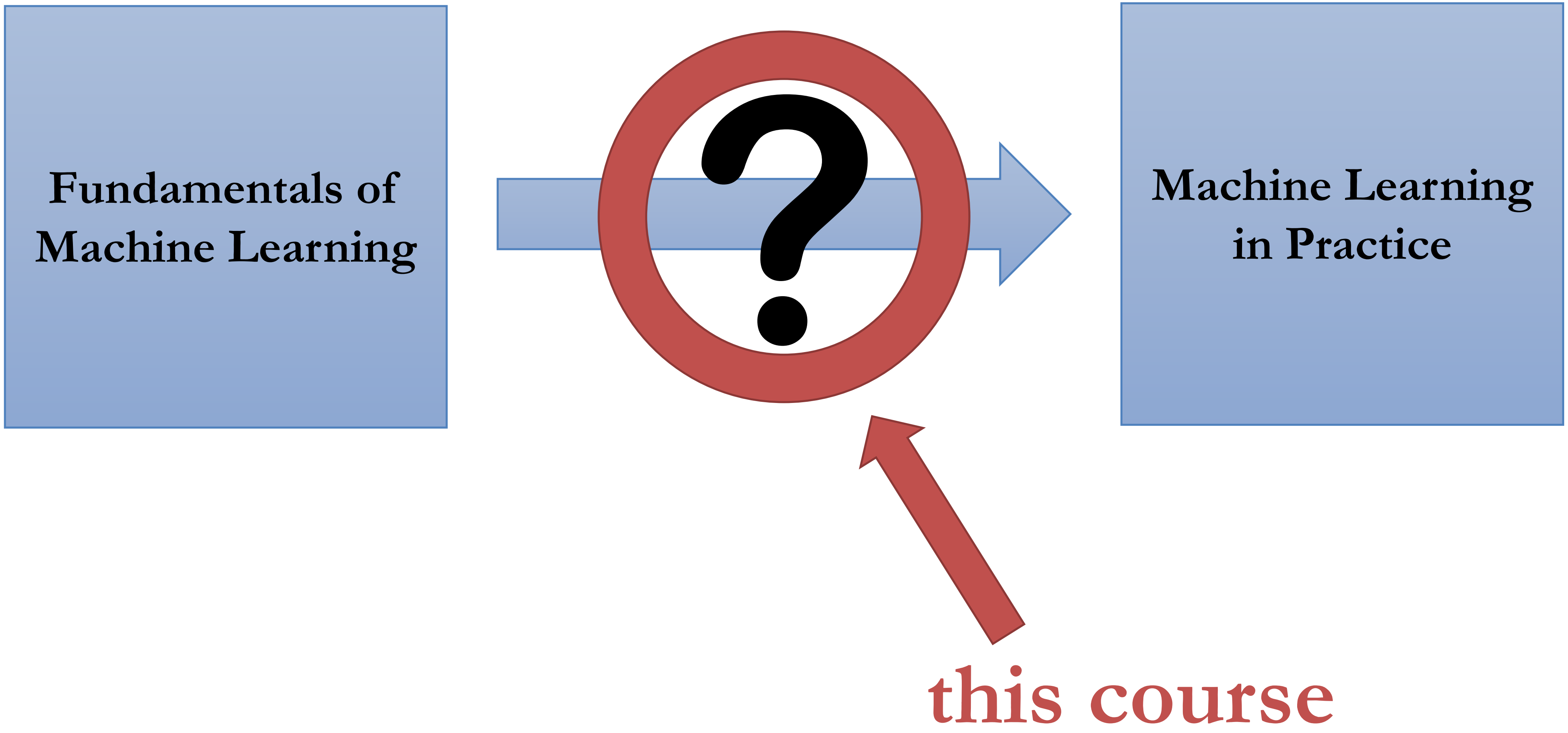
CS6787: Advanced Machine Learning Systems

CS6787 Lecture 1 — Fall 2019



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, and evaluate a machine 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 Friday!**
- Learning goal
  - Practice digesting and talking about other people's work

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
  - Learning goal: **practice how to deeply read and critique a paper in context, and get some window into how peer review works.**

Programming Assignments

- **New** by popular demand
- 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 2019

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

loss function

model

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

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:

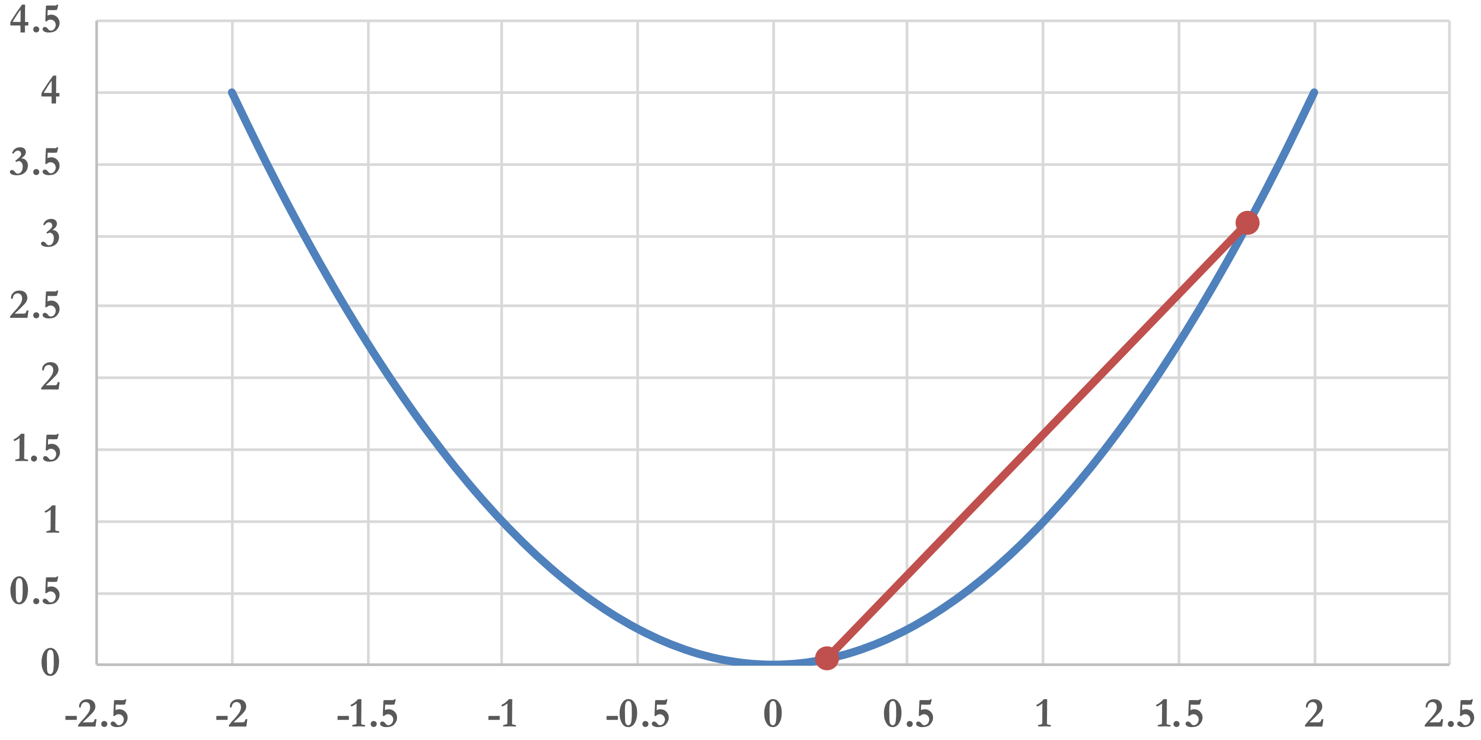
Build intuition about techniques from the convex case where we can prove things…

…and apply it to better understand more complicated systems.

An Abridged Introduction to Convex Functions

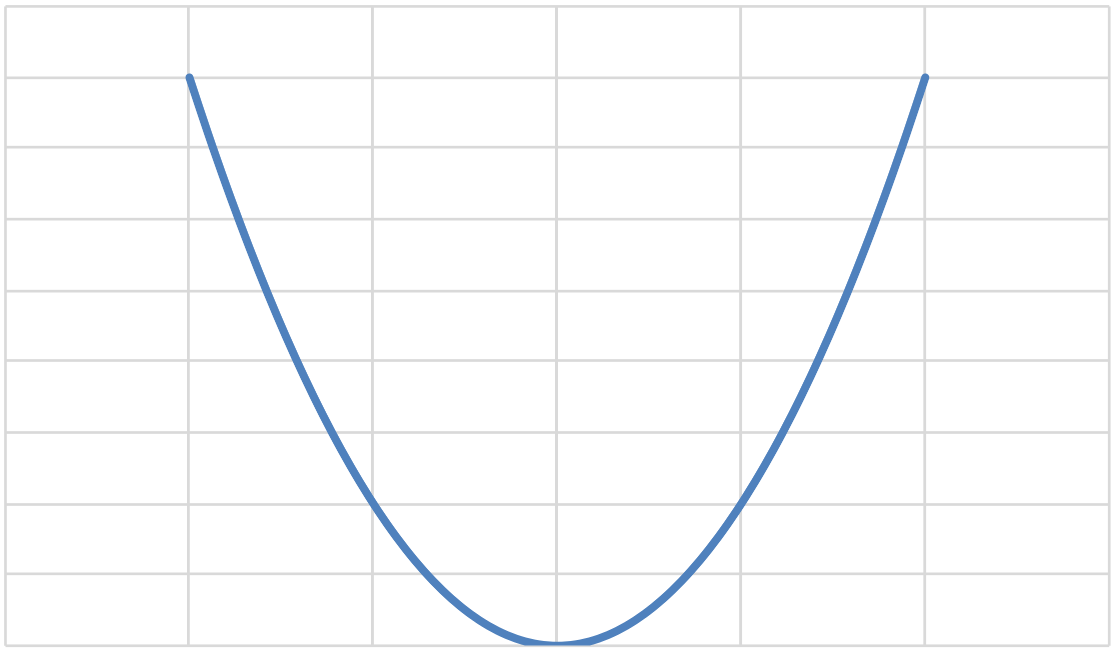
Convex Functions

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



$f(x) = x^2$

Example: Quadratic

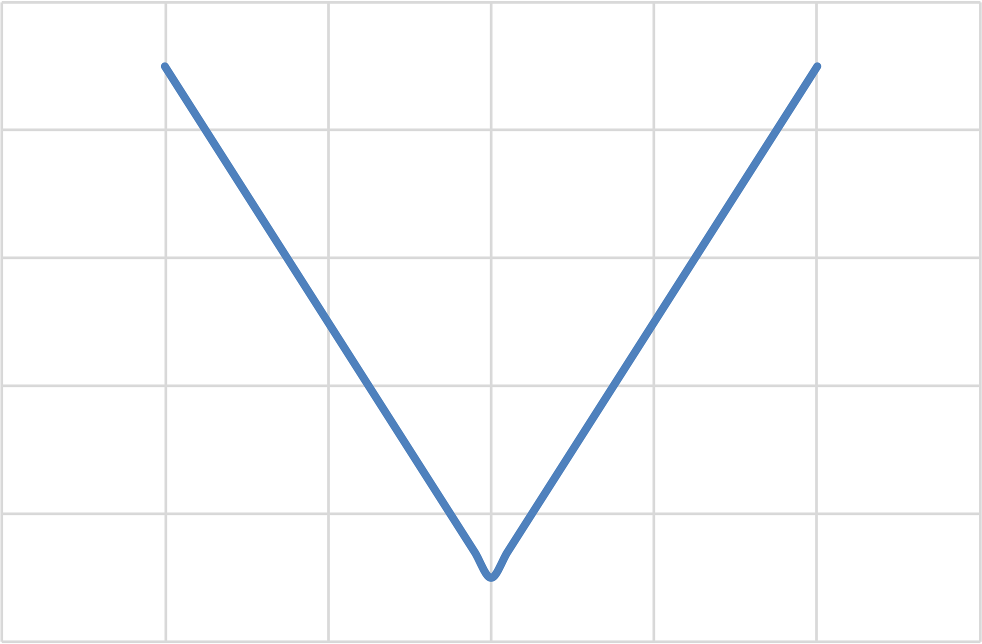


$$f(x) = x^2$$

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

Example: Abs

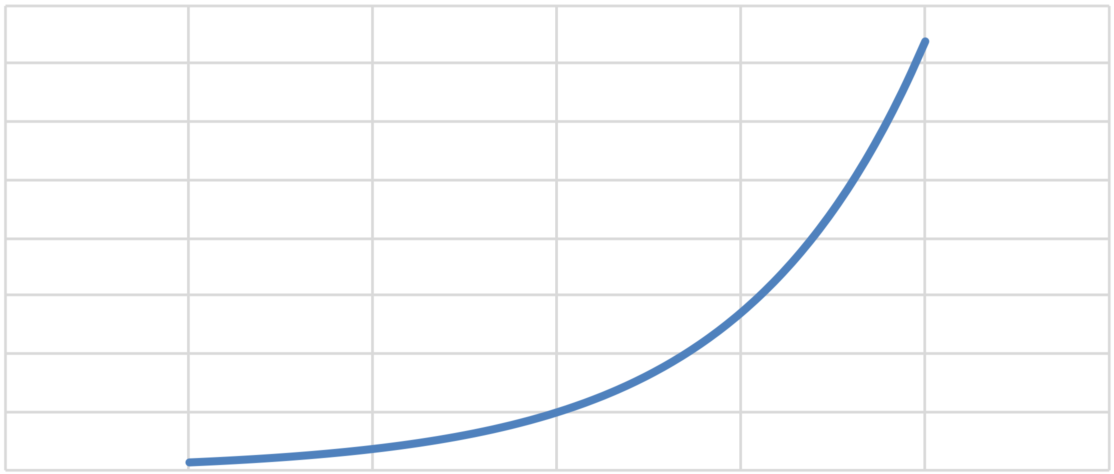
$$f(x) = |x|$$



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

Example: Exponential

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



$$e^{\alpha x + (1-\alpha) y} = e^y e^{\alpha(x-y)} = e^y \sum_{n=0}^{\infty} \frac{1}{n!} \alpha^n (x-y)^n$$

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

$$= e^y \left((1-\alpha) + \alpha e^{x-y} \right)$$

$$= (1-\alpha) e^y + \alpha e^x$$

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

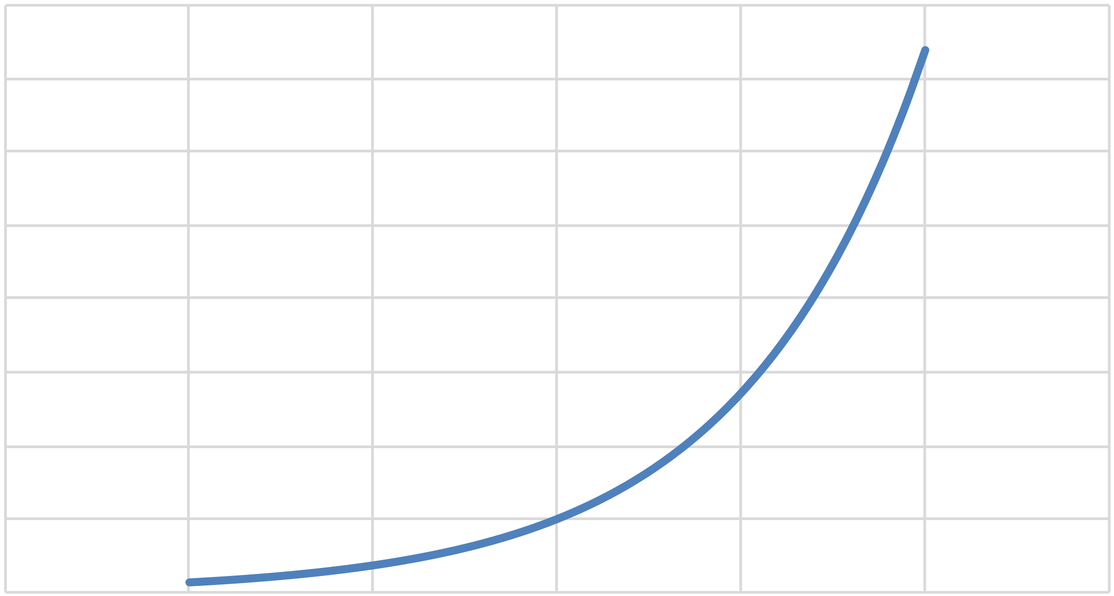
$$A \succeq 0 \Leftrightarrow \forall x,\ \langle x, Ax \rangle \geq 0$$

Example: Quadratic

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

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

Example: Exponential

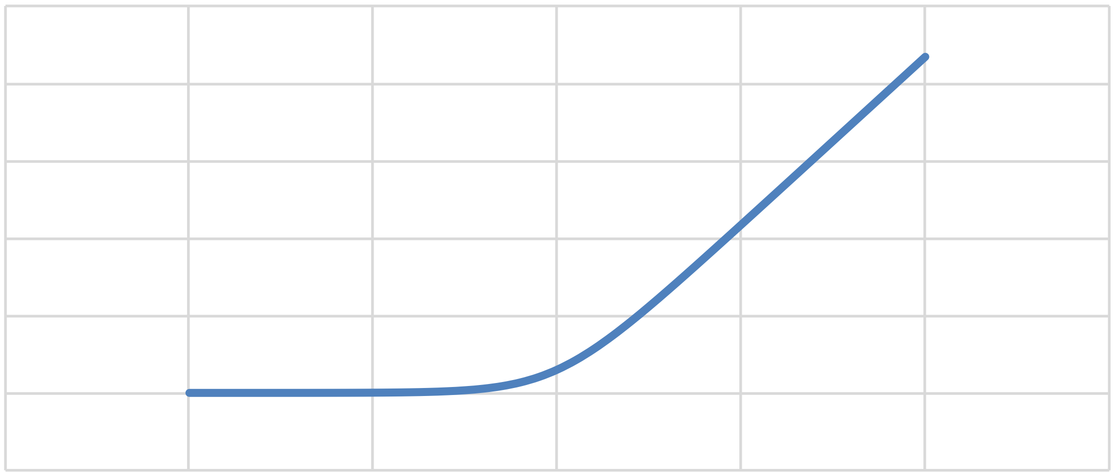


$$f(x) = e^x$$

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

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:

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

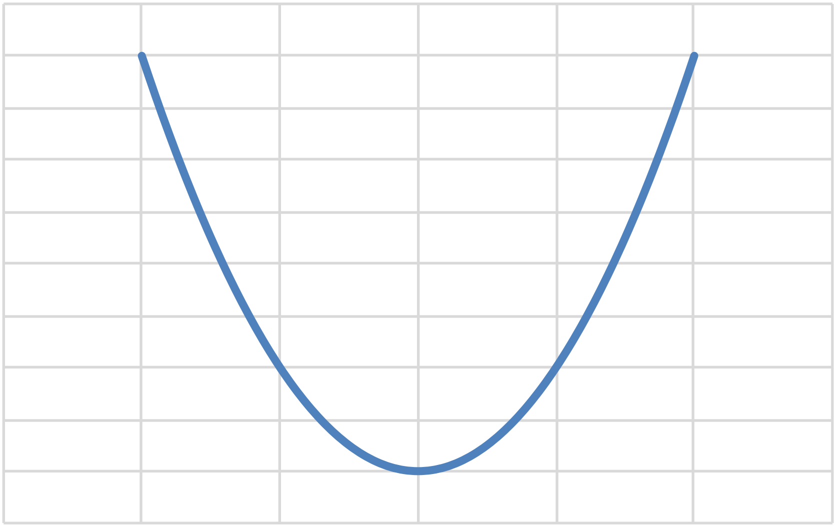
  - Second-order condition:

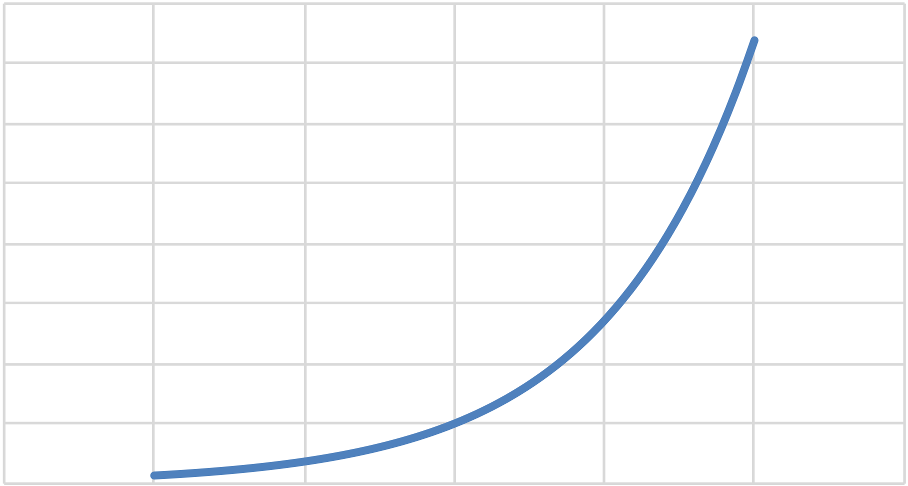
$$\nabla^2 f(x) \succeq \mu I$$

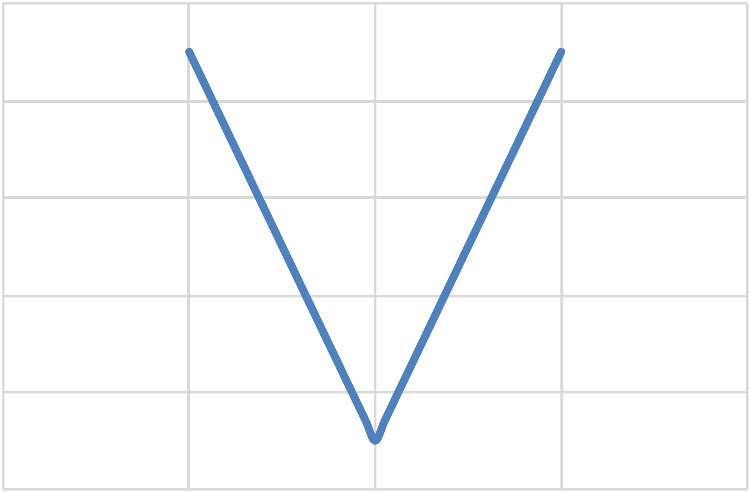
  - Equivalently:

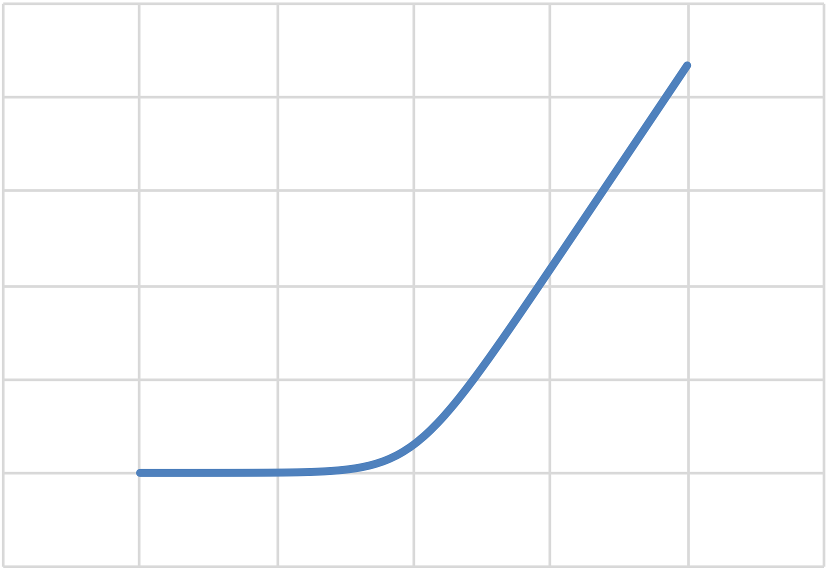
$$h(x) = f(x) - \frac{\mu}{2}\|x\|^2 \text{ is convex}$$

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

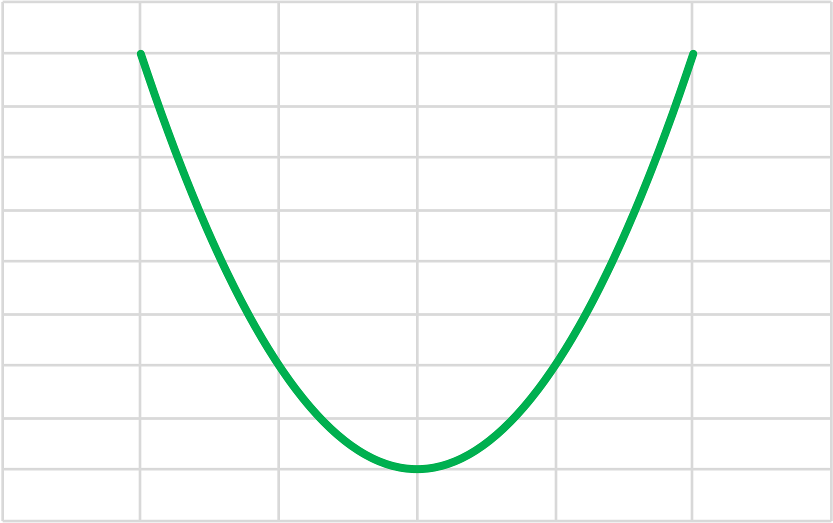


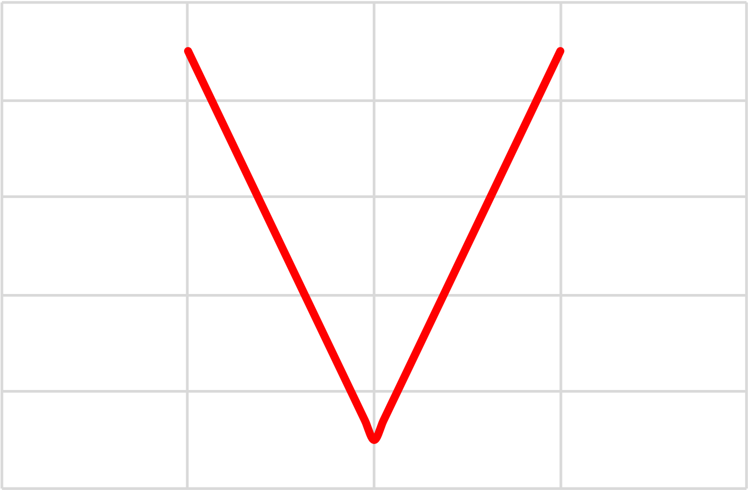


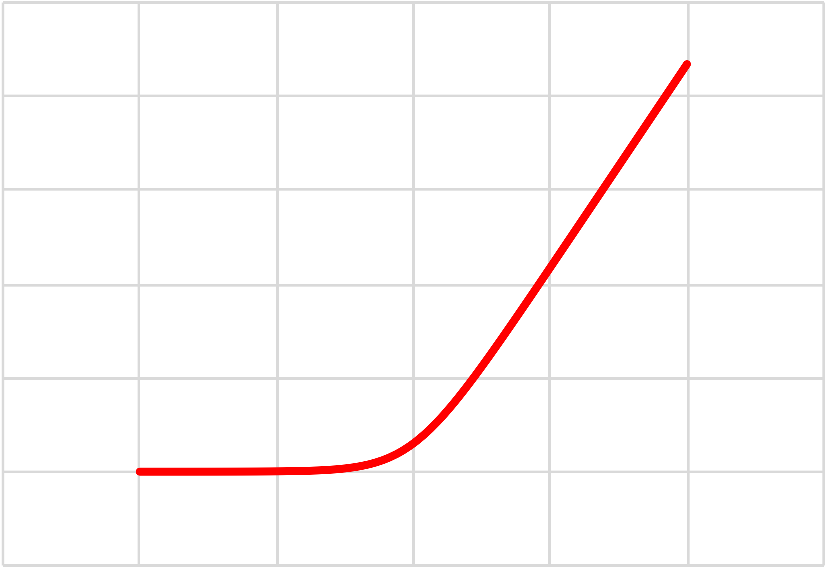




Which of the functions we've looked at are strongly convex?







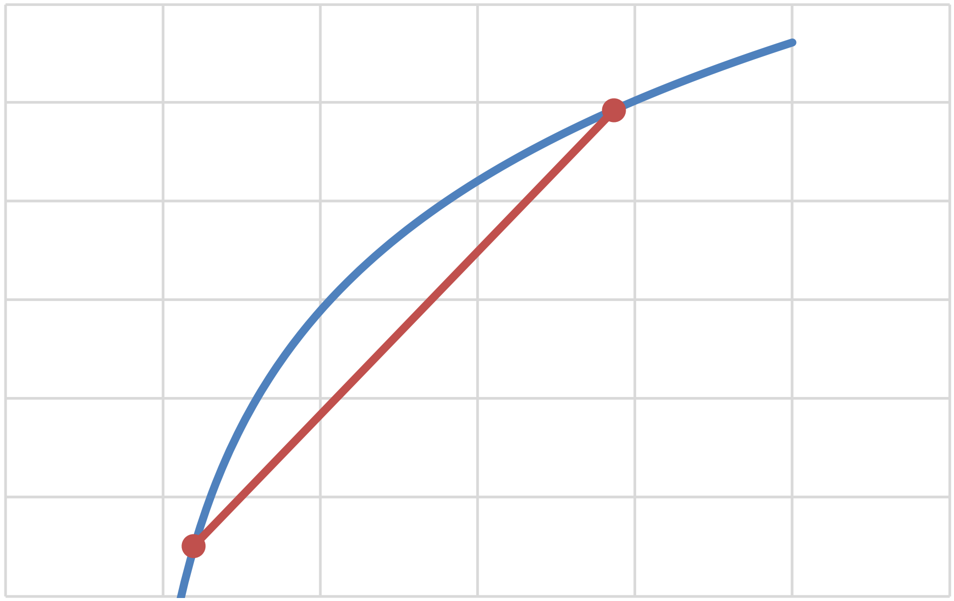
Concave functions

- A function is concave if its negation is convex

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

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

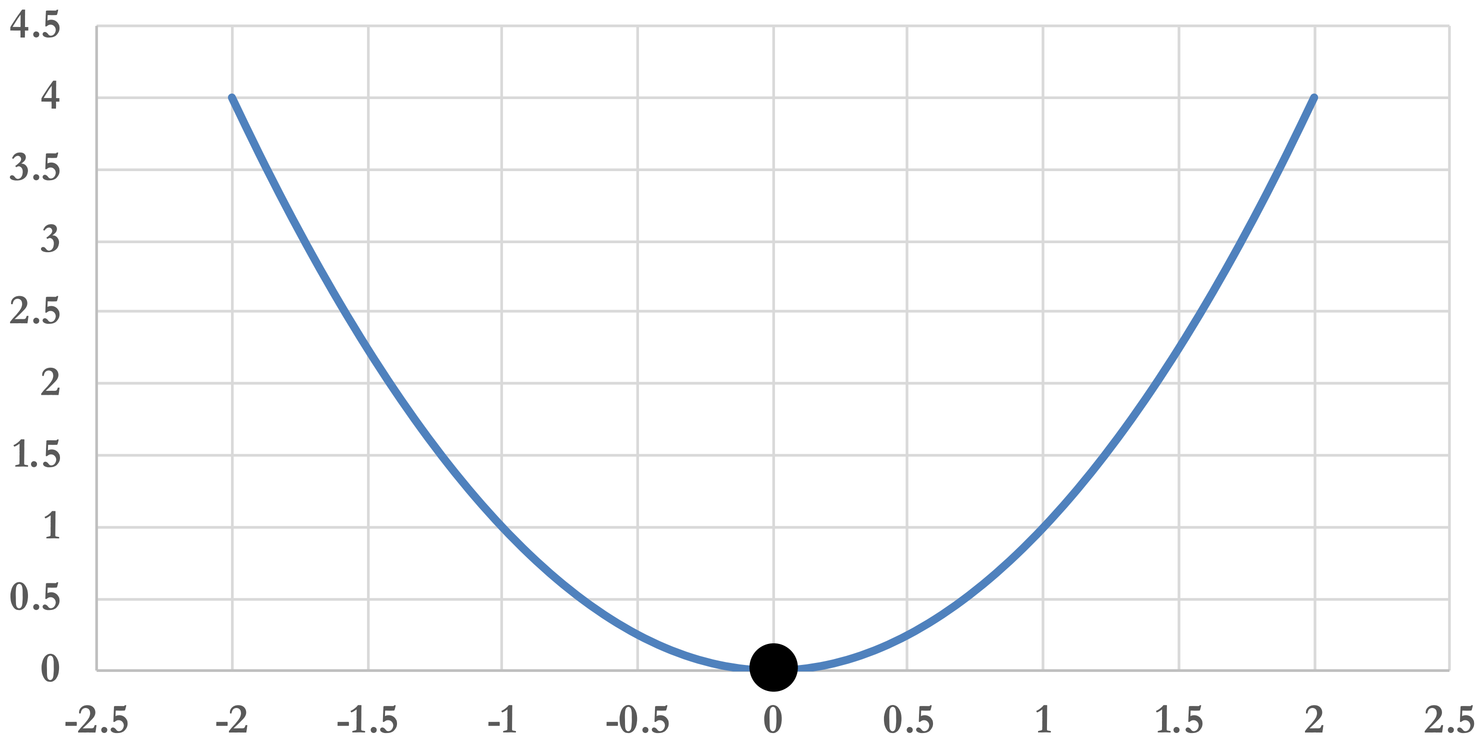
$$f''(x) = -\frac{1}{x^2} \leq 0$$



Why care about convex functions?

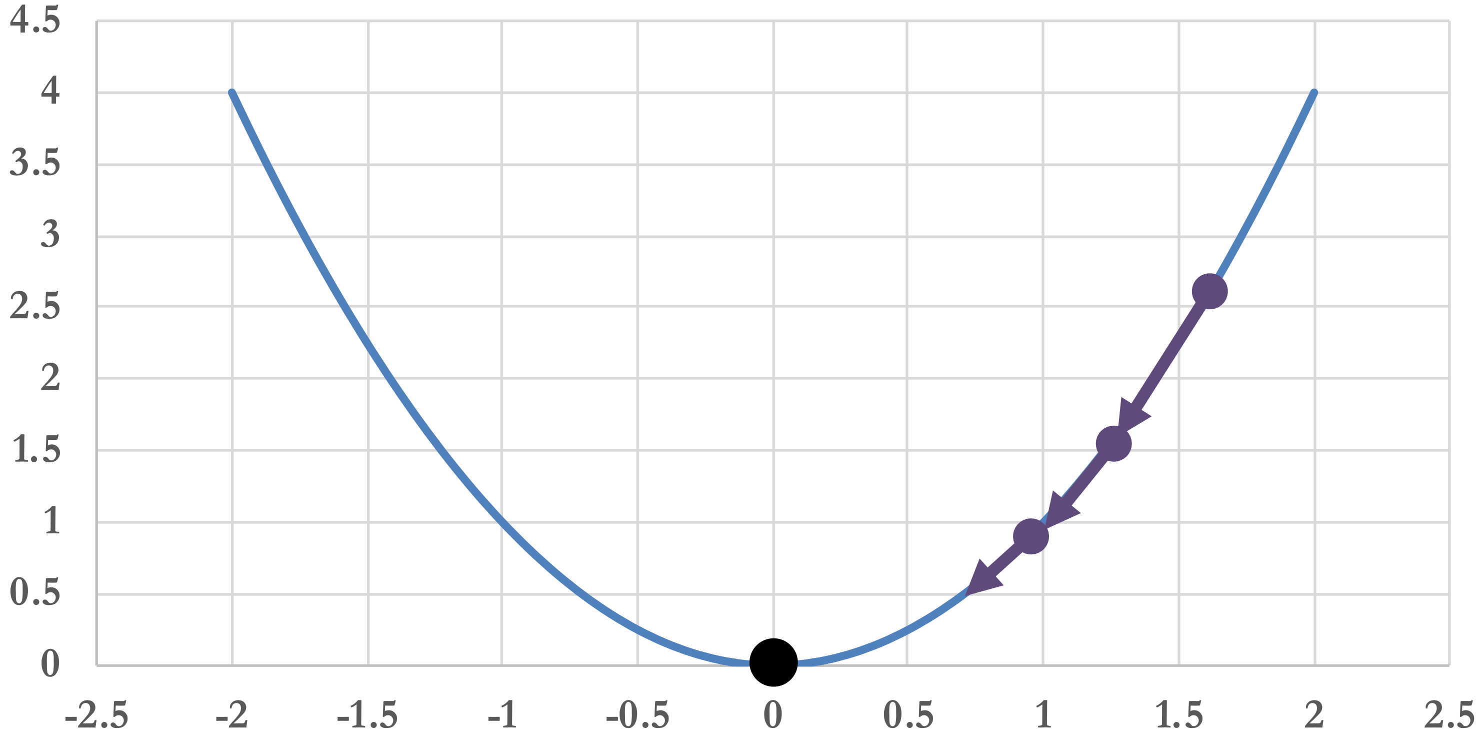
Convex Optimization

- Goal is to minimize a convex function



Gradient Descent

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



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?

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

- How do we handle this extra noise term?

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

Stochastic Gradient Descent Convergence

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

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

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!

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.