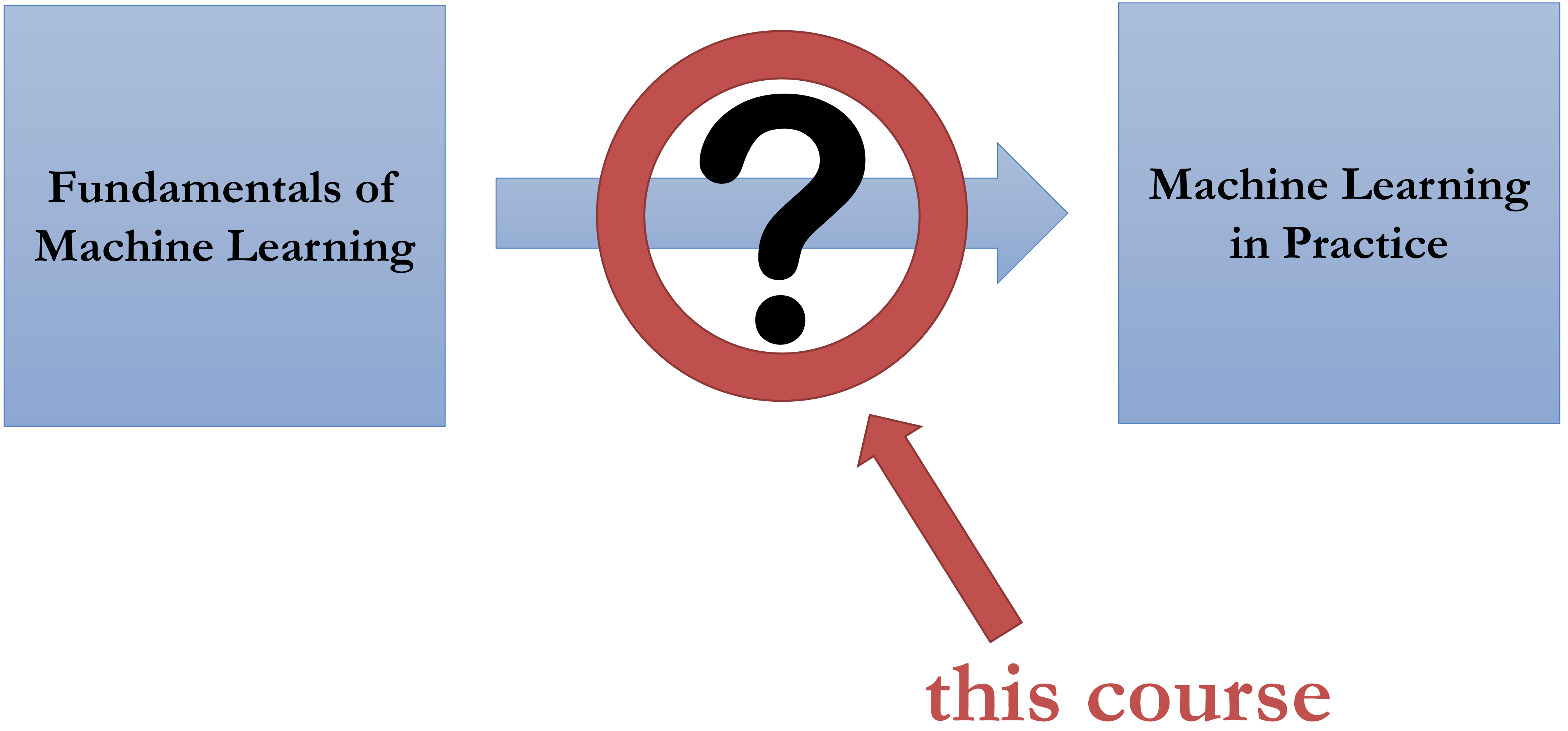
CS6787: Advanced Machine Learning Systems

CS6787 Lecture 1 — Fall 2020


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

- Build frameworks/software that make it easy to express & train a machine learning/deep learning model. **Part 1**
- Use methods for accelerating convergence of learning algorithms — learn in fewer iterations. **Part 2**
- Automatically configure learning systems by using hyperparameter optimization **Part 3**
- Use methods for improving hardware efficiency — run each iteration faster. **Part 4**
- Use specialized ML hardware accelerators and get our frameworks to do as much as possible automatically. **Part 5**

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
- Programming assignments
- Final project

Paper presentations

- Papers listed on the website
  - 20-minute presentation slot for each paper
  - Presenting in groups of two-to-three
- **Signups by Monday!**
  - Survey will be sent out over the next couple of days
- **Learning goal**
  - **Practice digesting and talking about other people's work**

Paper Reading and Discussion

- Each presentation is followed by questions and breakout discussion
- Please **read at least one of the papers** before attending class
  - And at least skim the other paper, so you know what to expect
- Note: grade is not for attendance, but rather on participation and bringing insightful ideas to the table — *full remote support*
- **Learning goal: practice how to deeply read and critique a paper in context**

Paper Reviews

- For each class period, **submit a review** of one of the two papers
  - (Only if you are not presenting.)

- Review the paper as if you were doing peer review on a newly submitted work

- Reviews due a few days after our in-class discussion

- **Learning goal: build technical reading and writing skills, and get some window into how peer review works.**

Programming Assignments

- Two assignments in the first part of the semester only
- **Learning goal: become familiar with ML frameworks/tools**
  - **…and the principles that underlie them**
  - **This will hopefully build skills for you to use in the final project**

Final Project

- **Open-ended**: work on what you think is interesting!
  - Learning goal: **do a small bit of non-trivial research on your own**
- 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 and programming assignments
- No late days on the final project
  - To make things easy on the graders
- No late days on the presentations (for obvious reasons)

Questions?

Today's Topic

Stochastic Gradient Descent: The Workhorse of Machine Learning

CS6787 Lecture 1 — Fall 2020

But first…an icebreaker activity!

For each person in order:

- What is your name?
- What are you studying?
- **What do you hope to learn from CS6787?**

After everyone is done, discuss together:

Why do people use stochastic gradient descent?

Today's Topic

Stochastic Gradient Descent: The Workhorse of Machine Learning

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Optimization

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

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f(w; x_i)$$

model (w) — **loss function** (f) — **training examples** (x_i)

- 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

<u>A good strategy:</u>

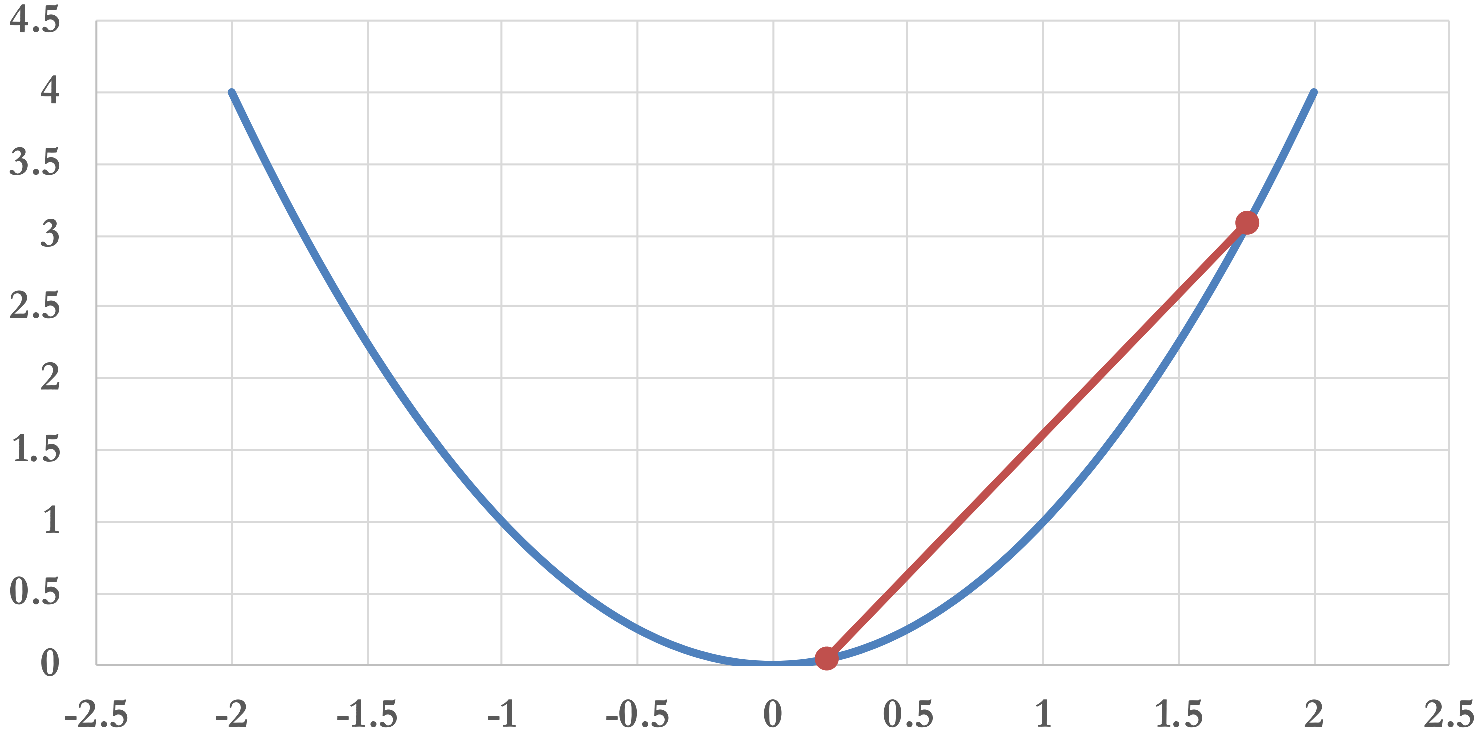
Build theoretical intuition about techniques from the convex case where we can prove things…

…and apply it to better understand more complicated systems.

An Abridged Introduction to Convex Functions

Convex Functions

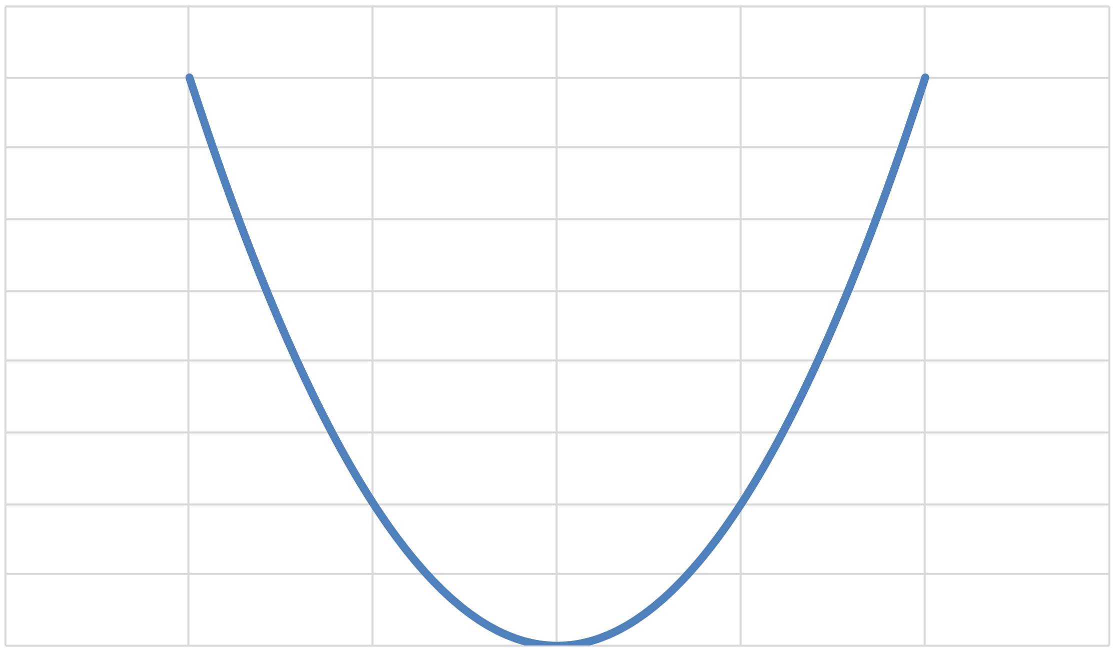
$$\forall \alpha \in [0,1],\ f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y)$$



$f(x) = x^2$

Example: Quadratic

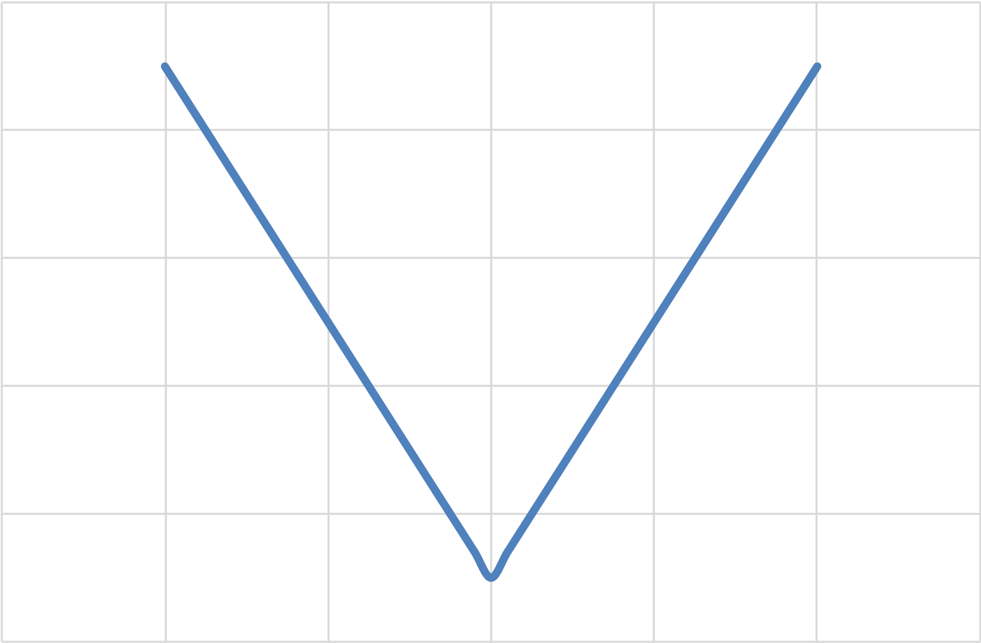
$$f(x) = x^2$$



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

Example: Abs

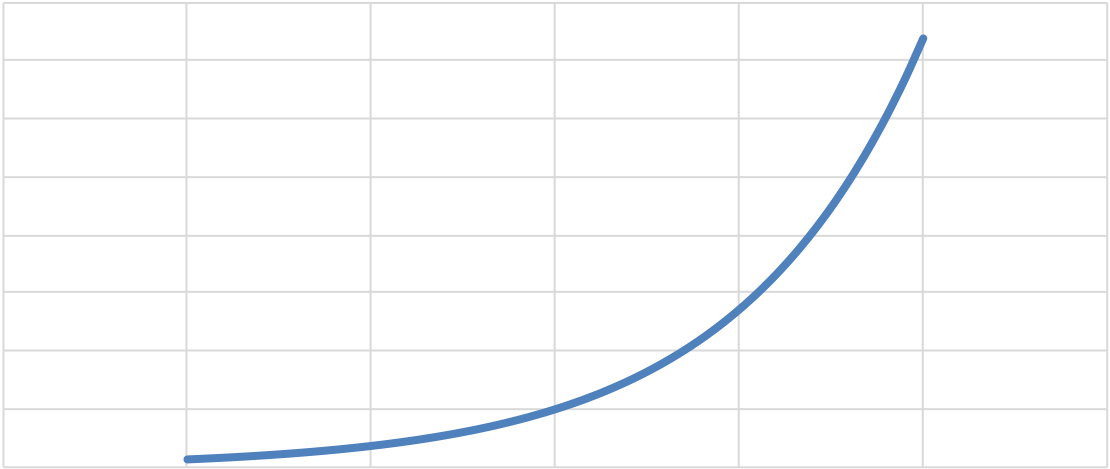
$$f(x) = |x|$$



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

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

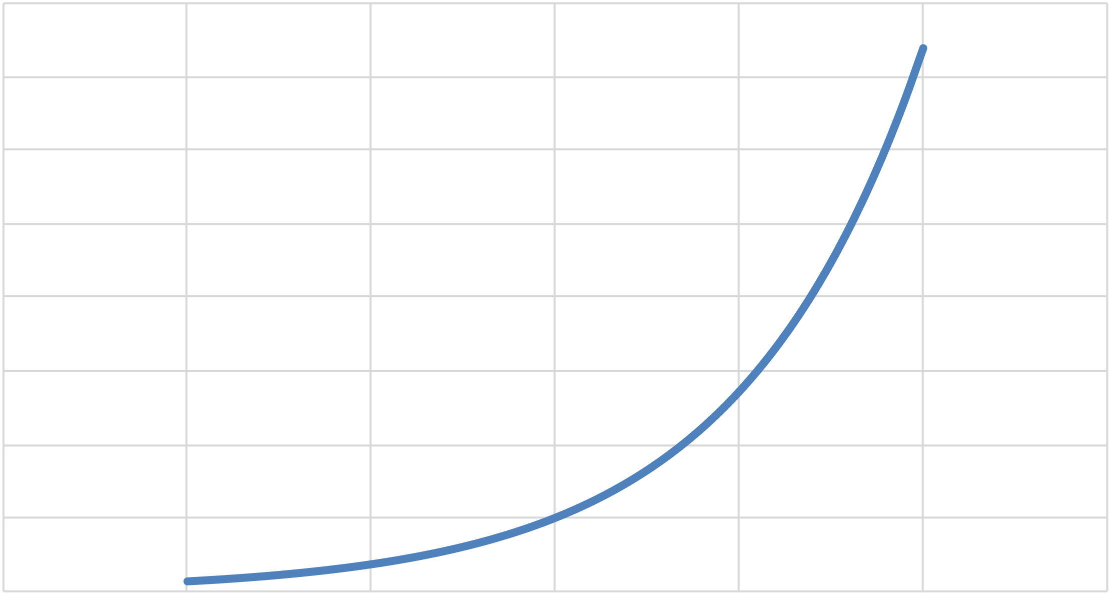
$$A \succeq 0 \Leftrightarrow \forall x,\ \langle x, Ax \rangle \geq 0$$

Example: Quadratic

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

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

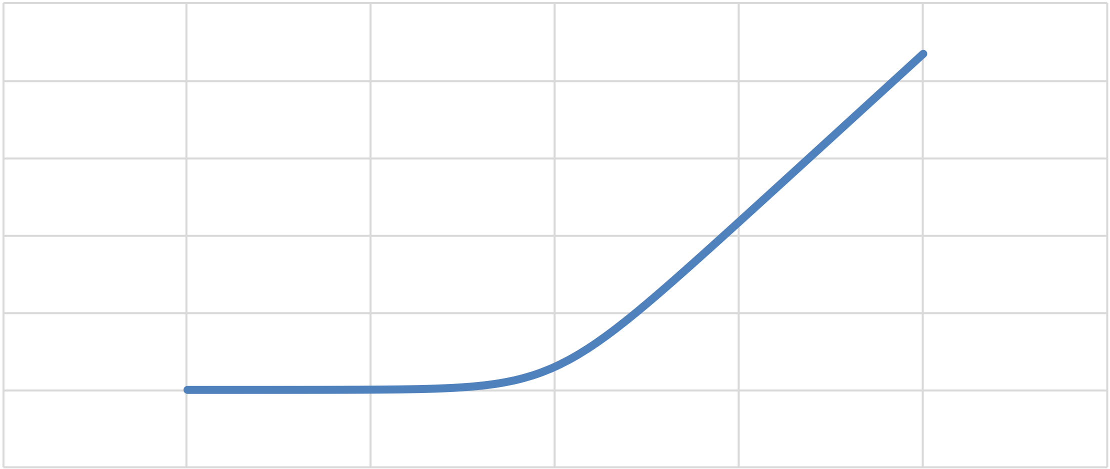
Example: Exponential



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

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

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:

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

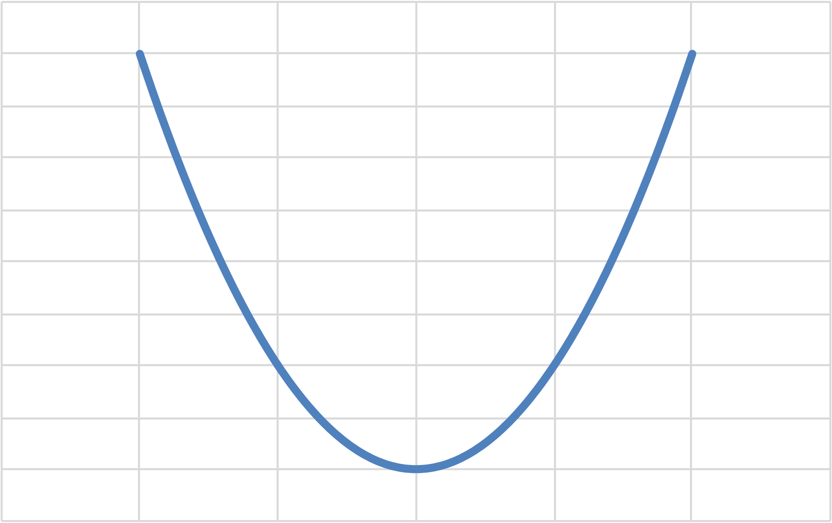
  - Second-order condition:

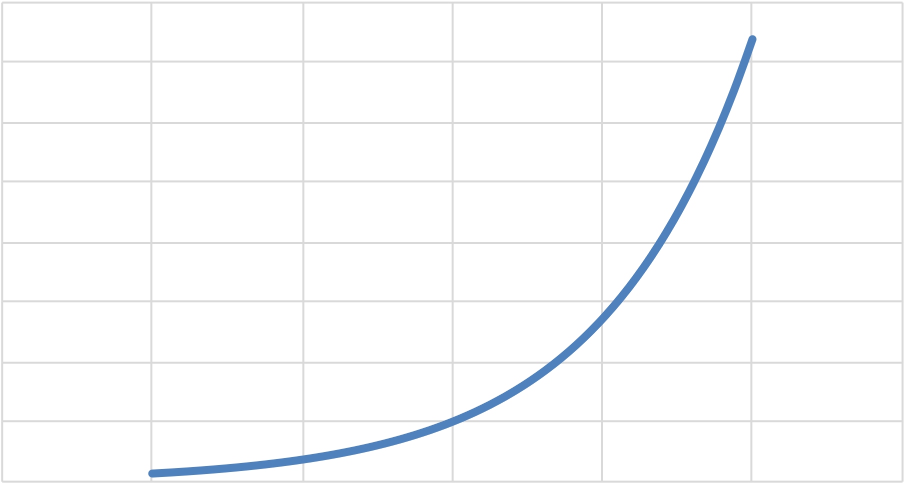
$$\nabla^2 f(x) \succeq \mu I$$

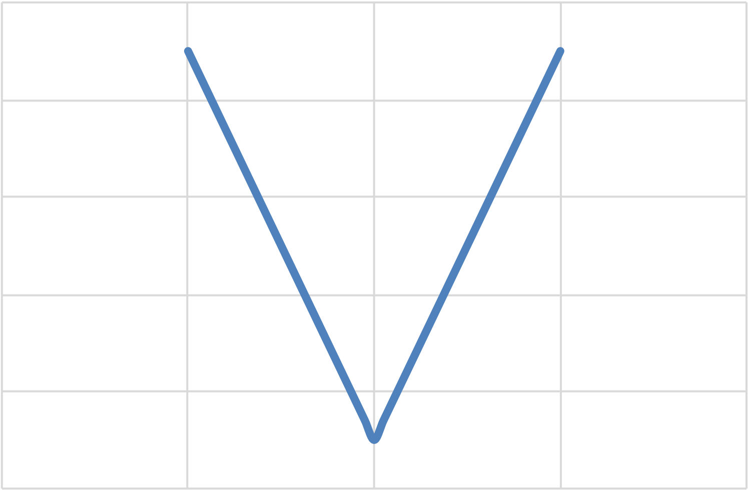
  - Equivalently:

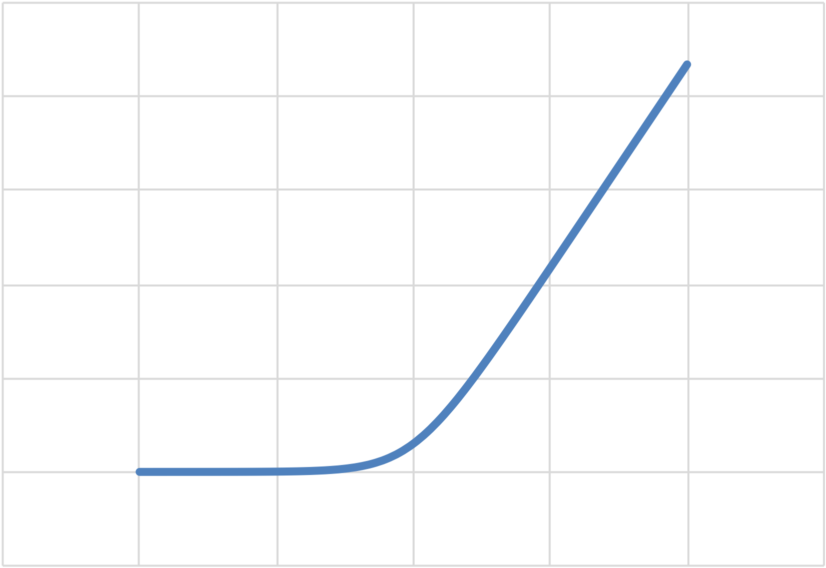
$$h(x) = f(x) - \tfrac{\mu}{2}\|x\|^2 \text{ is convex}$$

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

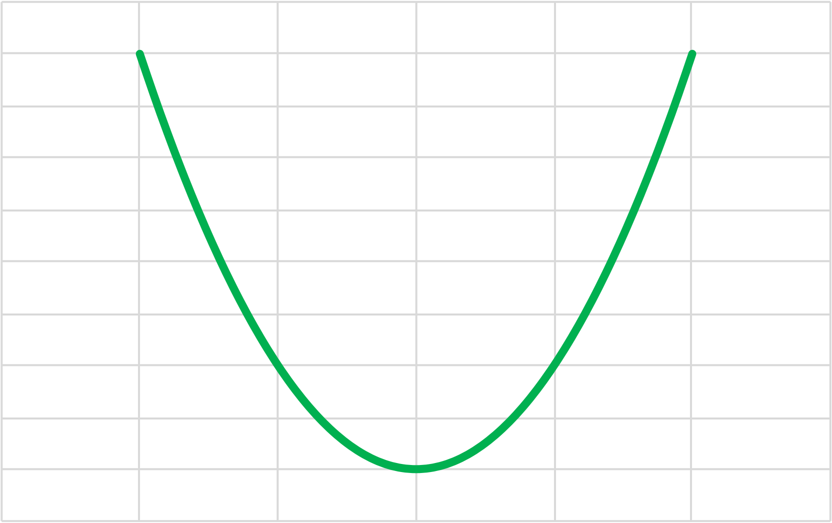


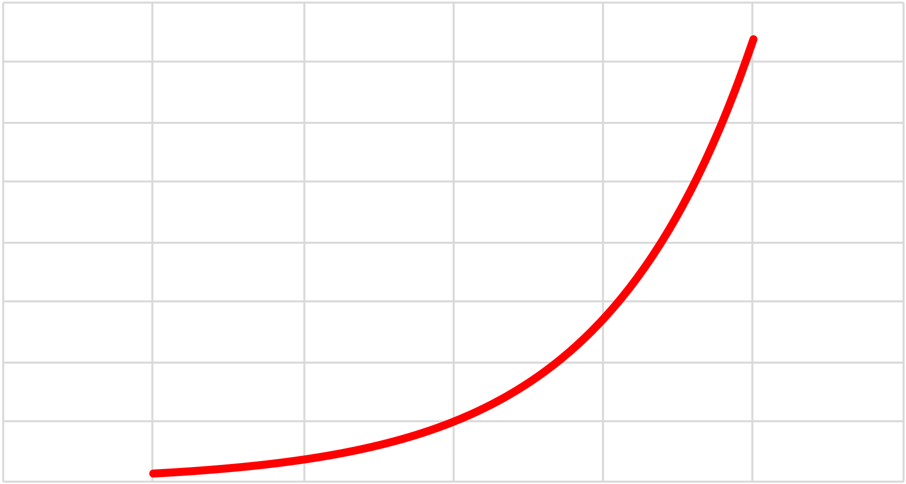


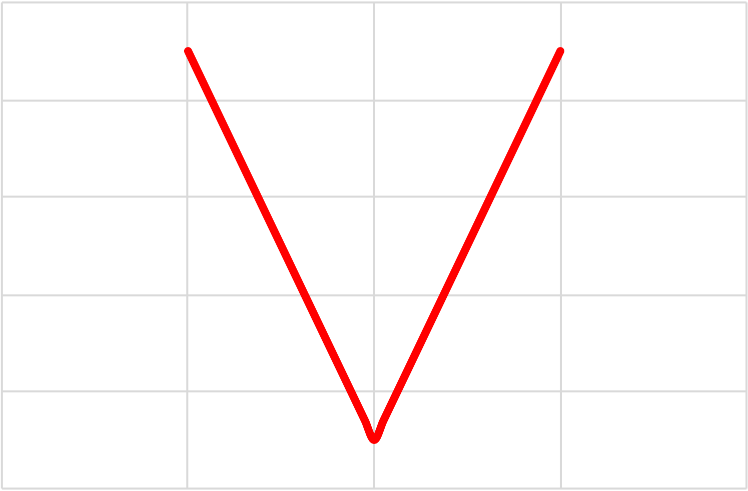


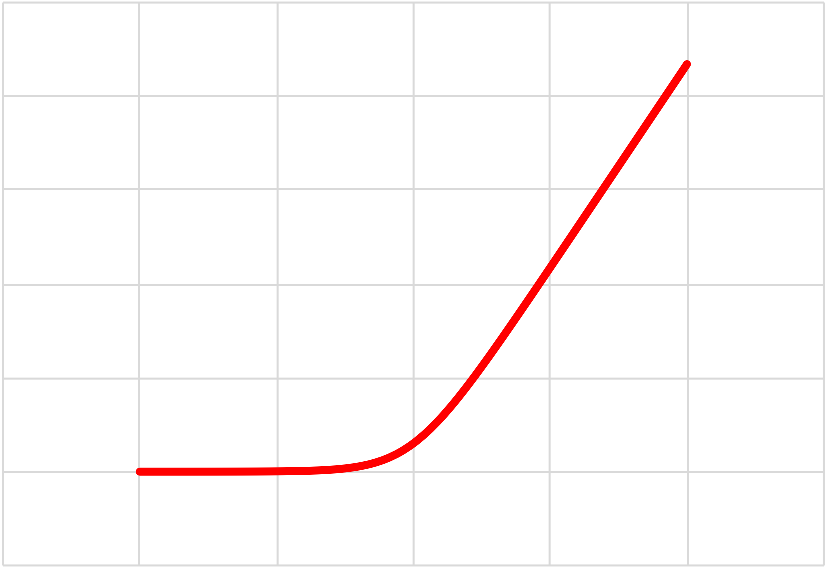


Which of the functions we've looked at are strongly convex?









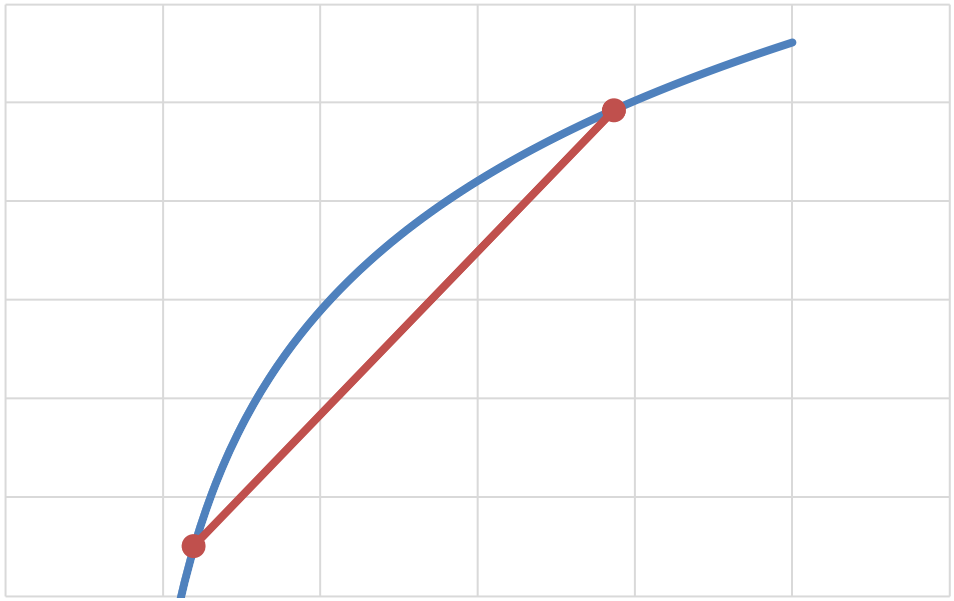
Concave functions

- A function is concave if its negation is convex

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

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

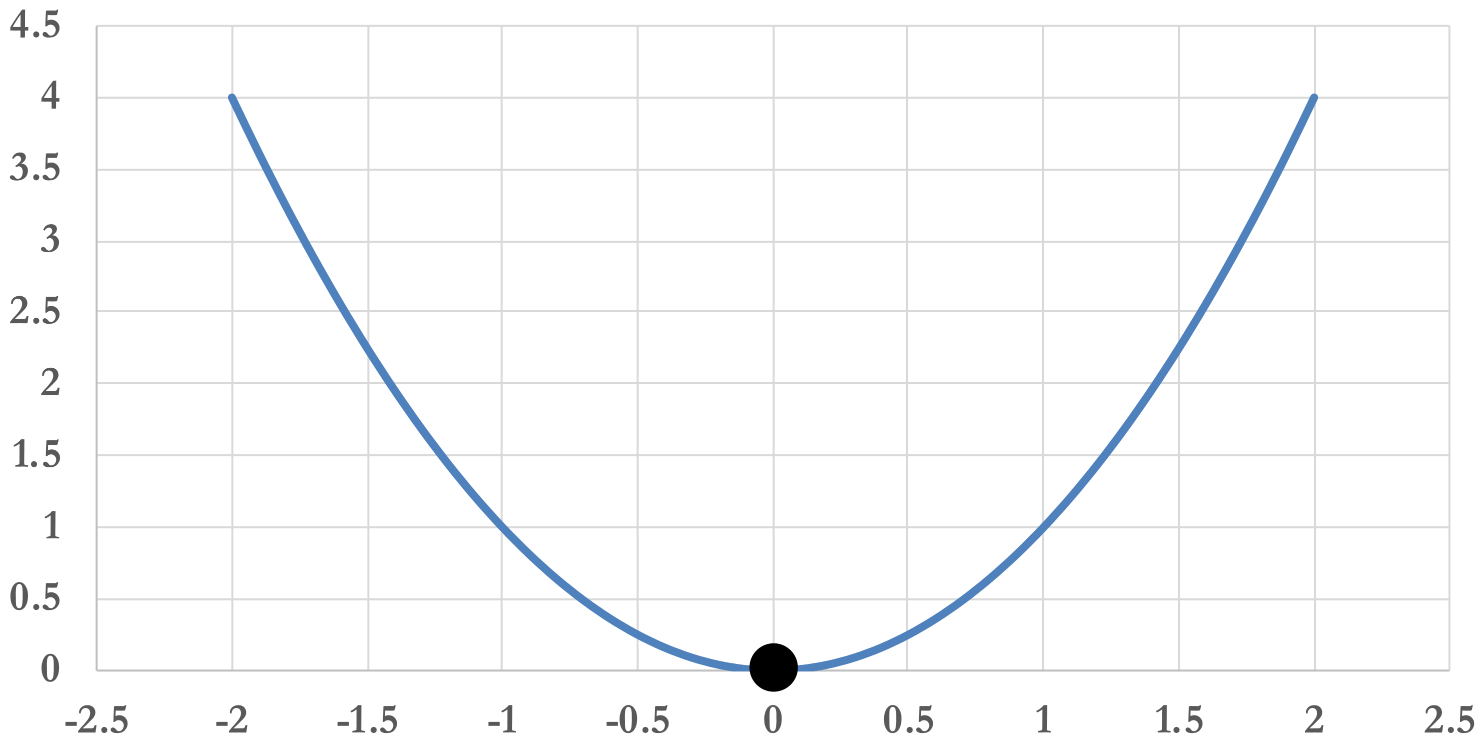
$$f''(x) = -\frac{1}{x^2} \leq 0$$



Why care about convex functions?

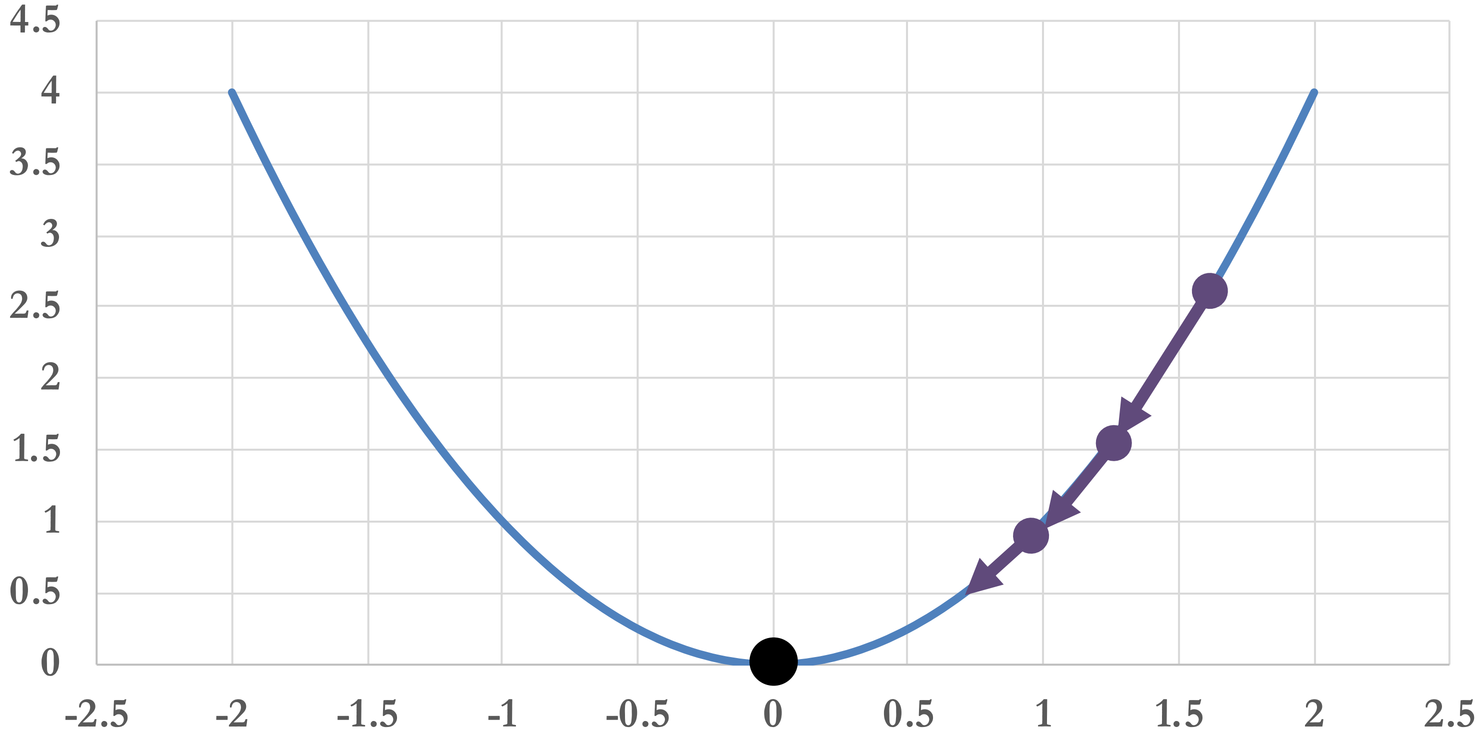
Convex Optimization

- Goal is to minimize a convex function



Gradient Descent

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



Gradient Descent Converges

- Iterative definition of gradient descent

$$w_{t+1} = w_t - \alpha \nabla f(w_t)$$

- 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)

$$\begin{aligned} w_{t+1} - w^* &= w_t - w^* - \alpha \left(\nabla f(w_t) - \nabla f(w^*) \right) \\ &= w_t - w^* - \alpha \nabla^2 f(\zeta_t) \left(w_t - w^* \right) \\ &= \left(I - \alpha \nabla^2 f(\zeta_t) \right) \left(w_t - w^* \right). \end{aligned}$$

Taking the norm

$$\begin{aligned} \| w_{t+1} - w^* \| &\leq \left\| I - \alpha \nabla^2 f(\zeta_t) \right\|_2 \cdot \| w_t - w^* \| \\ &\leq \max(|1 - \alpha \mu|, |1 - \alpha L|) \cdot \| w_t - w^* \|. \end{aligned}$$

Gradient Descent Converges (continued)

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

$$\|w_{t+1} - w^*\| \leq \frac{L-\mu}{L+\mu} \cdot \|w_t - w^*\|$$

- And recursively

$$\|w_K - w^*\| \leq \left(\frac{L-\mu}{L+\mu}\right)^K \cdot \|w_0 - w^*\|$$

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

The Problem with Gradient Descent

- Large-scale optimization

$$h(w) = \frac{1}{n} \sum_{i=1}^{n} f(w; x_i)$$

- Computing the gradient takes O(n) time

$$\nabla h(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla f(w; x_i)$$

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

$$\nabla h(w) = \frac{1}{2n} \sum_{i=1}^{n} \nabla f(w; x_i) + \frac{1}{2n} \sum_{i=1}^{n} \nabla f(w; x_i)$$

- **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

$$w_{t+1} = w_t - \alpha \nabla f(w_t, x_{i_t})$$

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

- In expectation, it's just gradient descent:

$$\begin{aligned} \mathbf{E}[w_{t+1}] &= \mathbf{E}[w_t] - \alpha \cdot \mathbf{E}[\nabla f(w_t, x_{i_t})] \\ &= \mathbf{E}[w_t] - \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} \nabla f(w_t, x_i) \end{aligned}$$

Stochastic Gradient Descent Convergence

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

$$w_{t+1} - w^* = w_t - w^* - \alpha \left(\nabla h(w_t) - \nabla h(w^*) \right) - \alpha \left(\nabla f(w_t; x_{i_t}) - \nabla h(w_t) \right)$$

$$= \left(I - \alpha \nabla^2 h(\zeta_t) \right) (w_t - w^*) - \underline{\alpha \left(\nabla f(w_t; x_{i_t}) - \nabla h(w_t) \right)}$$

- How do we handle this extra noise term?

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

Stochastic Gradient Descent Convergence

$$
\begin{aligned}
\mathbf{E}\left[\|w_{t+1} - w^*\|^2\right] &= \mathbf{E}\left[\left\|\left(I - \alpha \nabla^2 h(\zeta_t)\right)(w_t - w^*) - \alpha\left(\nabla f(w_t; x_{i_t}) - \nabla h(w_t)\right)\right\|^2\right] \\
&= \mathbf{E}\left[\left\|\left(I - \alpha \nabla^2 h(\zeta_t)\right)(w_t - w^*)\right\|^2\right] \\
&\quad - \alpha \mathbf{E}\left[\left(\nabla f(w_t; x_{i_t}) - \nabla h(w_t)\right)^T \left(I - \alpha \nabla^2 h(\zeta_t)\right)(w_t - w^*)\right] \\
&\quad + \alpha^2 \mathbf{E}\left[\|(\nabla f(w_t; x_{i_t}) - \nabla h(w_t))\|^2\right] \\
&= \mathbf{E}\left[\left\|\left(I - \alpha \nabla^2 h(\zeta_t)\right)(w_t - w^*)\right\|^2\right] + \alpha^2 \mathbf{E}\left[\|(\nabla f(w_t; x_{i_t}) - \nabla h(w_t))\|^2\right] \\
&\leq (1 - \alpha\mu)^2 \cdot \mathbf{E}\left[\|w_t - w^*\|^2\right] + \alpha^2 M
\end{aligned}
$$

assuming small enough α and the bound $\mathbf{E}\left[\|(\nabla f(w; x_i) - \nabla h(w))\|^2\right] \leq M$.

Stochastic Gradient Descent Convergence

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

$$\lim_{t \to \infty} \mathbf{E}\left[\left\| w_t - w^* \right\|^2 \right] \leq \frac{\alpha M}{2\mu - \alpha \mu^2}$$

- 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!

PyTorch

AlphaGo

scikit learn

theano

TensorFlow

Caffe

K

Caffe CON TROLL

KeystoneML

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.