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

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Agenda

1. Review
2. Quiz
3. Optimization
4. Calculus review
5. Deriving linear regression
6. Gradient descent
7. Backpropagation
8. Layer gradient
9. Full gradient
10. Practical considerations

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We can solve these problems using linear regression too

For multivariate problems, we will define the input dimension as d_x

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We will write the vectors as

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

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

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

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The solution is the same as before

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

Limitations of Linear Regression

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One-dimensional polynomial functions

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We introduced neural networks because they scale to larger problems

Brains and neural networks rely on **neurons**

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Brain: Biological neurons $\rightarrow$ Biological neural network

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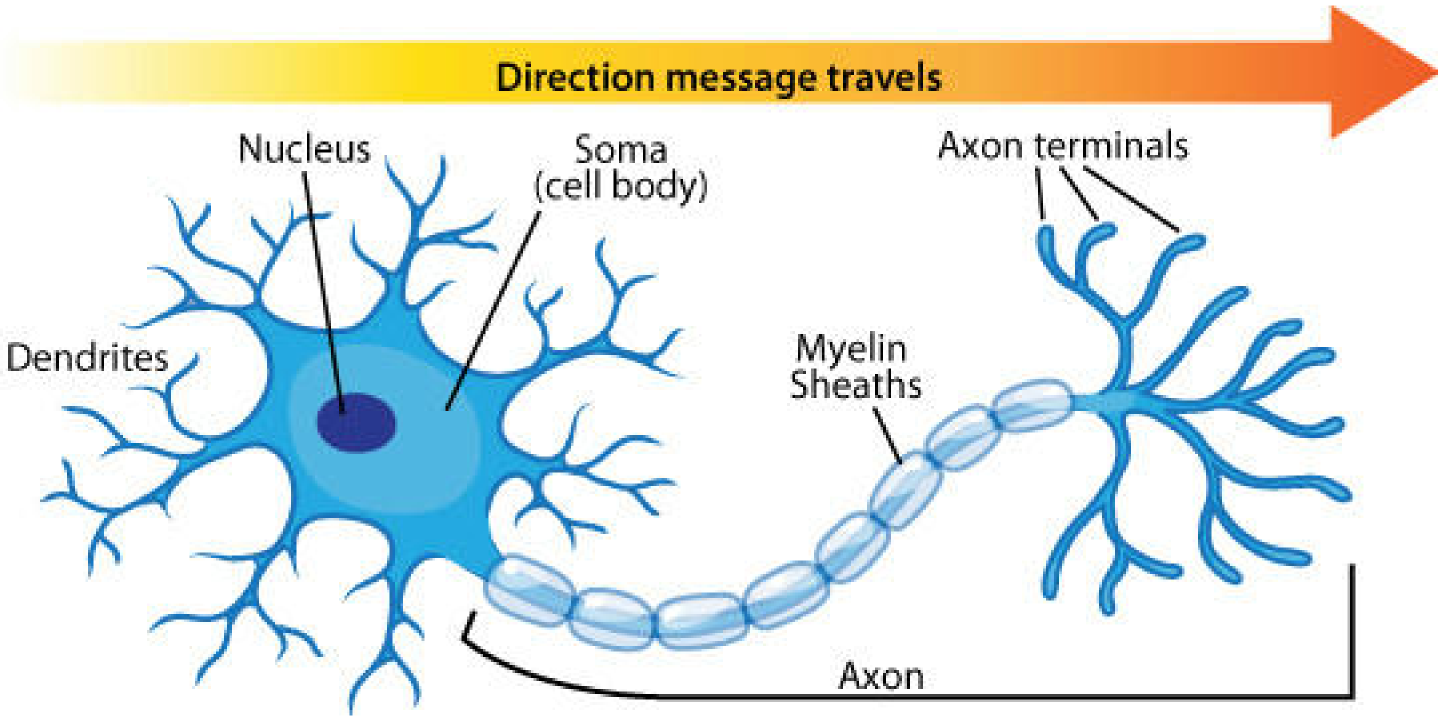
Brain: Biological neurons $\rightarrow$ Biological neural network

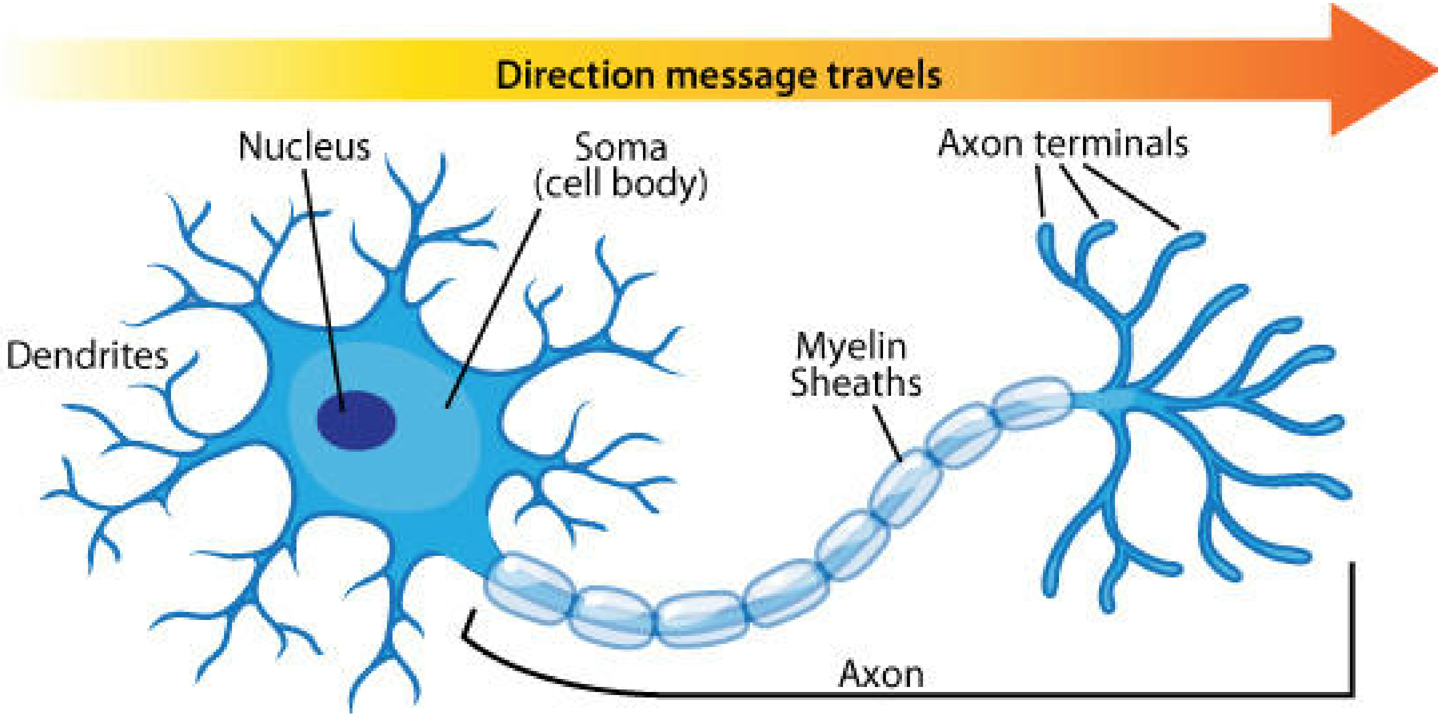
Computer: Artificial neurons $\rightarrow$ Artificial neural network

Review



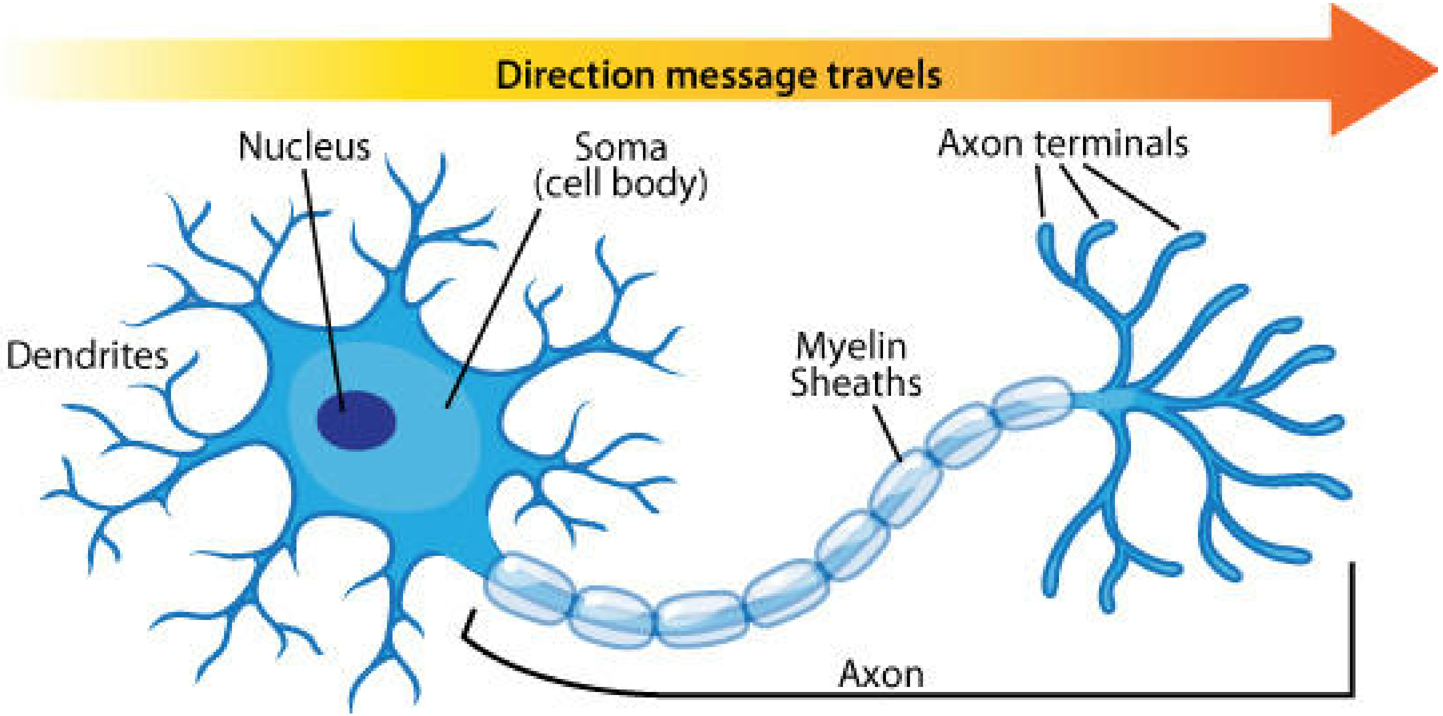
Neurons send messages based on messages received from other neurons

Review



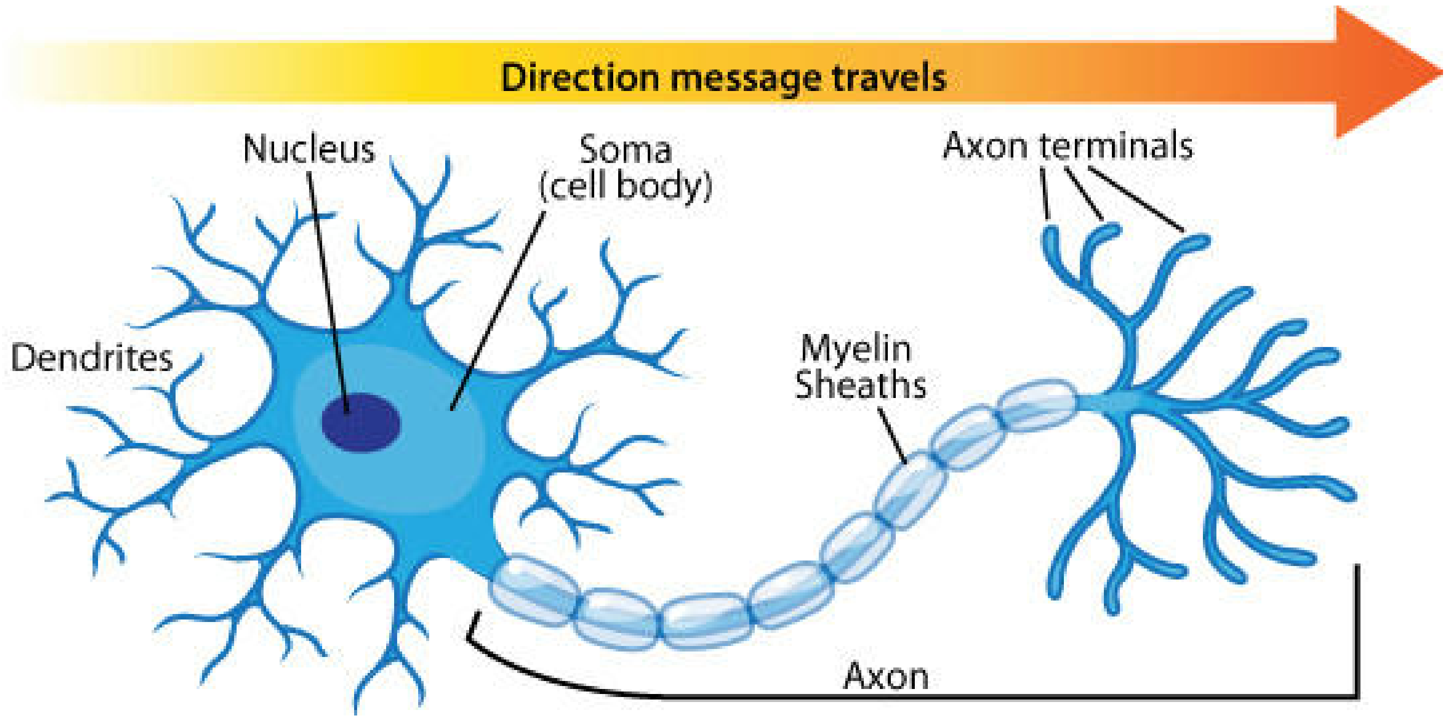
Incoming electrical signals travel along dendrites

Review



Electrical charges collect in the Soma (cell body)

Review



The axon outputs an electrical signal to other neurons

Biological Neurons

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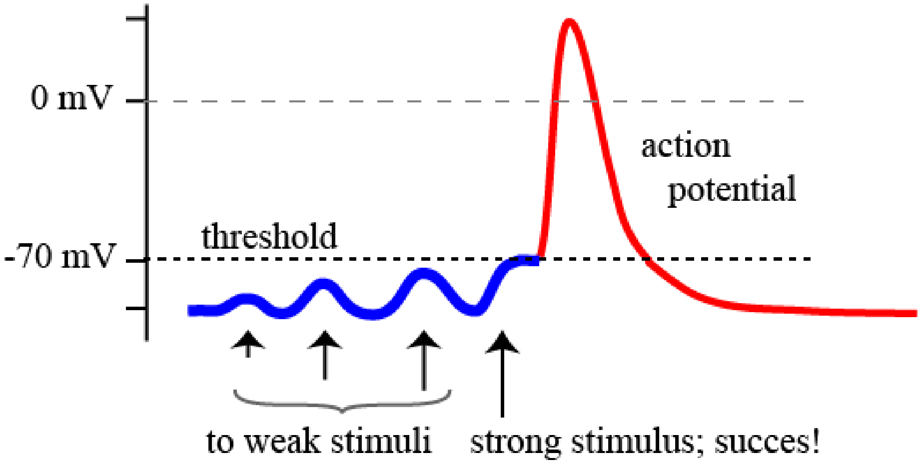

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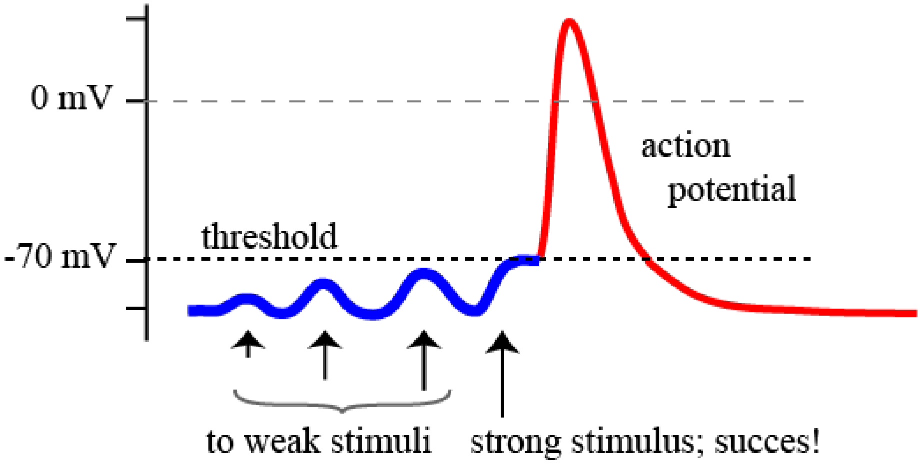

Many active dendrites will add together and trigger an impulse

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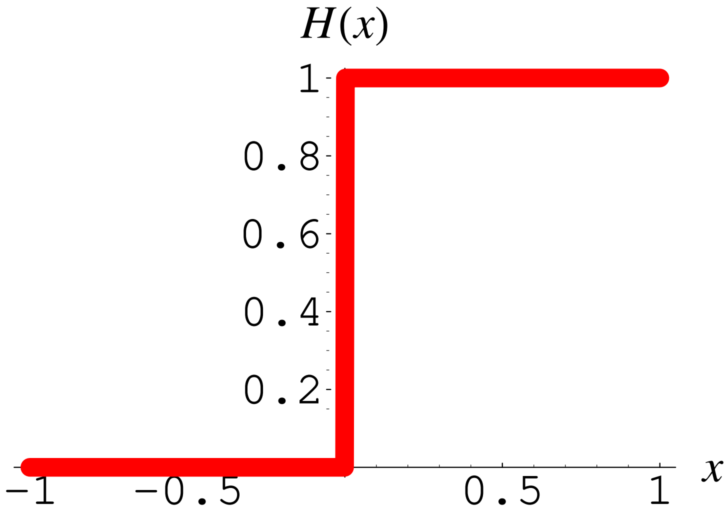

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\underbrace{\theta_0 1 + \theta_1 x_1 + \ldots + \theta_{d_x} x_{d_x}}_{\text{Linear model}}\right)$$

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

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A single neuron:

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

d_y neurons (wide):

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

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

For a wide network (also called a layer):

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

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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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I will take away your quiz, give zero points, and refer you to the Dean if:

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

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

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To start, let us consider how we find

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

in linear regression

Recall how we solved the linear regression problem

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We define the square error loss function

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Recall how we solved the linear regression problem

We define the square error loss function

$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} (f(x_i, \boldsymbol{\theta}) - y_i)^2$$

Then, I gave you a magical solution to this optimization problem

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

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

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

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We will briefly review basic calculus concepts

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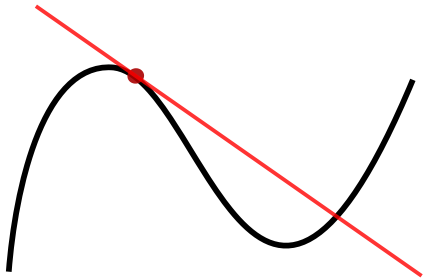

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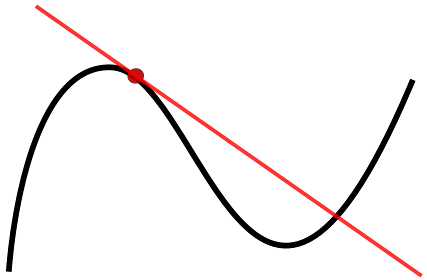

$f(x), f'(x = a)$

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

There are formulas for computing the derivative of various operations

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

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

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

Sum/Difference

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

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

Chain

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

For example, consider the function

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

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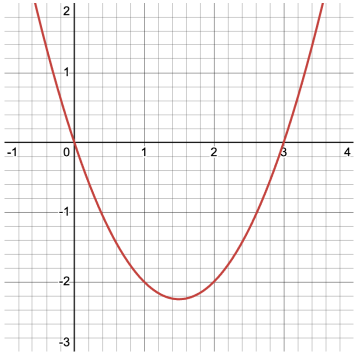
$$\left(\frac{d}{dx} f\right)(1) = 2 \cdot 1 - 3 = -1$$



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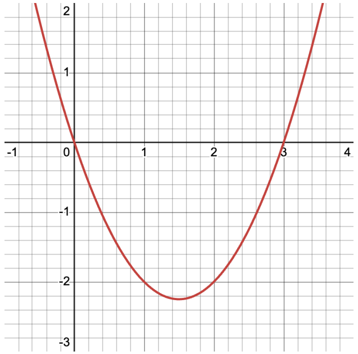

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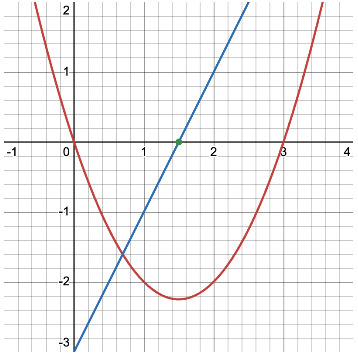

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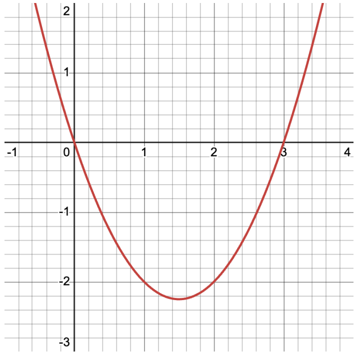

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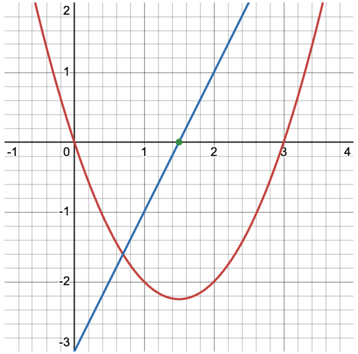

$$\frac{df}{dx} = 2x - 3$$

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

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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For our purposes, we treat partial derivatives like standard derivatives

$$\frac{\partial}{\partial x_1} f(x_1, \dots, x_n) = \frac{d}{d x_1} f(x_1, \dots, x_n)$$

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

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We can write the gradient as

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \nabla_{x_1, x_2} f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(x_1, x_2) \\ \frac{\partial}{\partial x_2} f(x_1, x_2) \end{bmatrix} = \begin{bmatrix} 2x_1 - 3x_2 \\ -3x_1 \end{bmatrix}$$

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$$\nabla_{\boldsymbol{x}} f\left(\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = \nabla_{x_1, x_2} f\left(\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(1, 0) \\ \frac{\partial}{\partial x_2} f(1, 0) \end{bmatrix} = \begin{bmatrix} 2 \cdot 1 - 3 \cdot 0 \\ -3 \cdot 1 \end{bmatrix} = \begin{bmatrix} -1 \\ -3 \end{bmatrix}$$

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

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

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

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Now that we remember calculus, let us revisit linear regression

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

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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We can write the square error loss in matrix form as

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

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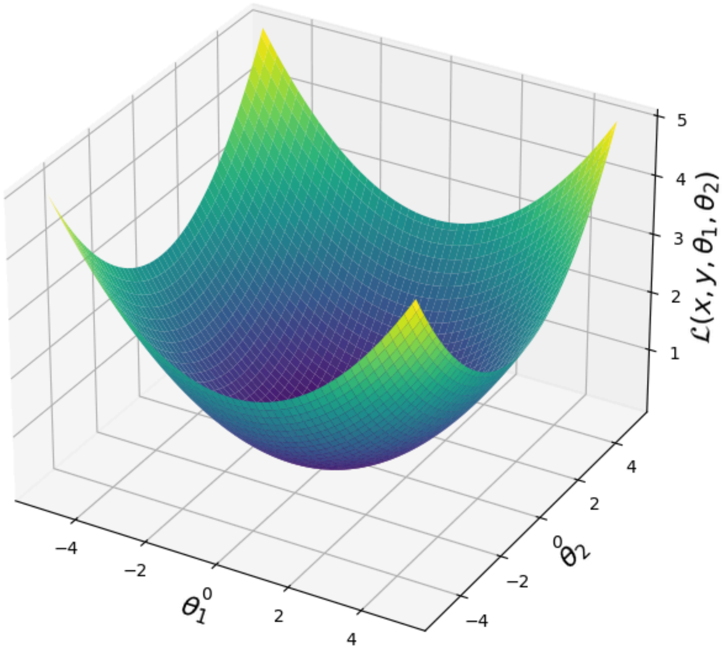
A quadratic function has a single minima! The minima must be at

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



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Also solves

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

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

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

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And so, the gradient of the loss is

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

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

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

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Now, we will do the same approach for neural networks

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Step 1: Write the loss function for a neural network

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

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Neural network model

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Neural network model

Now, we plug the model f into the loss function

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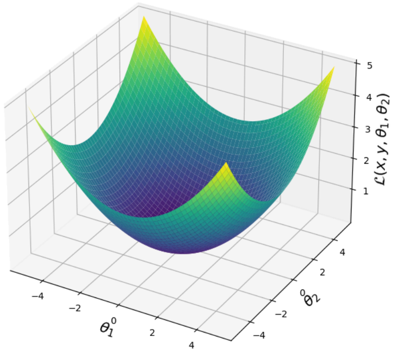
Linear regression loss function was quadratic with one minima



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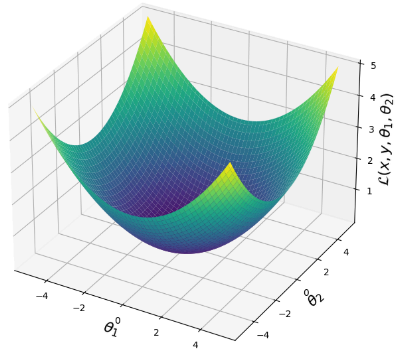

With a neural network, this is our loss function

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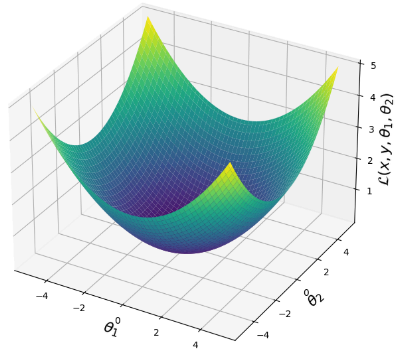

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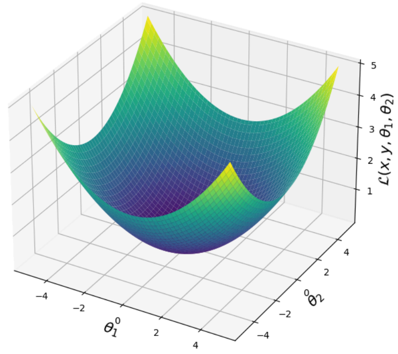

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Answer: We do not know

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Activation functions make the neural network powerful

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

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

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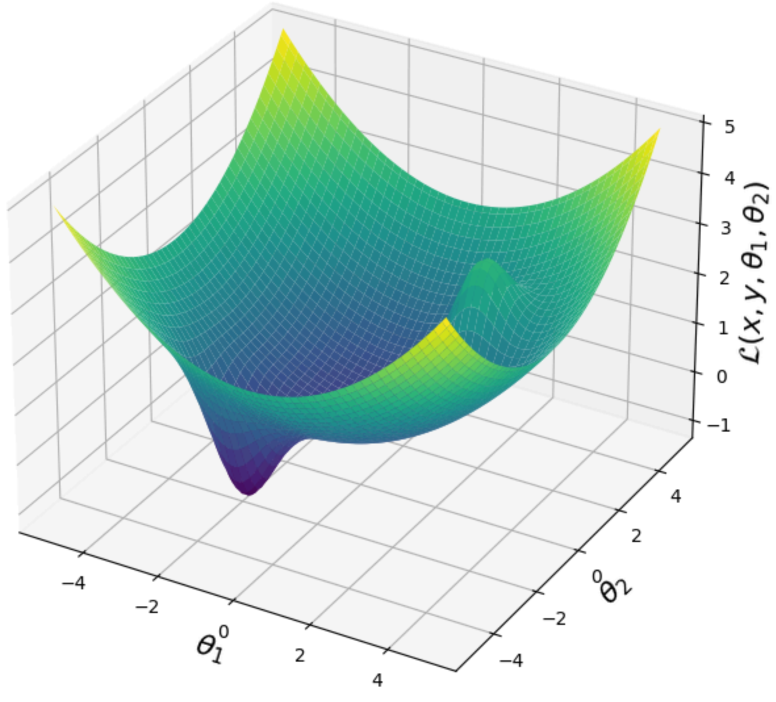
How does gradient descent work?

A differentiable loss function produces a manifold



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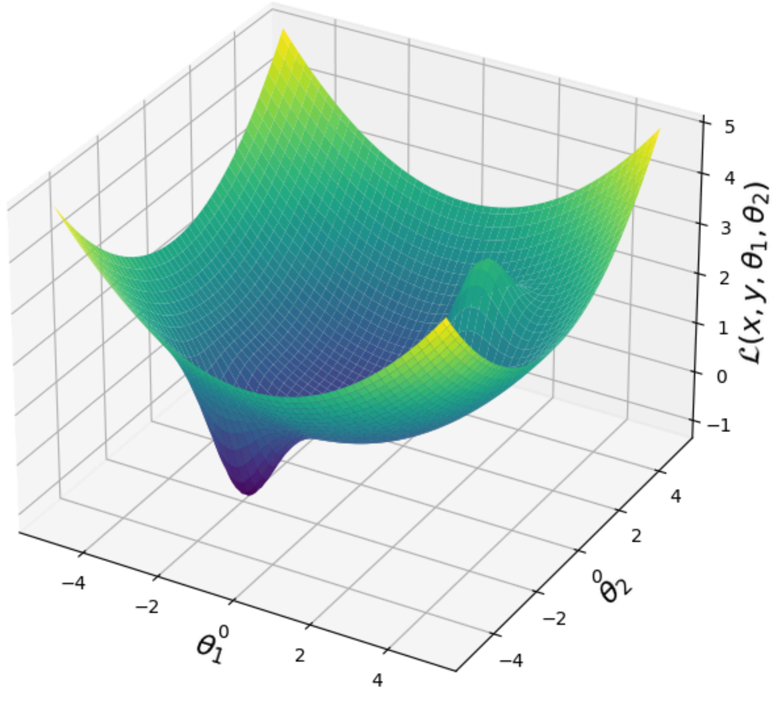

Our goal is to find the lowest point on this manifold

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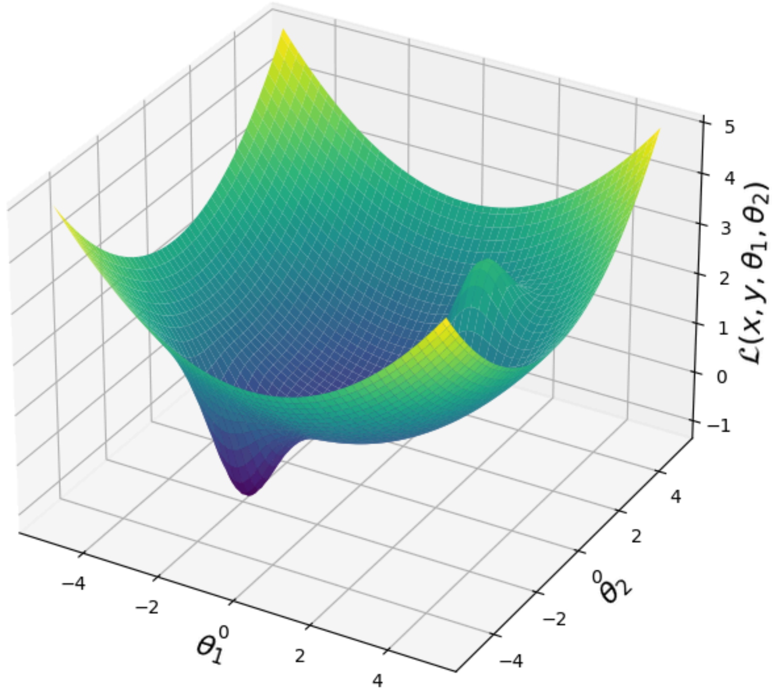

Our goal is to find the lowest point on this manifold

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

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

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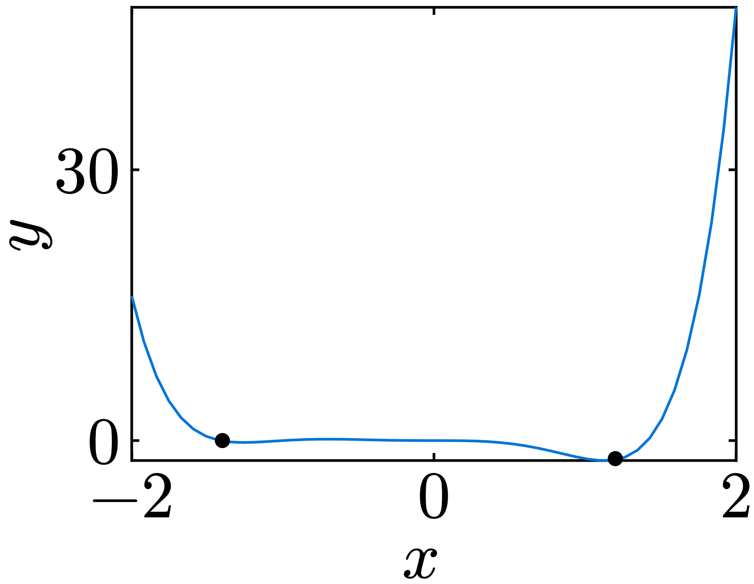

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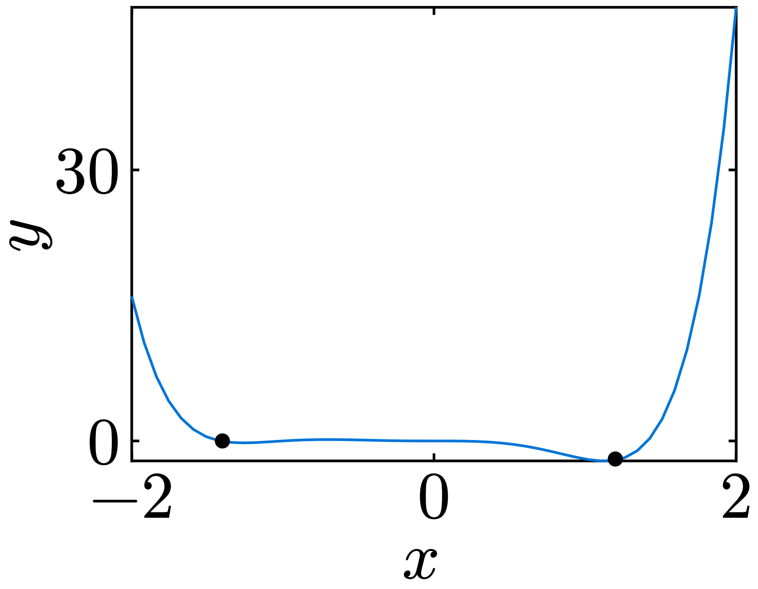

In practice, a local optima provides a good enough model

Let us define gradient descent without math

Let us define gradient descent without math

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

Let us define gradient descent without math

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

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

But you do not know the path down!

But you do not know the path down!

You see this, which way do you walk next?

This is 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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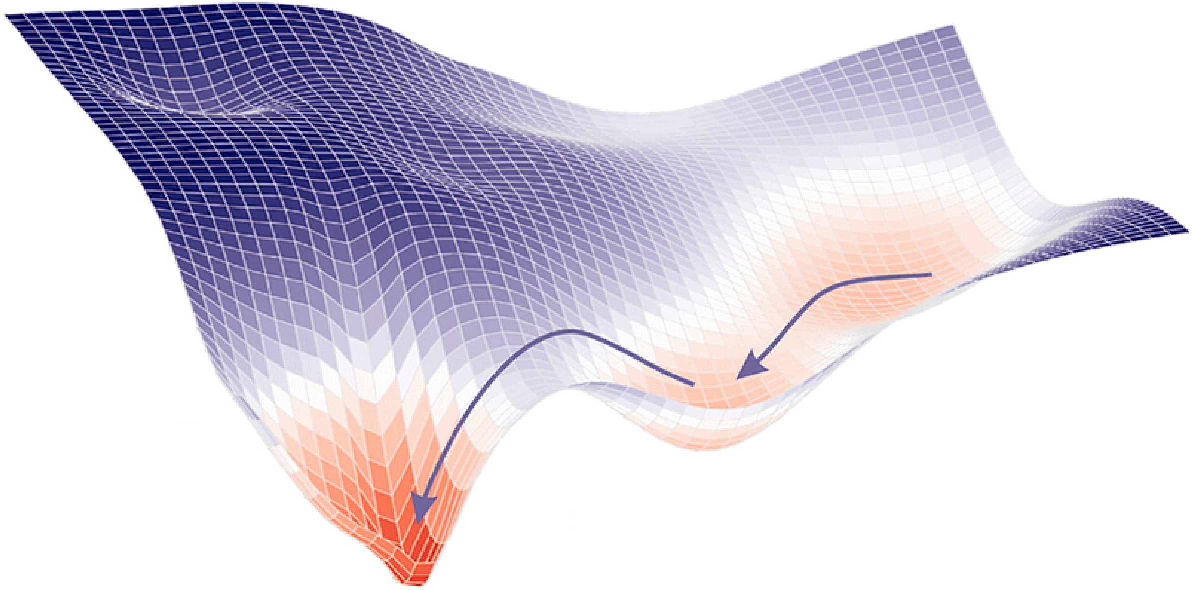

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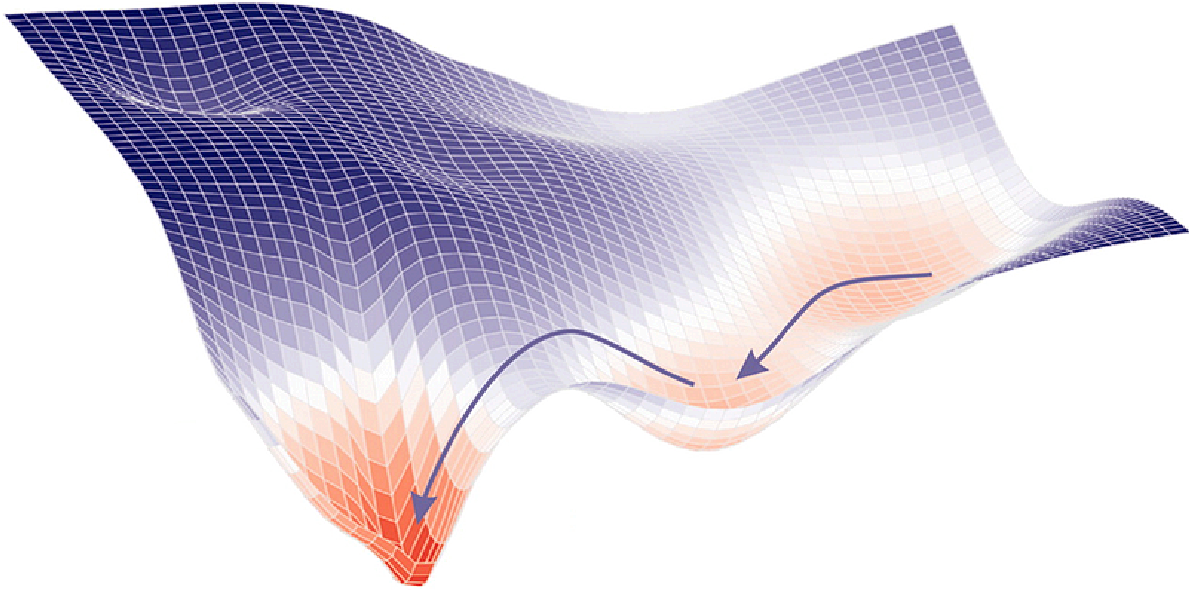
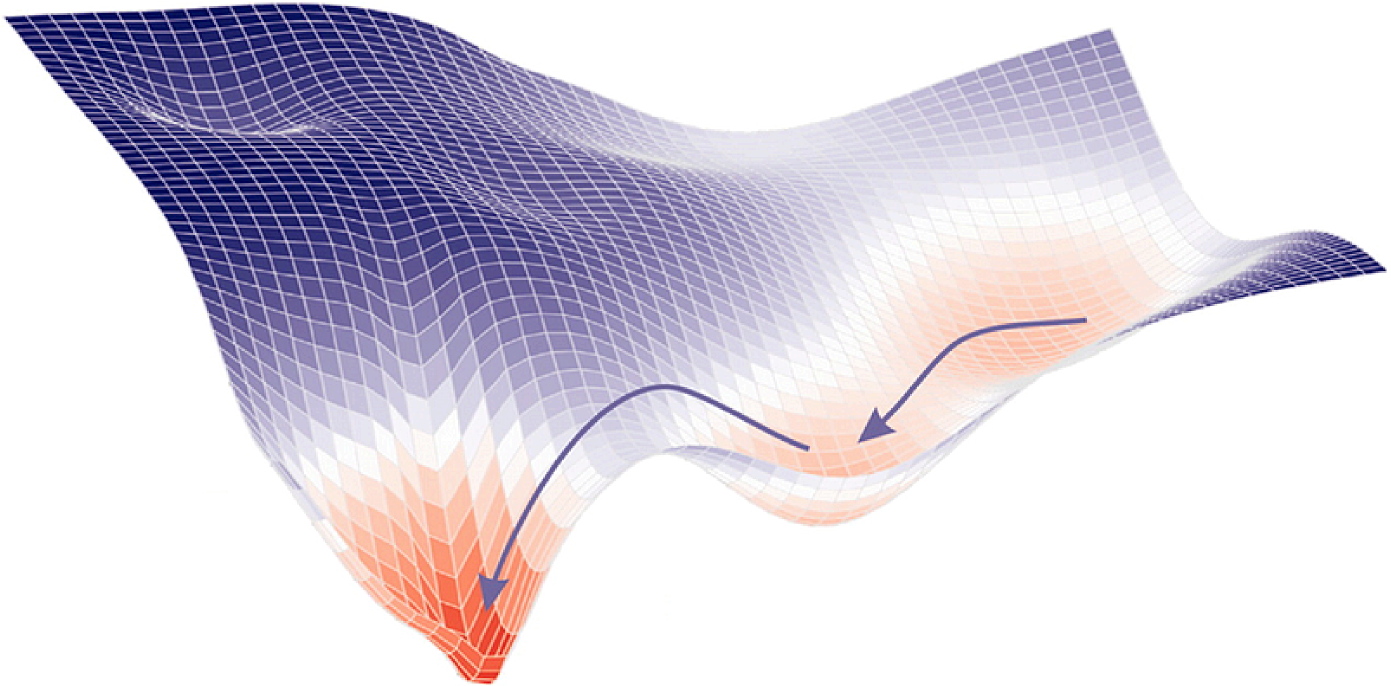
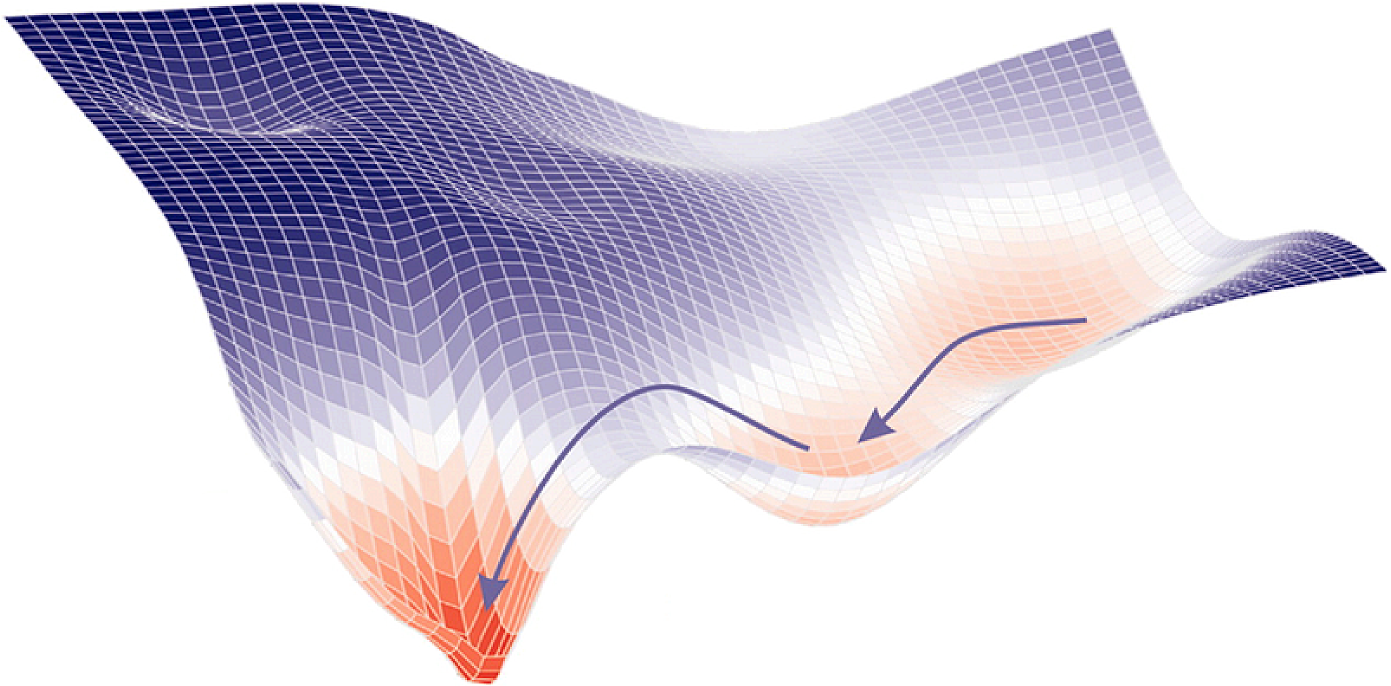
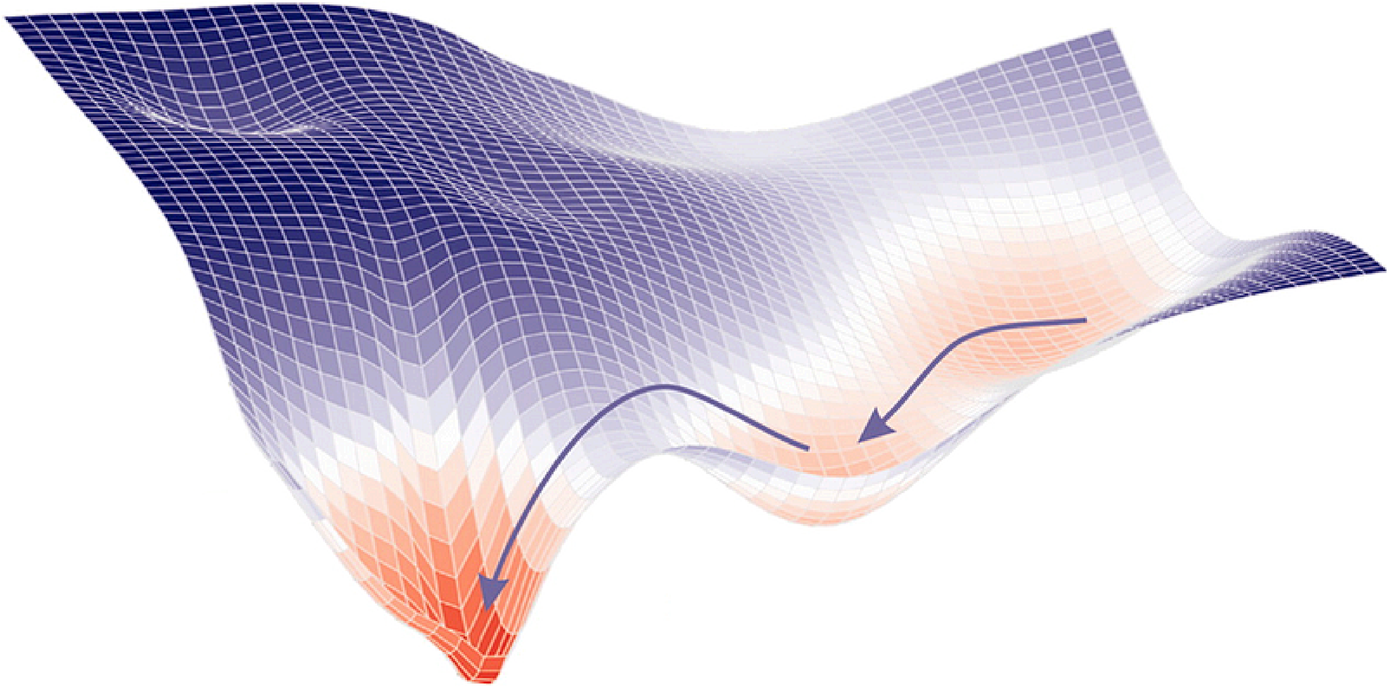


And then we repeat



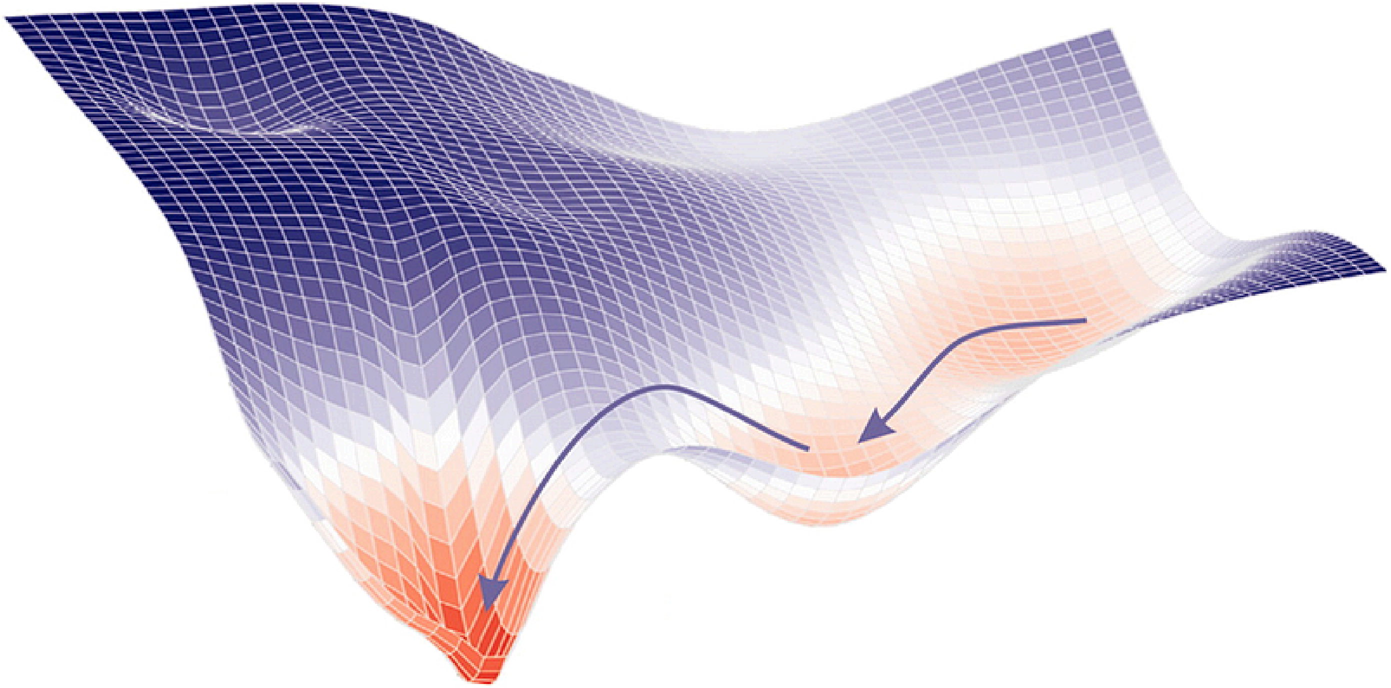


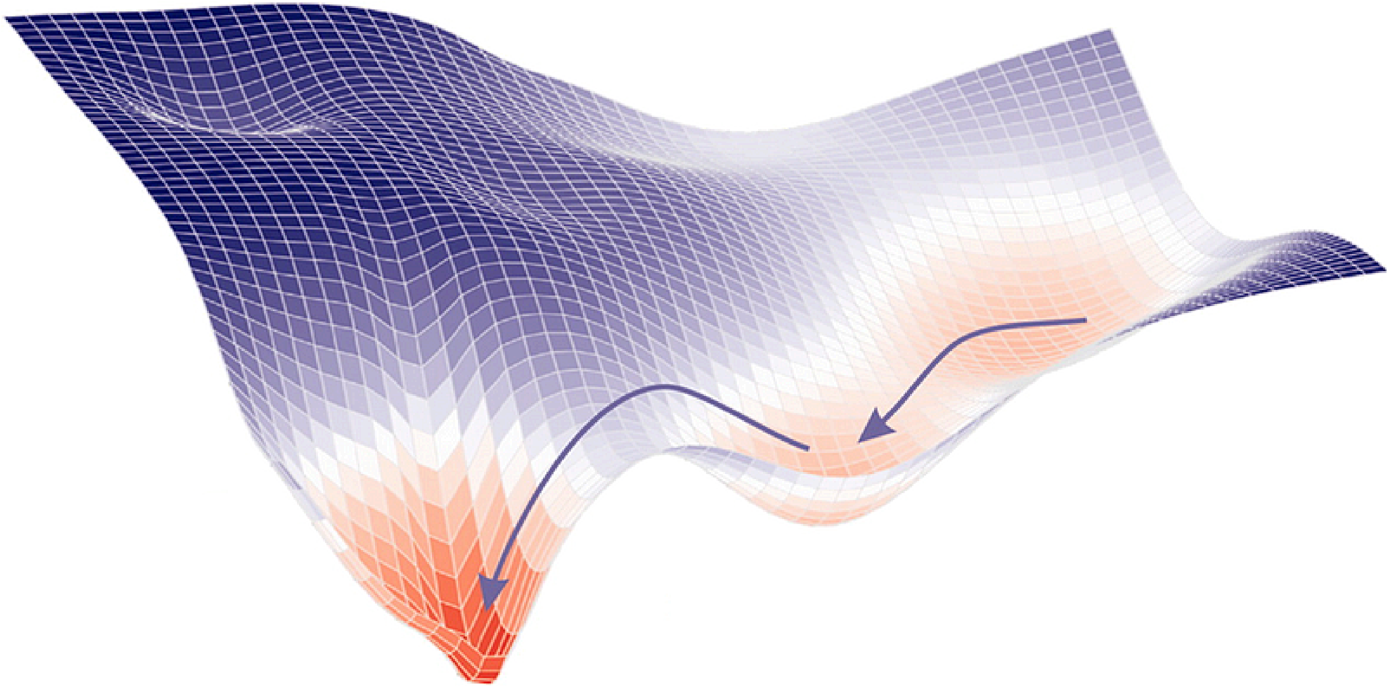
We find the gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$



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

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





Eventually, we arrive at the bottom

With gradient descent, the loss function must be differentiable

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

The gradient descent algorithm is as follows:

function GRADIENT DESCENT($\boldsymbol{x}$, $\boldsymbol{y}$, $\mathcal{L}$, t, α)

  $\triangleright$ Randomly initialize parameters

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

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

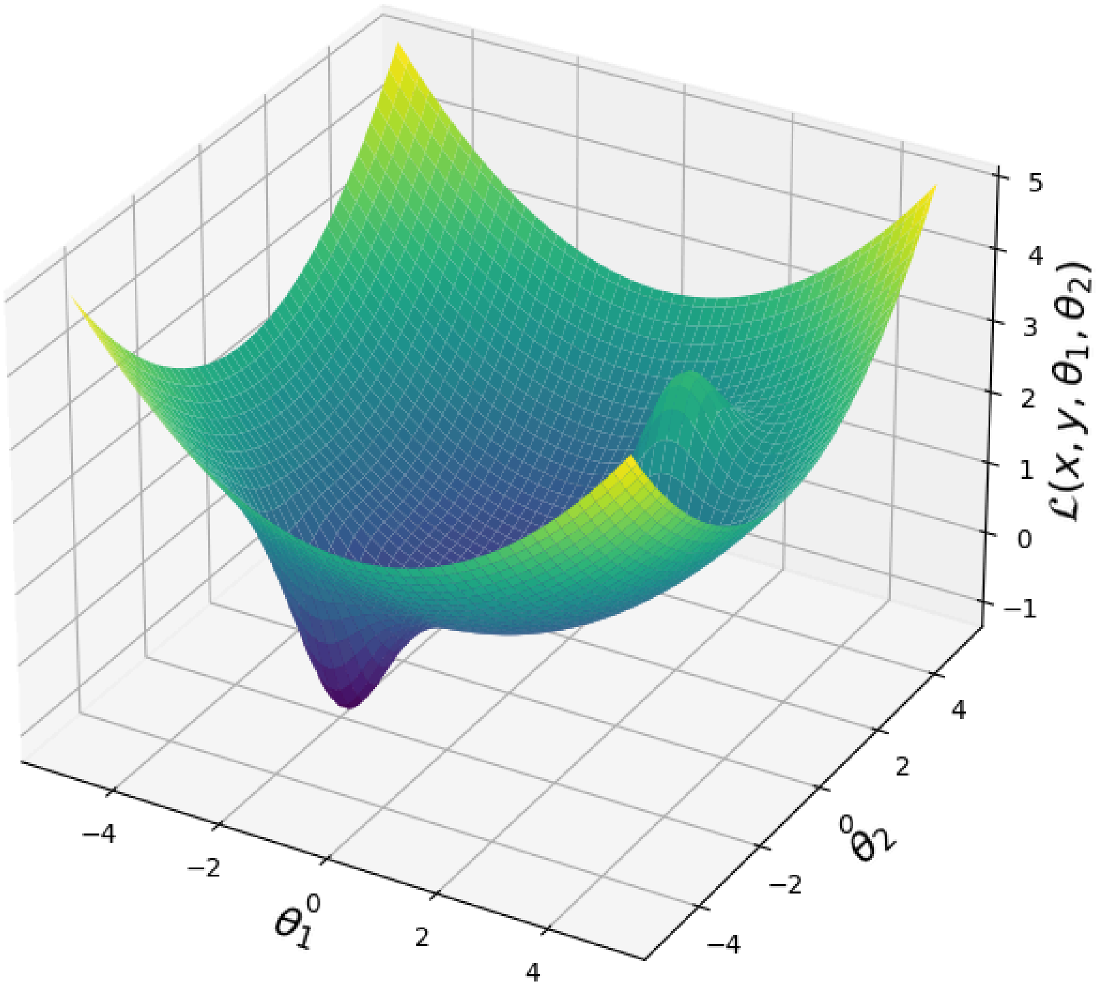
    $\triangleright$ Compute the gradient of the loss

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

    $\triangleright$ Update the parameters using the negative gradient

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

  return $\boldsymbol{\theta}$



5
4
3
2
1
0
−1
$\mathcal{L}(x, y, \theta_1, \theta_2)$
−4
−2
0
2
4
θ_1
4
2
0
−2
−4
θ_2

Two main steps in gradient descent:

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Let us start with step 1

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1. Review
2. Quiz
3. Optimization
4. Calculus review
5. **Deriving linear regression**
6. Gradient descent
7. Backpropagation
8. Layer gradient
9. Full gradient
10. Practical considerations

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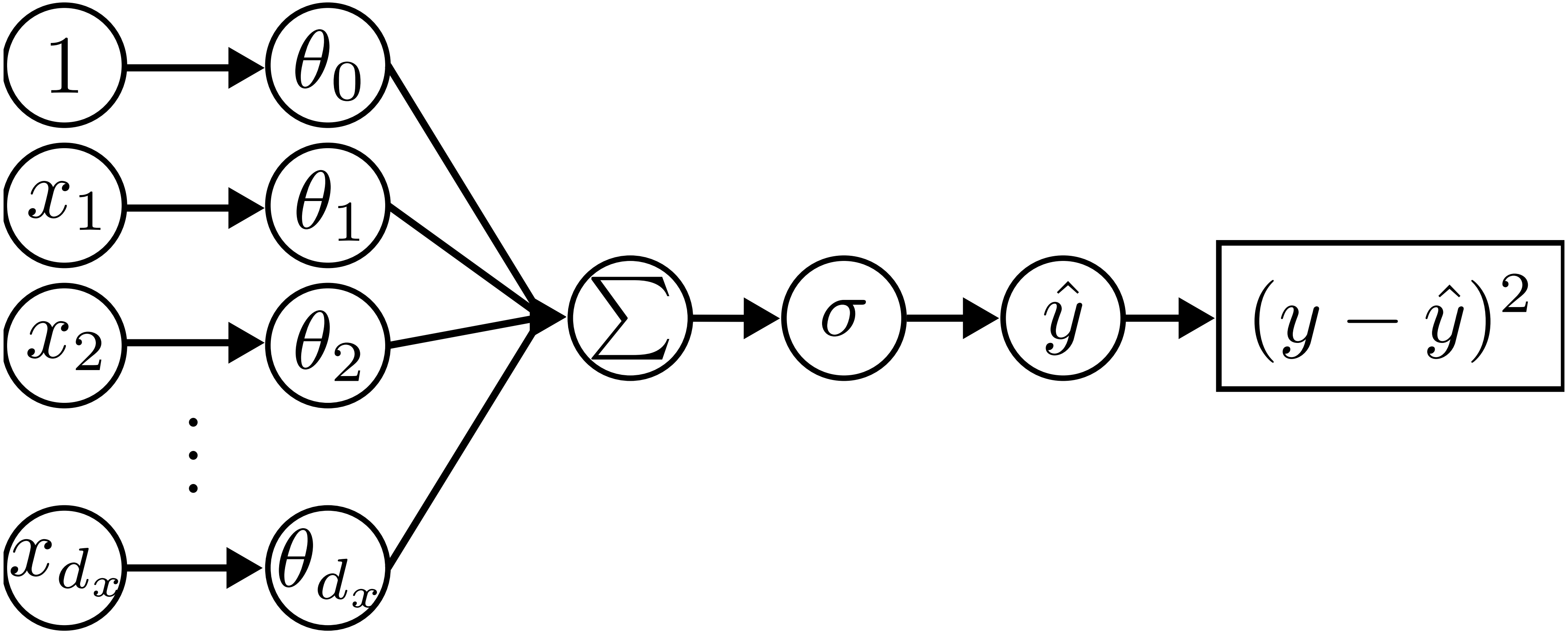
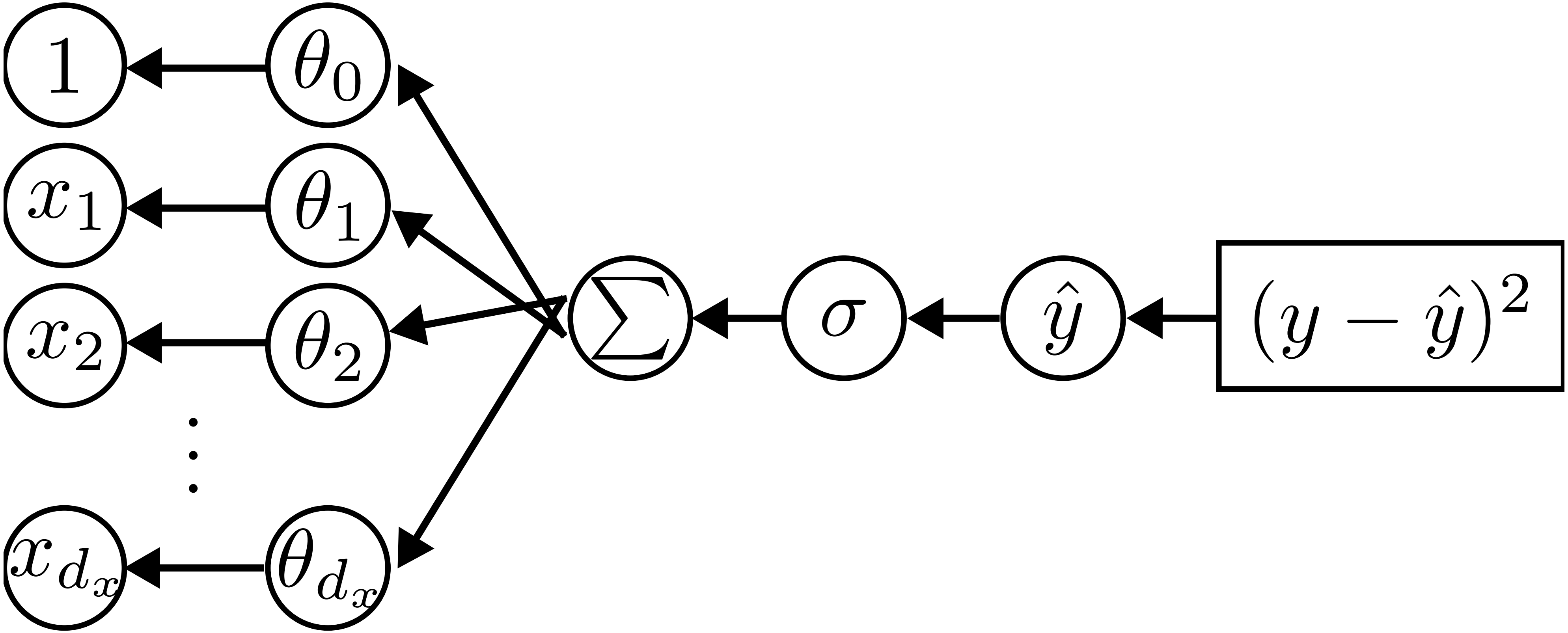
Forward propagation



Backward propagation



Finding the gradient is necessary to use gradient descent!

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We will use the gradient of layers to find the gradient of a deep neural network

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We will use the gradient of layers to find the gradient of a deep neural network

First, let us compute the gradient of a neural network layer

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

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$$\text{What is } \frac{\partial \sigma}{\partial z}(z)?$$

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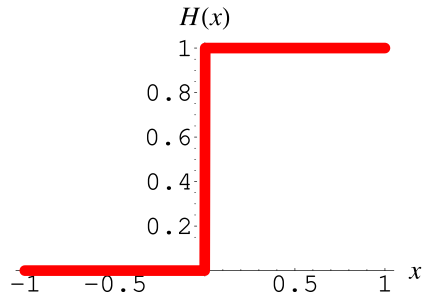

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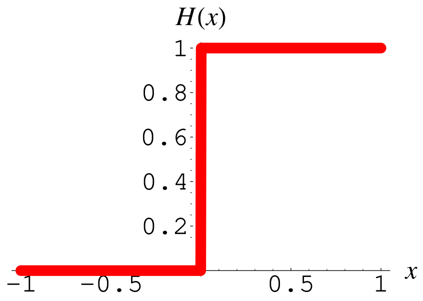

Derivative is zero everywhere and infinity at $x = 0$, so the derivative for a layer is either infinity or zero

We use a differentiable approximation of the heaviside step function

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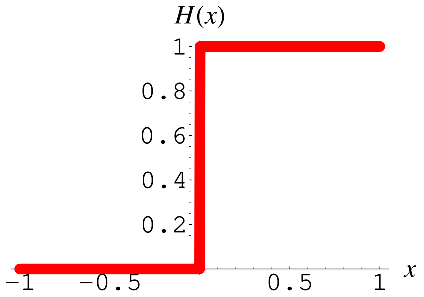
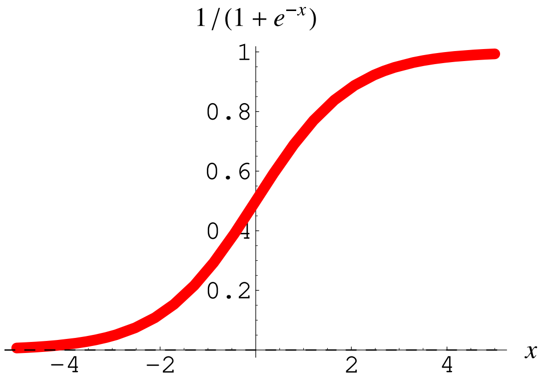
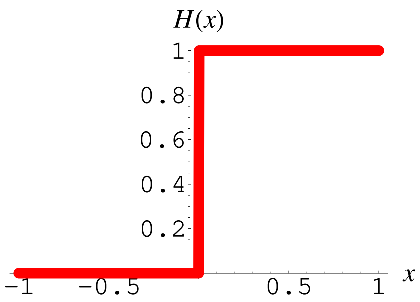
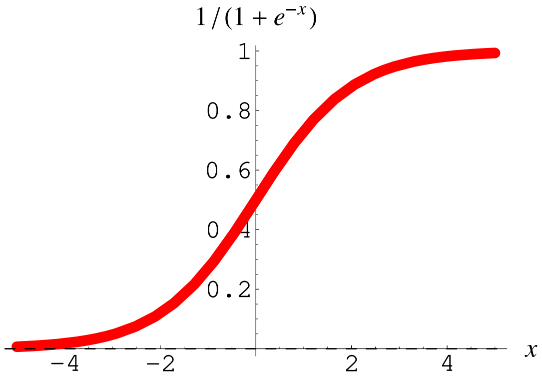




The sigmoid function has finite and nonzero derivative everywhere

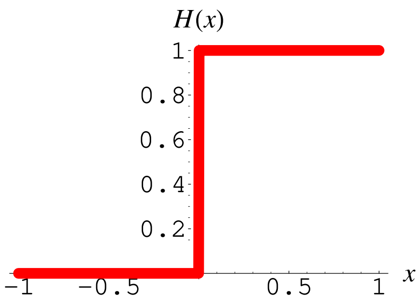


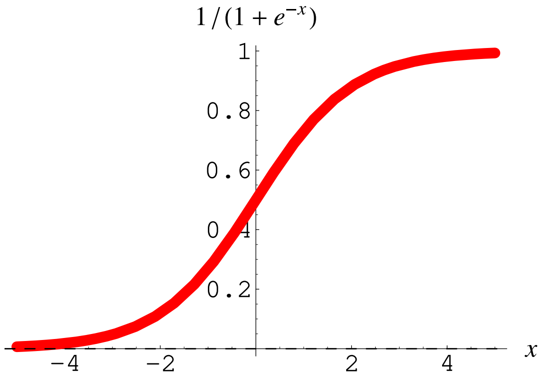


$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

The derivative of the sigmoid function is

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





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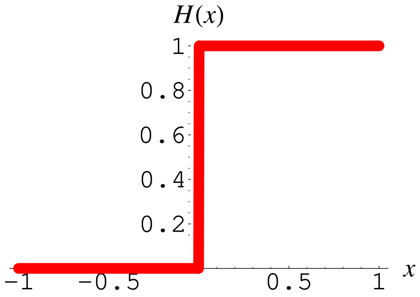

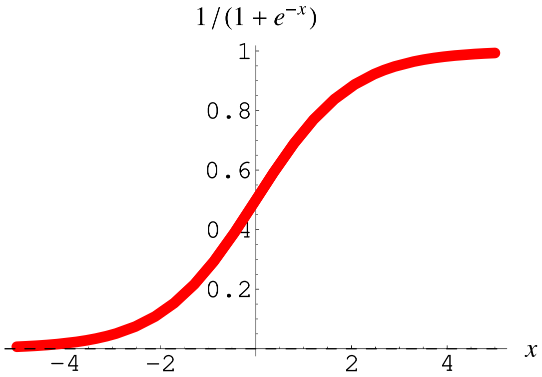

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Back to our layer

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

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Plug in the derivative of our new activation function

Back to our layer

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

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

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

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8. **Layer gradient**
9. Full gradient
10. Practical considerations

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Recall the deep neural network has many layers

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

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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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Take the gradient of both sides

$$\nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \ldots, \boldsymbol{\xi}} \boldsymbol{z}_1 = \nabla_{\boldsymbol{\varphi}, \boldsymbol{\psi}, \boldsymbol{\xi}} f_1(\boldsymbol{x}, \boldsymbol{\varphi})$$

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

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

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

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

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5: $\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \boldsymbol{J}$

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

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If you do research, you might have to derive your own analytical gradients like we did today

```python
import jax

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

# Returns a new function that is the gradient of L
gradient_L = jax.grad(L, argnums=2)
# Evaluate the gradient with our dataset
grads = gradient_L(X, Y, theta)
# Update parameters
alpha = 0.0001
theta = theta - alpha * grads
```

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

def L(X, Y, model):
  ...
# Pytorch will construct a graph of all operations
loss = L(X, Y, model) # compute gradient
# Backward will traverse the graph and compute the full
gradient
loss.backward()
optimizer.step() # Update the parameters
optimizer.zero_grad() # Always remember to do this
```