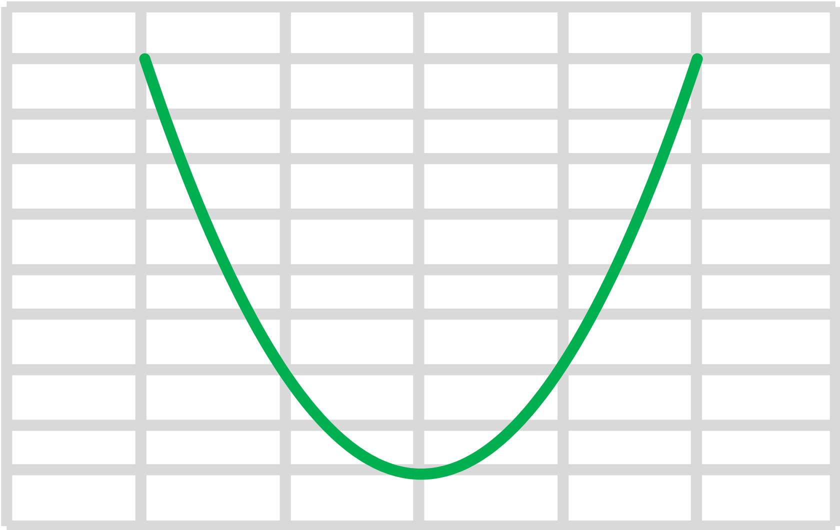


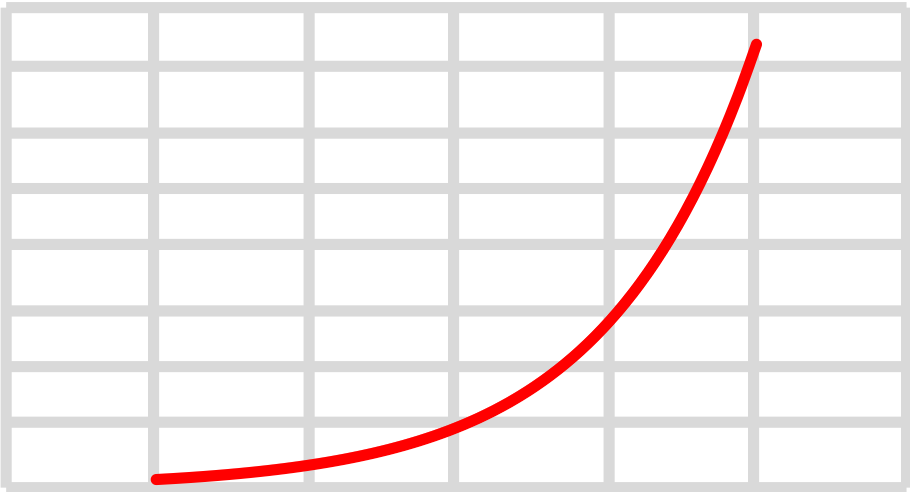


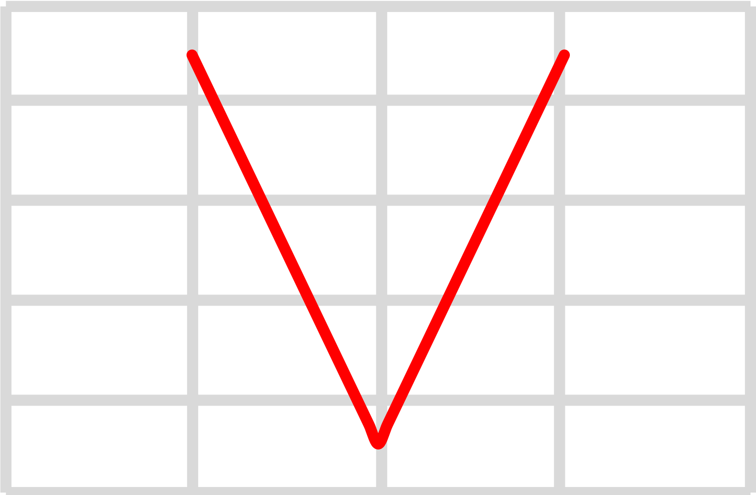


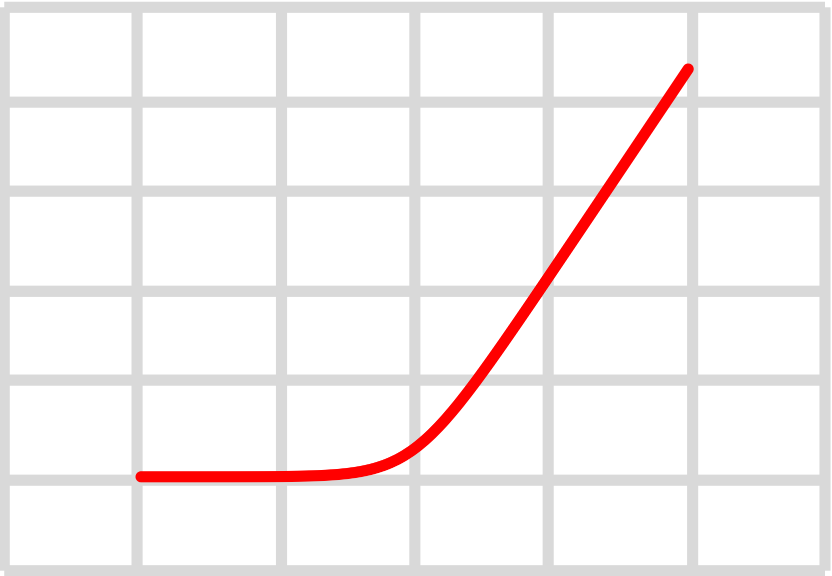


Which of the functions we've looked at are strongly convex?









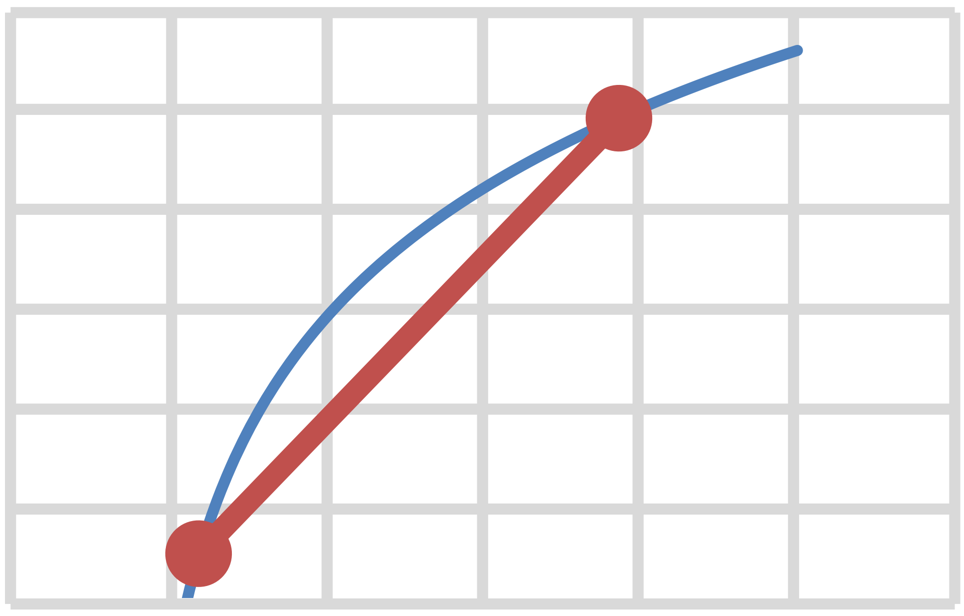
Concave functions

- A function is concave if its negation is convex

$$f \text{ is convex} \Leftrightarrow h(x) = -f(x) \text{ is concave}$$

- Example: $f(x) = \log(x)$

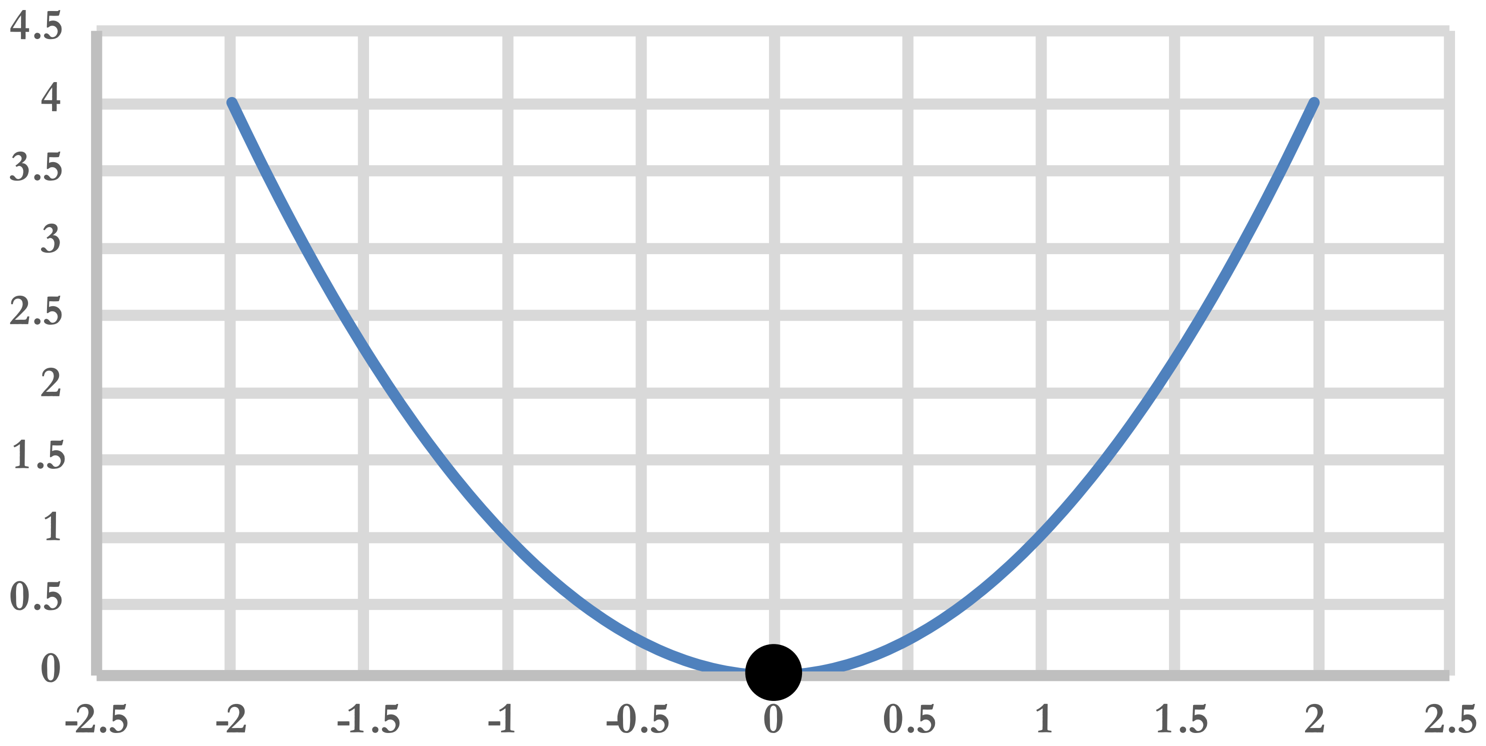
$$f''(x) = -\frac{1}{x^2} \leq 0$$



Why care about convex functions?

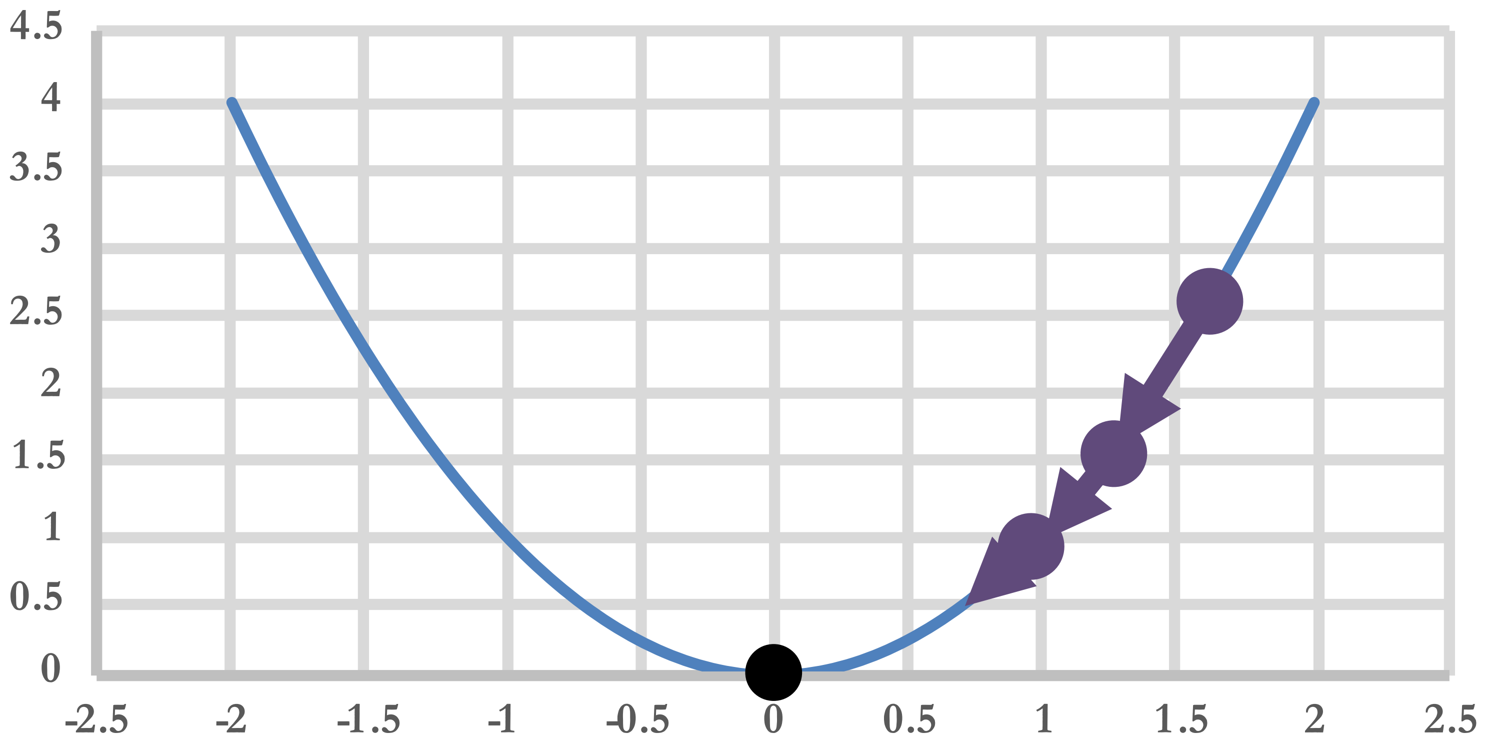
Convex Optimization

- Goal is to minimize a convex function



Gradient Descent

$$x \leftarrow x - \alpha \nabla f(x)$$



Gradient Descent Converges

- Iterative definition of gradient descent

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

- Assumptions/terminology:

$$\text{Global optimum is } x^*$$

$$\text{Bounded second derivative } \mu I \preceq \nabla^2 f(x) \preceq \text{Ł} I$$

Gradient Descent Converges (continued)

$$
\begin{aligned}
x_{t+1} - x^* &= x_t - x^* - \alpha(\nabla f(x_t) - \nabla f(x^*)) \\
&= x_t - x^* - \alpha \nabla^2 f(z_t)(x_t - x^*) \\
&= (I - \alpha \nabla^2 f(z_t))(x_t - x^*).
\end{aligned}
$$

- Taking the norm

$$
\begin{aligned}
\|x_{t+1} - x^*\| &\leq \left\| I - \alpha \nabla^2 f(z_t) \right\| \|x_t - x^*\| \\
&\leq \max\left(|1 - \alpha\mu|, |1 - \alpha L|\right) \|x_t - x^*\|
\end{aligned}
$$

Gradient Descent Converges (continued)

- So if we set $\alpha = 2/(L+\mu)$ then

$$\|x_{t+1} - x^*\| \leq \frac{L-\mu}{L+\mu} \|x_t - x^*\|$$

- And recursively

$$\|x_T - x^*\| \leq \left(\frac{L-\mu}{L+\mu}\right)^T \|x_0 - x^*\|$$

  - Called **convergence at a linear rate** or sometimes (confusingly) exponential rate

The Problem with Gradient Descent

- Large-scale optimization

$$h(x) = \frac{1}{N} \sum_{i=1}^{N} f(x; y_i)$$

- Computing the gradient takes O(N) time

$$\nabla h(x) = \frac{1}{N} \sum_{i=1}^{N} \nabla f(x; y_i)$$

Gradient Descent with More Data

- Suppose we add more examples to our training set
  - For simplicity, imagine we just add an extra copy of every training example

$$\nabla h(x) = \frac{1}{2N}\sum_{i=1}^{N}\nabla f(x; y_i) + \frac{1}{2N}\sum_{i=1}^{N}\nabla f(x; y_i)$$

- **Same objective function**
  - But gradients take **2x the time to compute** (unless we cheat)

- We want to **scale up to huge datasets**, so how can we do this?

Stochastic Gradient Descent

- Idea: rather than using the full gradient, just use one training example
  - Super fast to compute

$$x_{t+1} = x_t - \alpha \nabla f(x_t; y_{\tilde{i}_t})$$

This is an example selected uniformly at random from the dataset.

- In expectation, it's just gradient descent:

$$\mathbf{E}[x_{t+1}] = \mathbf{E}[x_t] - \alpha \mathbf{E}[\nabla f(x_t; y_{i_t})]$$
$$= \mathbf{E}[x_t] - \alpha \frac{1}{N} \sum_{i=1}^{N} \nabla f(x_t; y_i)$$

Stochastic Gradient Descent Convergence

- Can SGD converge using just one example to estimate the gradient?

$$x_{t+1} - x^* = x_t - x^* - \alpha \left(\nabla h(x_t) - \nabla h(x^*) \right) - \alpha \left(\nabla f(x_t; y_{i_t}) - \nabla h(x_t) \right)$$
$$= \left(I - \alpha \nabla^2 h(z_t) \right) (x_t - x^*) - \underline{\alpha \left(\nabla f(x_t; y_{i_t}) - \nabla h(x_t) \right)}$$

- How do we handle this extra noise term?

- **Answer: bound it using the second moment!**

Stochastic Gradient Descent Convergence

$$\begin{aligned}
\mathbf{E}\left[\|x_{t+1} - x^*\|^2\right] &= \mathbf{E}\left[\|(I - \alpha\nabla^2 h(z_t))(x_t - x^*) - \alpha(\nabla f(x_t; y_{i,t}) - \nabla h(x_t))\|^2\right] \\
&= \mathbf{E}\Big[\|(I - \alpha\nabla^2 h(z_t))(x_t - x^*)\|^2 \\
&\qquad - 2\alpha(\nabla f(x_t; y_{i,t}) - \nabla h(x_t))^T (I - \alpha\nabla^2 h(z_t))(x_t - x^*) \\
&\qquad + \alpha^2\|\nabla f(x_t; y_{i,t}) - \nabla h(x_t)\|^2\Big] \\
&= \mathbf{E}\Big[\|(I - \alpha\nabla^2 h(z_t))(x_t - x^*)\|^2 + \alpha^2\|\nabla f(x_t; y_{i,t}) - \nabla h(x_t)\|^2\Big] \\
&\leq (1 - \alpha\mu)^2\mathbf{E}\left[\|(x_t - x^*)\|^2\right] + \alpha^2 M
\end{aligned}$$

assuming the upper bound $\mathbf{E}\left[\|\nabla f(x; y) - \nabla h(x)\|^2\right] \leq M$

Stochastic Gradient Descent Convergence

- Already we can see that this converges to a fixed point of

$$\mathbf{E}\left[\|x_{t+1} - x^*\|^2\right] = \frac{\alpha M}{2\mu - \alpha\mu^2}$$

- This phenomenon is called converging to a **noise ball**
  - Rather than approaching the optimum, SGD (with a constant step size) converges to a region of low variance around the optimum
  - This is okay for a lot of applications that **only need approximate solutions**

Demo

Stochastic gradient descent is super popular.

What Does SGD Power?

- Everything!

But how SGD is implemented in practice is not exactly what I've just shown you…

…and we'll see how it's different in the upcoming lectures.

Questions?

- Upcoming things
  - Paper presentation signups **on Wednesday**