Lecture 05

Fitting Neurons with Gradient Descent

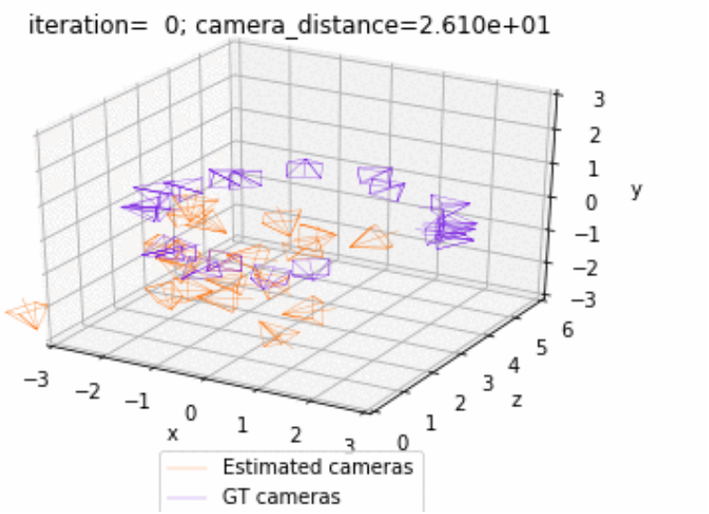
STAT 453: Deep Learning, Spring 2020

Sebastian Raschka

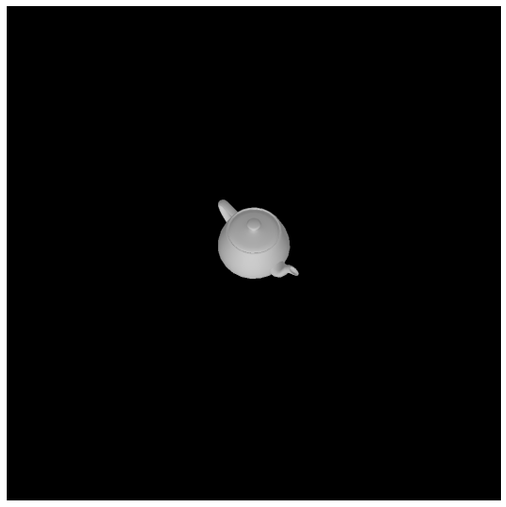
http://stat.wisc.edu/~sraschka/teaching/stat453-ss2020/

News

PyTorch3D



https://github.com/facebookresearch/pytorch3d



hardmaru
@hardmaru

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

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

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.

Also known as "graduate student descent"

Let's improve upon the perceptron & learn about a neural network model for which the training always converges

Our Goals

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

- 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!)

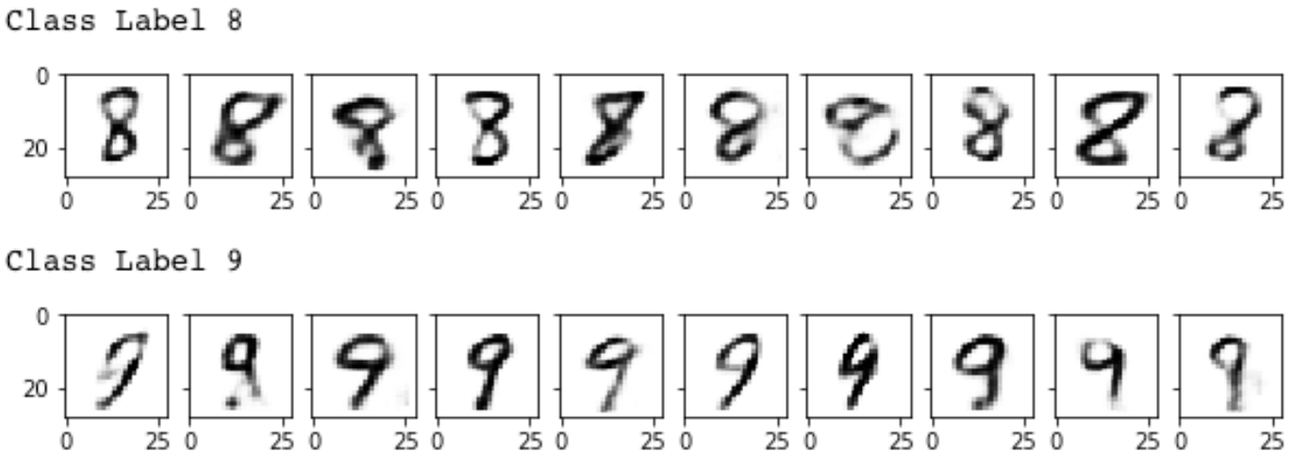
- Handle multiple categories (not just binary) in classification

- Do even fancier things like generating NEW images and text

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

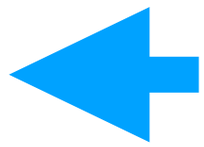
```
Probability Female 99.71%
```

Age: 30



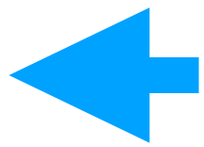
Our Goals

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



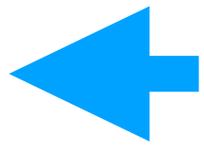
This lecture

- 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!)



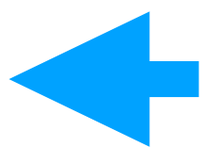
Next lecture(s)

- Handle multiple categories (not just binary) in classification

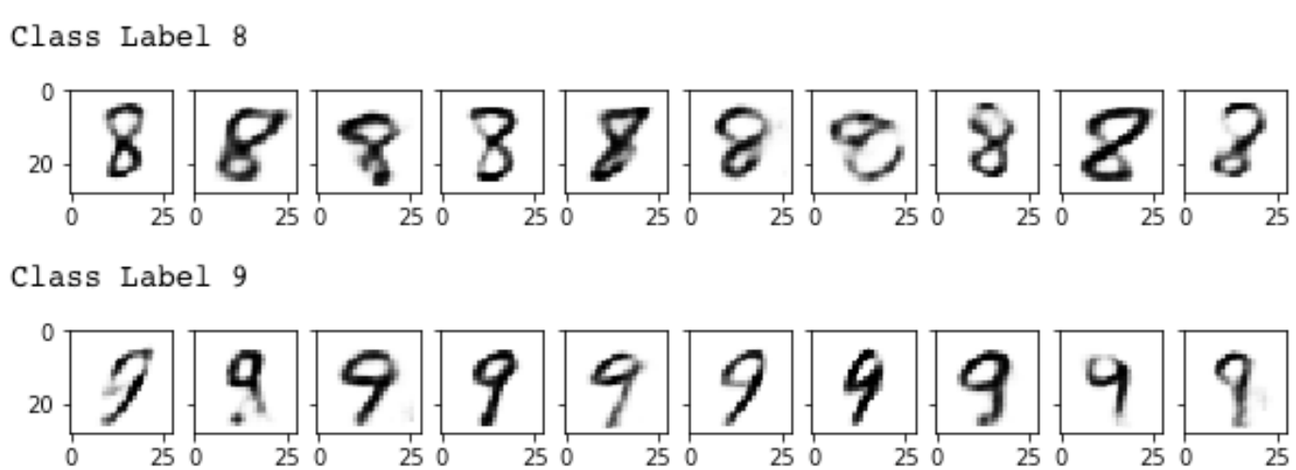


Next lecture(s)

- Do even fancier things like generating NEW images and text



More towards the end of the course

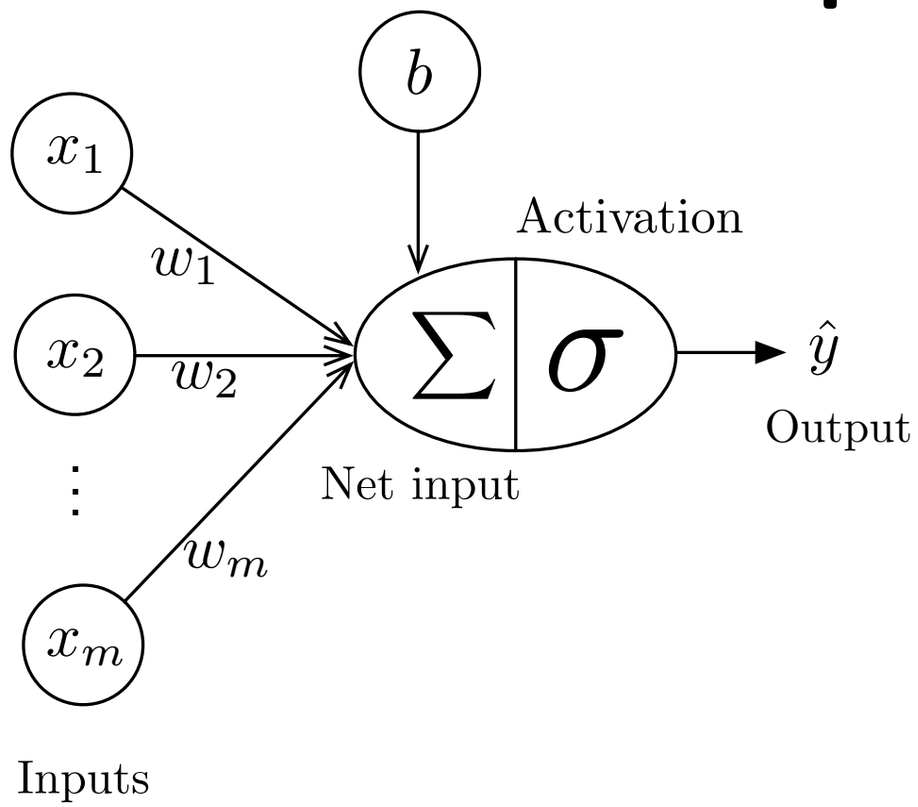


All based on the same learning algorithm and extensions thereof.
So, this is prob. the most fundamental lecture!

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 $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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) $\text{err} := (y^{[i]} - \hat{y}^{[i]})$ ← 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 $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
2. For every training epoch:
   - A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$:
     - (a) Compute output (prediction)
     - (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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Batch mode

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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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In practice, we usually shuffle the dataset prior to each epoch to prevent cycles

"On-line" mode II (alternative)

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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 $\mathbf{w}, b$

No shuffling required

(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 $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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

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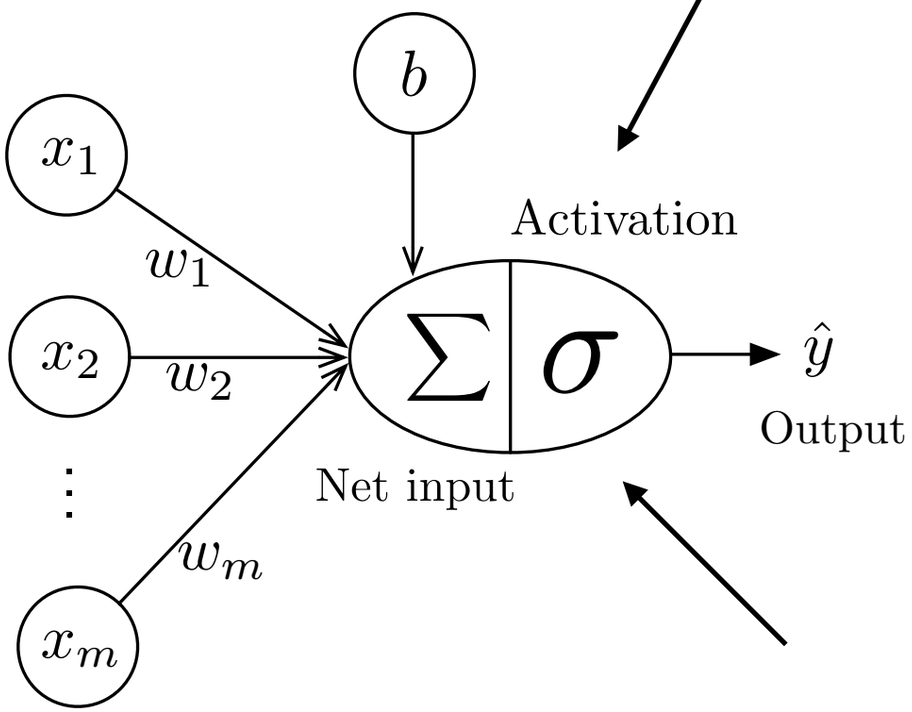
Most commonly used in DL, because

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

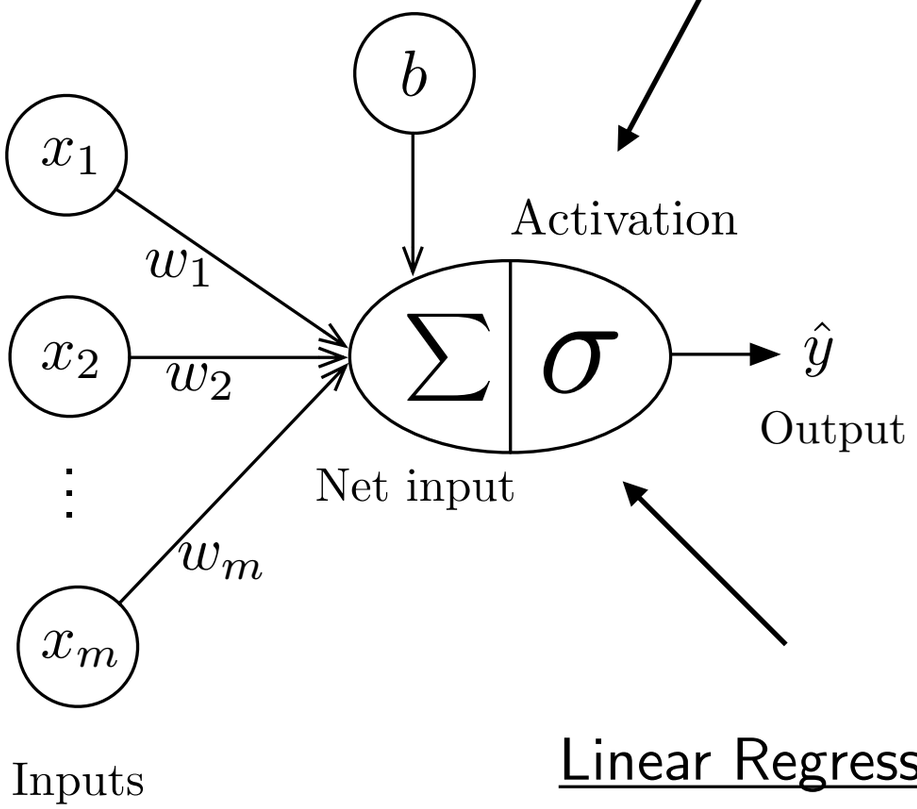
$$\sigma(x) = x$$

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

Linear Regression

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

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



You can think of linear regression as a linear neuron!

<u>Linear Regression:</u> 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 linear regression model model like this, using the "normal equations" (analytical solution):

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

(assuming that the bias is included in $\mathbf{w}$, 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:"

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

(assuming that the bias is included in $\mathbf{w}$, 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 -- iteratively with "brute force"

- A very naive way to fit a linear regression model (and any neural net) is to start with initializing the parameters to 0's or small random values
- 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 iteratively

- A very naive way to fit a linear regression model (and any neural net) is to start with initializing the parameters to 0's or small random values
- Then, for k rounds
  - Choose another random set of weights
  - If the model performs better, keep those weights
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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

Perceptron learning rule

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
2. For every training epoch:
   A. For every $\langle \mathbf{x}^{[i]}, y^{[i]} \rangle \in \mathcal{D}$
   (a) $\hat{y}^{[i]} := \sigma\left(\mathbf{x}^{[i]T}\mathbf{w} + b\right)$
   (b) $\text{err} := (y^{[i]} - \hat{y}^{[i]})$
   (c) $\mathbf{w} := \mathbf{w} + err \times \mathbf{x}^{[i]}$
   $b := b + err$

Stochastic gradient descent

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

learning rate

negative gradient

For-Loop

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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) $\frac{\partial \mathcal{L}}{\partial w_j} = \big(y^{[i]} - \hat{y}^{[i]}\big)x_j^{[i]}$
   (c) $w_j := w_j + \eta \times (-\frac{\partial \mathcal{L}}{\partial w_j})$
   C. $\frac{\partial \mathcal{L}}{\partial b} = \big(y^{[i]} - \hat{y}^{[i]}\big)$
   $b := b + \eta \times (-\frac{\partial \mathcal{L}}{\partial b})$

(Least-Squares) Linear Regression

The update rule turns out to be this:

"On-line" mode

1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
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   - 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.

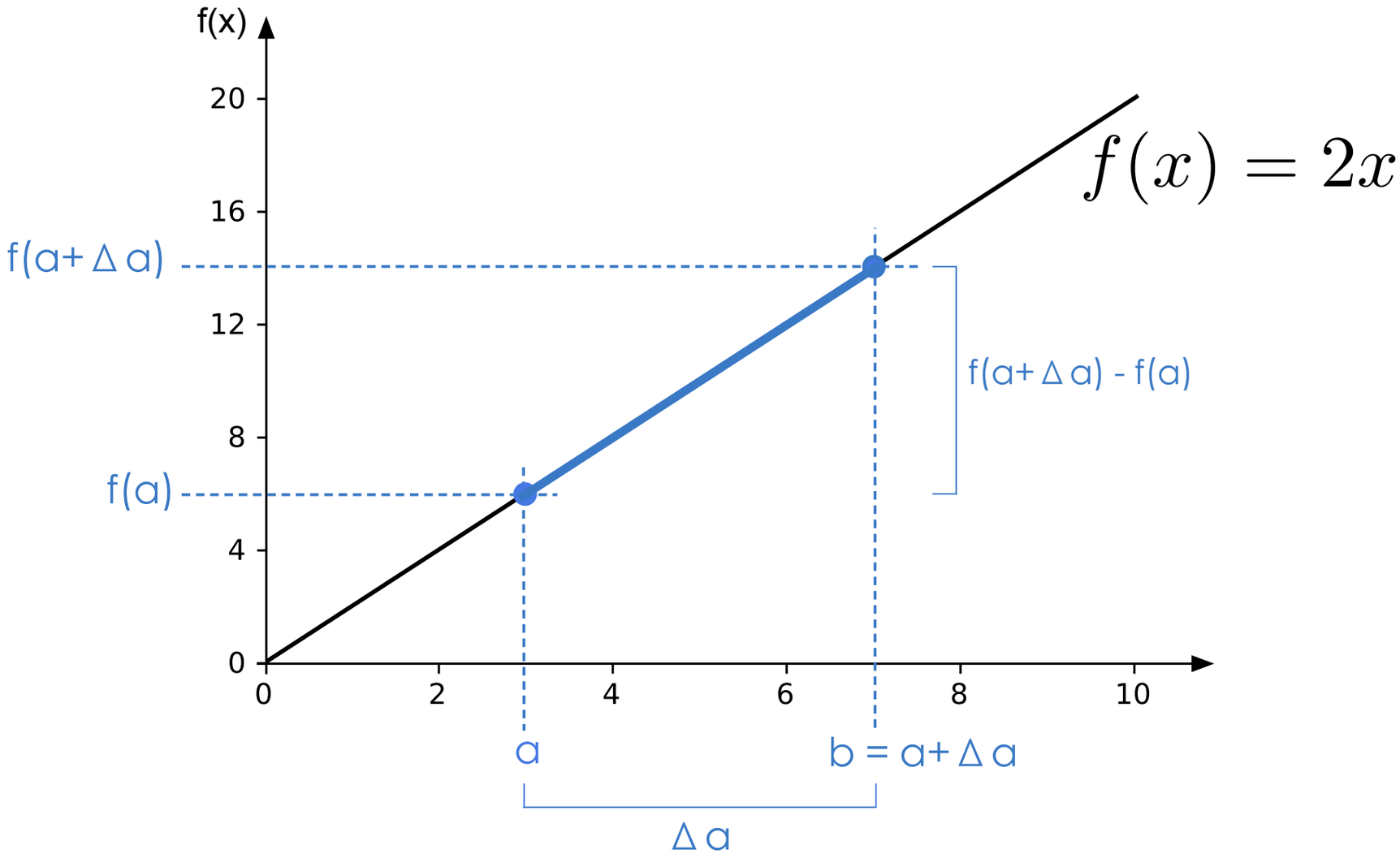
So, how did we get there?

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

(Optional section)

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

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

Example 1: $f(x) = 2x$

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

Numerical vs Analytical/Symbolical Derivatives

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

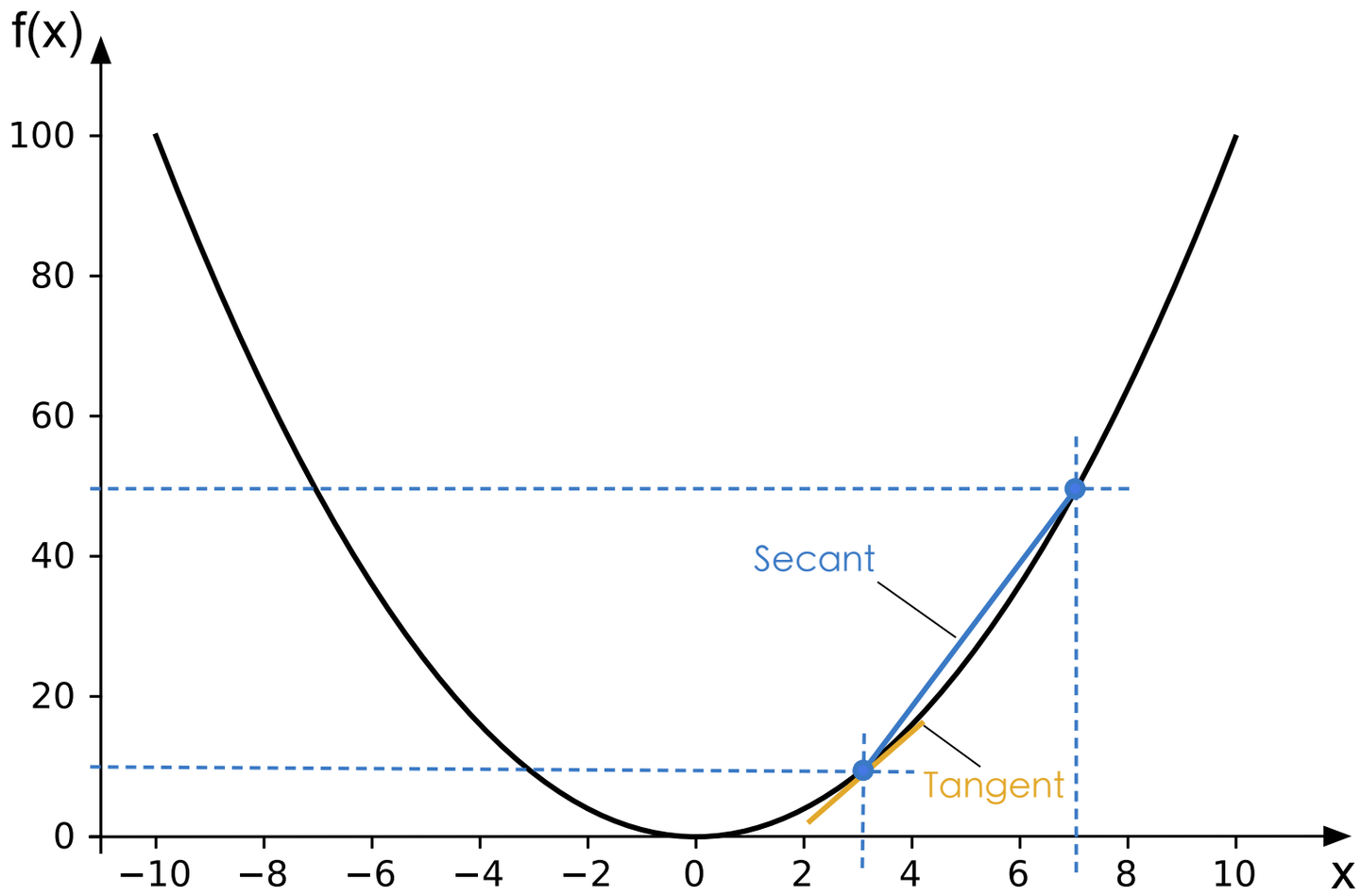
Example 2: $f(x) = x^2$

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

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	$f(g(x))$	$f'(g(x))g'(x)$

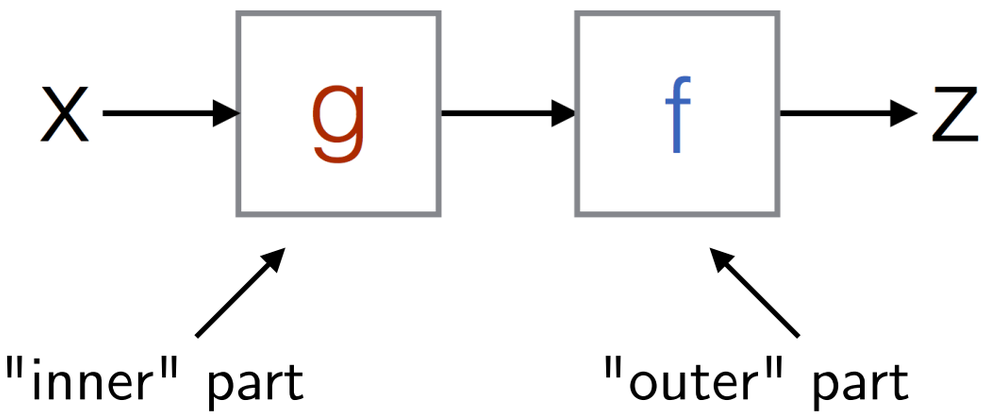
Chain Rule

- 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

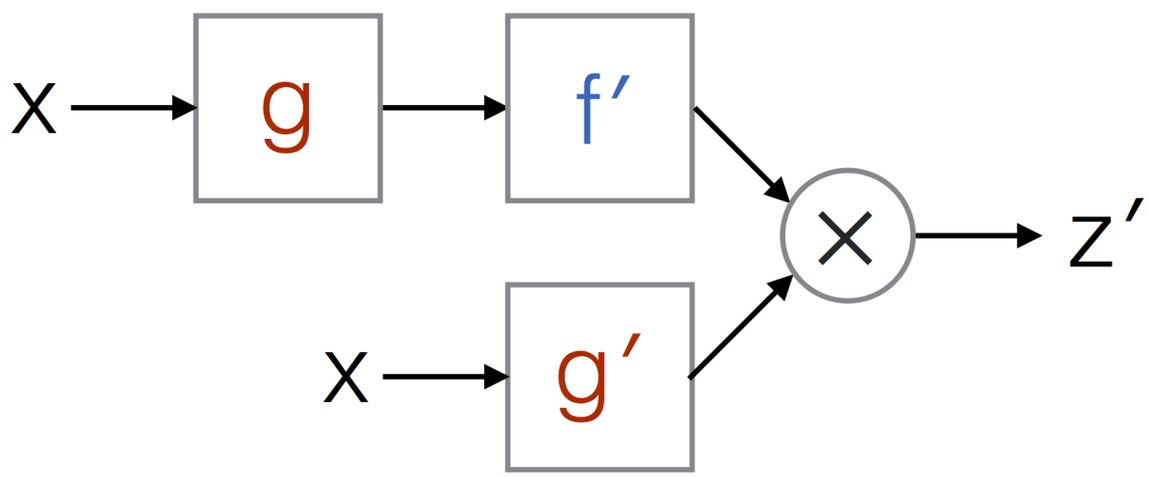
$$F(x) = f\,(\,g(x)\,) = z$$

Decomposition of some (nested) function:



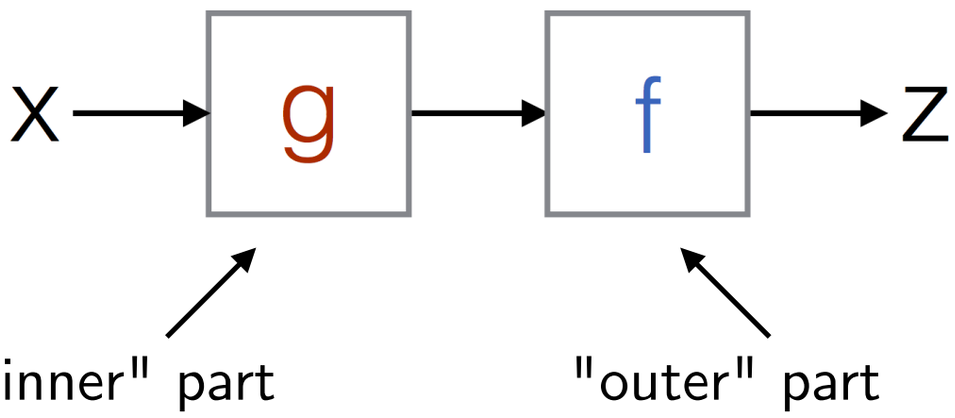
$$F'(x) = f'(\,g(x)\,)\,g'(x) = z'$$

Derivative of that nested function:



Chain Rule & "Computation Graph" Intuition

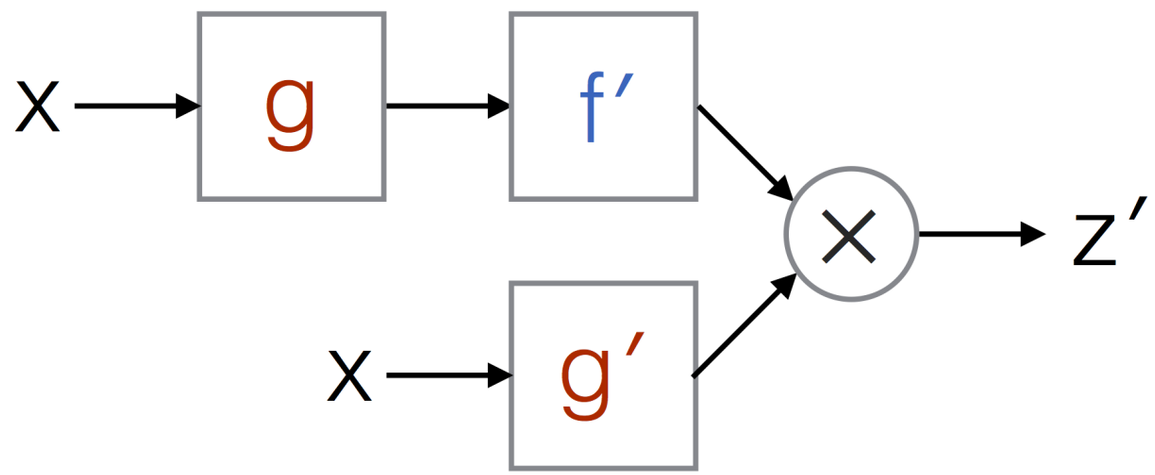
$$F(x) = f(\,g(x)\,) = z$$



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

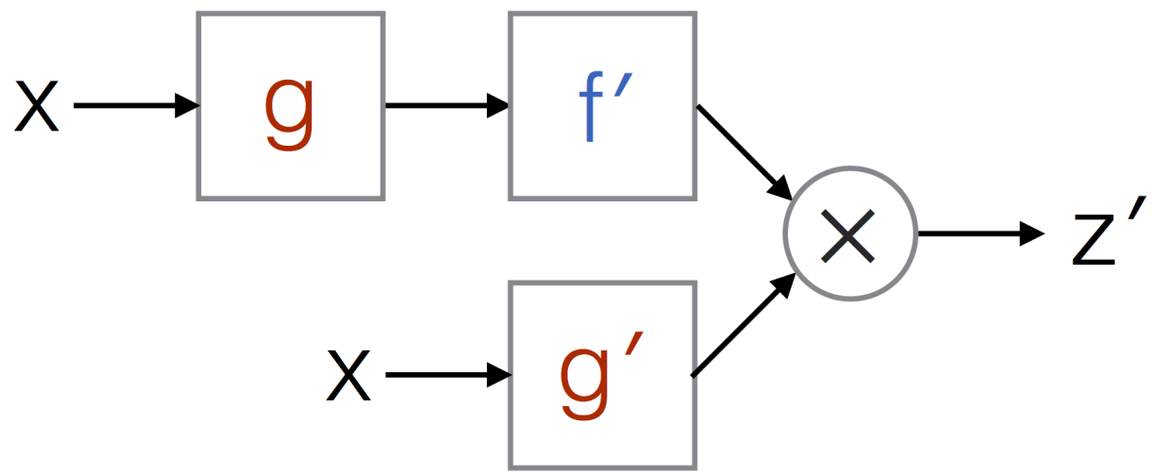
Also, PyTorch can compute the derivatives of most (differentiable) functions automatically

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



Chain Rule & "Computation Graph" Intuition

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



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

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

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

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

Chain Rule for Arbitrarily Long Function Compositions

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

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

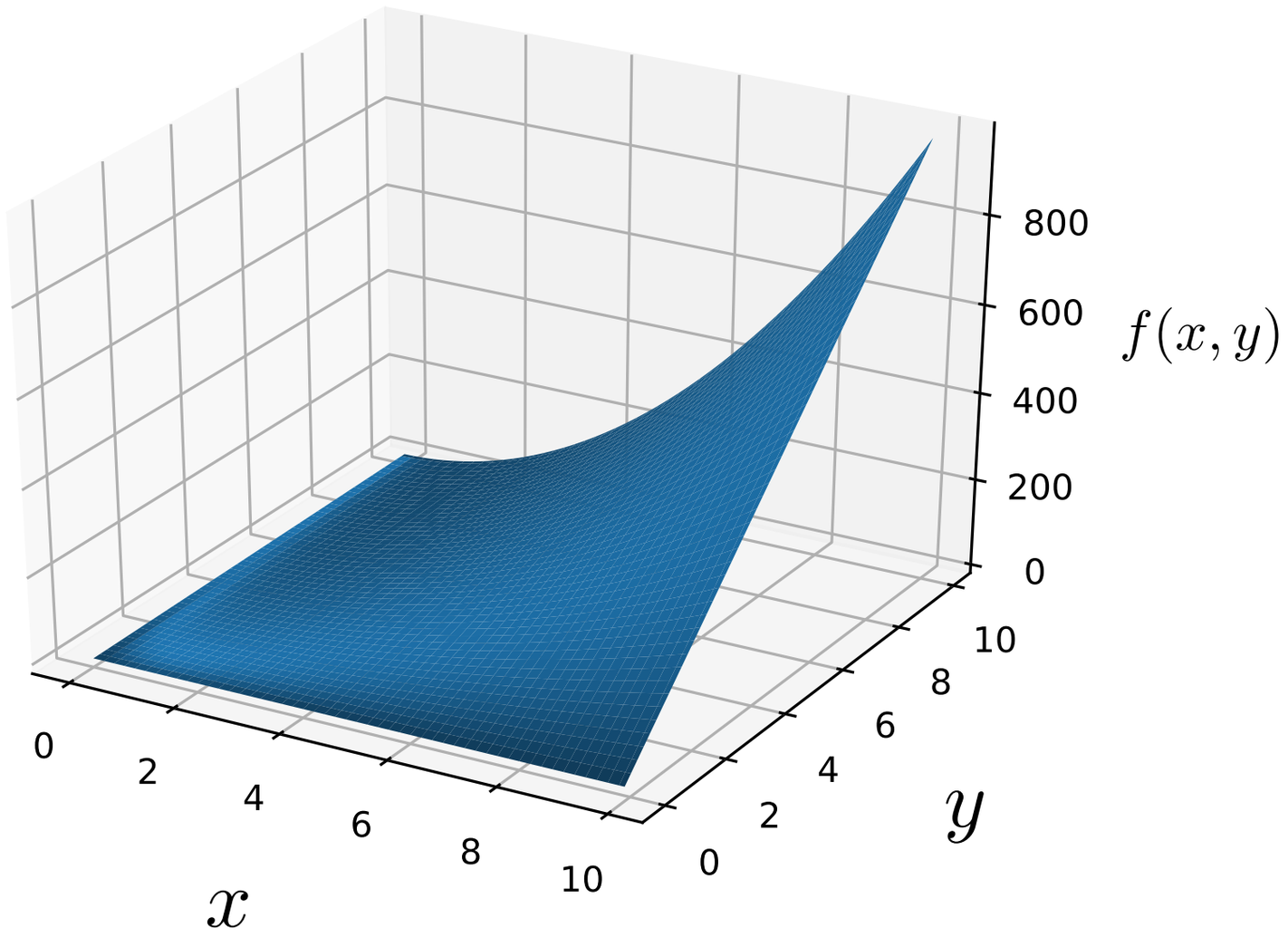
$$f(x, y, z, ...)$$

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

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

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

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

where

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

(via the power rule and constant rule), and

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

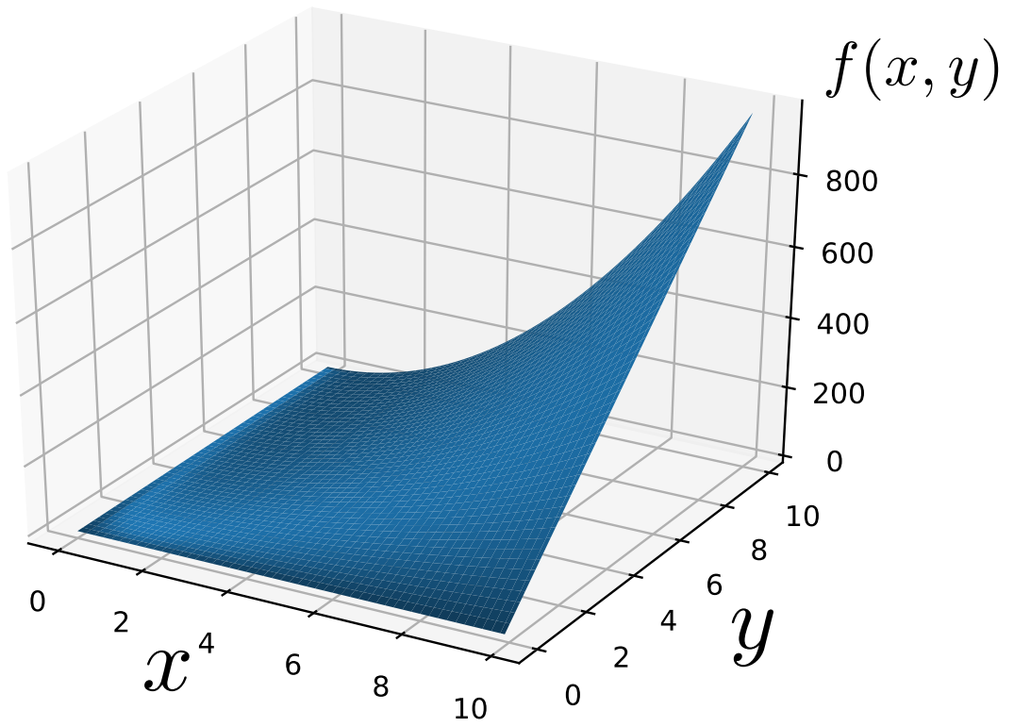
So, the gradient of the function f is defined as

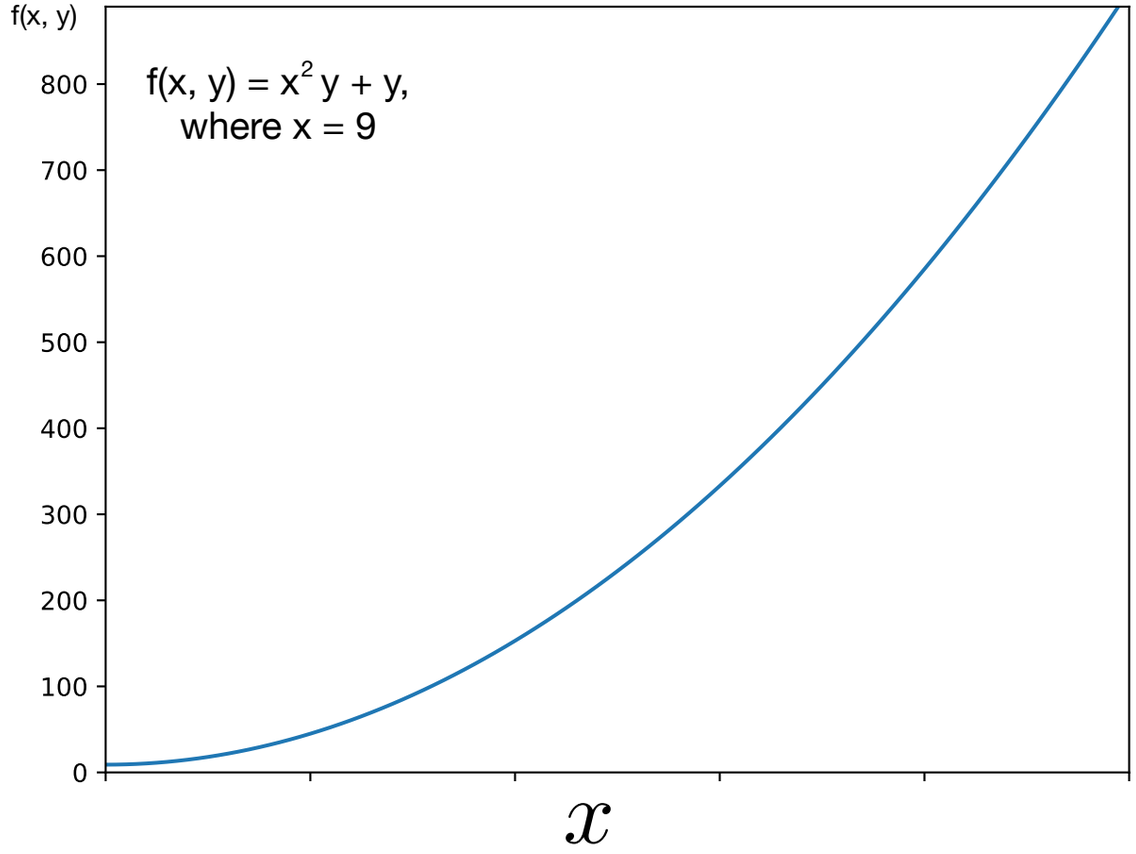
$$\nabla f(x, y) = \begin{bmatrix} 2xy \\ x^2 + 1 \end{bmatrix}.$$

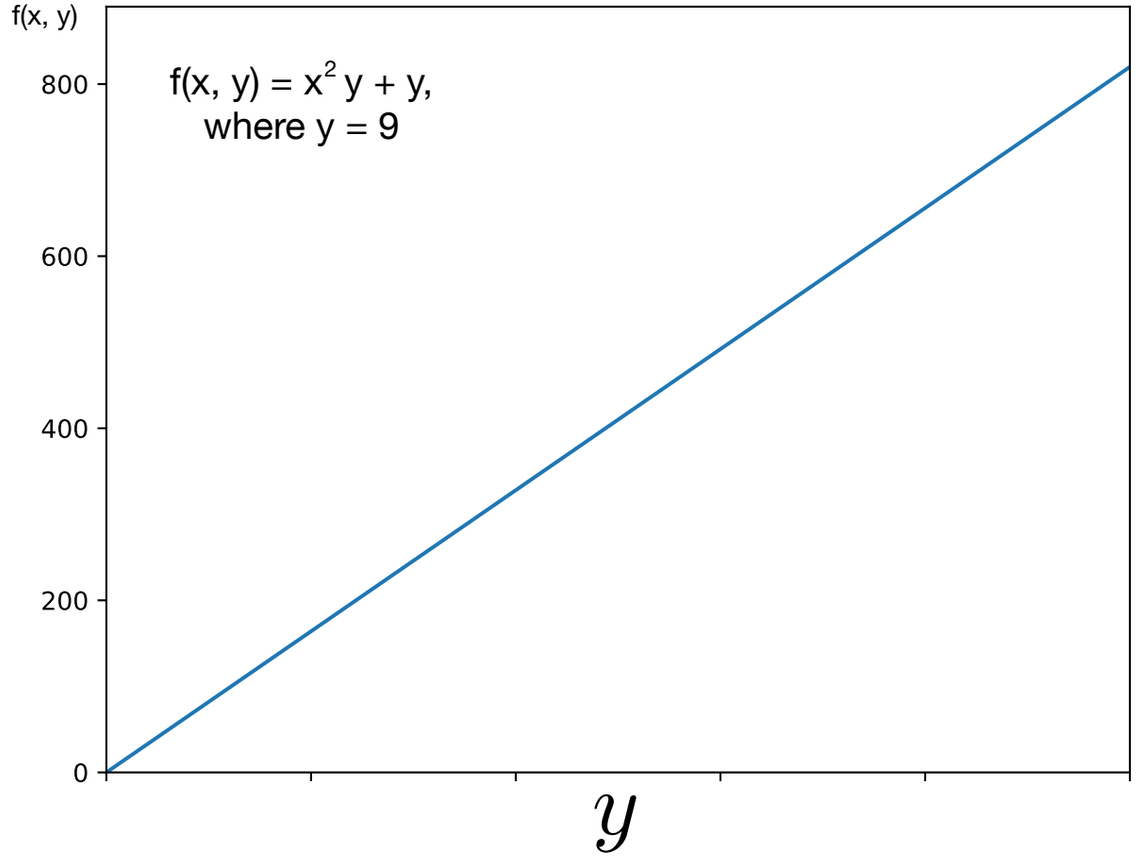
Gradients: Derivative of Multivariable Functions

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

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







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:

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

For two inputs, we now have

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

Gradients & the Multivariable Chain Rule

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

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

Example:

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

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

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

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

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

$$= 2xg^2 + 6gh + 2x$$

Gradients & the Multivariable Chain Rule in Vector Form

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

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

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)

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

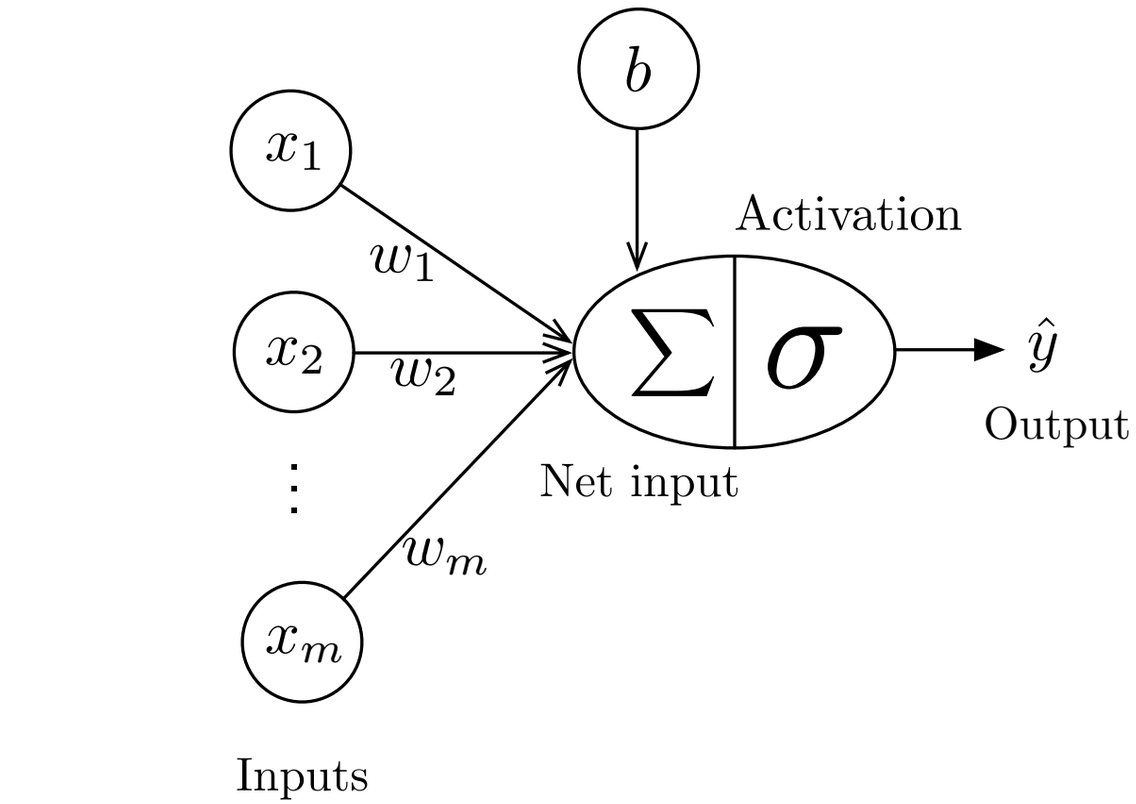
$$J\left(x_1, x_2, x_3, \cdots x_m\right) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial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

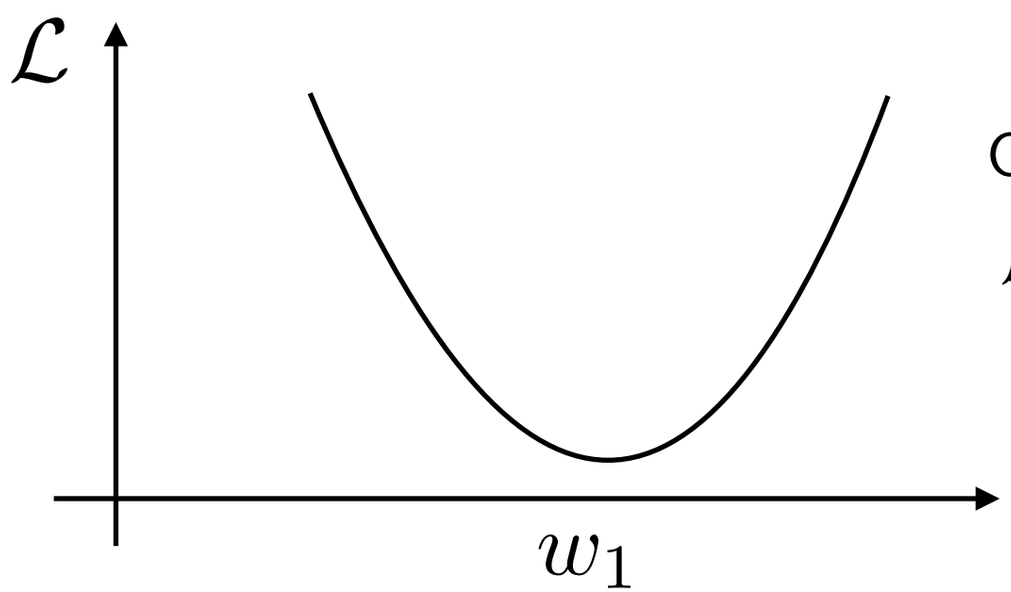
Second Order Derivatives

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

(End of the optional section)

Back to Linear Regression



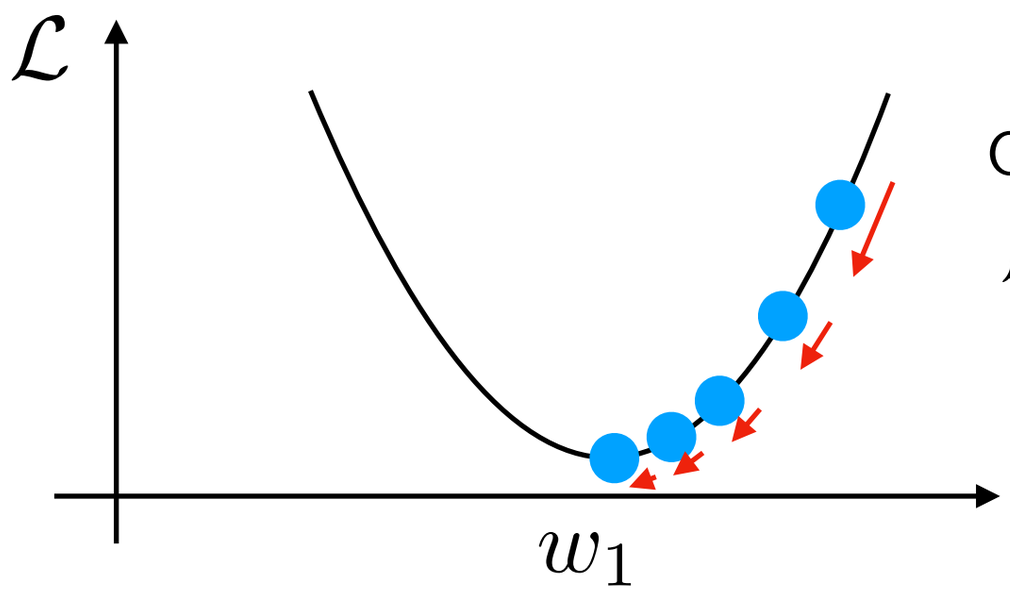


Convex loss function

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

Gradient Descent

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

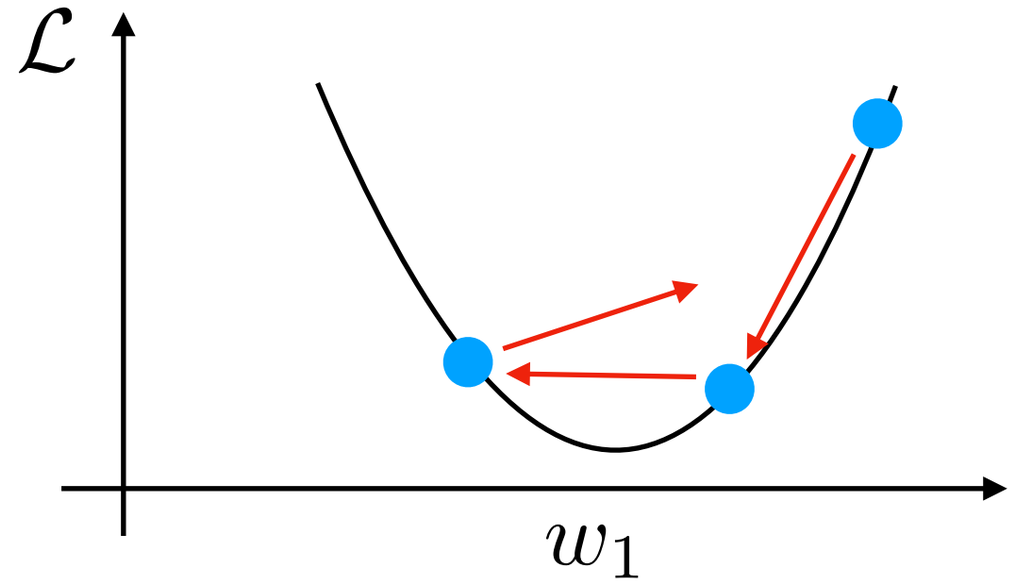


Convex loss function

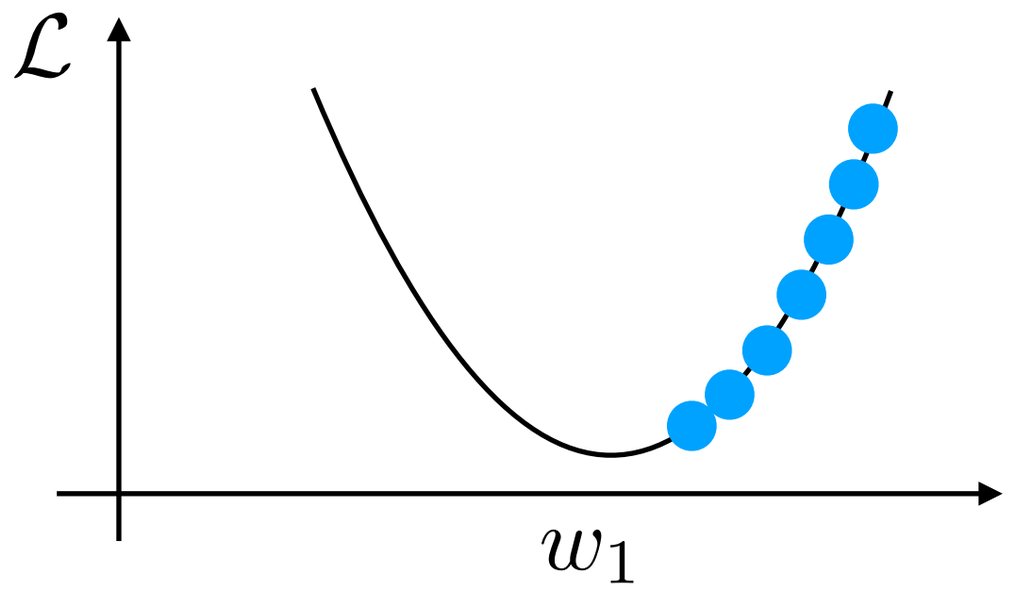
$$\mathcal{L}(\mathbf{w}, b) = \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

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

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial}{\partial w_j} \sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

$$= \frac{\partial}{\partial w_j} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]})^2$$

$$= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{\partial}{\partial w_j} (\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]})$$

$$= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} \frac{\partial}{\partial w_j} \mathbf{w}^T \mathbf{x}^{[i]}$$

$$= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) \frac{d\sigma}{d(\mathbf{w}^T \mathbf{x}^{[i]})} x_j^{[i]}$$

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

$$= \sum_i 2(\sigma(\mathbf{w}^T \mathbf{x}^{[i]}) - y^{[i]}) x_j^{[i]}$$

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

$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial}{\partial w_j}\frac{1}{2n}\sum_i (\hat{y}^{[i]} - y^{[i]})^2$$

$$= \frac{\partial}{\partial w_j}\sum_i \frac{1}{2n}(\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})^2$$

$$= \sum_i \frac{1}{n}(\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})\frac{\partial}{\partial w_j}(\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})$$

$$= \frac{1}{n}\sum_i (\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})\frac{d\sigma}{d(\mathbf{w}^T\mathbf{x}^{[i]})}\frac{\partial}{\partial w_j}\mathbf{w}^T\mathbf{x}^{[i]}$$

$$= \frac{1}{n}\sum_i (\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})\frac{d\sigma}{d(\mathbf{w}^T\mathbf{x}^{[i]})}x_j^{[i]}$$

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

$$= \frac{1}{n}\sum_i (\sigma(\mathbf{w}^T\mathbf{x}^{[i]}) - y^{[i]})x_j^{[i]}$$

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)

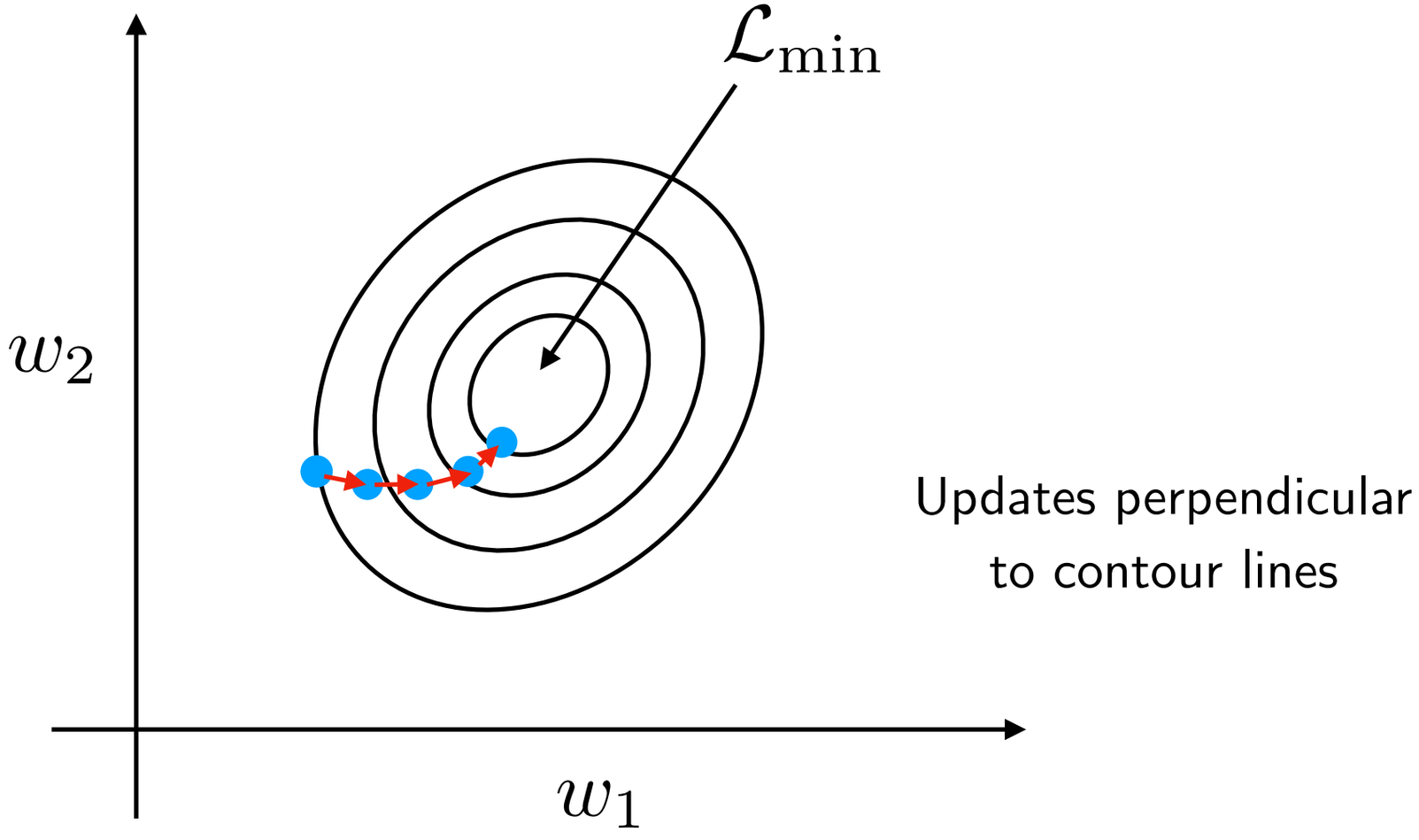
1. Initialize $\mathbf{w} := \mathbf{0} \in \mathbb{R}^m$, $\mathbf{b} := 0$
2. For every training epoch:
   - A. Initialize $\Delta\mathbf{w} := 0,\ \Delta b := 0$
   - B. For every $\{\langle \mathbf{x}^{[i]}, y^{[i]} \rangle, ..., \langle \mathbf{x}^{[i+k]}, y^{[i+k]} \rangle\} \subset \mathcal{D}$: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

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

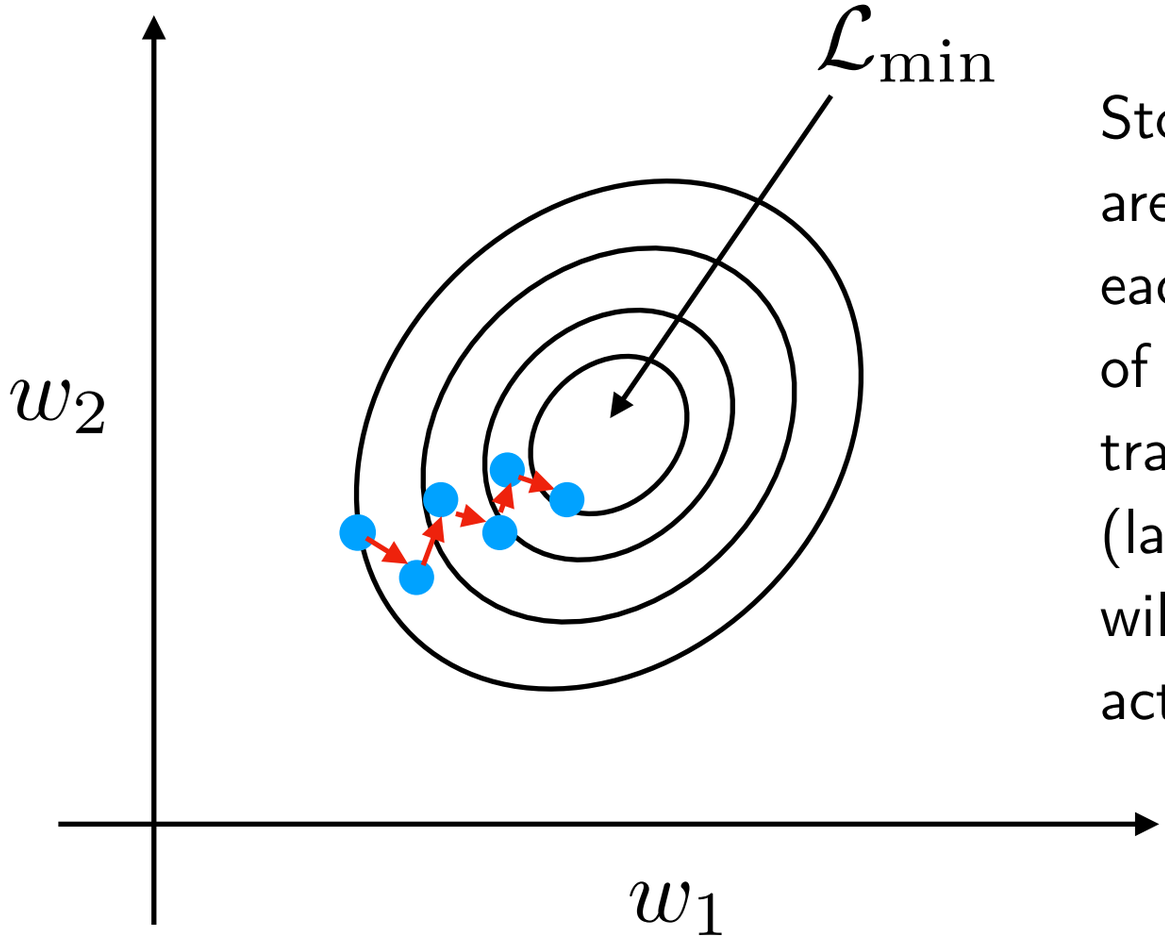
Most commonly used in DL, because

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

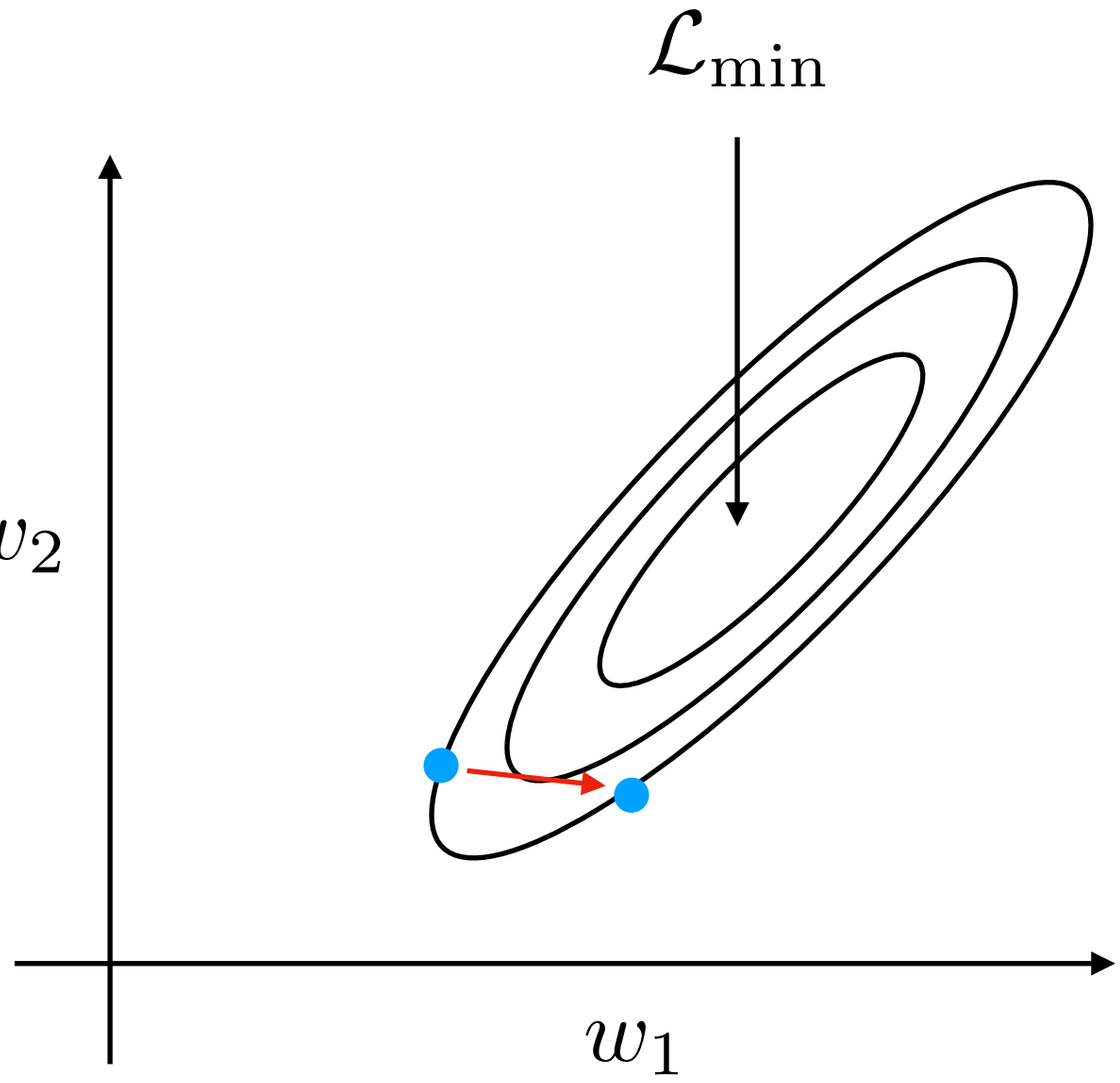


Stochastic Gradient Descent as Surface Plot



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!)

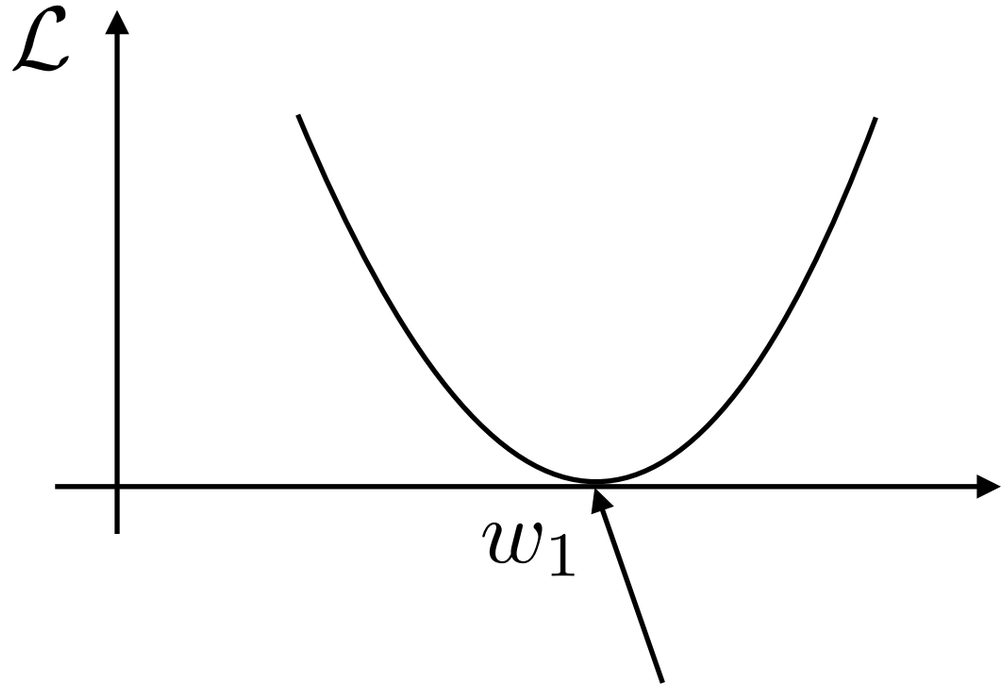
https://github.com/rasbt/stat453-deep-learning-ss20/blob/master/extras/good-andor-common-questions/L05-faq.pdf

Thu, Feb 13	Day 8	L05: Fitting Neurons with Gradient Descent	[L05 Slides] [L05 Code] [L05 Questions]	
Tue, Feb 18	Day 9	L06: Automatic Differentiation with PyTorch	[L06 Slides] [L06 Code]	
Thu, Feb 20	Day 10			
Tue,	Day 11			

Follow-up Explanations 1 (From Office Hours)

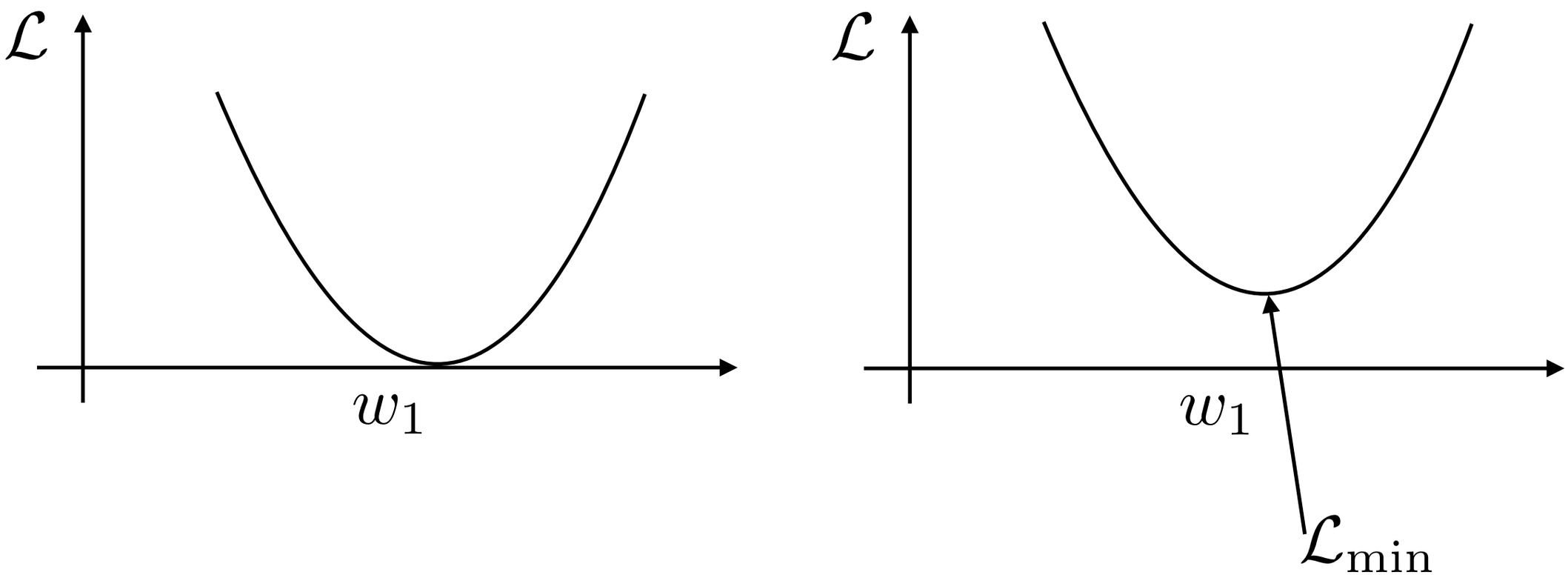
Why is the Loss convex?
Because we assumed it's the
Sum Squared Error (SSE) or Mean Squared Error (MSE)
(Not every loss is convex.)

$$SSE(y, \hat{y}) = \sum_i (y - \hat{y})^2$$



In Adaline (or linear regression), the SSE is 0 if we have a weight such that $y = \hat{y}$ for all y and $\hat{y}$. Also, note that the loss is symmetric because of the exponent "2."

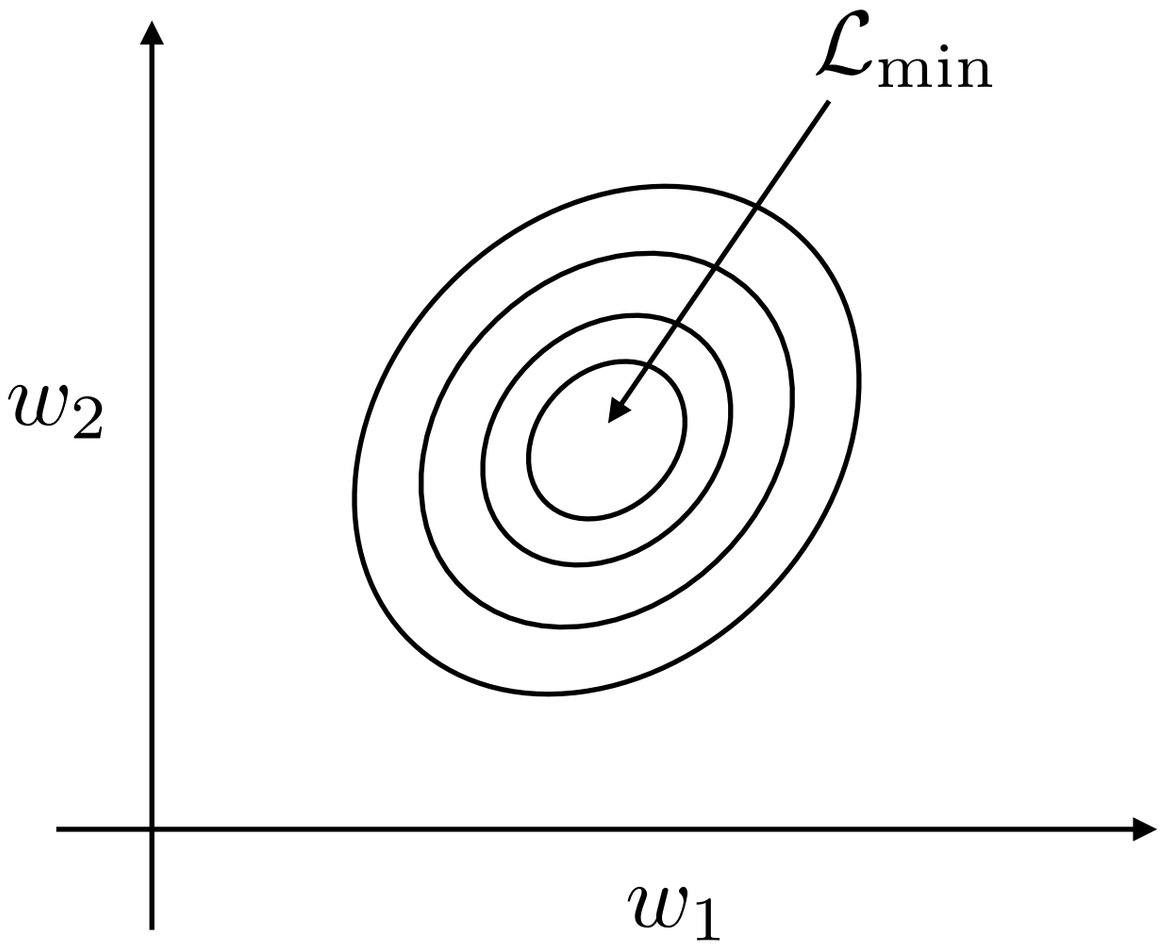
Follow-up Explanations 2 (From Office Hours)



Esp. for linear models, it is often not possible to achieve a zero loss even on the training data

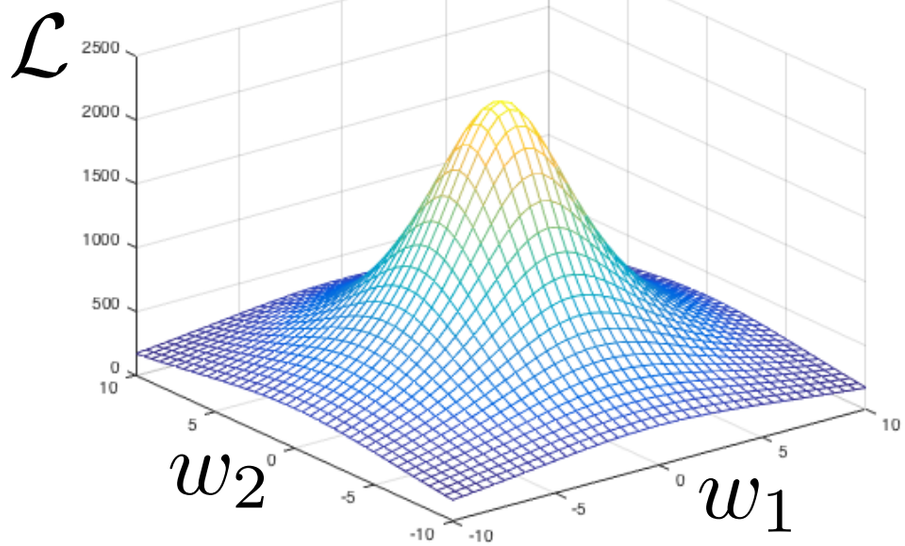
Follow-up Explanations 3 (From Office Hours)

What does this figure mean/show?

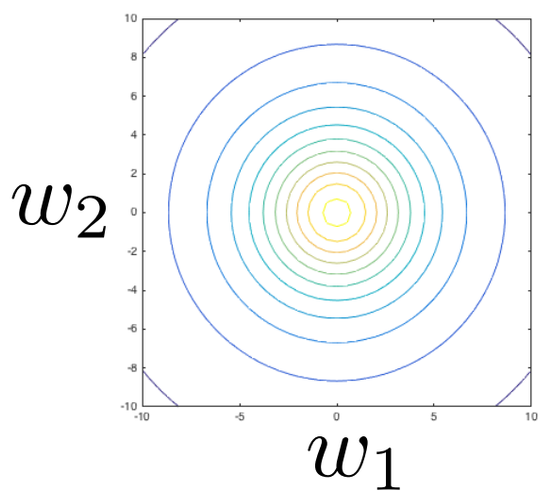


It's simply showing the loss plot (previous slide) for 2 instead of 1 weight

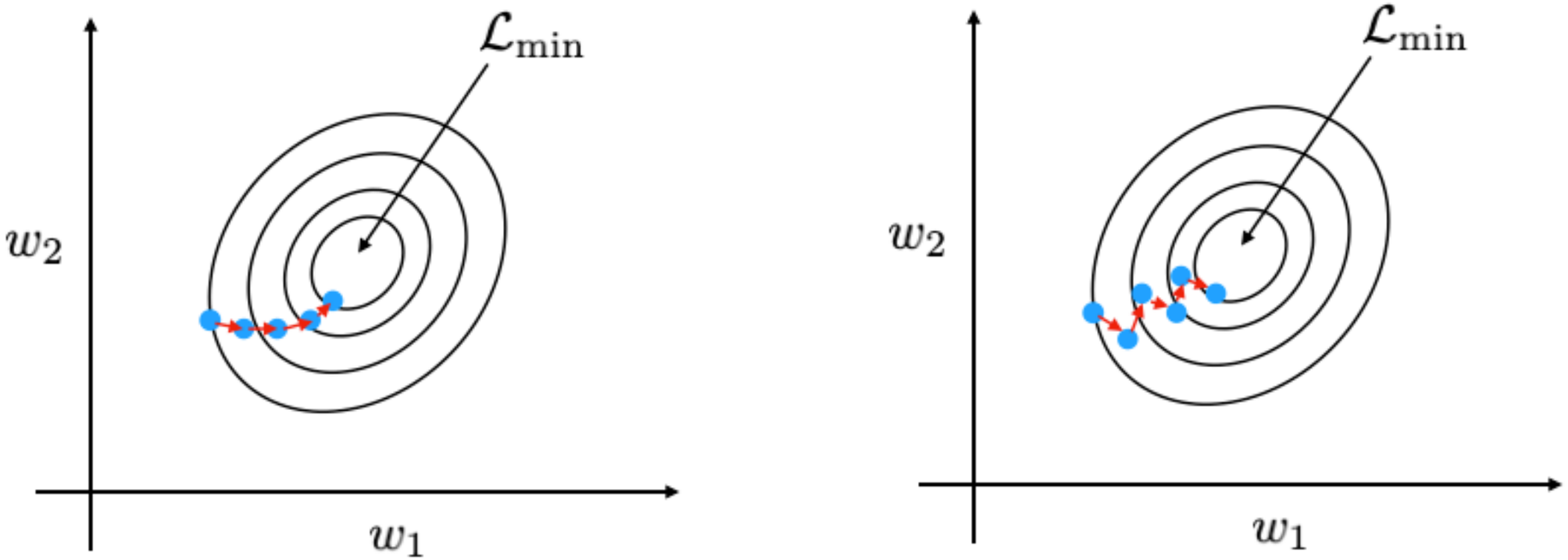
It's like this



It's like this but flattened



Follow-up Explanations 4 (From Office Hours)



Why is stochastic (on-line or minibatch) noisier than batch ("whole-training-set") gradient descent?

Follow-up Explanations 5 (From Office Hours)

Why is stochastic (on-line or minibatch) noisier than batch ("whole-training-set") gradient descent?

1. Imagine you are a scientist who develops a new pharmaceutical drug.
2. You want to know its average efficiency to further improve the formula.
3. In order to know the average effectiveness, you would have to test this on all patients in the world.
4. This would be very expensive and take a long time before you get feedback! (Like "batch gradient descent").
5. Instead, you select a smaller group of patients (like a "minibatch").
6. Your estimate will be an estimate of the true average effectiveness. The larger the sample size, the better your estimate but the higher the cost; assume a certain sample size is enough such that the estimate is accurate enough that it will point you in the right direction when developing your drug...

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."*.

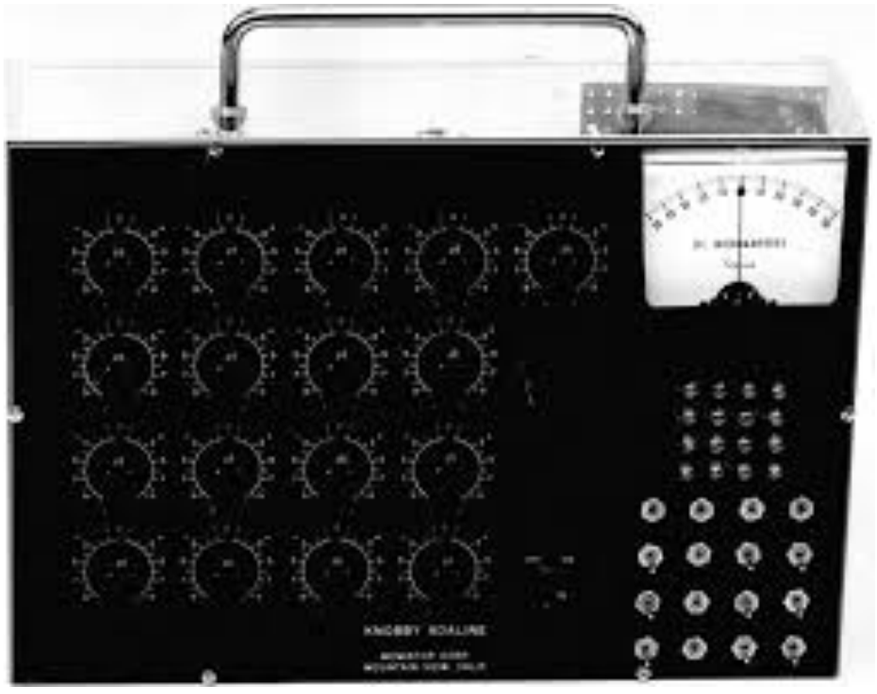
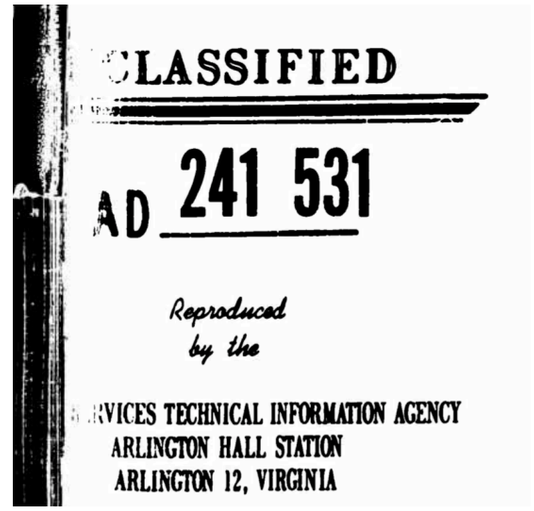


Image source: https://www.researchgate.net/profile/Alexander_Magoun2/publication/265789430/figure/fig2/AS:392335251787780@1470551421849/ADALINE-An-adaptive-linear-neuron-Manually-adapted-synapses-Designed-and-built-by-Ted.png



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ADALINE

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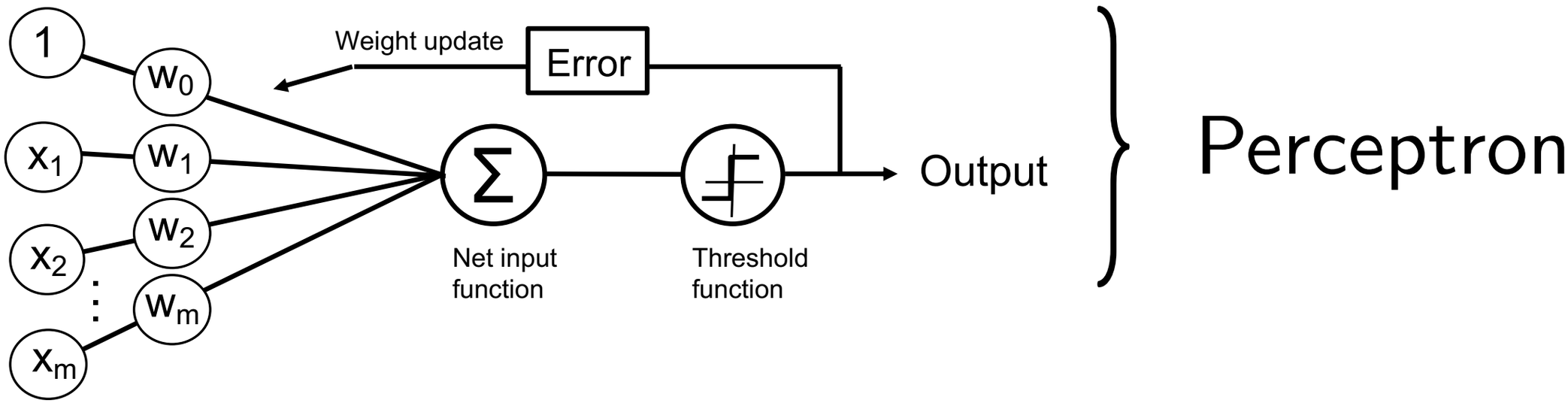

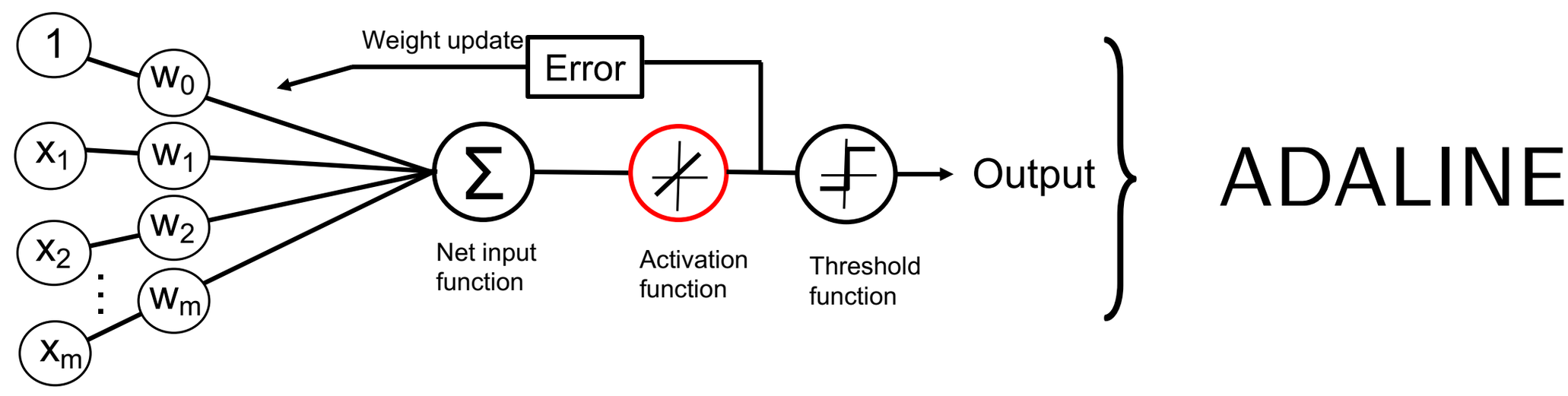

Code Examples

https://github.com/rasbt/stat453-deep-learning-ss20/tree/master/L05-grad-descent/code

(if link does not work yet, I haven't finished the examples; will do so soon)

Reading Assignments

Single-layer artificial neural networks

S. Raschka. *Python Machine Learning* (1st, 2nd, or 3rd ed.): Chapter 2

Calculus refresher

https://sebastianraschka.com/pdf/books/dlb/appendix_d_calculus.pdf

Fitting a model via closed-form equations vs. Gradient Descent vs Stochastic Gradient Descent vs Mini-Batch Learning. What is the difference?

https://sebastianraschka.com/faq/docs/closed-form-vs-gd.html

Next Lecture:

Neurons with non-linear activation functions