Lecture 05

Fitting Neurons with Gradient Descent

STAT 479: Deep Learning, Spring 2019

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http://stat.wisc.edu/~sraschka/teaching/stat479-ss2019/

DISCUSS HOMEWORK

hardmaru
@hardmaru

How do people come up with all these crazy deep learning architectures?
reddit.com/r/MachineLearn...

Brudaks 153 points

A popular method for designing deep learning architectures is GDGS (gradient descent by grad student).

This is an iterative approach, where you start with a straightforward baseline architecture (or possibly an earlier SOTA), measure its effectiveness; apply various modifications (e.g. add a highway connection here or there), see what works and what does not (i.e. where the gradient is pointing) and iterate further on from there in that direction until you reach a (local?) optimum.

https://twitter.com/hardmaru/status/876303574900264960

Also known as "graduate student descent"

Our Goals

- A learning rule that is more robust than the perceptron: always converges even if the data is not (linearly) separable

```
model.eval()
logits, probas = model(features.to(device)[0, None])
print('Probability Female %.2f%%' % (probas[0][0]*100))
```

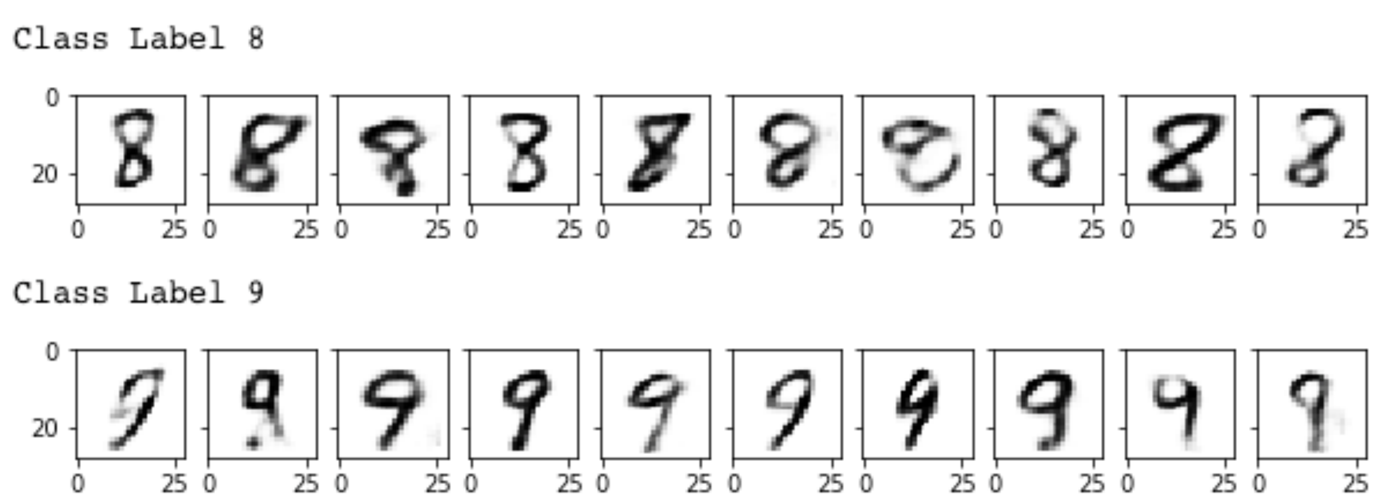
```
Probability Female 99.71%
```

- Combine multiple neurons and layers of neurons ("deep neural nets") to learn more complex decision boundaries (because most real-world problems are not "linear" problems!)

- Handle multiple categories (not just binary) in classification

- Do even fancier things like generating NEW images and text

Age: 30



Our Goals

- A learning rule that is more robust than the perceptron: <u>always converges</u> even if the data is not (linearly) separable

This lecture

- <u>Combine multiple neurons</u> and layers of neurons ("deep neural nets") to learn more complex decision boundaries (because most real-world problems are not "linear" problems!)

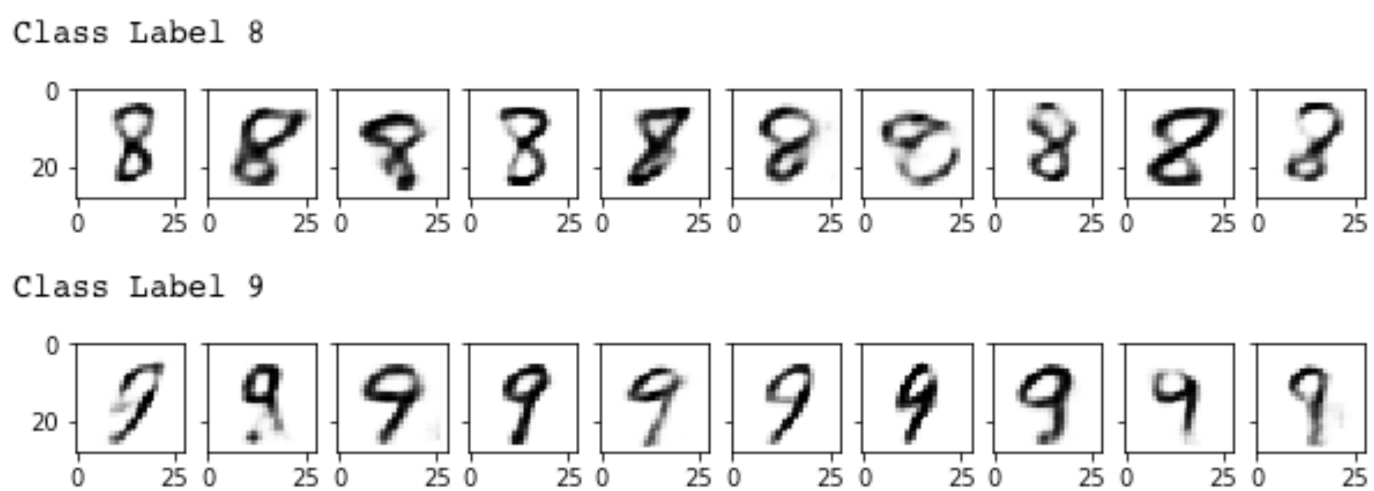
Next lecture(s)

- Handle <u>multiple categories</u> (not just binary) in classification

Next lecture(s)

- Do even <u>fancier things</u> like generating NEW images and text

More towards the end of the course

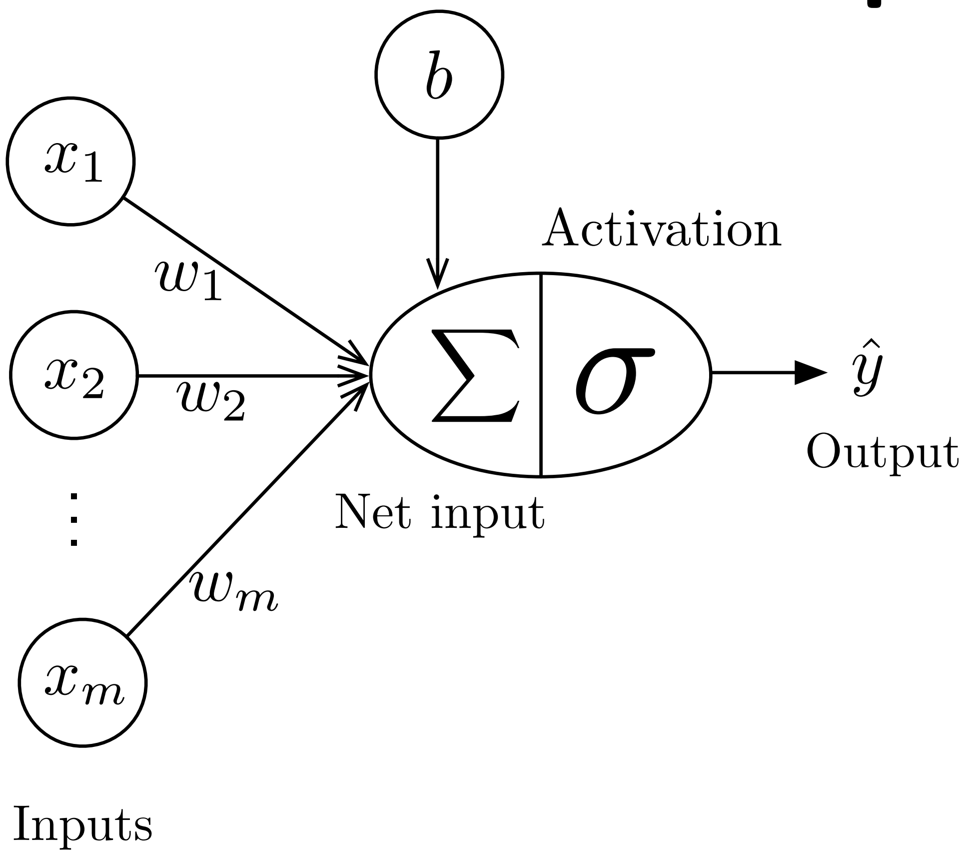


All based on the same learning algorithm and extensions thereof.
So, this is prob. the most fundamental lecture!

Good news:

- After this lecture, there won't be any "new" mathematical concepts.
- Everything in DL will be extensions & applications of these basic concepts.

Perceptron Recap



$$\sigma\left(\sum_{i=1}^{m} x_i w_i + b\right) = \sigma\left(\mathbf{x}^T\mathbf{w} + b\right) = \hat{y}$$

$$\sigma(z) = \begin{cases} 0, & z \leq 0 \\ 1, & z > 0 \end{cases}$$

$$b = -\theta$$

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
      (a) $\hat{y}^{[i]} := \sigma\left(\mathbf{x}^{[i]T}\mathbf{w} + b\right)$ ← Compute output (prediction)
      (b) $\mathrm{err} := (y^{[i]} - \hat{y}^{[i]})$ ← Calculate error
      (c) $\mathbf{w} := \mathbf{w} + err \times \mathbf{x}^{[i]}$, $b := b + err$ ← Update parameters

General Learning Principle

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

"On-line" mode

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
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   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
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      (b) Calculate error
      (c) Update $\mathbf{w}, b$

This applies to all common neuron models and (deep) neural network architectures!

There are some variants of it, namely the "batch mode" and the "minibatch mode" which we will briefly go over in the next slides and then discuss more later

General Learning Principle

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

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      (c) Update $\mathbf{w}, b$

Batch mode

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. Initialize $\Delta\mathbf{w} := 0, \ \Delta b := 0$
   B. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
      (a) Compute output (prediction)
      (b) Calculate error
      (c) Update $\Delta\mathbf{w}, \Delta b$
   C. Update $\mathbf{w}, b$:
      $\mathbf{w} := \mathbf{w} + \Delta\mathbf{w}, b := +\Delta b$

General Learning Principle

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

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In practice, we usually shuffle the dataset prior to each epoch to prevent cycles

Batch mode

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"On-line" mode

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"semi"-stochastic

"On-line" mode II (alternative)

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For for t iterations:
   A. Pick random $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
      (a) Compute output (prediction)
      (b) Calculate error
      (c) Update $\mathbf{w}, b$

stochastic
(actually, not really stochastic because a fixed training set instead of sampling from the population)

General Learning Principle

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

Minibatch mode

(mix between on-line and batch)

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. Initialize $\Delta \mathbf{w} := 0, \ \Delta b := 0$
   B. For every $\{\langle \mathbf{x}^{[i]}, y^{[i]} \rangle, ..., \langle \mathbf{x}^{[i+k]}, y^{[i+k]} \rangle\} \subset \mathcal{D}$:
      (a) Compute output (prediction)
      (b) Calculate error
      (c) Update $\Delta \mathbf{w}, \Delta b$
   C. Update $\mathbf{w}, b$:
      $\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}, b := +\Delta b$

The most common mode in deep learning. Any ideas why?

General Learning Principle

Let $\mathcal{D} = (\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, \langle \mathbf{x}^{[2]}, y^{[2]} \rangle, ..., \langle \mathbf{x}^{[n]}, y^{[n]} \rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$

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   - C. Update $\mathbf{w}, b$:

     $\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}, b := +\Delta b$

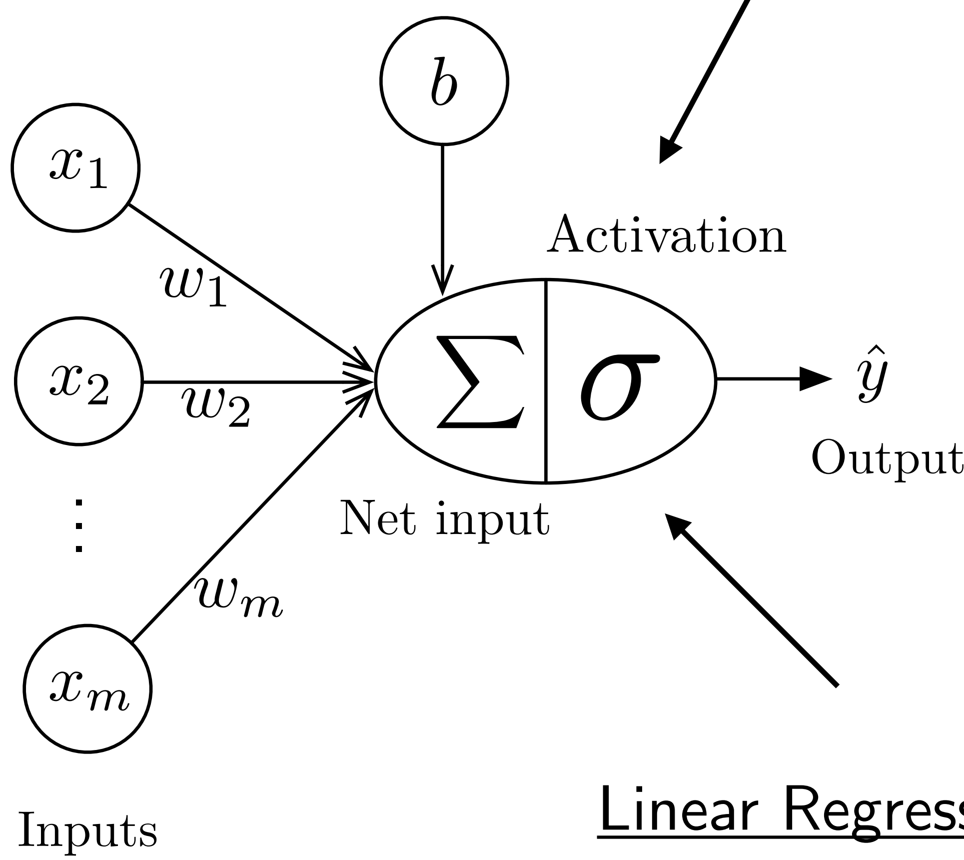
Most commonly used in DL, because

1. Choosing a subset (vs 1 example at a time) takes advantage of vectorization (faster iteration through epoch than on-line)
2. having fewer updates than "on-line" makes updates less noisy
3. makes more updates/ epoch than "batch" and is thus faster

Linear Regression

<u>Perceptron:</u> Activation function is the threshold function

The output is a binary label $\hat{y} \in \{0, 1\}$



<u>Linear Regression:</u> Activation function is the identity function

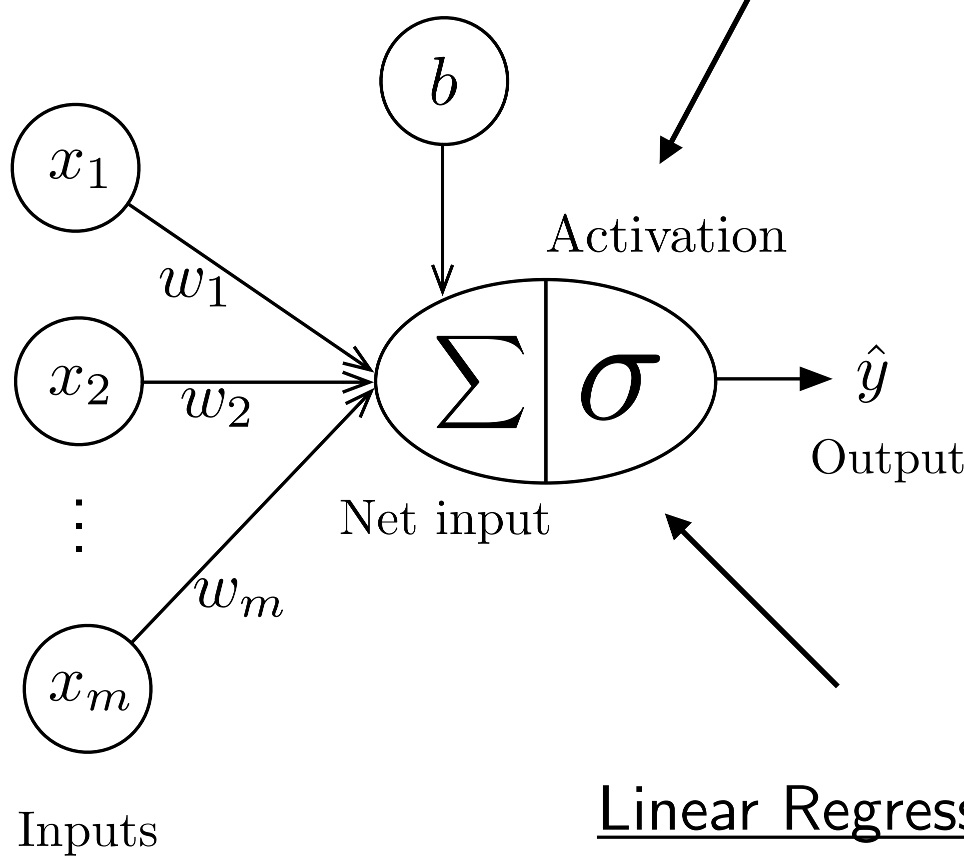
$$\sigma(x) = x$$

The output is a real number $\hat{y} \in \mathbb{R}$

Linear Regression

Perceptron: Activation function is the threshold function

The output is a binary label $\hat{y} \in \{0, 1\}$



You can think of this as a linear neuron!

Linear Regression: Activation function is the identity function

$$\sigma(x) = x$$

The output is a real number $\hat{y} \in \mathbb{R}$

(Least-Squares) Linear Regression

In earlier statistics classes, you probably fit a model like this:
using the "normal equations:"

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top y$$

(implying that the bias is included, and the design matrix has an additional vector of 1's)

(Least-Squares) Linear Regression

In earlier statistics classes, you probably fit a model like this: using the "normal equations:"

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top y$$

(implying that the bias is included, and the design matrix has an additional vector of 1's)

- Generally, this is the best approach for linear regression (although, the matrix inversion might be problematic on large datasets)
- However, we will now learn about another way to learn these parameters iteratively
- Why? Because this is what we will be doing in deep neural nets later, where we have large datasets, many connections, and non-convex loss functions

(Least-Squares) Linear Regression

- A very naive way to fit a linear regression model (and any neural net) is to start with all-zero or random parameters
- Then, for k rounds
  - Choose another random set of weights
  - If the model performs better, keep those weights
  - If the model performs worse, discard the weights

This approach is guaranteed to find the optimal solution for very large k, but it would be terribly slow.

(Least-Squares) Linear Regression

- A very naive way to fit a linear regression model (and any neural net) is to start with all-zero or random parameters
- Then, for *k* rounds
  - Choose another random set of weights
  - If the model performs better, keep those weights
  - If the model performs worse, discard the weights

- There's a better way!
- We will analyze what effect a change of a parameter has on the predictive performance (loss) of the model
  then, we change the weight a little bit in the direction that improves the performance (minimizes the loss) the most
- We do this in several (small) steps until the loss does not further decrease

(Least-Squares) Linear Regression

The update rule turns out to be this:

"On-line" mode

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$
      (a) $\hat{y}^{[i]} := \sigma\big(\mathbf{x}^{[i]T}\mathbf{w} + b\big)$
      (b) $\mathrm{err} := (y^{[i]} - \hat{y}^{[i]})$
      (c) $\mathbf{w} := \mathbf{w} + err \times \mathbf{x}^{[i]}$
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   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$
      (a) $\hat{y}^{[i]} := \sigma\big(\mathbf{x}^{[i]T}\mathbf{w} + b\big)$
      (b) $\nabla_{\mathbf{w}}\mathcal{L} = \big(y^{[i]} - \hat{y}^{[i]}\big)\mathbf{x}^{[i]}$
          $\nabla_{b}\mathcal{L} = \big(y^{[i]} - \hat{y}^{[i]}\big)$
      (c) $\mathbf{w} := \mathbf{w} + \eta \times (-\nabla_{\mathbf{w}}\mathcal{L})$
          $b := b + \eta \times \underbrace{(-\nabla_{b}\mathcal{L})}$

learning rate

negative gradient

(Least-Squares) Linear Regression

The update rule turns out to be this:

"On-line" mode:

Vectorized

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:

   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$

   (a) $\hat{y}^{[i]} := \sigma\big(\mathbf{x}^{[i]T}\mathbf{w} + b\big)$

   (b) $\nabla_{\mathbf{w}} \mathcal{L} = \big(y^{[i]} - \hat{y}^{[i]}\big)\mathbf{x}^{[i]}$
   $\nabla_{b} \mathcal{L} = \big(y^{[i]} - \hat{y}^{[i]}\big)$

   (c) $\mathbf{w} := \mathbf{w} + \eta \times (-\nabla_{\mathbf{w}} \mathcal{L})$
   $b := b + \eta \times \underbrace{(-\nabla_{b} \mathcal{L})}$

learning rate

negative gradient

$\Longleftrightarrow$

For-Loop

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:

   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$

   (a) $\hat{y}^{[i]} := \sigma\big(\mathbf{x}^{[i]T}\mathbf{w} + b\big)$

   B. For weight j in $\{1, \ldots, m\}$:

   (b) $\dfrac{\partial \mathcal{L}}{\partial w_j} = -\big(y^{[i]} - \hat{y}^{[i]}\big)x_j^{[i]}$

   (c) $w_j := w_j + \eta \times (-\dfrac{\partial \mathcal{L}}{\partial w_j})$

   C. $\dfrac{\partial \mathcal{L}}{\partial b} = -\big(y^{[i]} - \hat{y}^{[i]}\big)$
   $b := b + \eta \times (-\dfrac{\partial \mathcal{L}}{\partial b})$

(Least-Squares) Linear Regression

The update rule turns out to be this:

"On-line" mode

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$
      (a) $\hat{y}^{[i]} := \sigma\big(\mathbf{x}^{[i]T}\mathbf{w} + b\big)$
   B. For weight j in {1, ..., m}:
      (b) $\dfrac{\partial \mathcal{L}}{\partial w_j} = \boxed{-\big(y^{[i]} - \hat{y}^{[i]}\big)x_j^{[i]}}$
      (c) $w_j := w_j + \boxed{\eta \times (-\dfrac{\partial \mathcal{L}}{\partial w_j})}$
   C. $\dfrac{\partial \mathcal{L}}{\partial b} = -\big(y^{[i]} - \hat{y}^{[i]}\big)$
      $b := b + \eta \times (-\dfrac{\partial \mathcal{L}}{\partial b})$

Coincidentally, this appears almost to be the same as the perceptron rule, except that the prediction is a real number and we have a learning rate

This learning rule (from the previous slide) is called (stochastic) gradient descent. So, how did we get there?

DISCUSS HOMEWORK

Due next Thursday (Feb 21) 11:59 pm

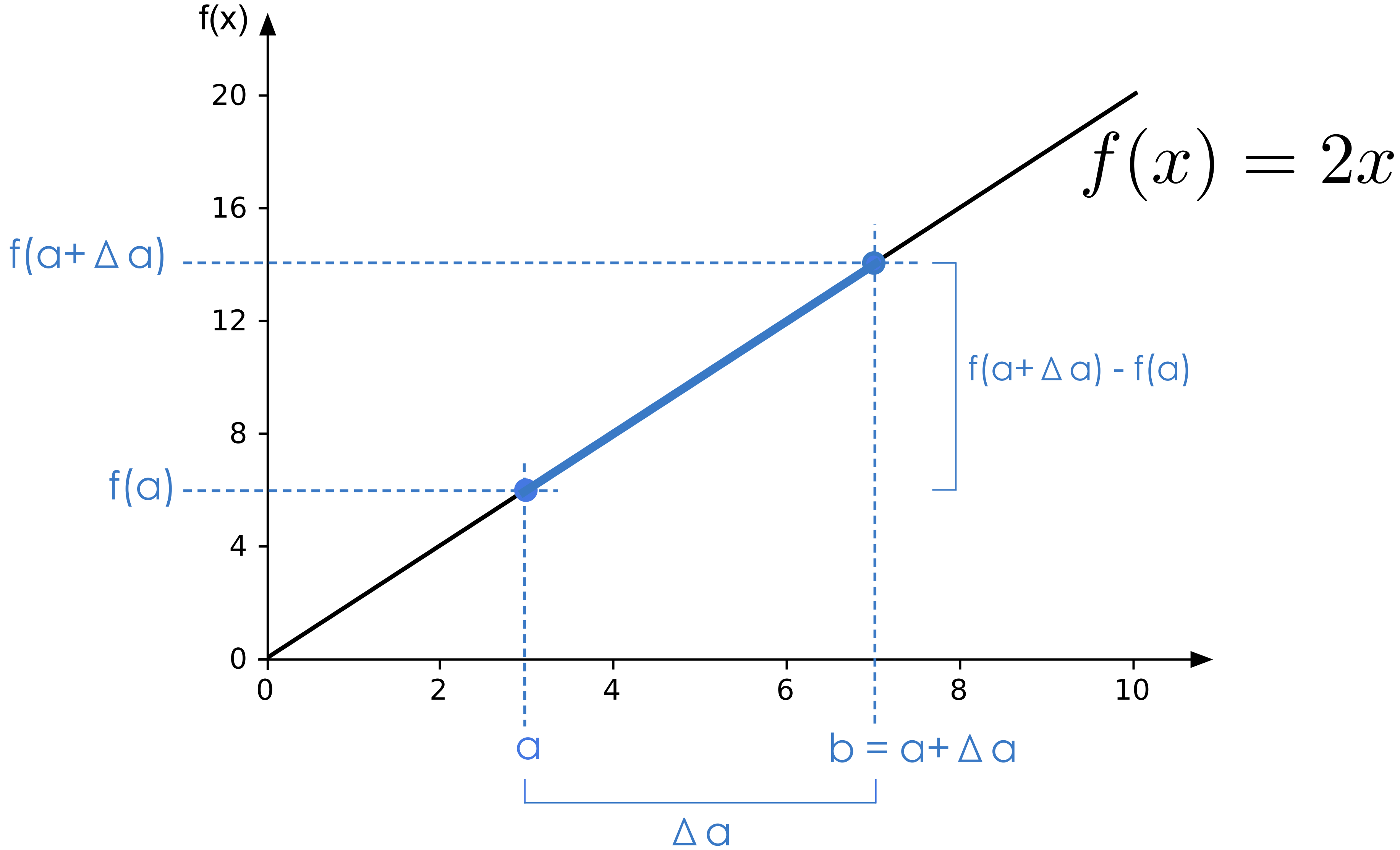
https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/hw2/hw2.ipynb

(explain LaTeX editing)

First, let's briefly cover relevant background info ...

Differential Calculus Refresher

Derivative of a function = "rate of change" = "slope"



$$\text{Slope} = \frac{f(a + \Delta a) - f(a)}{a + \Delta a - a} = \frac{f(a + \Delta a) - f(a)}{\Delta a}$$

Function Derivative

$$f'(x) = \frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

<u>Example 1:</u> $f(x) = 2x$

$$\begin{aligned}
\frac{df}{dx} &= \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \\
&= \lim_{\Delta x \to 0} \frac{2x + 2\Delta x - 2x}{\Delta x} \\
&= \lim_{\Delta x \to 0} \frac{2\Delta x}{\Delta x} \\
&= \lim_{\Delta x \to 0} 2.
\end{aligned}$$

Numerical vs Analytical/Symbolical Derivatives

$$f'(x) = \frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

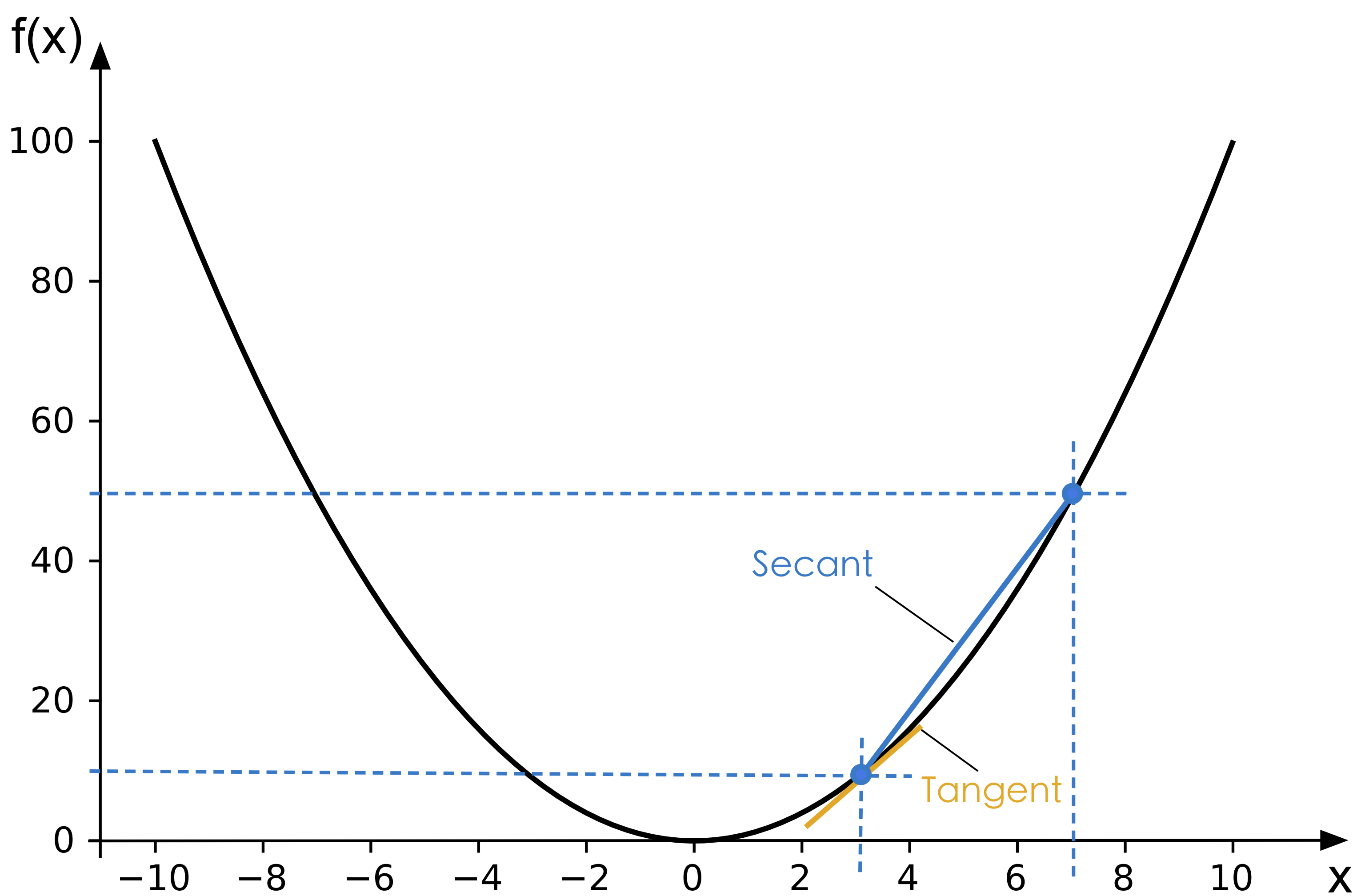
<u>Example 2:</u> $f(x) = x^2$

$$\begin{aligned}
\frac{df}{dx} &= \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \\
&= \lim_{\Delta x \to 0} \frac{x^2 + 2x\Delta x + (\Delta x)^2 - x^2}{\Delta x} \\
&= \lim_{\Delta x \to 0} \frac{2x\Delta x + (\Delta x)^2}{\Delta x} \\
&= \lim_{\Delta x \to 0} 2x + \Delta x.
\end{aligned}$$

Numerical vs Analytical/Symbolical Derivatives

Conceptually, we obtained the derivative $\frac{d}{dx}x^2 = 2x$

By approximating the slope (tangent) by a second between two points (as before)



A Cheatsheet for You (1)

	Function $f(x)$	Derivative with respect to x
1	a	0
2	x	1
3	ax	a
4	x^2	$2x$
5	x^a	ax^{a-1}
6	a^x	$\log(a)a^x$
7	$\log(x)$	$1/x$
8	$\log_a(x)$	$1/(x\log(a))$
9	$\sin(x)$	$\cos(x)$
10	$\cos(x)$	$-\sin(x)$
11	$\tan(x)$	$\sec^2(x)$

A Cheatsheet for You (2)

	Function	Derivative
Sum Rule	$f(x) + g(x)$	$f'(x) + g'(x)$
Difference Rule	$f(x) - g(x)$	$f'(x) - g'(x)$
Product Rule	$f(x)g(x)$	$f'(x)g(x) + f(x)g'(x)$
Quotient Rule	$f(x)/g(x)$	$[g(x)f'(x) - f(x)g'(x)]/[g(x)]^2$
Reciprocal Rule	$1/f(x)$	$-[f'(x)]/[f(x)]^2$
Chain Rule	$f(g(x))$	$f'(g(x))g'(x)$

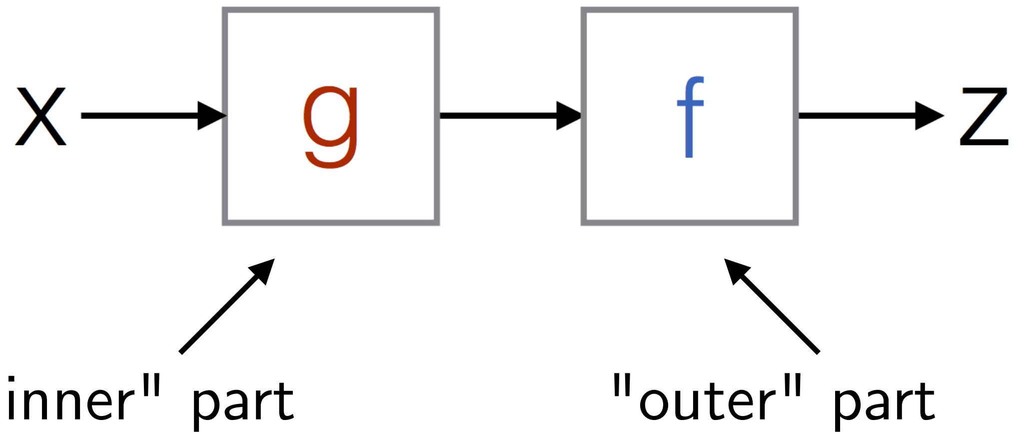
Chain Rule

- The chain rule is basically the essence of training (deep) neural networks
- If you understand and learn how to apply the chain rule to various function decompositions, deep learning will be super easy and even seem trivial to you from now on
- In fact, neural networks will become even easier to understand than any algorithm you learned about in my previous ML class

Chain Rule & "Computation Graph" Intuition

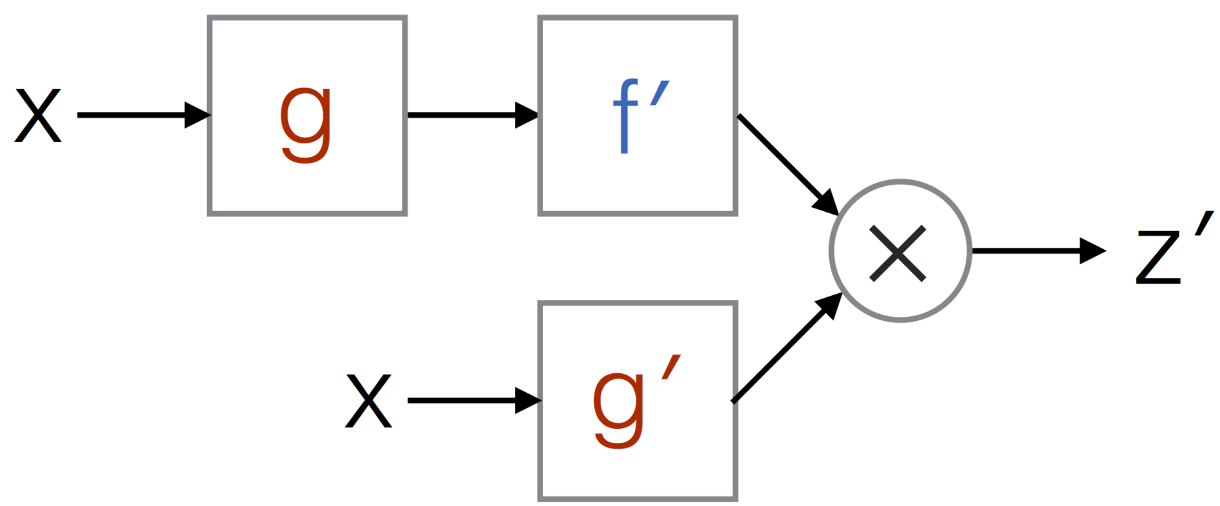
$$F(x) = f\,(\,g(x)\,) = z$$

Decomposition of some (nested) function:



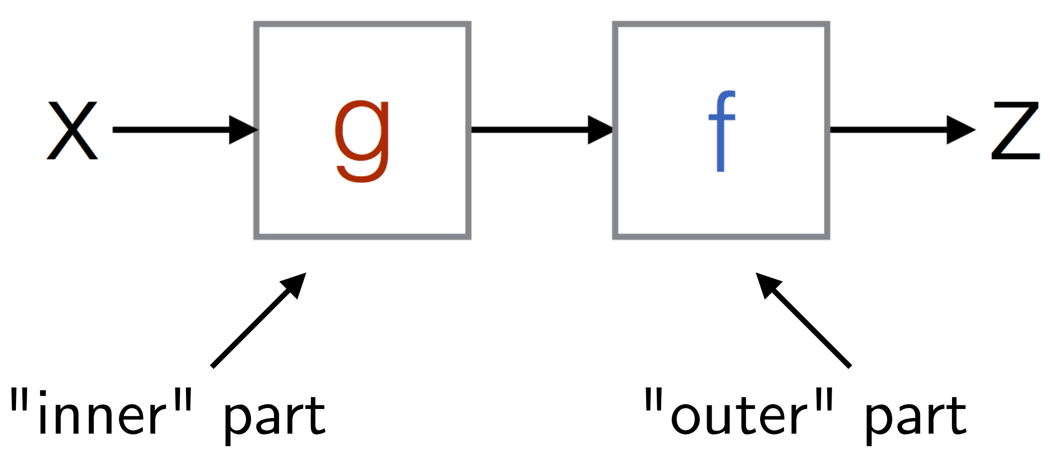
$$F'(x) = f'(\,g(x)\,)\,g'(x) = z'$$

Derivative of that nested function:



Chain Rule & "Computation Graph" Intuition

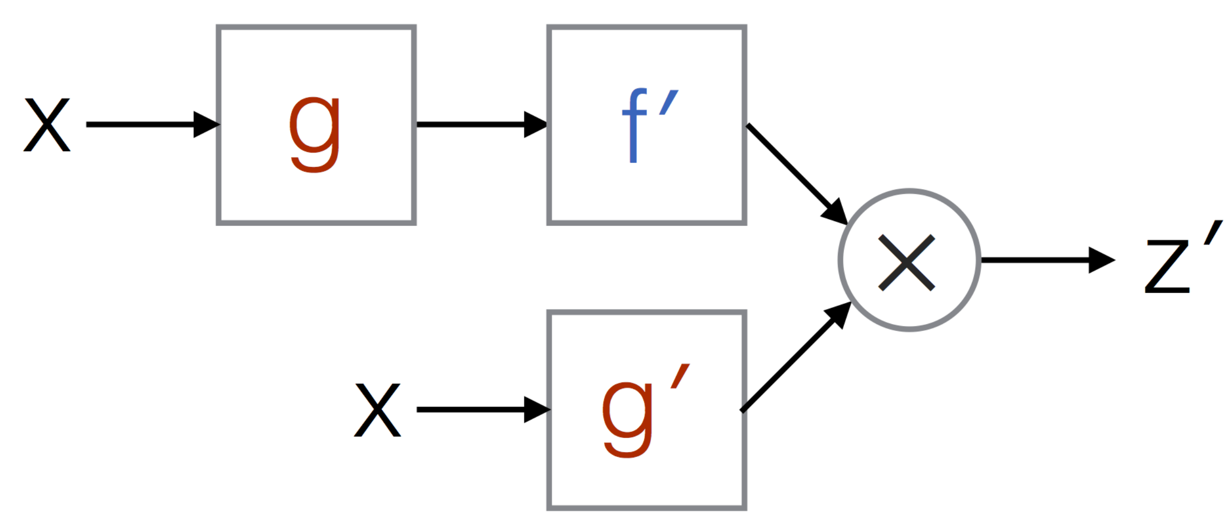
$$F(x) = f(\,g(x)\,) = z$$



Later, we will see that PyTorch can do that automatically for us :) (PyTorch literally keeps a computation graph in the background)

$$F'(x) = f'(\,g(x)\,)\,g'(x) = z'$$

Also, PyTorch can compute the derivatives of most (differentiable) functions automatically



Chain Rule & "Computation Graph" Intuition

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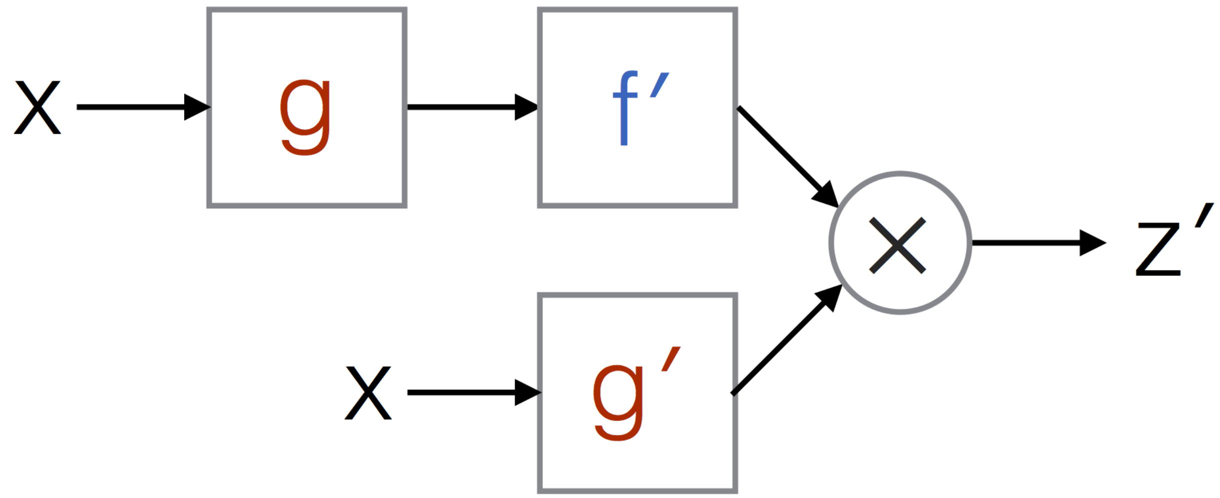


In text, for efficiency, we will mostly use the Leibniz notation:

$$\frac{d}{dx}\left[f(g(x))\right] = \frac{df}{dg} \cdot \frac{dg}{dx}$$

Chain Rule Example

$$\frac{d}{dx}\left[f(g(x))\right] = \frac{df}{dg} \cdot \frac{dg}{dx}$$

Example: $f(x) = \log(\sqrt{x})$

substituting $$\frac{df}{dx} = \frac{d}{dg}\log(g) \cdot \frac{d}{dx}\sqrt{x}$$

with $\frac{d}{dg}\log(g) = \frac{1}{g} = \frac{1}{\sqrt{x}}$ and $\frac{d}{dx}x^{1/2} = \frac{1}{2}x^{-1/2} = \frac{1}{2\sqrt{x}}$

leads us to the solution $$\frac{df}{dx} = \frac{1}{\sqrt{x}} \cdot \frac{1}{2\sqrt{x}} = \frac{1}{2x}$$

Chain Rule for Arbitrarily Long Function Compositions

$$F(x) = f(g(h(u(v(x)))))$$

$$\begin{aligned}\frac{dF}{dx} = \frac{d}{dx}F(x) &= \frac{d}{dx}f(g(h(u(v(x))))) \\ &= \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{du} \cdot \frac{du}{dv} \cdot \frac{dv}{dx}\end{aligned}$$

Chain Rule for Arbitrarily Long Function Compositions

$$\frac{dF}{dx} = \frac{d}{dx}F(x) = \frac{d}{dx}f(g(h(u(v(x)))))$$

$$\boxed{= \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{du} \cdot \frac{du}{dv} \cdot \frac{dv}{dx}}$$

Also called "reverse mode" as we start
with the outer function. In neural nets, this will be from
right to left.

We could also start from the inner parts ("forward mode")

$$\frac{dv}{dx} \cdot \frac{du}{dv} \cdot \frac{dh}{du} \cdot \frac{dg}{dh} \cdot \frac{df}{dg}$$

- Backpropagation (covered later) is basically "reverse" mode auto-differentiation
- It is cheaper than forward mode if we work with gradients, since then we have matrix-"vector" multiplications instead of matrix multiplications

Gradients: Derivatives of Multivariable* Functions

*note that in some fields, the terms "multivariable" and "multivariate" are used interchangeably, but here, we really mean "multivariable" because "multivariate" means "multiple outputs", which is not the case here -- similarly, in most DL applications output one prediction value, or one prediction value per training example

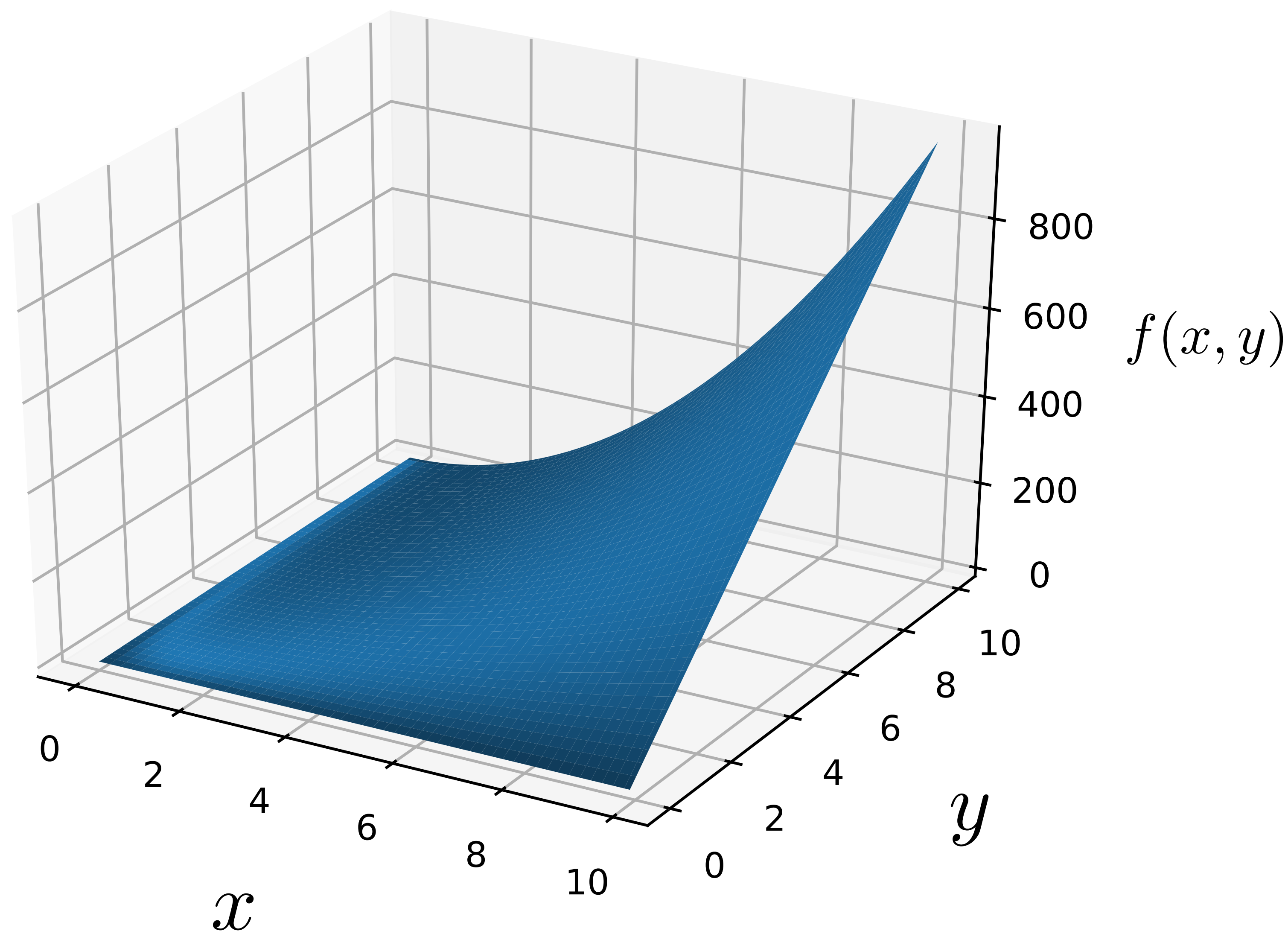
$$f(x, y, z, \ldots)$$

$$\nabla f = \begin{bmatrix} \partial f / \partial x \\ \partial f / \partial y \\ \partial f / \partial z \\ \vdots \end{bmatrix}$$

For gradients, we use the "partial" symbol to denote partial derivatives; more of a notational convention and the concept is the same as before when we were computing ordinary derivatives (denoted them as "d")

Gradients: Derivatives of Multivariable Functions

Example: $f(x, y) = x^2 y + y$



Gradients: Derivatives of Multivariable Functions

<u>Example:</u> $f(x, y) = x^2 y + y$

$$\nabla f(x, y) = \begin{bmatrix} \partial f / \partial x \\ \partial f / \partial y \end{bmatrix},$$

where

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x} x^2 y + y = 2xy$$

(via the power rule and constant rule), and

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y} x^2 y + y = x^2 + 1.$$

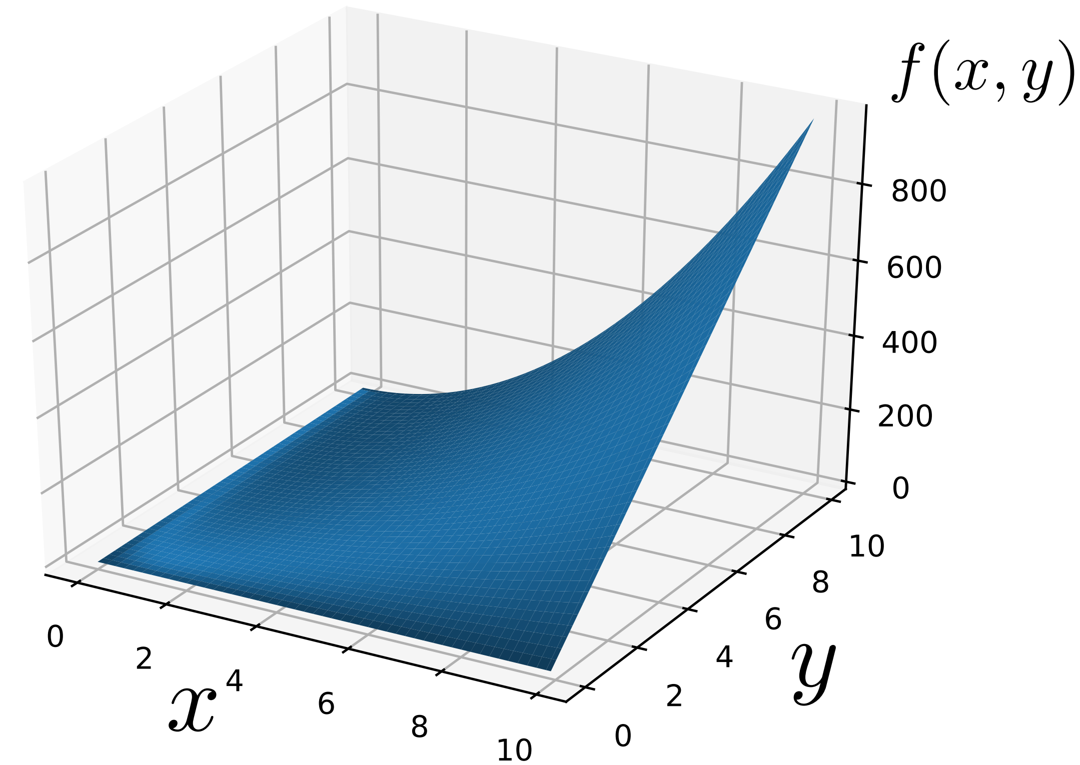
So, the gradient of the function f is defined as

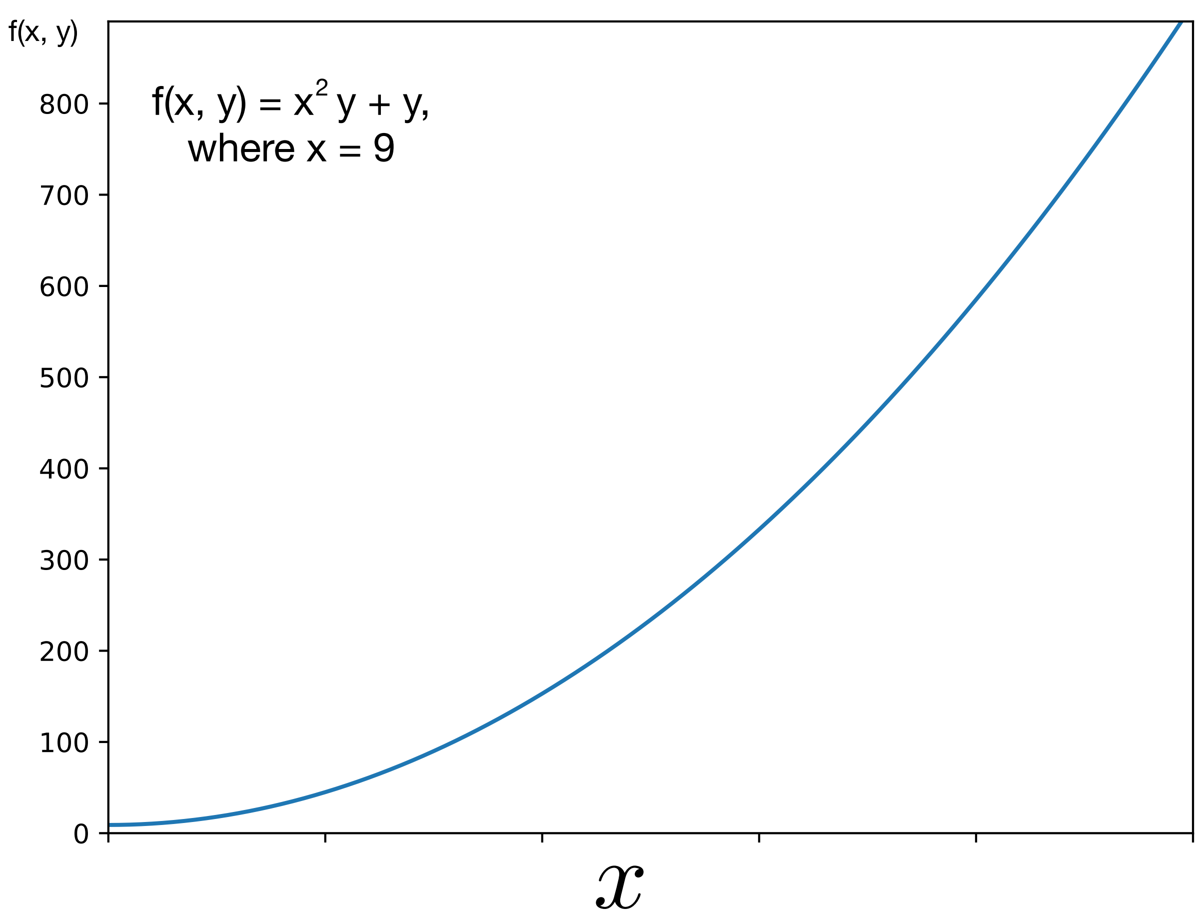
$$\nabla f(x, y) = \begin{bmatrix} 2xy \\ x^2 + 1 \end{bmatrix}.$$

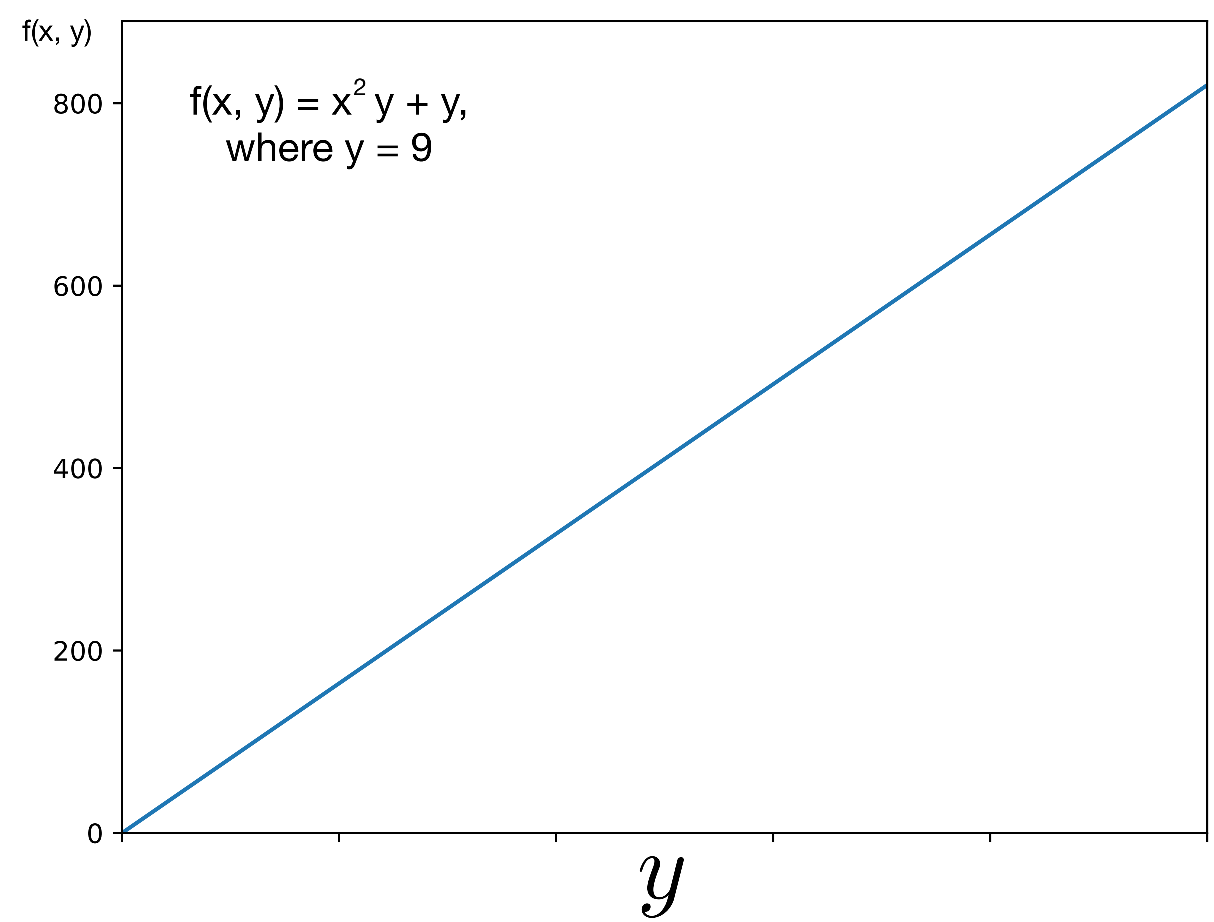
Gradients: Derivative of Multivariable Functions

<u>Example:</u> $f(x, y) = x^2 y + y$

$$\nabla f(x, y) = \begin{bmatrix} 2xy \\ x^2 + 1 \end{bmatrix}$$







Gradients & the Multivariable Chain Rule

Suppose we have a composite function like this:

$$f\Big(g(x), h(x)\Big)$$

Remember the regular chain rule for a single input:

$$\frac{d}{dx}\Big[f\big(g(x)\big)\Big] = \frac{df}{dg} \cdot \frac{dg}{dx}$$

For two inputs, we now have

$$\frac{d}{dx}\Big[f\big(g(x), h(x)\big)\Big] = \frac{\partial f}{\partial g} \cdot \frac{dg}{dx} + \frac{\partial f}{\partial h} \cdot \frac{dh}{dx}$$

Gradients & the Multivariable Chain Rule

$$f\big(g(x), h(x)\big)$$

$$\frac{d}{dx}\big[f(g(x), h(x))\big] =$$

$$\frac{\partial f}{\partial g} \cdot \frac{dg}{dx} + \frac{\partial f}{\partial h} \cdot \frac{dh}{dx}$$

<u>Example:</u>

$$f\big(g, h\big) = g^2 h + h$$

where $g(x) = 3x,$ and $h(x) = x^2$

$$\frac{\partial f}{\partial g} = 2gh \qquad \frac{\partial f}{\partial h} = g^2 + 1$$

$$\frac{dg}{dx} = \frac{d}{dx} 3x = 3 \qquad \frac{dh}{dx} = \frac{d}{dx} x^2 = 2x$$

$$\begin{aligned}\frac{d}{dx}\big[f(g(x))\big] &= [2gh \cdot 3] + [(g^2 + 1) \cdot 2x] \\ &= g^2 + 6gh + 2x\end{aligned}$$

Gradients & the Multivariable Chain Rule in Vector Form

$$f\big(g(x), h(x)\big)$$

$$\begin{aligned}\frac{d}{dx}\big[f(g(x), h(x))\big] &= \frac{\partial f}{\partial g} \cdot \frac{dg}{dx} + \frac{\partial f}{\partial h} \cdot \frac{dh}{dx} \\ &= \nabla f \cdot \mathbf{v}'(x).\end{aligned}$$

Where

$$\mathbf{v}(x) = \begin{bmatrix} g(x) \\ h(x) \end{bmatrix} \qquad \mathbf{v}'(x) = \frac{d}{dx}\begin{bmatrix} g(x) \\ h(x) \end{bmatrix} = \begin{bmatrix} dg/dx \\ dh/dx \end{bmatrix}$$

Putting it together:

$$\nabla f \cdot \mathbf{v}'(x) = \begin{bmatrix} \partial f/\partial g \\ \partial f/\partial h \end{bmatrix} \cdot \begin{bmatrix} dg/dx \\ dh/dx \end{bmatrix} = \frac{\partial f}{\partial g} \cdot \frac{dg}{dx} + \frac{\partial f}{\partial h} \cdot \frac{dh}{dx}$$

The Jacobian (Matrix)

$$\mathbf{f}(x_1, x_2, ..., x_m) = \begin{bmatrix} f_1\left(x_1, x_2, x_3, \cdots x_m\right) \\ f_2\left(x_1, x_2, x_3, \cdots x_m\right) \\ f_3\left(x_1, x_2, x_3, \cdots x_m\right) \\ \vdots \\ f_m\left(x_1, x_2, x_3, \cdots x_m\right) \end{bmatrix}$$

$$J\left(x_1, x_2, x_3, \cdots x_m\right) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} & \cdots & \frac{\partial f_3}{\partial x_m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \frac{\partial f_m}{\partial x_3} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix}$$

The Jacobian (Matrix)

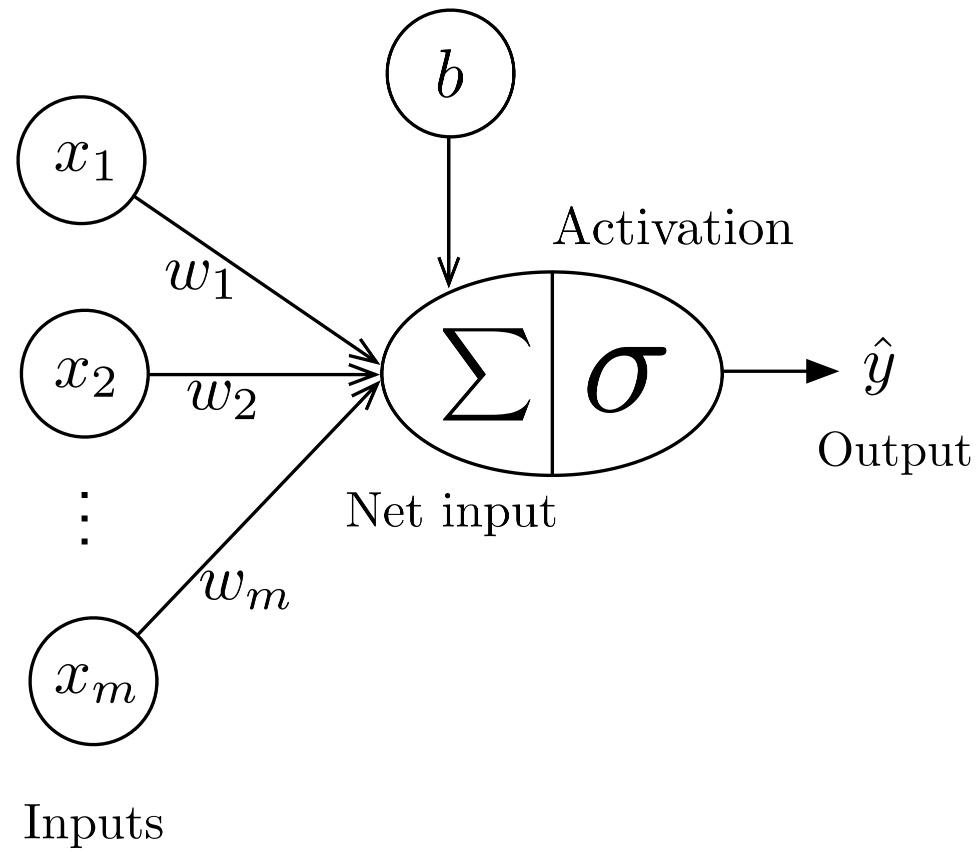
$$\mathbf{f}(x_1, x_2, ..., x_m) = \begin{bmatrix} f_1\left(x_1, x_2, x_3, \cdots x_m\right) \\ f_2\left(x_1, x_2, x_3, \cdots x_m\right) \\ f_3\left(x_1, x_2, x_3, \cdots x_m\right) \\ \vdots \\ f_m\left(x_1, x_2, x_3, \cdots x_m\right) \end{bmatrix}$$

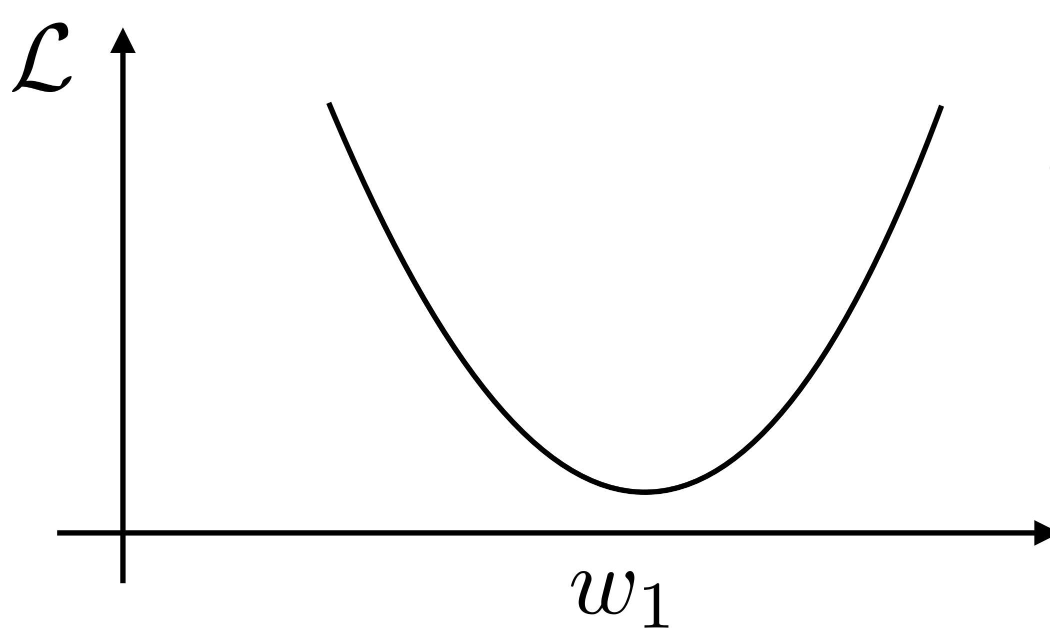
$$J\left(x_1, x_2, x_3, \cdots x_m\right) = \begin{array}{cc} \begin{bmatrix} \boxed{\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \cdots & \frac{\partial f_1}{\partial x_m}} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} & \cdots & \frac{\partial f_3}{\partial x_m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \frac{\partial f_m}{\partial x_3} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix} & \begin{matrix} \left(\nabla f_1\right)^\top \\ \\ \\ \\ \\ \end{matrix} \end{array}$$

Second Order Derivatives

Lucky for you, we won't need second order derivatives in this class ;)

Back to Linear Regression



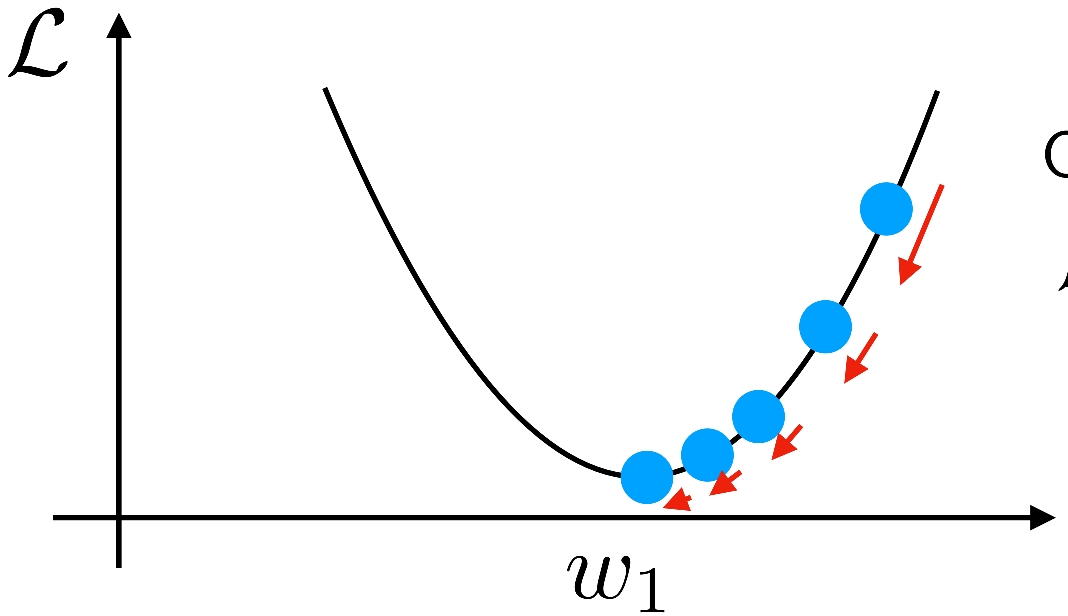


Convex loss function

$$\mathcal{L}(\mathbf{w}, b) = \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

Gradient Descent

Learning rate and steepness of the gradient determine how much we update

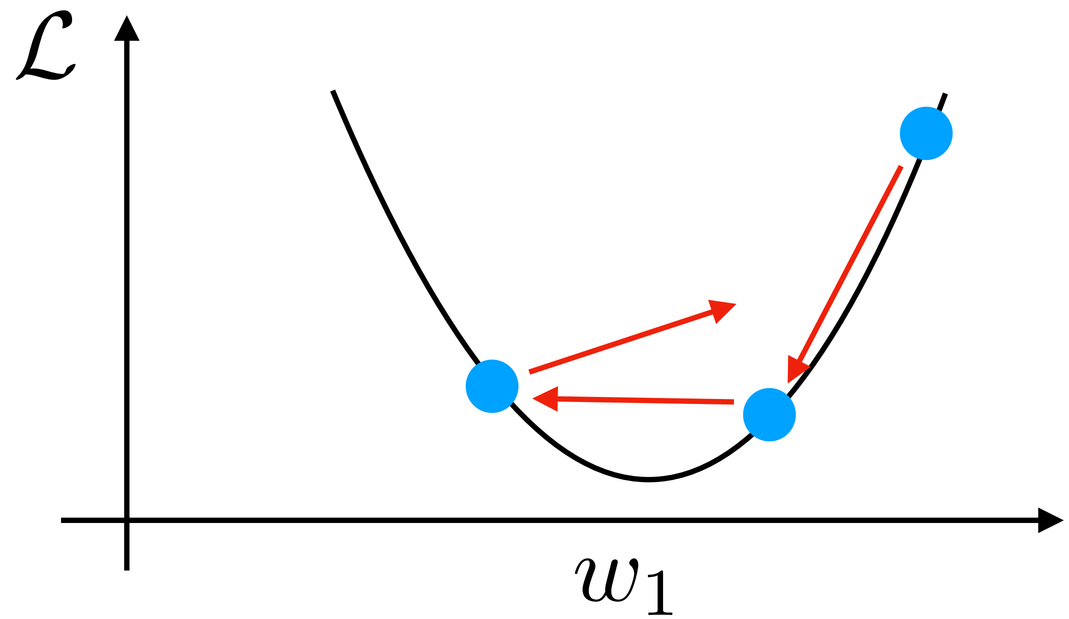


Convex loss function

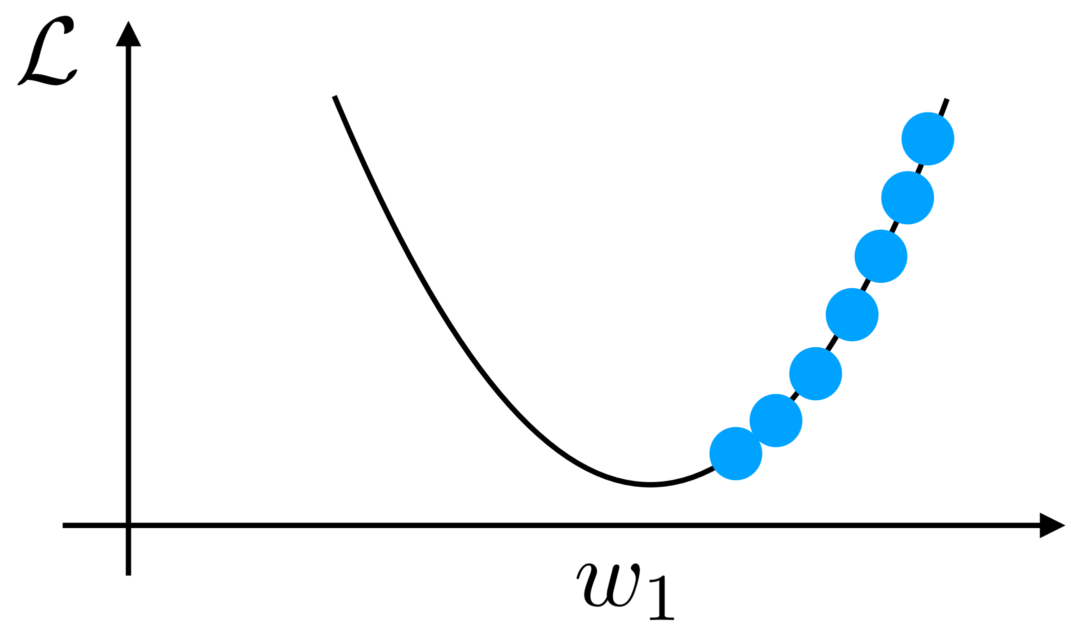
$$\mathcal{L}(\mathbf{w}, b) = \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

Gradient Descent

If the learning rate is too large, we can overshoot



If the learning rate is too small, convergence is very slow



Linear Regression Loss Derivative

$$\mathcal{L}(\mathbf{w}, b) = \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

Sum Squared Error (SSE) loss

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\partial}{\partial w_j} \sum_i (\hat{y}^{[i]} - y^{[i]})^2 \\
&= \frac{\partial}{\partial w_j} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]})^2 \\
&= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{\partial}{\partial w_j} (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \\
&= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} \frac{\partial}{\partial w_j} \mathbf{w}^T \mathbf{x}^{[i]} \\
&= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} x_j^{[i]} \\
&= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) x_j^{[i]}
\end{aligned}$$

(Note that the activation function is the identity function in linear regression)

Linear Regression Loss Derivative (alt.)

$$\mathcal{L}(\mathbf{w}, b) = \frac{1}{2n} \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

Mean Squared Error (MSE) loss often scaled by factor 1/2 for convenience

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\partial}{\partial w_j} \frac{1}{2n} \sum_i (\hat{y}^{[i]} - y^{[i]})^2 \\
&= \frac{\partial}{\partial w_j} \sum_i \frac{1}{2n} (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]})^2 \\
&= \sum_i \frac{1}{n} (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{\partial}{\partial w_j} (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \\
&= \frac{1}{n} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} \frac{\partial}{\partial w_j} \mathbf{w}^T \mathbf{x}^{[i]} \\
&= \frac{1}{n} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} x_j^{[i]} \\
&= \frac{1}{n} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) x_j^{[i]}
\end{aligned}$$

(Note that the activation function is the identity function in linear regression)

Batch vs Stochastic

The minibatch and on-line modes are stochastic versions of gradient descent (batch mode)

Minibatch mode

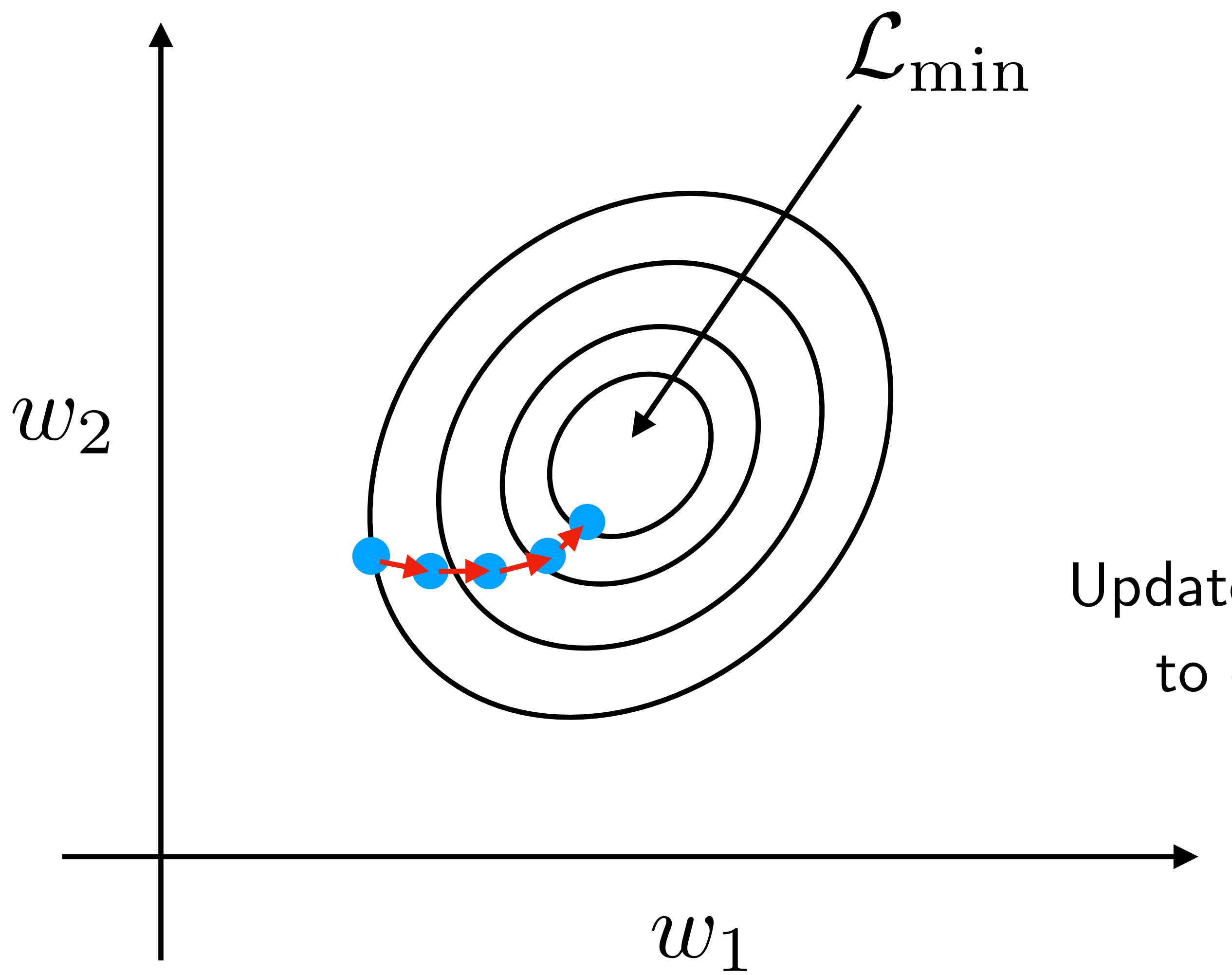
(mix between on-line and batch)

1. Initialize $\mathbf{w} := 0^{m-1}$, $\mathbf{b} := 0$
2. For every training epoch:
   A. Initialize $\Delta\mathbf{w} := 0, \ \Delta b := 0$
   B. For every $\{\langle \mathbf{x}^{[i]}, y^{[i]}\rangle, ..., \langle \mathbf{x}^{[i+k]}, y^{[i+k]}\rangle\} \subset \mathcal{D}$:
      (a) Compute output (prediction)
      (b) Calculate error
      (c) Update $\Delta\mathbf{w}, \Delta b$
   C. Update $\mathbf{w}, b$:
   $$\mathbf{w} := \mathbf{w} + \Delta\mathbf{w}, b := +\Delta b$$

Most commonly used in DL, because

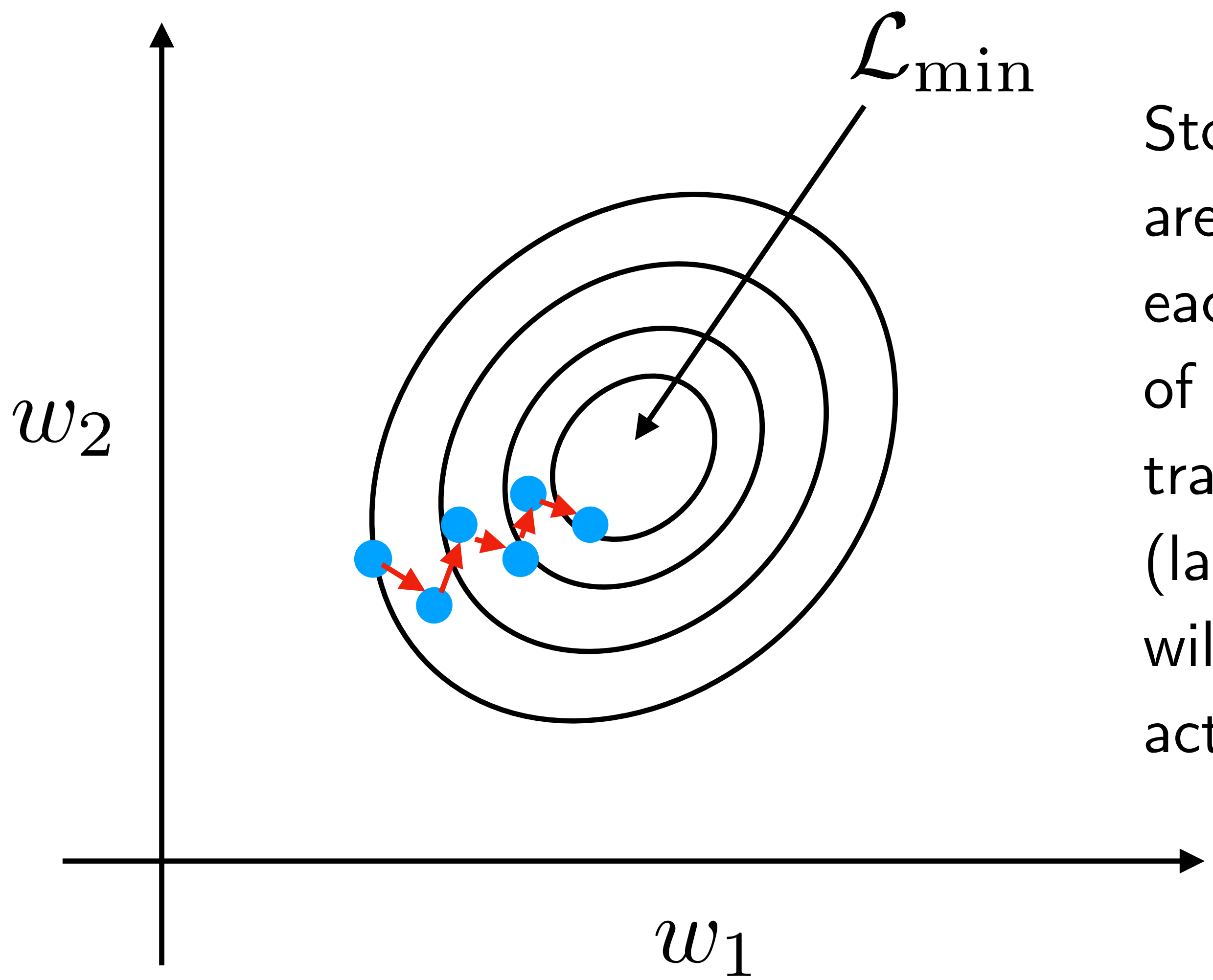
1. Choosing a subset (vs 1 example at a time) takes advantage of vectorization (faster iteration through epoch than on-line)
2. having fewer updates than "on-line" makes updates less noisy
3. makes more updates/ epoch than "batch" and is thus faster

Batch Gradient Descent as Surface Plot



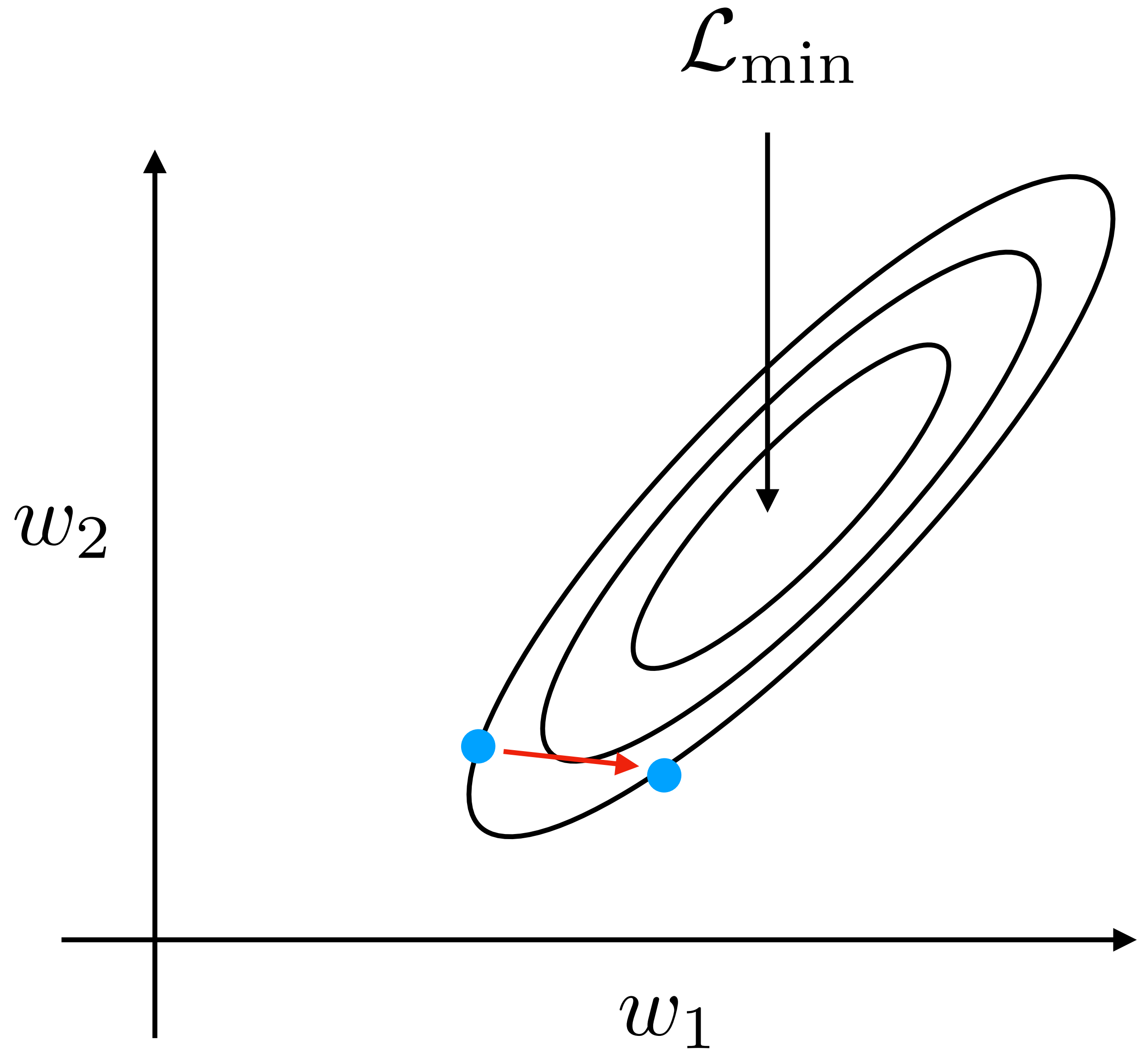
Updates perpendicular to contour lines

Stochastic Gradient Descent as Surface Plot



Stochastic updates
are a bit noisier, because
each batch is an approximation
of the overall loss on the
training set
(later, in deep neural nets, we
will see why noisier updates are
actually helpful)

Batch Gradient Descent as Surface Plot



If inputs are on very different scales
some weights will update more than
others ... and it will also harm convergence
(always normalize inputs!)

Linear Regression

Code example:

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L05_grad-descent/code/linear-regr-gd.ipynb

ADALINE

Widrow and Hoff's ADALINE (1960)

A nicely differentiable neuron model

Widrow, B., & Hoff, M. E. (1960). *Adaptive switching circuits* (No. TR-1553-1). Stanford Univ Ca Stanford Electronics Labs.

Widrow, B. (1960). *Adaptive" adaline" Neuron Using Chemical" memistors."*.

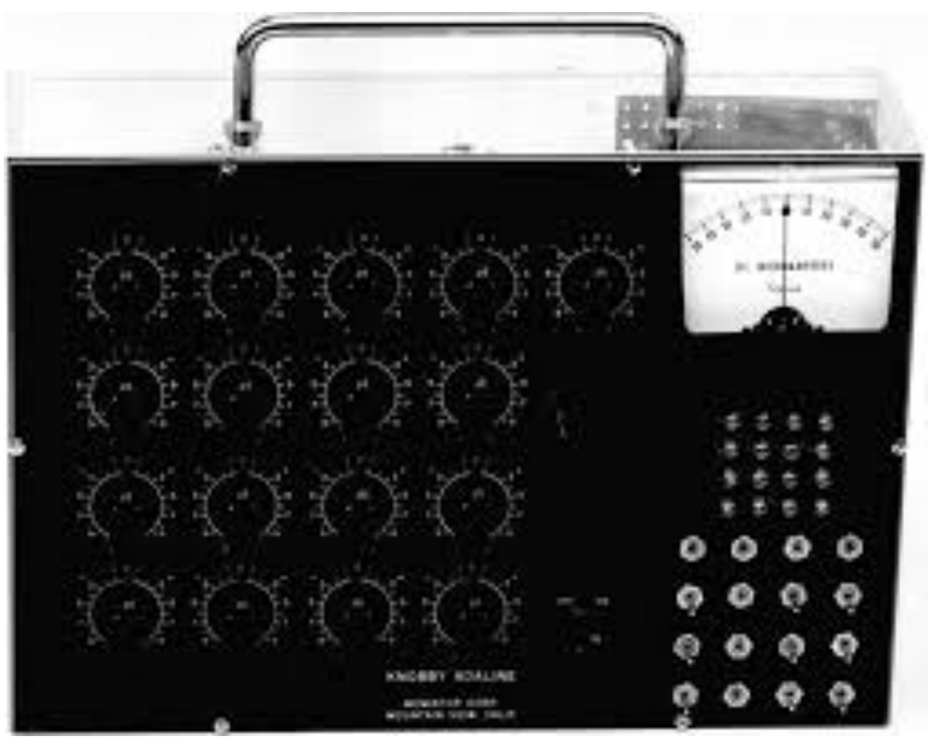
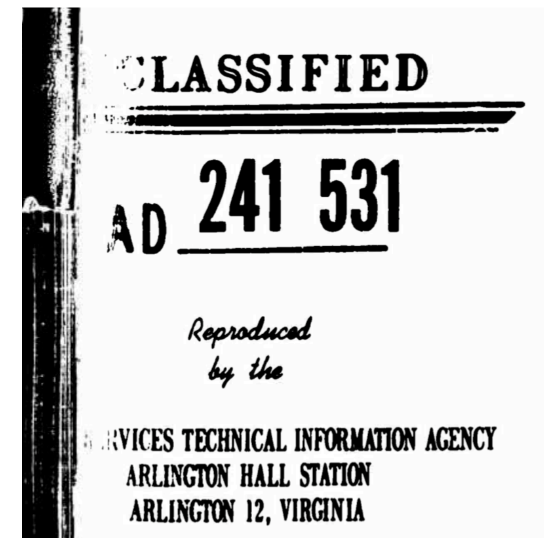


Image source: https://www.researchgate.net/profile/Alexander_Magoun2/publication/265789430/figure/fig2/AS:392335251787780@1470551421849/ADALINE-An-adaptive-linear-neuron-Manually-adapted-synapses-Designed-and-built-by-Ted.png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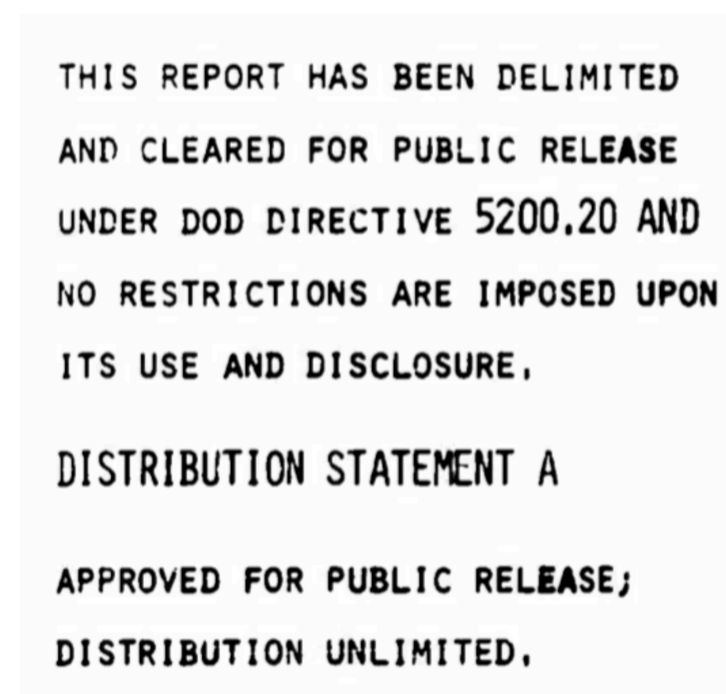
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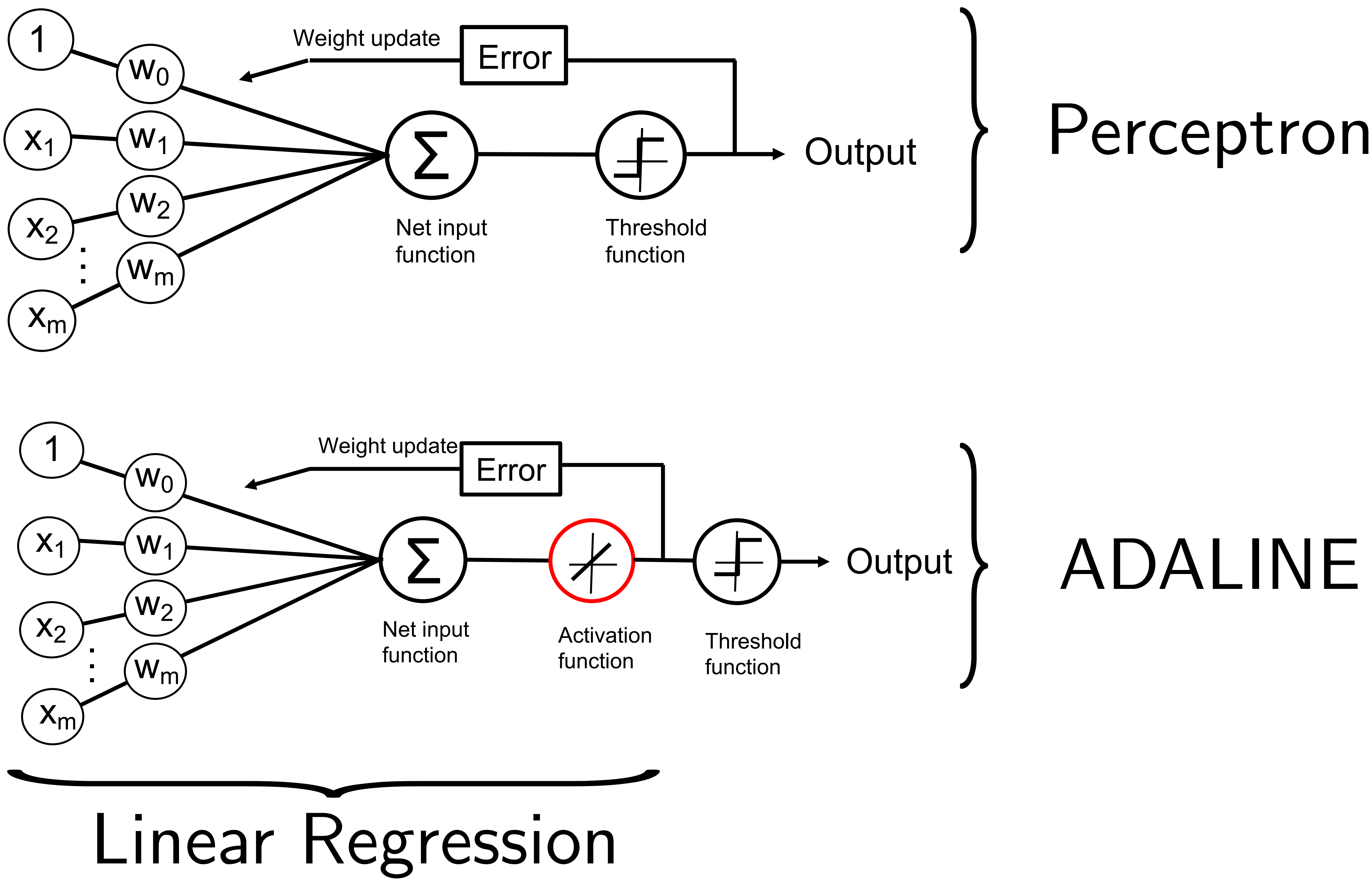
ADALINE

ADAptive LInear NEuron



ADALINE

Code example:

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L05_grad-descent/code/adaline-sgd.ipynb

Next Lecture:

Neurons with non-linear activation functions

Ungraded HW assignment

See last cell in the linear regression Jupyter Notebook

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L05_grad-descent/code/linear-regr-gd.ipynb