Optimization

CISC 7026: Introduction to Deep Learning

University of Macau

Previous Quiz

Quiz 1 grades are on moodle (mean 2.75 / 4)

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When I have a function called g that maps some inputs $a \in A, b \in B, c \in C$ to outputs $d \in D, e \in E$ I would write

$$g : A \times B \times C \mapsto D \times E$$

or

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In my code, I would write

$$d, e = g(a, b, c)$$

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So $f : \mathbb{R}^{d_x} \mapsto \mathbb{R}^{d_y}$ is a function that maps d_x numbers to d_y numbers

Admin

Assignment one should be graded next week

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Agenda

1. Review
2. Quiz
3. Optimization
4. Calculus review
5. Deriving linear regression
6. Gradient descent
7. Backpropagation
8. Coding

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We can solve these problems using linear regression too

Review

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We will write the vectors as

$$\boldsymbol{x}_{[i]} = \begin{bmatrix} x_{[i],1} \\ x_{[i],2} \\ \vdots \\ x_{[i],d_x} \end{bmatrix}$$

Review

The design matrix for a **multivariate** linear system is

$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1],d_x} & x_{[1],d_x-1} & \dots & x_{[1],1} & 1 \\ x_{[2],d_x} & x_{[2],d_x-1} & \dots & x_{[2],1} & 1 \\ \vdots & \vdots & \ddots & \vdots & \\ x_{[n],d_x} & x_{[n],d_x-1} & \dots & x_{[n],1} & 1 \end{bmatrix}$$

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The solution is the same as before

$$\boldsymbol{\theta} = \left(\boldsymbol{X}_D^\top \boldsymbol{X}_D\right)^{-1} \boldsymbol{X}_D^\top \boldsymbol{y}$$

Review

We combined **polynomial** and **multivariate** design matrices:

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One-dimensional polynomial functions

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Multi-dimensional linear functions

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$$\boldsymbol{X}_D = \begin{bmatrix} \boldsymbol{x}_{D,[1]} & \cdots & \boldsymbol{x}_{D,[n]} \end{bmatrix}^\top$$

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$$\begin{bmatrix} \underbrace{x^m_{[i],d_x} x^m_{[i],d_x-1} \dots x^m_{[i],1}}_{(d_x \Rightarrow 1, x^m)} & \underbrace{x^m_{[i],d_x} x^m_{[i],d_x-1} \dots x^m_{[i],2}}_{(d_x \Rightarrow 2, x^m)} & \cdots & \underbrace{x^{m-1}_{[i],d_x} x^{m-1}_{[i],d_x-1} \dots x^m_{[i],1}}_{(d_x \Rightarrow 1, x^{m-1})} & \cdots \end{bmatrix}$$

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The resulting design matrix is too large to solve

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We introduced neural networks because they scale to larger problems

Review

Brains and neural networks rely on **neurons**

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Brain: Biological neurons $\rightarrow$ Biological neural network

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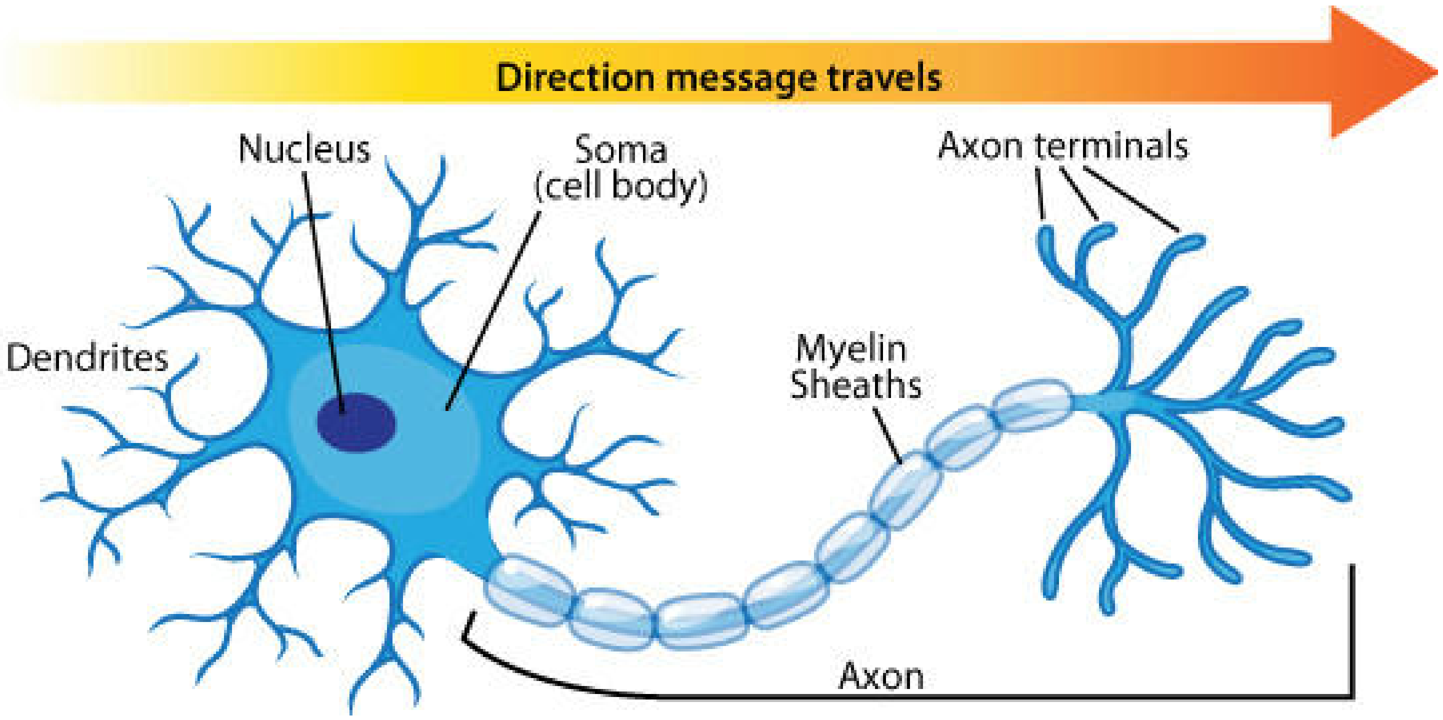
Brains and neural networks rely on **neurons**

Brain: Biological neurons $\rightarrow$ Biological neural network

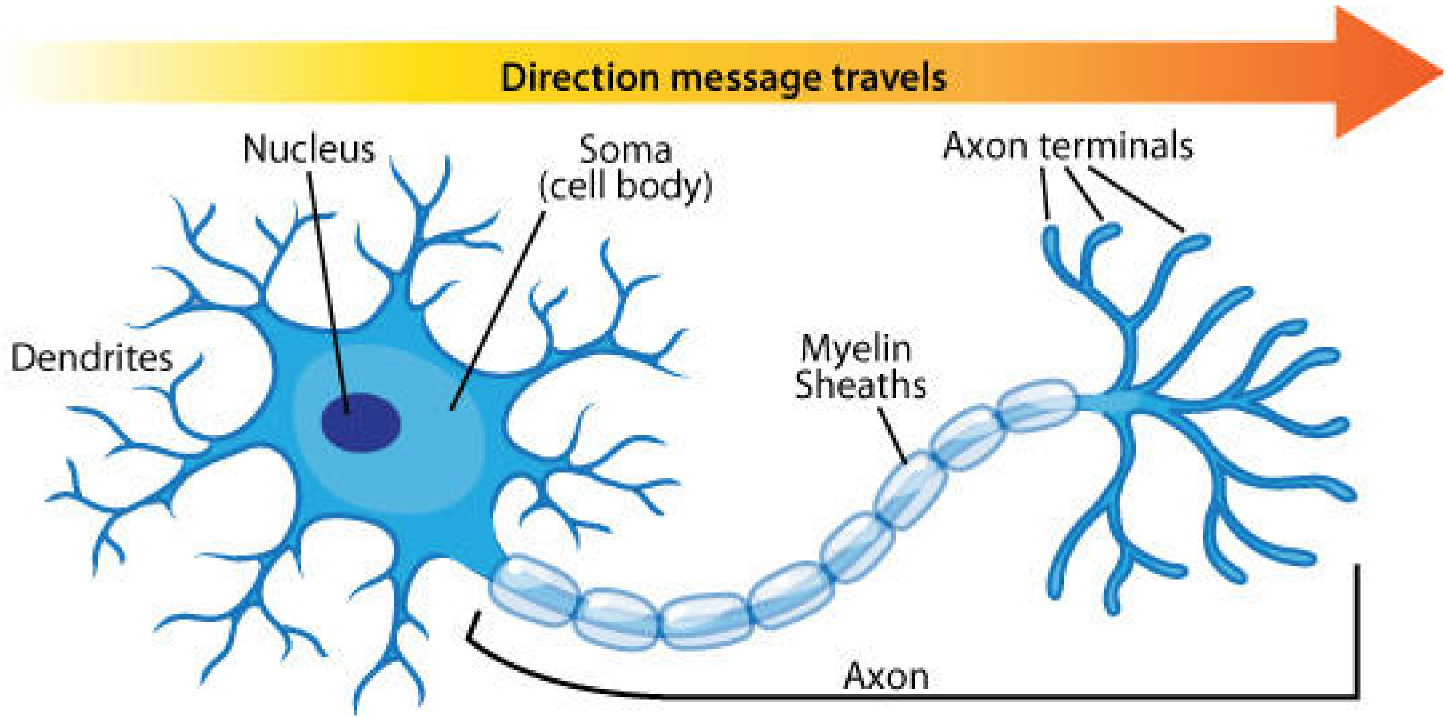
Computer: Artificial neurons $\rightarrow$ Artificial neural network

Review



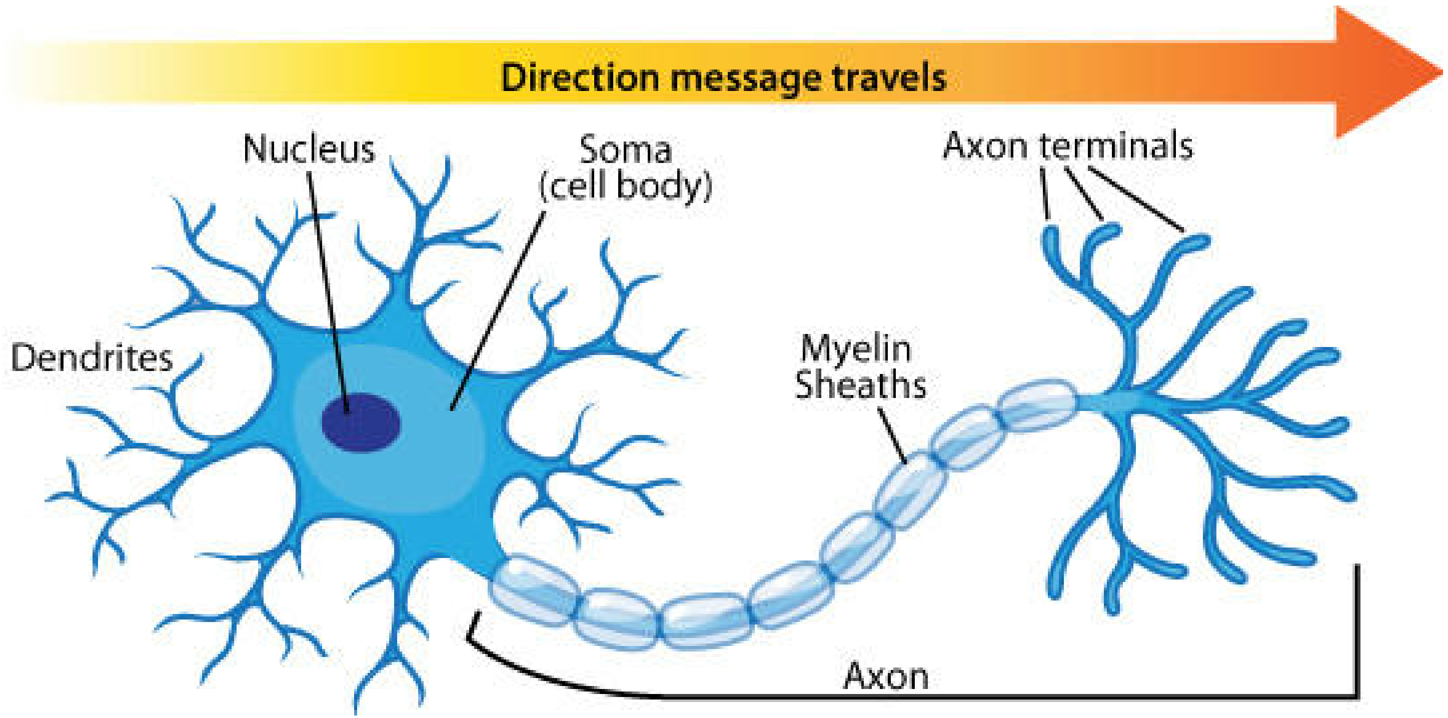
Neurons send messages based on messages received from other neurons

Review



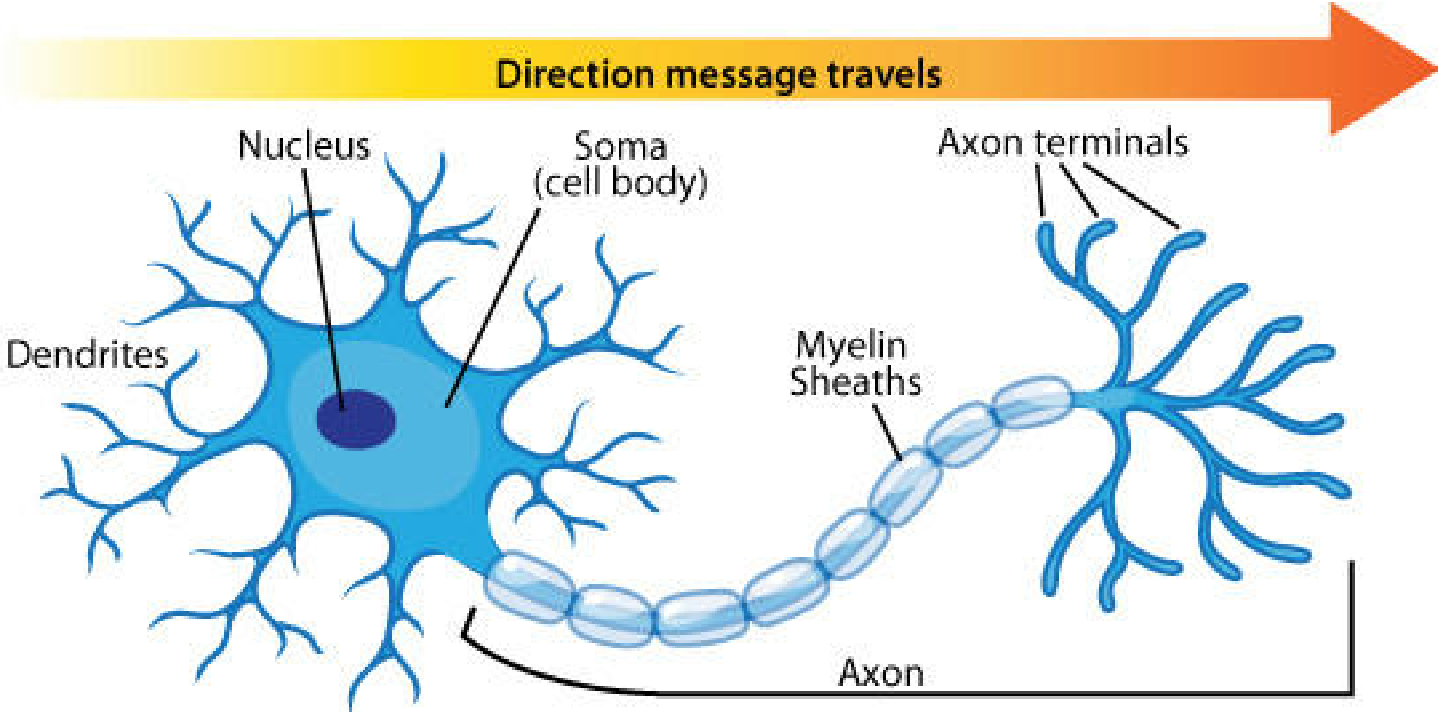
Incoming electrical signals travel along dendrites

Review



Electrical charges collect in the Soma (cell body)

Review



The axon outputs an electrical signal to other neurons

Review

How does a neuron decide to send an impulse (“fire”)?

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Dendrites form a parallel circuit

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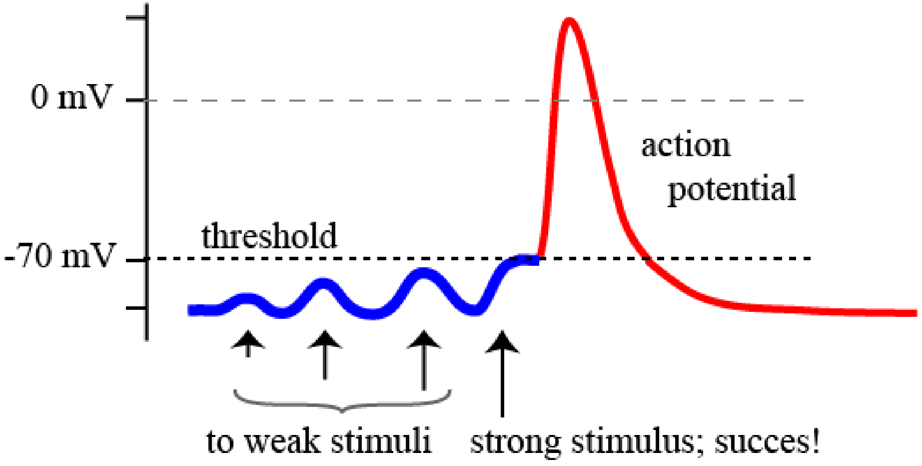

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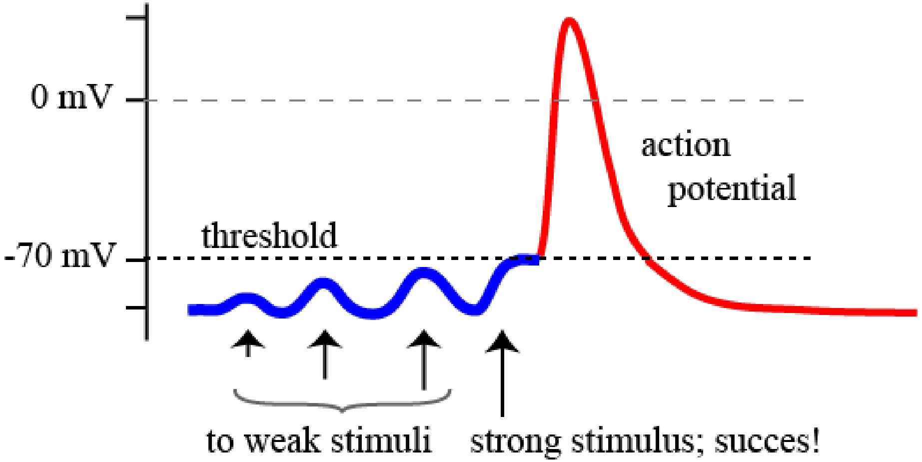

Many active dendrites will add together and trigger an impulse

Review

We model the neuron “firing” using an activation function σ

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Last time, we used the heaviside step function as the activation function

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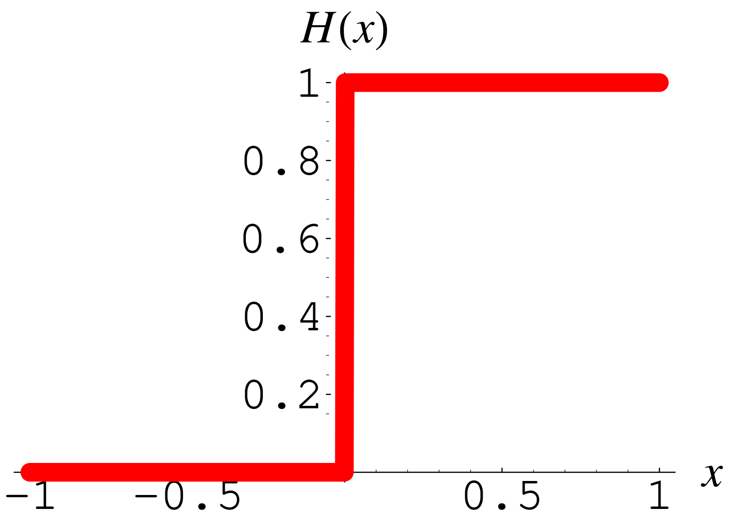

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We modeled a neuron mathematically, creating an artificial neuron

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}); \quad \overline{\boldsymbol{x}} = \begin{bmatrix} 1 \\ \boldsymbol{x} \end{bmatrix}$$

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$$f\left(\boldsymbol{x}, \begin{bmatrix} b \\ \boldsymbol{w} \end{bmatrix}\right) = \sigma(b + \boldsymbol{w}^\top \boldsymbol{x})$$

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An artificial neuron is a linear model with an activation function σ

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\underbrace{\theta_0 1 + \theta_1 x_1 + \ldots + \theta_{d_x} x_{d_x}}_{\text{Linear model}}\right)$$

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We can represent AND and OR boolean operators using a neuron

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So we take many neurons and create a neural network

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So we take many neurons and create a neural network

We discussed **wide** neural networks and **deep** neural networks

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How do we express a **wide** neural network mathematically?

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A single neuron:

$$f : \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}$$

$$\Theta \in \mathbb{R}^{d_x + 1}$$

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How do we express a **wide** neural network mathematically?

A single neuron:

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$$\Theta \in \mathbb{R}^{d_x + 1}$$

d_y neurons (wide):

$$f : \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}^{d_y}$$

$$\Theta \in \mathbb{R}^{(d_x + 1) \times d_y}$$

Review

For a wide network (also called a layer):

$$f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_{0,1} & \theta_{0,2} & \cdots & \theta_{0,d_y} \\ \theta_{1,1} & \theta_{1,2} & \cdots & \theta_{1,d_y} \\ \vdots & \vdots & \ddots & \vdots \\ \theta_{d_x,1} & \theta_{d_x,2} & \cdots & \theta_{d_x,d_y} \end{bmatrix}\right) = \begin{bmatrix} \sigma\left(\sum_{i=0}^{d_x} \theta_{i,1} \overline{x}_i\right) \\ \sigma\left(\sum_{i=0}^{d_x} \theta_{i,2} \overline{x}_i\right) \\ \vdots \\ \sigma\left(\sum_{i=0}^{d_x} \theta_{i,d_y} \overline{x}_i\right) \end{bmatrix}$$

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}); \quad \boldsymbol{\theta} \in \mathbb{R}^{(d_x+1) \times d_y}$$

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$$f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{W} \end{bmatrix}\right) = \sigma(\boldsymbol{b} + \boldsymbol{W}^\top \boldsymbol{x}); \quad \boldsymbol{b} \in \mathbb{R}^{d_y}, \boldsymbol{W} \in \mathbb{R}^{d_x \times d_y}$$

Review

A **wide** neural network is also called a **layer**

Review

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A **wide** neural network is also called a **layer**

A layer is a linear operation and an activation function

$$f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{W} \end{bmatrix}\right) = \sigma(\boldsymbol{b} + \boldsymbol{W}^\top \boldsymbol{x})$$

Review

Many layers makes a deep neural network

$$\boldsymbol{z}_1 = f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{b}_1 \\ \boldsymbol{W}_1 \end{bmatrix}\right)$$

$$\boldsymbol{z}_2 = f\left(\boldsymbol{z}_1, \begin{bmatrix} \boldsymbol{b}_2 \\ \boldsymbol{W}_2 \end{bmatrix}\right)$$

$$\boldsymbol{y} = f\left(\boldsymbol{z}_2, \begin{bmatrix} \boldsymbol{b}_2 \\ \boldsymbol{W}_2 \end{bmatrix}\right)$$

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Take out a paper and pen, write your name and student ID

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After I explain the questions, you will have 15 minutes to finish the quiz

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Optimization

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g can be a mapping from pictures to text, English to Chinese, etc

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But how do we find the $\boldsymbol{\theta}$ that makes $f(x, \boldsymbol{\theta}) = g(x) + \varepsilon$?

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Goal: Find the parameters $\boldsymbol{\theta}$ a neural network

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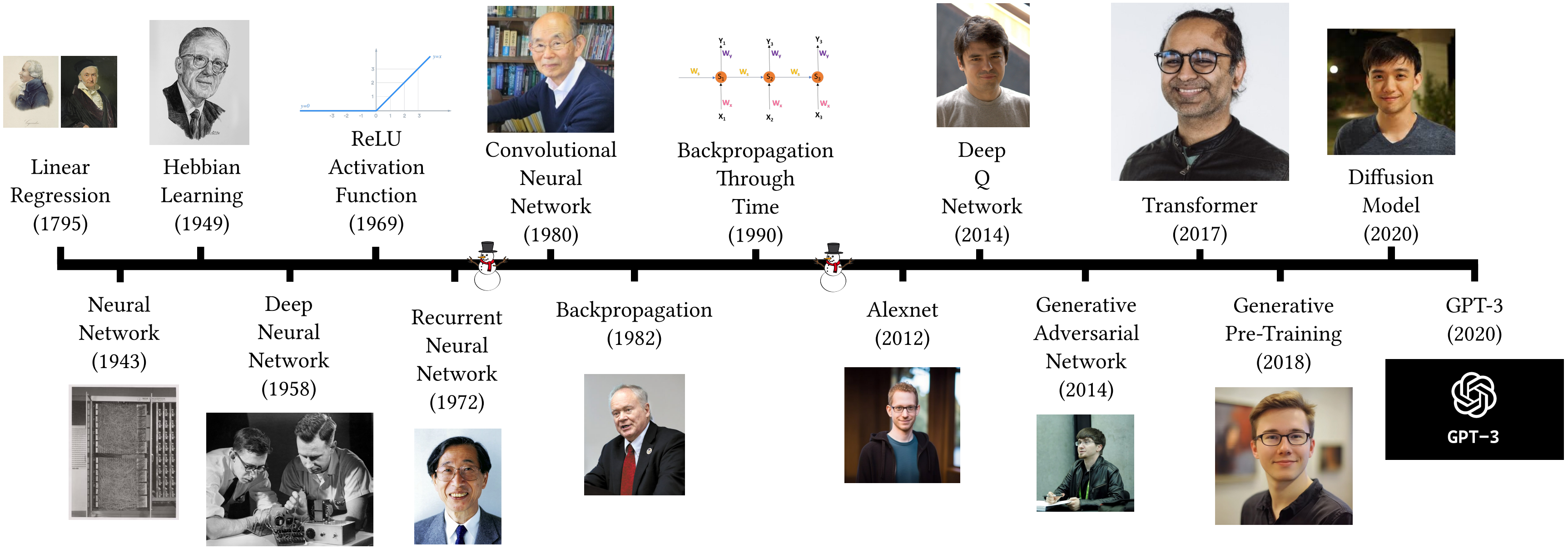
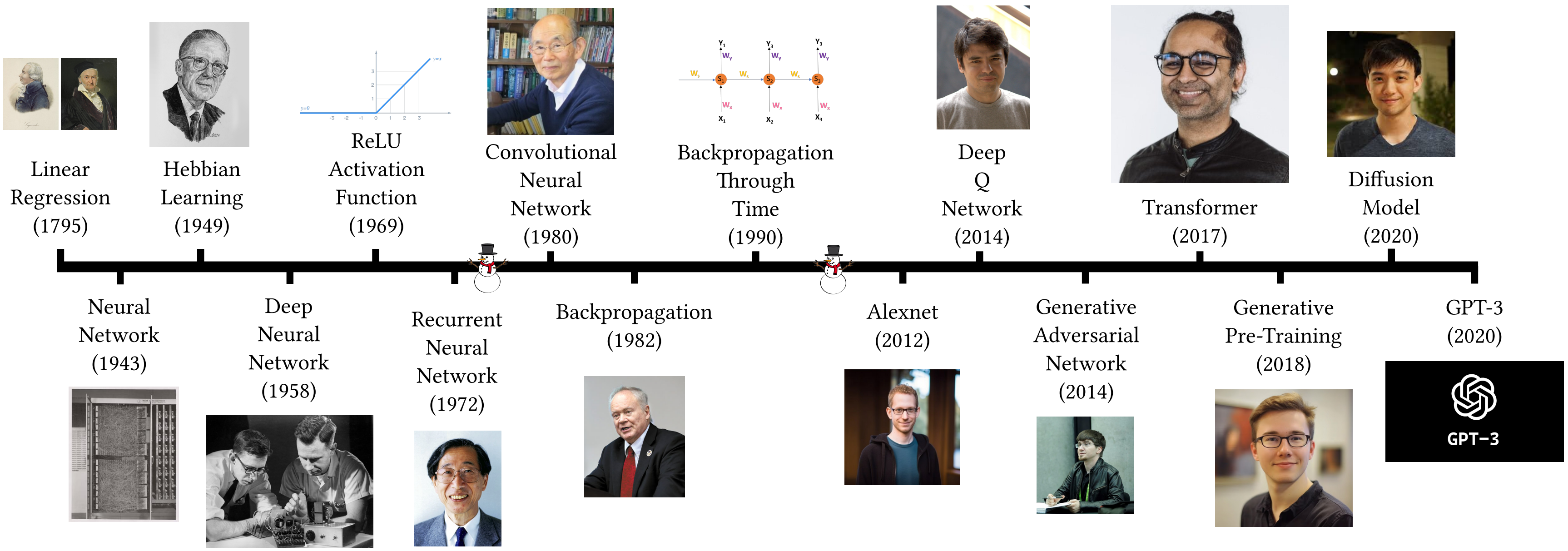
This expression looks very simple, but it can be very hard to evaluate

Optimization



Neural networks were discovered in 1943, but we could not train them until 1982!

Optimization



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This is why theory is important

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Recall how we found $\boldsymbol{\theta}$ in the linear regression problem

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We define the square error loss function

$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\right) - \boldsymbol{y}_{[i]} \right)^2$$

Optimization

Recall how we found $\boldsymbol{\theta}$ in the linear regression problem

We define the square error loss function

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Where does this solution come from? Can we do the same for neural networks?

Optimization

The solution for linear regression and neural networks comes from **calculus**

Optimization

The solution for linear regression and neural networks comes from **calculus**

The solution for neural networks also comes from calculus

Optimization

The solution for linear regression and neural networks comes from **calculus**

The solution for neural networks also comes from calculus

Let us review basic calculus concepts

Agenda

1. Review
2. Quiz
3. **Optimization**
4. Calculus review
5. Deriving linear regression
6. Gradient descent
7. Backpropagation
8. Coding

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Calculus Review

We write the **derivative** of a function f with respect to an input x as

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

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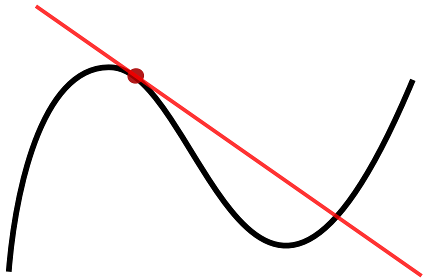

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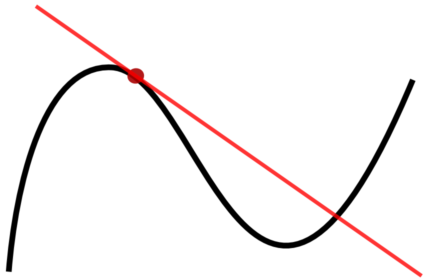

$$f(x), {\color{red} f'(x = a)}$$

Calculus Review

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The derivative takes a function f and outputs a new function f'

$$\frac{d}{dx} : [f : X \mapsto Y] \mapsto [f' : X \mapsto Y]$$

Calculus Review

There are formulas for computing the derivative of various operations

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Constant $$\frac{d}{dx} c = 0$$

Calculus Review

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Constant $$\frac{d}{dx} c = 0$$

Power $$\frac{d}{dx} x^n = n x^{n-1}$$

Calculus Review

Sum/Difference

$$\frac{d}{dx}[f(x) + g(x)] = f'(x) + g'(x)$$

Calculus Review

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Chain $$\frac{d}{dx}[f(g(x))] = f'(g(x))g'(x)$$

Calculus Review

For example, consider the function

$$f(x) = x^2 - 3x$$

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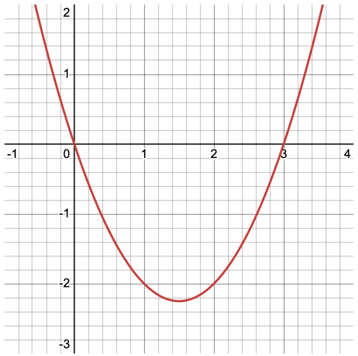
$$\frac{d}{dx}[f](1) = 2 \cdot 1 - 3 = -1$$

Calculus Review



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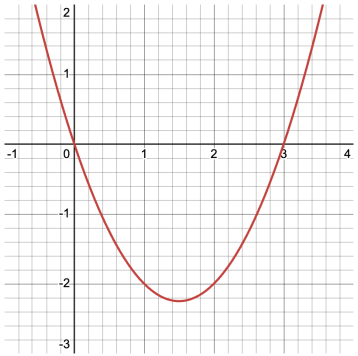

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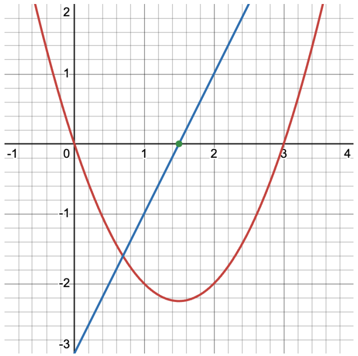

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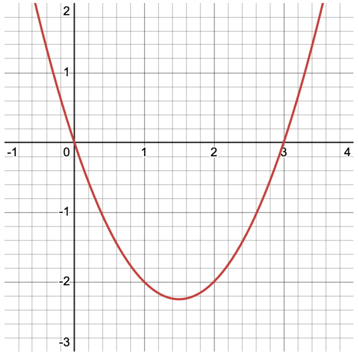
Calculus Review



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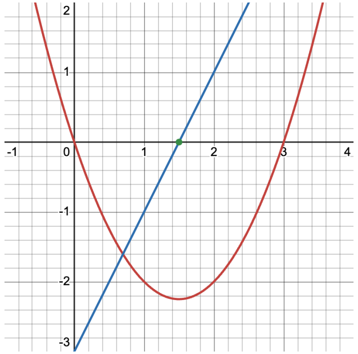

$$\frac{df}{dx} = 2x - 3$$

$$0 = 2x - 3 \quad \Rightarrow \quad x = \frac{3}{2}$$

Calculus Review

We can expand the definition of derivative to multivariate functions. We call this the **gradient**

$$\nabla_{\boldsymbol{x}} f\left(\begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}^\top\right) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \dots & \frac{\partial f}{\partial x_n} \end{bmatrix}^\top$$

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Partial derivatives behave similarly to standard derivatives

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$$\frac{\partial}{\partial x_1} f(x_1, ..., x_n) \approx \frac{d}{d x_1} f(x_1, ..., x_n)$$

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$$\frac{\partial}{\partial x_1} f(x_1, ..., x_n) \approx \frac{d}{d x_1} f(x_1, ..., x_n)$$

When computing $\frac{\partial}{\partial x_i} f(x_1, ..., x_n)$, we treat $x_1, ..., x_{i-1}, x_{i+1}, ..., x_n$ as constant

Calculus Review

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Calculus Review

In calculus, we can find the local extrema of a function $f(x)$ by finding where the derivative is zero

$$f'(x) = \frac{d}{dx} f(x) = 0$$

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With a multivariate function, the extrema lies where the gradient is zero

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \dots & \frac{\partial f}{\partial x_n} \end{bmatrix}^\top = \begin{bmatrix} 0 & 0 & \dots & 0 \end{bmatrix}^\top$$

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Deriving Linear Regression

Now that we remember calculus, let us revisit linear regression

Deriving Linear Regression

Now that we remember calculus, let us revisit linear regression

If we can derive the solution for linear regression, maybe we can apply it to deep neural networks

Deriving Linear Regression

In linear regression, our loss function is

$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta} \right) - \boldsymbol{y}_{[i]} \right)^2$$

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Deriving Linear Regression

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Deriving Linear Regression

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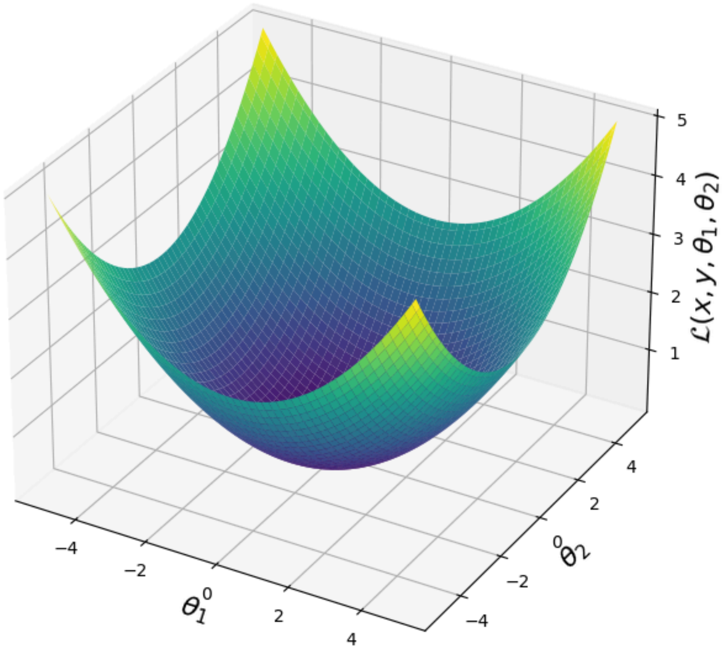
A quadratic function has a single minima! The minima must be at

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = 0$$



Deriving Linear Regression

Therefore, we know that the $\boldsymbol{\theta}$ that solves

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Also solves

$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$$

Deriving Linear Regression

Using calculus, let us derive the solution to linear regression

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$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \left[(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta}) \right]$$

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$$= \nabla_{\boldsymbol{\theta}} \left[\boldsymbol{Y}^\top \boldsymbol{Y} - \boldsymbol{Y}^\top \boldsymbol{X}_D \boldsymbol{\theta} - (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{Y} + (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{X}_D \boldsymbol{\theta} \right]$$

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$$= \boldsymbol{0} - \boldsymbol{Y}^\top \boldsymbol{X}_D \boldsymbol{I} - (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{Y} + (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{X}_D \boldsymbol{\theta} + (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{X}_D \boldsymbol{I}$$

Deriving Linear Regression

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Deriving Linear Regression

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Deriving Linear Regression

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Remember, $(\boldsymbol{A}\boldsymbol{B})^\top = \boldsymbol{B}^\top \boldsymbol{A}^\top$, and so $\boldsymbol{Y}^\top \boldsymbol{X}_D = \boldsymbol{Y}^\top \left(\boldsymbol{X}_D^\top\right)^\top = \boldsymbol{X}_D^\top \boldsymbol{Y}$

Deriving Linear Regression

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Deriving Linear Regression

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$$= -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X} \boldsymbol{\theta}$$

Deriving Linear Regression

$$= \mathbf{0} - \boldsymbol{Y}^\top \boldsymbol{X}_D \boldsymbol{I} - (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{Y} + (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{X}_D \boldsymbol{\theta} + (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{X}_D \boldsymbol{I}$$

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$$= -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X} \boldsymbol{\theta}$$

And so, the gradient of the loss is

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X}_D \boldsymbol{\theta}$$

Deriving Linear Regression

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = -2 \boldsymbol{X}_D^\top \boldsymbol{Y} + 2 \boldsymbol{X}_D^\top \boldsymbol{X}_D \boldsymbol{\theta}$$

Deriving Linear Regression

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X}_D \boldsymbol{\theta}$$

We want to find the $\boldsymbol{\theta}$ that makes the gradient of the loss zero

Deriving Linear Regression

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X}_D \boldsymbol{\theta}$$

We want to find the $\boldsymbol{\theta}$ that makes the gradient of the loss zero

$$\boldsymbol{0} = -2\boldsymbol{X}_D^\top \boldsymbol{Y} + 2\boldsymbol{X}_D^\top \boldsymbol{X}_D \boldsymbol{\theta}$$

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Great! We derived the solution to linear regression

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Step 1: Write the loss function for a neural network

Deriving Linear Regression

Like linear regression, we can use square error for a neural network

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Linear regression: $$f(x, y, \boldsymbol{\theta}) = \theta_0 + \theta_1 x$$

Perceptron: $$f(x, y, \boldsymbol{\theta}) = \sigma(\theta_0 + \theta_1 x)$$

Deriving Linear Regression

$$\mathcal{L}(x, y, \boldsymbol{\theta}) = (f(x, \boldsymbol{\theta}) - y)^2$$

Loss function

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Neural network model

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Now, we plug the model f into the loss function

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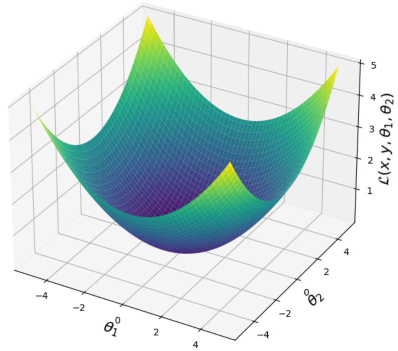
Deriving Linear Regression

Linear regression loss function was quadratic with one minima



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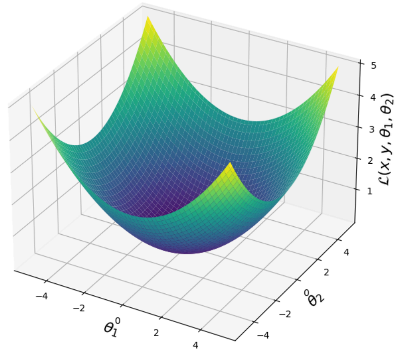

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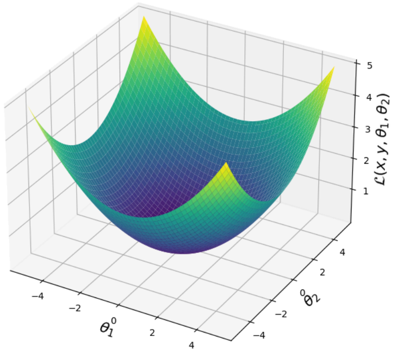

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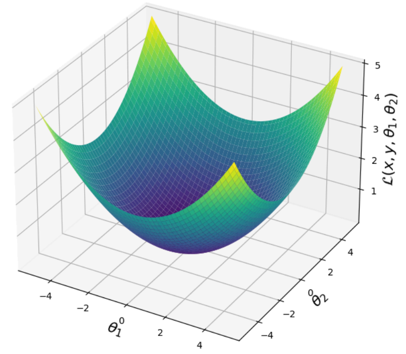

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Question: How many minima does this function have?

Answer: We do not know

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Activation functions make the neural network powerful

Deriving Linear Regression

Linear regression: analytical solution for $\boldsymbol{\theta}$

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Neural network: no analytical solution for $\boldsymbol{\theta}$

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So how to find $\boldsymbol{\theta}$ for a neural network?

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Gradient Descent

To find $\boldsymbol{\theta}$ for a neural network, we use **gradient descent**

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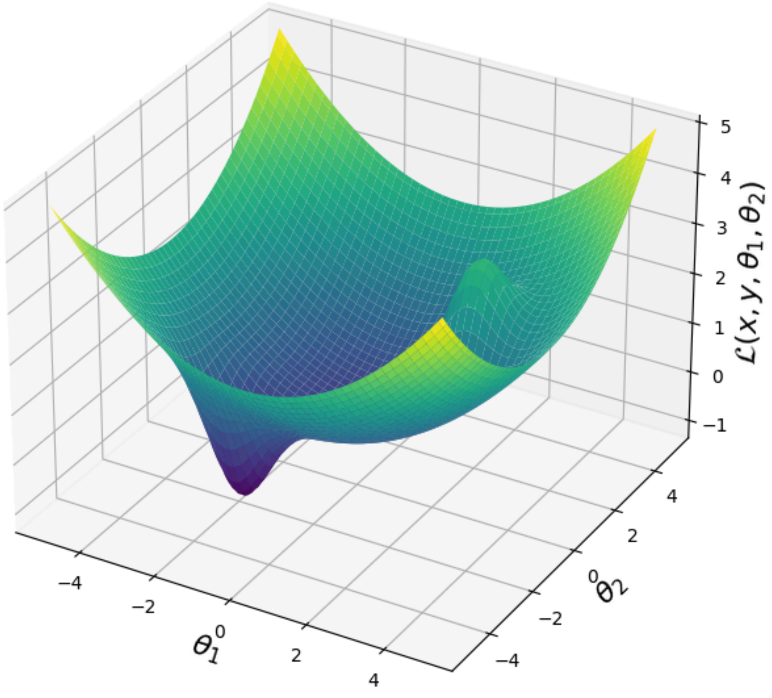
How does gradient descent work?

Gradient Descent

A differentiable loss function produces a manifold



Gradient Descent

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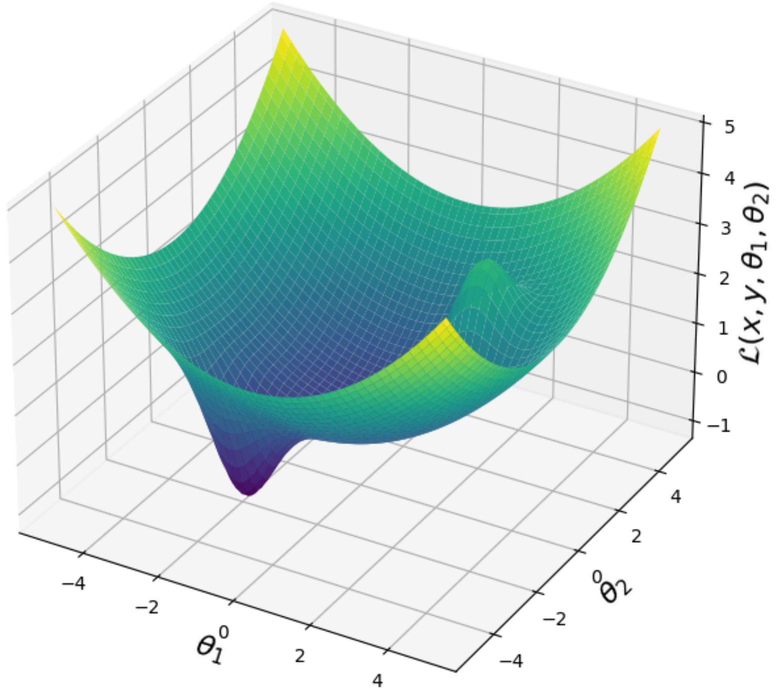

Our goal is to find the lowest point on this manifold

Gradient Descent

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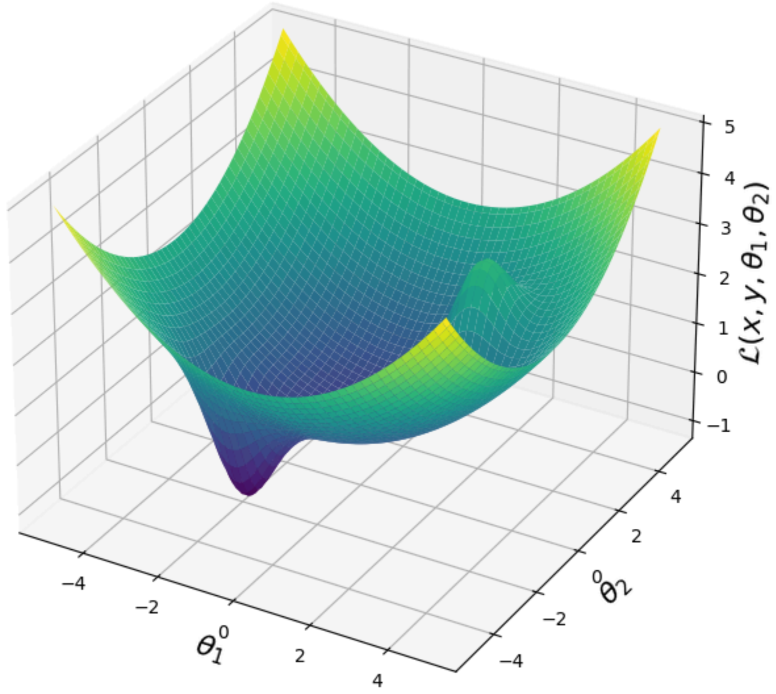

Our goal is to find the lowest point on this manifold

The lowest point solves $\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

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Note: Gradient descent provides a **local** optima, not necessarily a **global** optima

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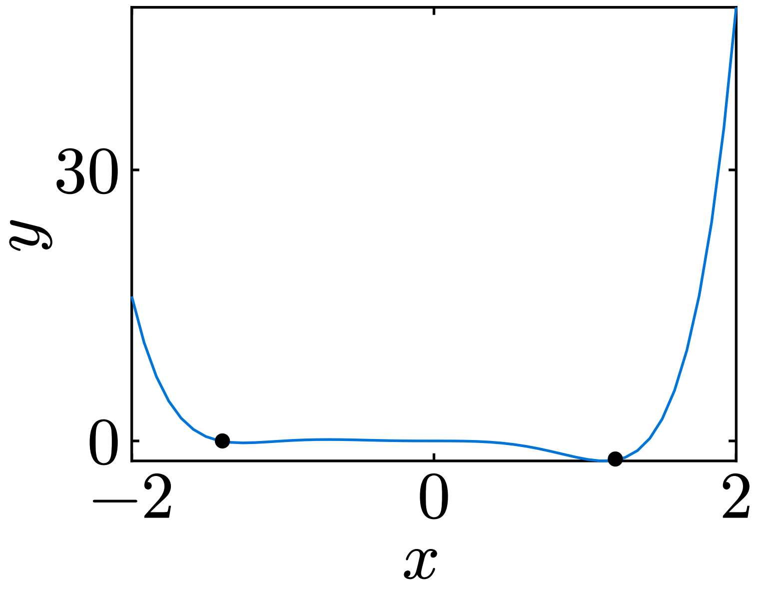
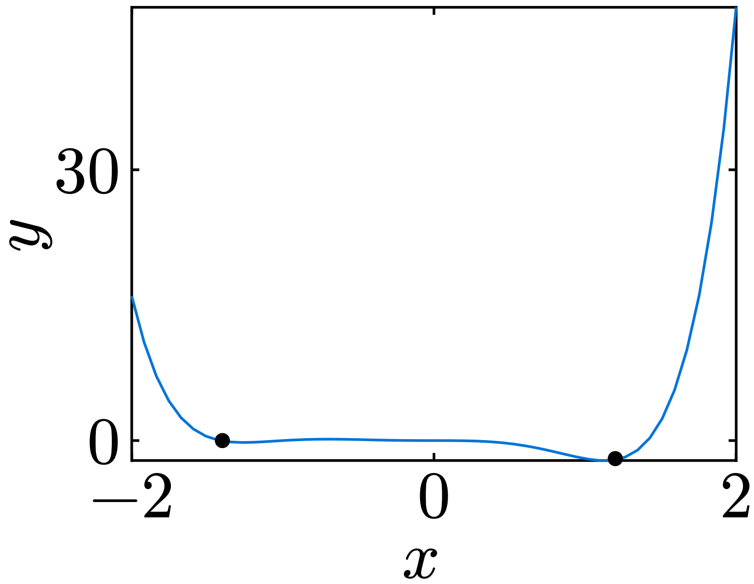


Gradient Descent

Note: Gradient descent provides a **local** optima, not necessarily a **global** optima



In practice, a local optima provides a good enough model

Relax

Gradient Descent

Let us define gradient descent without math

Gradient Descent

Let us define gradient descent without math

You are on the top of a mountain and there is lightning storm

Gradient Descent

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Let us define gradient descent without math

You are on the top of a mountain and there is lightning storm

For safety, you should walk down the mountain to escape the lightning

Gradient Descent

But you do not know the path down!

Gradient Descent

But you do not know the path down!

You see this, which way do you walk next?

Gradient Descent

This is gradient descent

Gradient Descent

In gradient descent, we look at the **slope** of the loss function

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And we walk in the steepest direction

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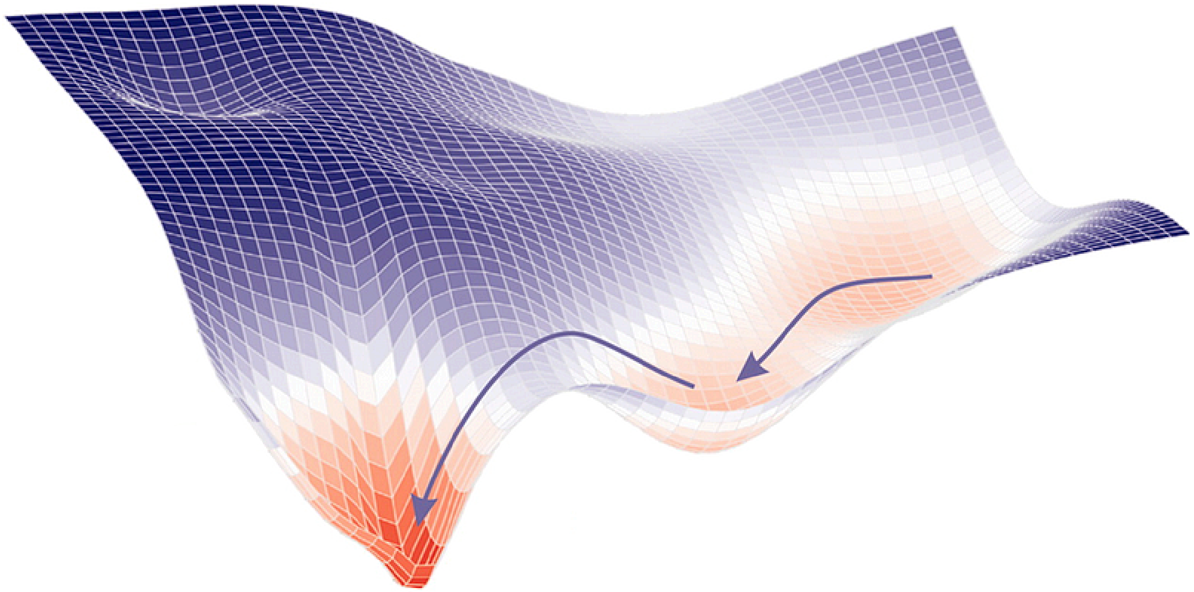

Gradient Descent

In gradient descent, we look at the **slope** of the loss function

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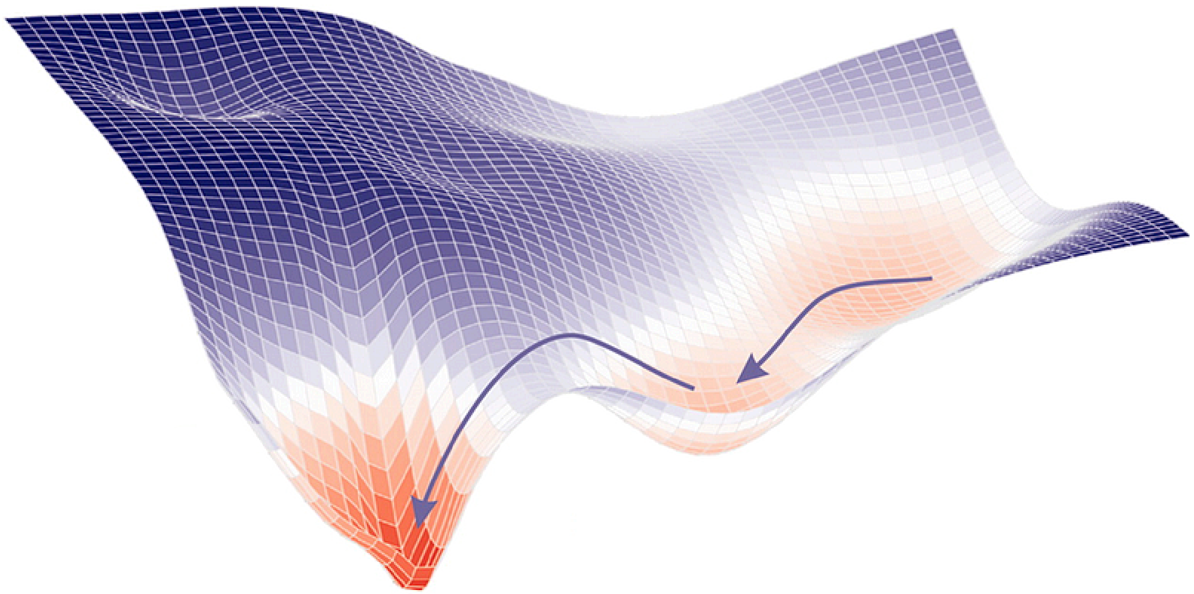
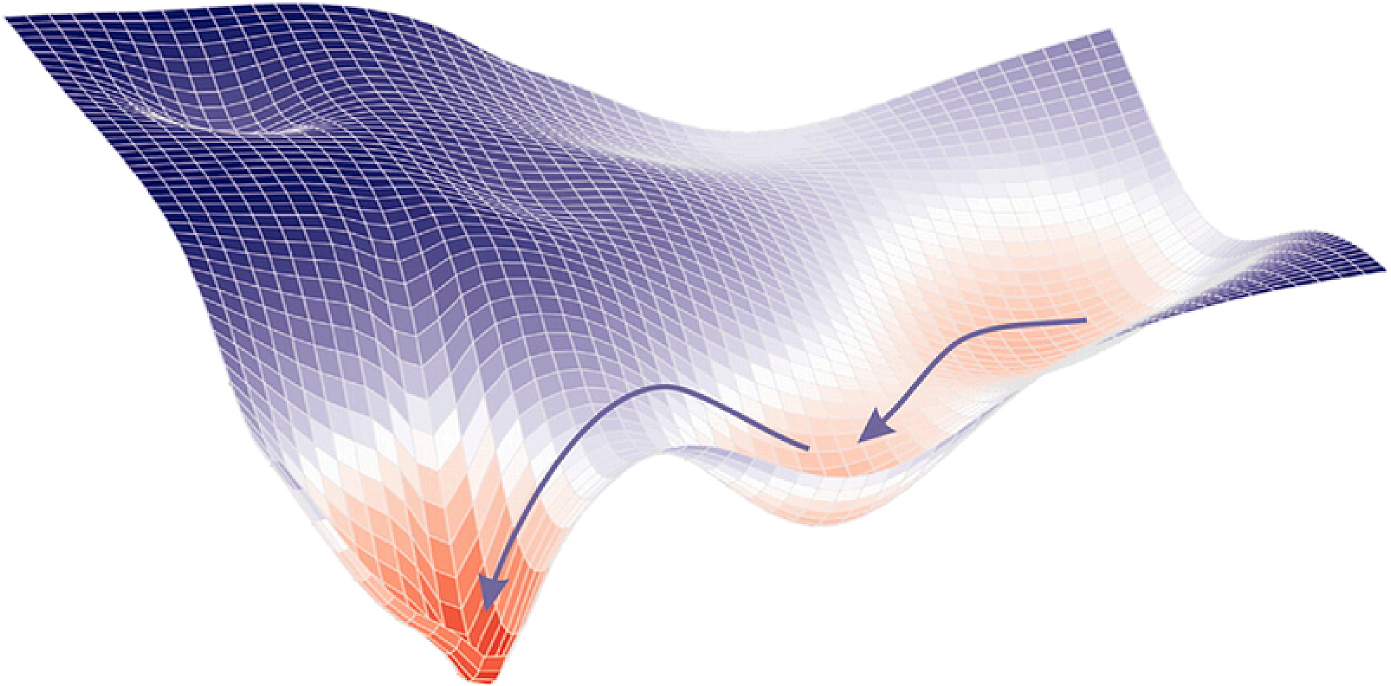
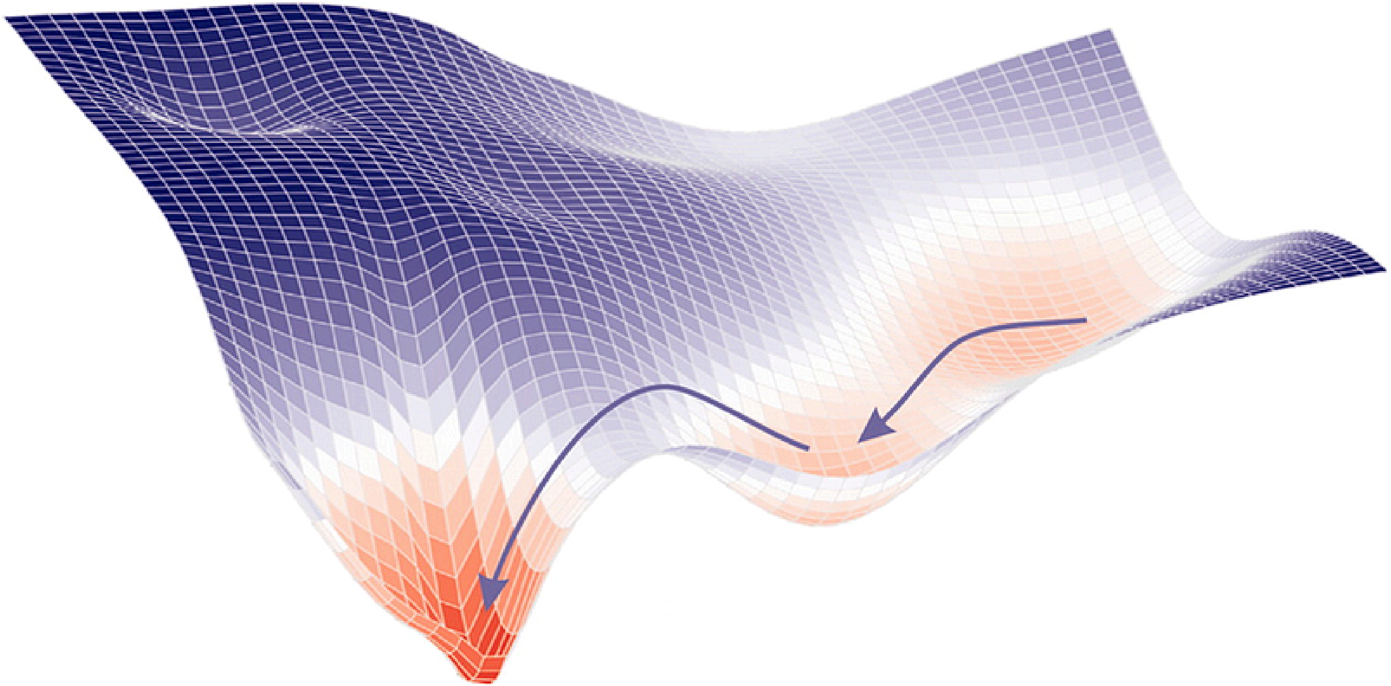


And then we repeat

Gradient Descent

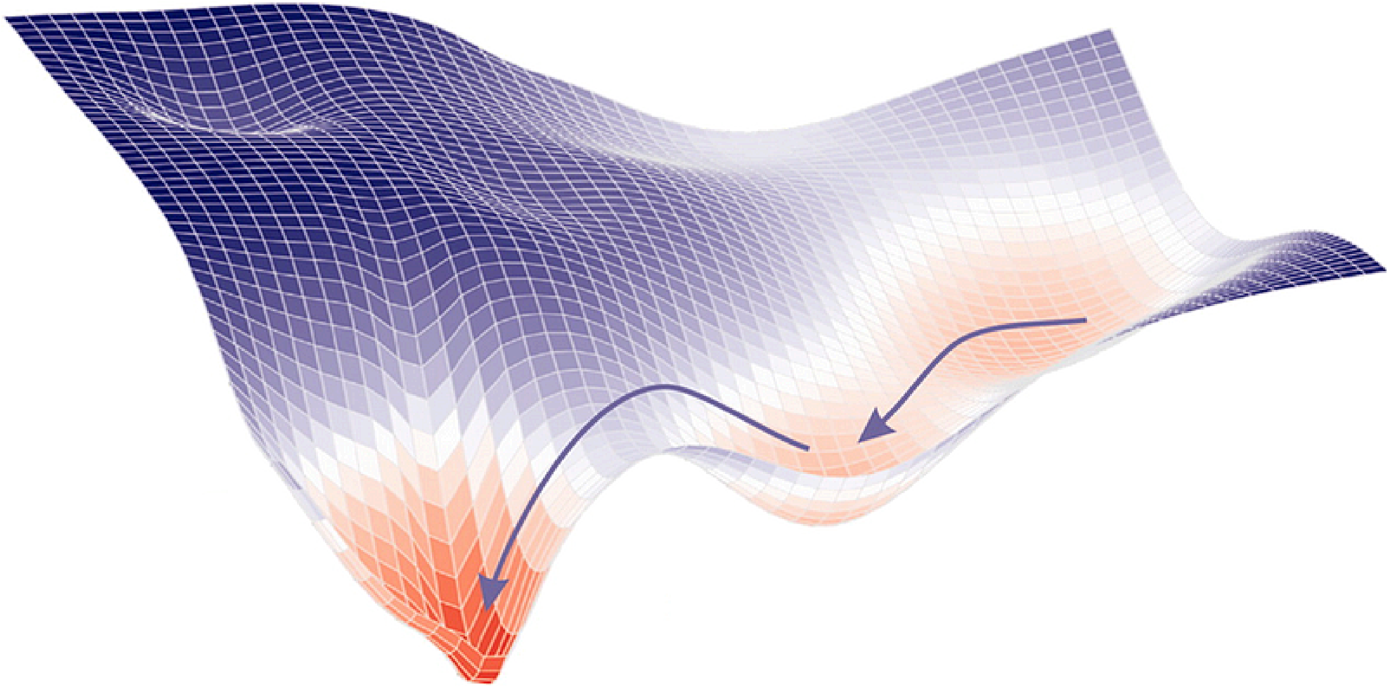


Gradient Descent



We find the gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

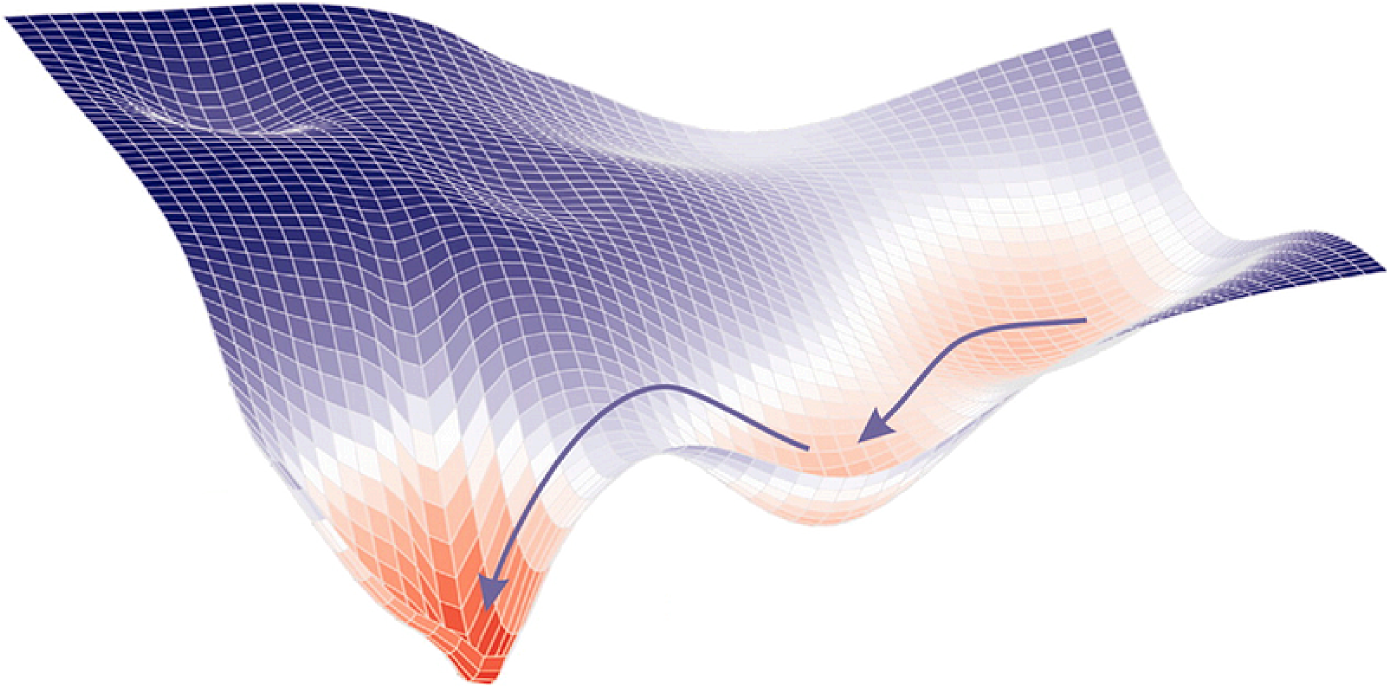
Gradient Descent



We find the gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

And update $\boldsymbol{\theta}$ in the steepest direction

Gradient Descent



Eventually, we arrive at the bottom

Gradient Descent

With gradient descent, the loss function must be differentiable

Gradient Descent

With gradient descent, the loss function must be differentiable

If we cannot compute the derivative/gradient, then we do not know which way to walk!

Gradient Descent

The gradient descent algorithm:

function Gradient Descent($\boldsymbol{X}$, $\boldsymbol{Y}$, $\mathcal{L}$, t, α)

  ▷ Randomly initialize parameters

  $\boldsymbol{\theta} \leftarrow \mathcal{N}(0, 1)$

  for $i \in 1...t$ **do**

    ▷ Compute the gradient of the loss

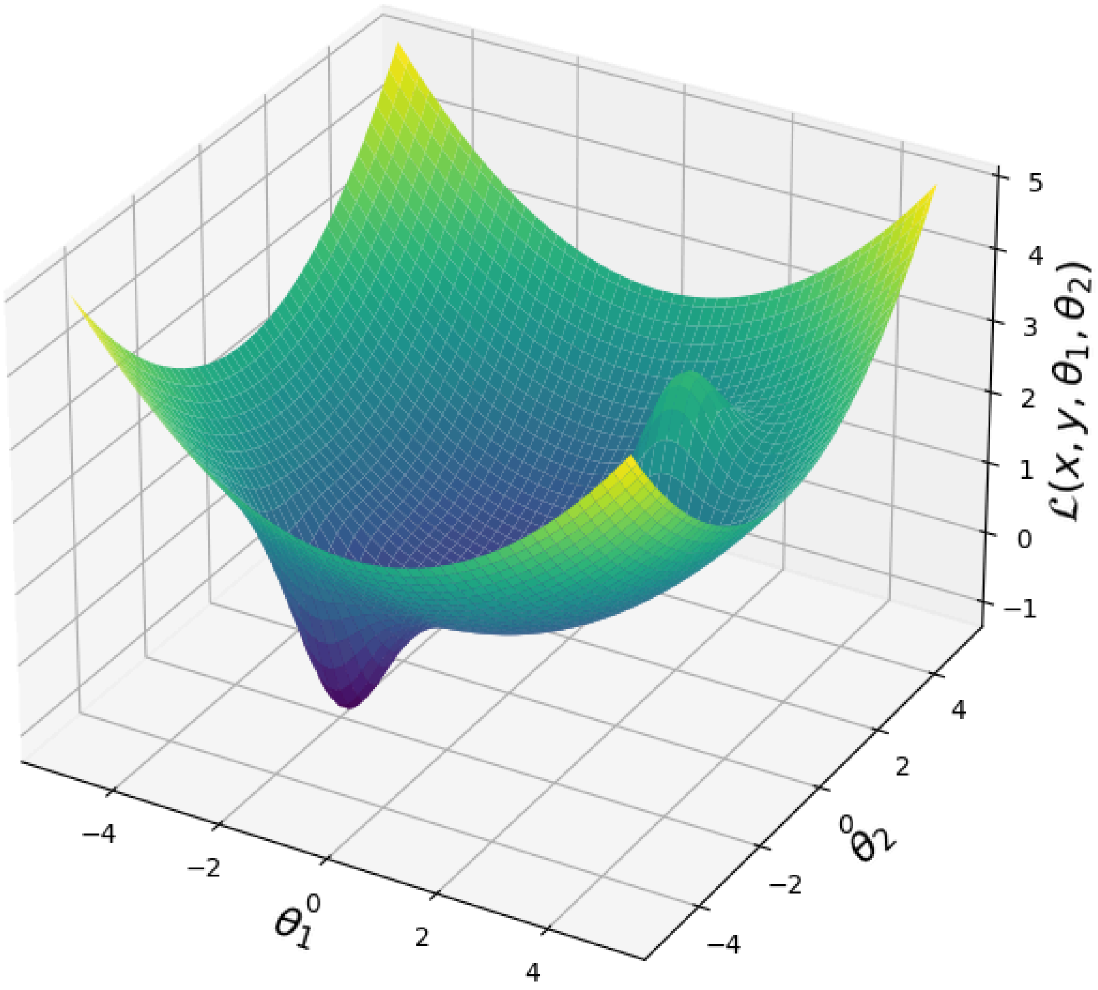
    $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

    ▷ Update the parameters using the negative gradient

    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$

  return $\boldsymbol{\theta}$

Gradient Descent



Gradient Descent

Two main steps in gradient descent:

Gradient Descent

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Step 1: Compute the gradient of the loss

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Step 2: Update the parameters using the gradient

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Step 2: Update the parameters using the gradient

Let us start with step 1

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Backpropagation

Goal: Compute the gradient of the loss $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

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We propagate errors from the loss function **backward** through each layer of the neural network

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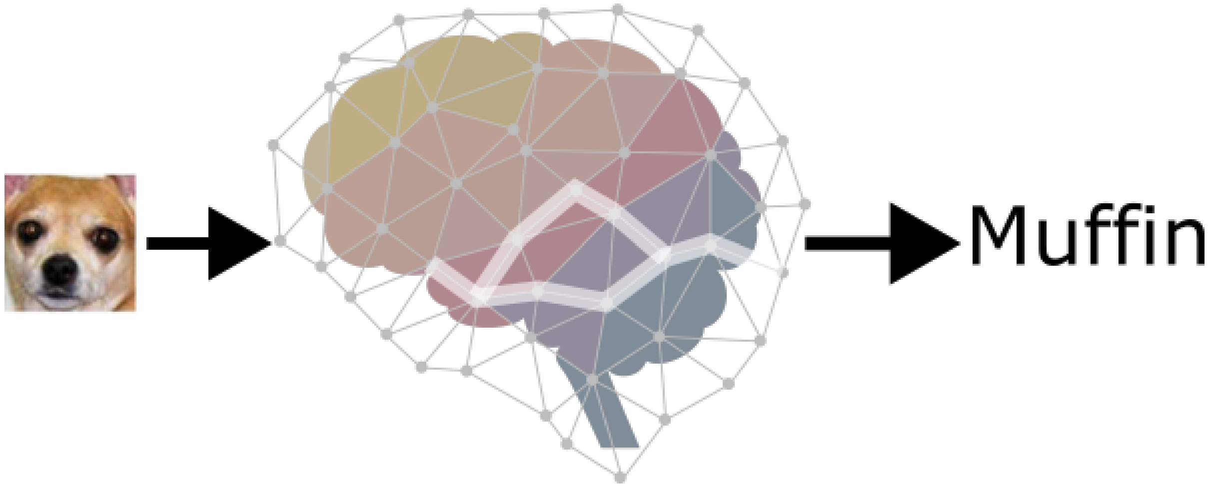
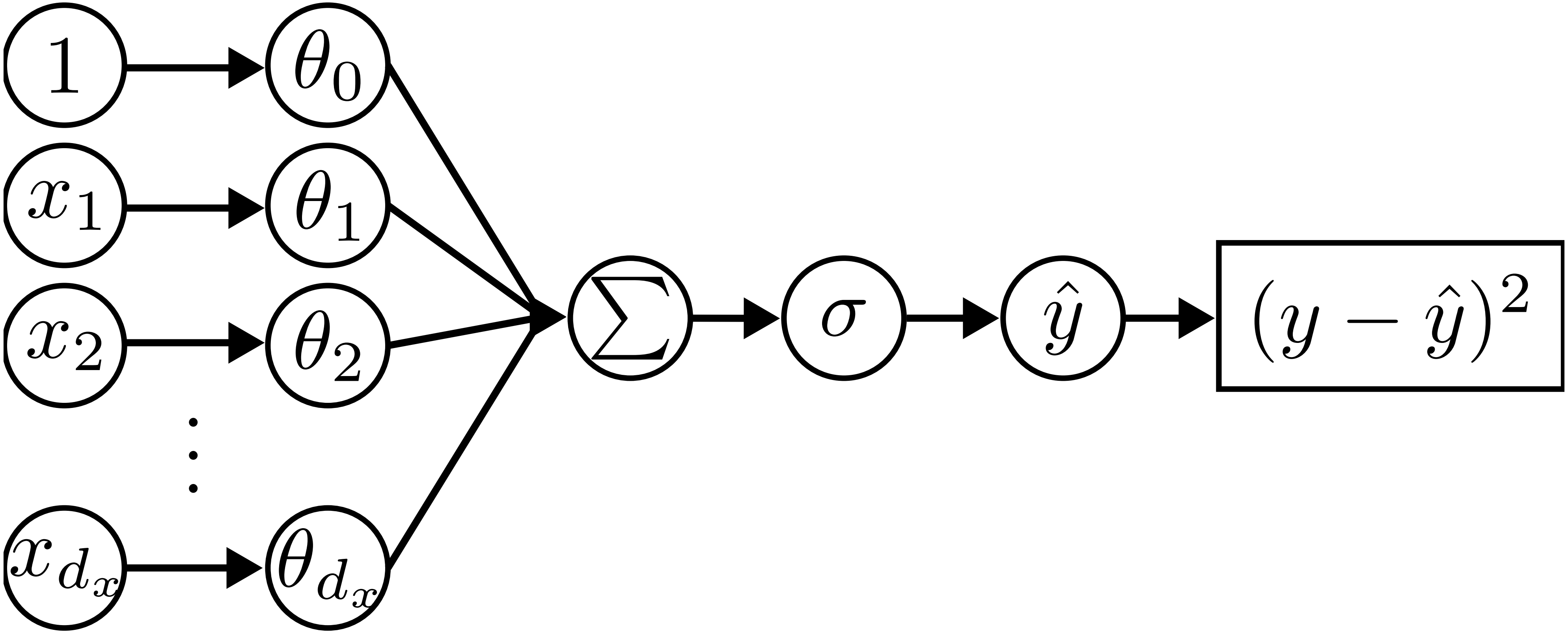


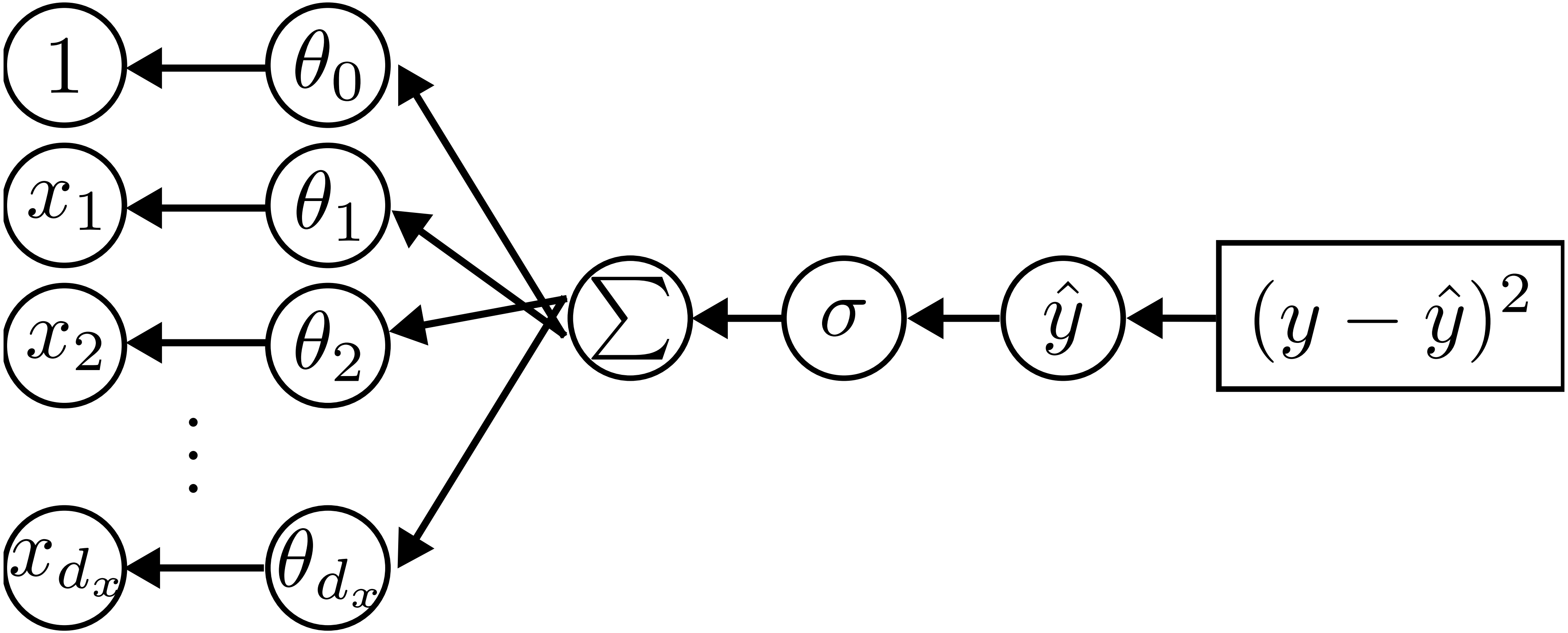
Backpropagation

Forward propagation



Backpropagation

Backward propagation



Backpropagation

Finding the gradient is necessary to use gradient descent!

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First, we will find the gradient of a neural network layer

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Backpropagation

Finding the gradient is necessary to use gradient descent!

First, we will find the gradient of a neural network layer

Then, we will find the gradient of a deep neural network

Finally, we will find the gradient of the loss function

Backpropagation

Start with the equation of a neural network layer

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}})$$

Backpropagation

Start with the equation of a neural network layer

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Take the gradient of both sides

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}})$$

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$$\text{Chain: } \frac{d}{dx} f(g(x)) = f'(g(x)) \cdot g'(x)$$

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$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} [\sigma](\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}) \cdot \nabla_{\boldsymbol{\theta}} (\boldsymbol{\theta}^\top \overline{\boldsymbol{x}})$$

Backpropagation

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What is $\nabla_{\boldsymbol{\theta}} \sigma$?

Backpropagation

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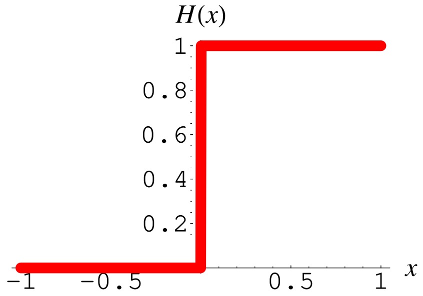

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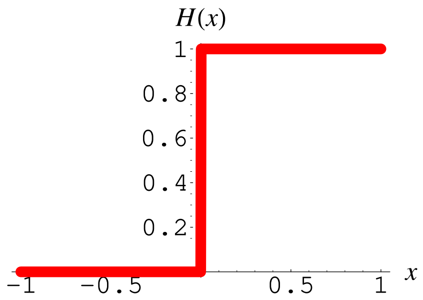

Derivative is zero everywhere and infinity at $x = 0$, so the derivative for a layer is either infinity or zero

Backpropagation

We use a differentiable approximation of the heaviside step function

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$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

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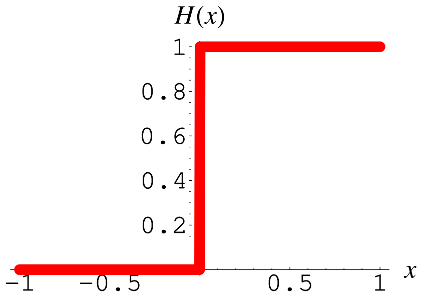
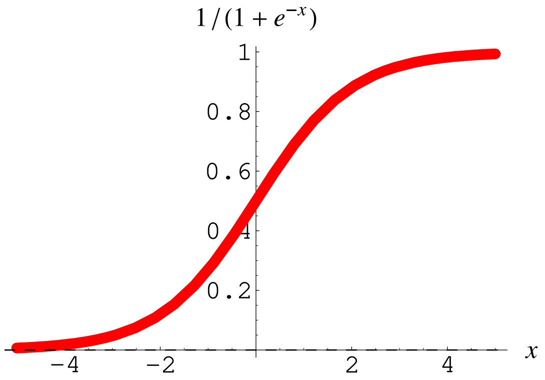
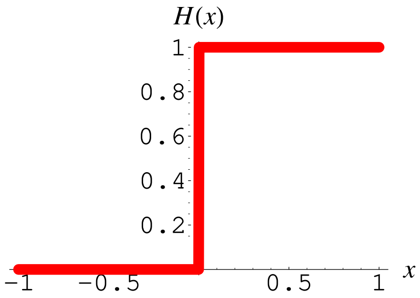
We call this approximation the **sigmoid function**

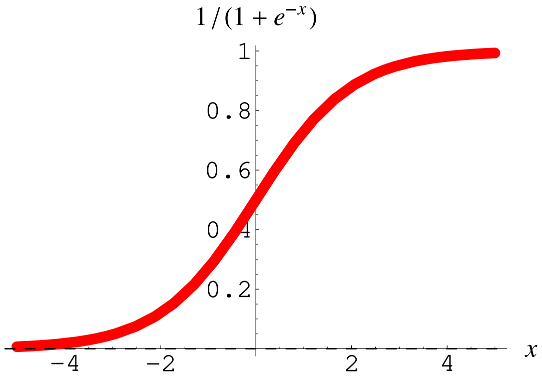




The sigmoid function has finite and nonzero derivative everywhere

Backpropagation



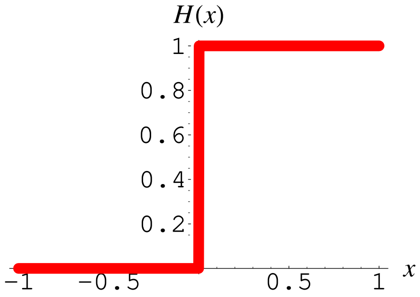


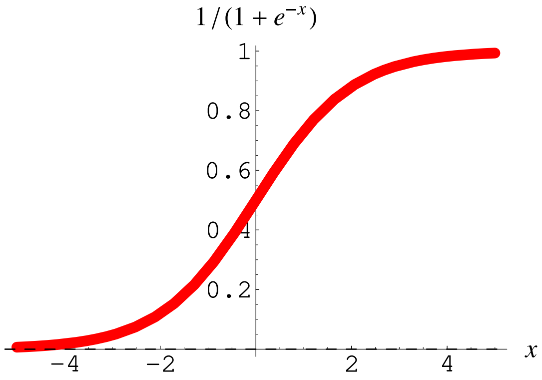
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

The derivative of the sigmoid function is

$$\frac{d}{dz}\sigma(z) = \sigma(z) \cdot (1 - \sigma(z))$$

Backpropagation





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Backpropagation

Back to our layer

Backpropagation

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Plug in the gradient of our new activation function

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Evalute the final term

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Backpropagation

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \left(\sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}) \odot (1 - \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}))\right)\overline{\boldsymbol{x}}^\top$$

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This is the gradient for the layer of a neural network!

Backpropagation

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \left(\sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}) \odot (1 - \sigma(\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}))\right)\overline{\boldsymbol{x}}^\top$$

This is the gradient for the layer of a neural network!

We will use this to compute the gradient of a deep neural network

Backpropagation

Recall the deep neural network has many layers

$$f_1(\boldsymbol{x}, \boldsymbol{\varphi}) = \sigma(\boldsymbol{\varphi}^\top \overline{\boldsymbol{x}}) \quad f_2(\boldsymbol{x}, \boldsymbol{\psi}) = \sigma(\boldsymbol{\psi}^\top \overline{\boldsymbol{x}}) \quad \dots \quad f_\ell(\boldsymbol{x}, \boldsymbol{\xi}) = \sigma(\boldsymbol{\xi}^\top \overline{\boldsymbol{x}})$$

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And that we call them in series

$$\begin{aligned} \boldsymbol{z}_1 &= f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\ \boldsymbol{z}_2 &= f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\ &\vdots \\ \boldsymbol{z}_\ell &= f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) \end{aligned}$$

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Backpropagation

Take the gradient of both sides

$$\nabla_{\varphi, \psi, \dots, \xi} z_1 = \nabla_{\varphi, \psi, \xi} f_1(x, \varphi)$$

$$\nabla_{\varphi, \psi, \dots, \xi} z_2 = \nabla_{\varphi, \psi, \xi} f_2(z_1, \psi)$$

$$\vdots$$

$$\nabla_{\varphi, \psi, \dots, \xi} z_\ell = \nabla_{\varphi, \psi, \xi} f_\ell(z_{\ell-1}, \xi)$$

Backpropagation

Take the gradient of both sides

$$\begin{aligned}
\nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} \boldsymbol{z}_1 &= \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \boldsymbol{\xi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\
\nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} \boldsymbol{z}_2 &= \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \boldsymbol{\xi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\
&\vdots \\
\nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} \boldsymbol{z}_\ell &= \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi})
\end{aligned}$$

Each layer only uses one set of parameters

$$\begin{aligned}
\nabla_{\boldsymbol{\varphi}} \boldsymbol{z}_1 &= \nabla_{\boldsymbol{\varphi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\
\nabla_{\boldsymbol{\psi}} \boldsymbol{z}_2 &= \nabla_{\boldsymbol{\psi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\
&\vdots \\
\nabla_{\boldsymbol{\xi}} \boldsymbol{z}_\ell &= \nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi})
\end{aligned}$$

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Take the gradient of both sides

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Backpropagation

The gradient of a deep neural network is

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} f\left(\boldsymbol{x}, [\boldsymbol{\varphi} \ \ \boldsymbol{\psi} \ \ \ldots \ \ \boldsymbol{\xi}]^\top\right) = \begin{bmatrix} \nabla_{\boldsymbol{\varphi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\ \nabla_{\boldsymbol{\psi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\ \vdots \\ \nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) \end{bmatrix}$$

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Where each layer gradient is

$$\nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) = (\sigma(\boldsymbol{\xi}^\top \overline{\boldsymbol{z}}_{\ell-1}) \odot (1 - \sigma(\boldsymbol{\xi}^\top \overline{\boldsymbol{z}}_{\ell-1}))) \overline{\boldsymbol{z}}_{\ell-1}^\top$$

Backpropagation

We computed the gradient of a neural network layer

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Now, we must compute gradient of the loss function

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$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta} \right) - \boldsymbol{y}_{[i]} \right)^2$$

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$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} 2 \left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta} \right) - \boldsymbol{y}_{[i]} \right) \nabla_{\boldsymbol{\theta}} f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta} \right)$$

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$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} 2\Big(f\Big(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\Big) - \boldsymbol{y}_{[i]}\Big) \nabla_{\boldsymbol{\theta}} f\Big(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\Big)$$

$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) = \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} f\Big(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{\varphi} & \boldsymbol{\psi} & \ldots & \boldsymbol{\xi} \end{bmatrix}^\top\Big) = \begin{bmatrix} \nabla_{\boldsymbol{\varphi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) \\ \nabla_{\boldsymbol{\psi}} f_2(\boldsymbol{z}_1, \boldsymbol{\psi}) \\ \vdots \\ \nabla_{\boldsymbol{\xi}} f_\ell(\boldsymbol{z}_{\ell-1}, \boldsymbol{\xi}) \end{bmatrix}$$

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for $i \in 1 ... t$ **do**

$\qquad \triangleright$ Compute the gradient of the loss

$\qquad \boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

$\qquad \triangleright$ Update the parameters using the negative gradient

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$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}_t)$$

Agenda

1. Review
2. Quiz
3. Optimization
4. Calculus review
5. Deriving linear regression
6. Gradient descent
7. **Backpropagation**
8. Coding

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Now, let us look at `jax` and `torch` optimization code

```python
import jax

def L(theta, X, Y):
  ...

# Create a new function that is the gradient of L
# Then compute gradient of L for given inputs
J = jax.grad(L)(X, Y, theta)
# Update parameters
alpha = 0.0001
theta = theta - alpha * J
```

```python
import torch
optimizer = torch.optim.SGD(lr=0.0001)

def L(model, X, Y):
  ...
# Pytorch will record a graph of all operations
# Everytime you do theta @ x, it stores inputs and outputs
loss = L(X, Y, model) # compute gradient
# Traverse the graph backward and compute the gradient
loss.backward() # Sets .grad attribute on each parameter
optimizer.step() # Update the parameters using .grad
optimizer.zero_grad() # Set .grad to zero, DO NOT FORGET!!
```

Time for some interactive coding

https://colab.research.google.com/drive/1W8WVZ8n_9yJCcOqkPVURp_wJUx3EQc5w