Optimization

CISC 7026: Introduction to Deep Learning

University of Macau

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

or

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

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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

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$$asg1 = 60$$
, $asg2 = 90$, $asg3 = 70$, total $score = \frac{160}{200}$

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$$asg1 = 60$$
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- 1. Review
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- 4. Calculus review
- 5. Deriving linear regression
- 6. Gradient descent
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We can solve these problems using linear regression too

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$$x \in X; X \in \mathbb{R}^{d_x}$$

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We will write the vectors as

$$oldsymbol{x}_{[i]} = egin{bmatrix} x_{[i],1} \ x_{[i],2} \ dots \ x_{[i],d_x} \end{bmatrix}$$

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

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

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The solution is the same as before

$$oldsymbol{ heta} = oldsymbol{\left(X_D^ op X_D^ op X_D^ op oldsymbol{y}
ight)}^{-1} oldsymbol{X}_D^ op oldsymbol{y}$$

Limitations of Linear Regression

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

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

One-dimensional polynomial functions

$$m{X}_D = egin{bmatrix} x_{[1]}^m & x_{[1]}^{m-1} & \dots & x_{[1]} & 1 \ x_{[2]}^m & x_{[2]}^{m-1} & \dots & x_{[2]} & 1 \ dots & dots & \ddots & \ x_{[n]}^m & x_{[n]}^{m-1} & \dots & x_{[n]} & 1 \end{bmatrix}$$

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We introduced neural networks because they scale to larger problems

Brains and neural networks rely on **neurons**

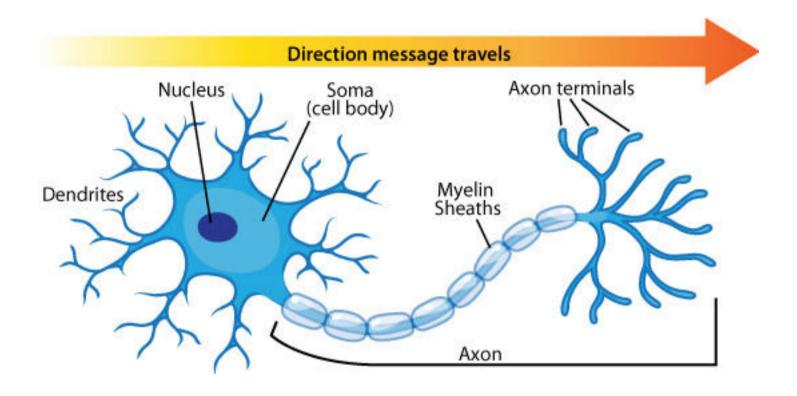
Brains and neural networks rely on **neurons**

Brain: Biological neurons \rightarrow Biological neural network

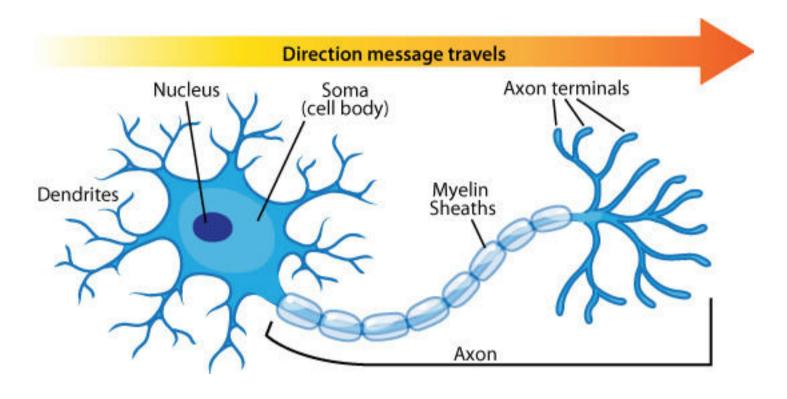
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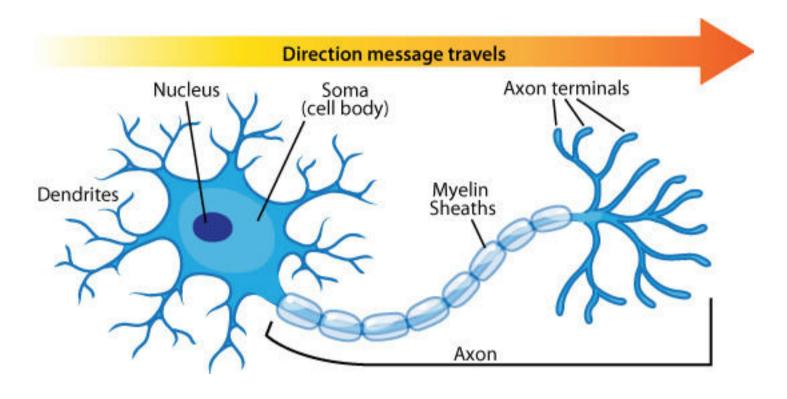
Computer: Artificial neurons \rightarrow Artificial neural network



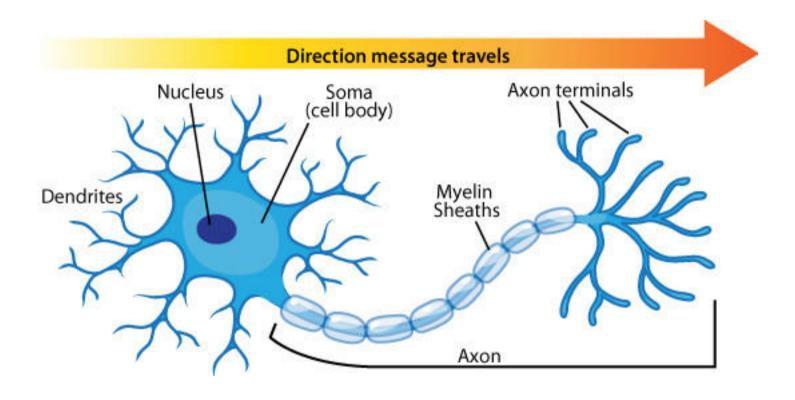
Neurons send messages based on messages received from other neurons



Incoming electrical signals travel along dendrites



Electrical charges collect in the Soma (cell body)



The axon outputs an electrical signal to other neurons

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Dendrites form a parallel circuit

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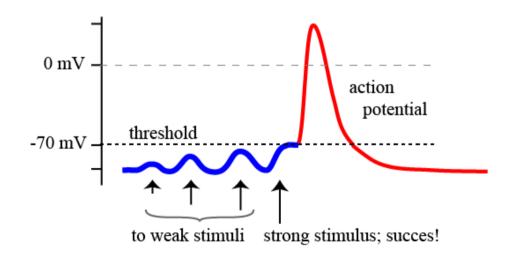
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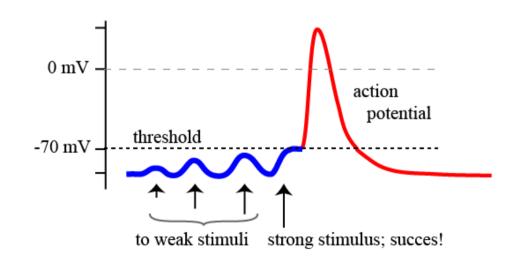


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Many active dendrites will add together and trigger an impulse

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We model the neuron "firing" using an activation function σ

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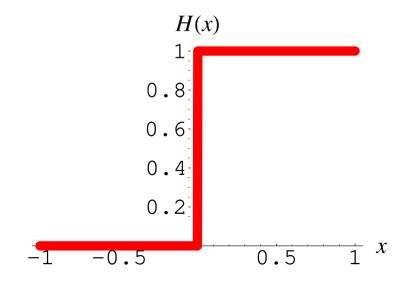
$$\sigma(x) = H(x) = \begin{cases} 0 & \text{if } x \le 0 \\ 1 & \text{if } x > 0 \end{cases}$$

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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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 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):

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

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

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A layer is a linear operation and an activation function

$$f\Big(oldsymbol{x}, egin{bmatrix} oldsymbol{b} \ oldsymbol{W} \end{bmatrix}\Big) = \sigma(oldsymbol{b} + oldsymbol{W}^ op oldsymbol{x})$$

Many layers makes a deep neural network

$$egin{align} oldsymbol{z}_1 &= figg(oldsymbol{x}, egin{bmatrix} oldsymbol{b}_1 \ oldsymbol{w}_1 \end{bmatrix}igg) \ oldsymbol{z}_2 &= figg(oldsymbol{z}_1, egin{bmatrix} oldsymbol{b}_2 \ oldsymbol{W}_2 \end{bmatrix}igg) \ oldsymbol{y} &= figg(oldsymbol{z}_2, egin{bmatrix} oldsymbol{b}_2 \ oldsymbol{W}_2 \end{bmatrix}igg) \end{aligned}$$

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Put away your phones and laptops

Quiz

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

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

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 θ for a neural network

We optimize a loss function by computing

$$\operatorname*{arg\;min}_{\pmb{\theta}} \mathcal{L}(\pmb{X}, \pmb{Y}, \pmb{\theta})$$

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To start, let us consider how we find

$$\operatorname*{arg\ min}_{m{ heta}} \mathcal{L}(m{X},m{Y},m{ heta})$$

in linear regression

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

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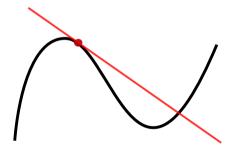
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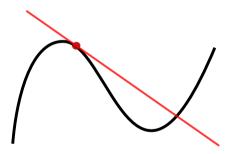
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$$f(x), f'(x = a)$$

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

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

There are formulas for computing the derivative of various operations

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Constant

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

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Power

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

Sum/Difference

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

Sum/Difference

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

Product

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

Sum/Difference

Product

Chain

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

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

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

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

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We can write the derivative as

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We can evaluate the derivative at specific points

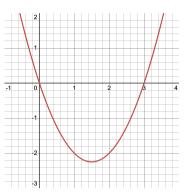
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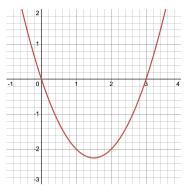
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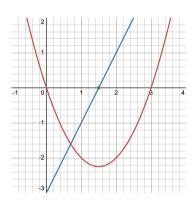
We can evaluate the derivative at specific points

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



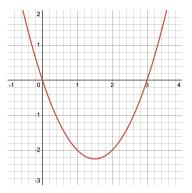
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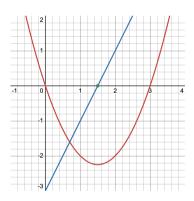


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$$\frac{df}{dx} = 2x - 3$$

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

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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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

$$f(x_1,x_2) = x_1^2 - 3x_1x_2$$

$$f(x_1, x_2) = x_1^2 - 3x_1x_2$$

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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We can evaluate the gradient at specific points

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

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

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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

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

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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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}(oldsymbol{X},oldsymbol{Y},oldsymbol{ heta}) = \sum_{i=1}^n \left(fig(oldsymbol{x}_{[i]},oldsymbol{ heta}ig) - oldsymbol{y}_{[i]}
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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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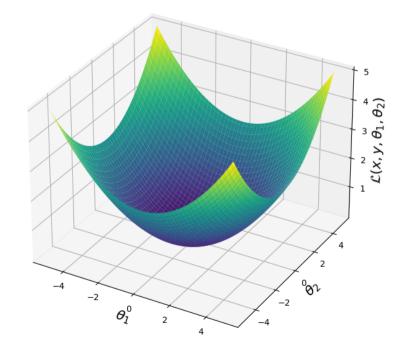
$$\mathcal{L}(\boldsymbol{X},\boldsymbol{Y},\boldsymbol{\theta}) = \underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D\boldsymbol{\theta})^\top}_{\text{Linear function of }\boldsymbol{\theta}} \underbrace{(\boldsymbol{Y} - \boldsymbol{X}_D\boldsymbol{\theta})}_{\text{Quadratic function of }\boldsymbol{\theta}}$$

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

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



Therefore, we know that the heta that solves

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = 0$$

Therefore, we know that the $oldsymbol{ heta}$ that solves

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Also solves

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

Using calculus, let us derive the solution to linear regression

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Using calculus, let us derive the solution to linear regression

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

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

Using calculus, let us derive the solution to linear regression

$$\begin{split} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) &= (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta}) \\ \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) &= \nabla_{\boldsymbol{\theta}} \Big[(\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta})^\top (\boldsymbol{Y} - \boldsymbol{X}_D \boldsymbol{\theta}) \Big] \\ &= \nabla_{\boldsymbol{\theta}} \Big[\boldsymbol{Y}^\top \boldsymbol{Y} - \boldsymbol{Y}^\top \boldsymbol{X}_D \boldsymbol{\theta} - (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{Y} + (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{X}_D \boldsymbol{\theta} \Big] \\ &= \boldsymbol{0} - \boldsymbol{Y}^\top \boldsymbol{X}_D \boldsymbol{I} - (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{Y} + (\boldsymbol{X}_D \boldsymbol{I})^\top \boldsymbol{X}_D \boldsymbol{\theta} + (\boldsymbol{X}_D \boldsymbol{\theta})^\top \boldsymbol{X}_D \boldsymbol{I} \end{split}$$

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

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Lecture 1: Introduction

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

$$= -\mathbf{Y}^{\top} \mathbf{X}_{D} - \mathbf{X}_{D}^{\top} \mathbf{Y} + \mathbf{X}_{D}^{\top} \mathbf{X}_{D} \boldsymbol{\theta} + (\mathbf{X}_{D} \boldsymbol{\theta})^{\top} \mathbf{X}_{D}$$

Remember, $({m A}{m B})^{ op} = {m B}^{ op} {m A}^{ op}$, and so ${m Y}^{ op} {m X}_D = {m X}_D^{ op} {m Y}$

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

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

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

Lecture 1: Introduction

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

$$= -\mathbf{Y}^{\top} \mathbf{X}_{D} - \mathbf{X}_{D}^{\top} \mathbf{Y} + \mathbf{X}_{D}^{\top} \mathbf{X}_{D} \boldsymbol{\theta} + (\mathbf{X}_{D} \boldsymbol{\theta})^{\top} \mathbf{X}_{D}$$
Remember, $(\mathbf{A} \mathbf{B})^{\top} = \mathbf{B}^{\top} \mathbf{A}^{\top}$, and so $\mathbf{Y}^{\top} \mathbf{X}_{D} = \mathbf{X}_{D}^{\top} \mathbf{Y}$

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$$= -2 \mathbf{X}_{D}^{\top} \mathbf{Y} + 2 \mathbf{X}_{D}^{\top} \mathbf{X} \boldsymbol{\theta}$$

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$$= -2 \mathbf{X}_{D}^{\top} \mathbf{Y} + 2 \mathbf{X}_{D}^{\top} \mathbf{X} \boldsymbol{\theta}$$

And so, the gradient of the loss is

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

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Lecture 1: Introduction

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$$2\boldsymbol{X}_D^{ op} \boldsymbol{Y} = 2\boldsymbol{X}_D^{ op} \boldsymbol{X}_D \boldsymbol{ heta}$$

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

$$\left(oldsymbol{X}_D^ op oldsymbol{X}_D^ op oldsymbol{X}_D^ op oldsymbol{Y} = oldsymbol{ heta}$$

This was the "magic" solution I gave you for linear regression

$$\left(oldsymbol{X}_D^ op oldsymbol{X}_D^ op oldsymbol{X}_D^ op oldsymbol{Y} = oldsymbol{ heta}$$

This was the "magic" solution I gave you for linear regression

$$oldsymbol{ heta} = ig(oldsymbol{X}_D^ op oldsymbol{X}_D^{-1} oldsymbol{X}_D^ op oldsymbol{Y}$$

Now, we will do the same approach for neural networks

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To make it simple, we assume $d_x=1, d_y=1, n=1$

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One input dimension, one output dimension, one datapoint

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One input dimension, one output dimension, one datapoint

Step 1: Write the loss function for a neural network

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

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All that changes is the model f

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All that changes is the model f

Linear regression:

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

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

All that changes is the model f

Linear regression:

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

Perceptron:

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

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

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

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

Neural network model

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

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

Neural network model

Now, we plug the model f into the loss function

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

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

Neural network model

Now, we plug the model *f* into the loss function

$$\mathcal{L}(x,y,\boldsymbol{\theta}) = \left(\sigma(\theta_0 + \theta_1 x) - y\right)^2$$

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

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

Neural network model

Now, we plug the model f into the loss function

$$\mathcal{L}(x,y,\boldsymbol{\theta}) = \left(\sigma(\theta_0 + \theta_1 x) - y\right)^2$$

Rewrite

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

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Neural network model

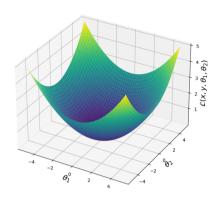
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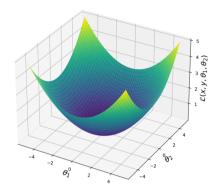
$$\mathcal{L}(x,y,\theta) = \underbrace{(\sigma(\theta_0 + \theta_1 x) - y)(\sigma(\theta_0 + \theta_1 x) - y)}_{\text{Nonlinear function of }\theta} \underbrace{(\sigma(\theta_0 + \theta_1 x) - y)(\sigma(\theta_0 + \theta_1 x) - y)}_{\text{Nonlinear function of }\theta}$$

Linear regression loss function was quadratic with one minima



Lecture 1: Introduction

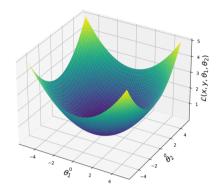
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With a neural network, this is our loss function

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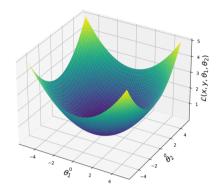
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Question: How many minima does this function have?

Lecture 1: Introduction

Linear regression loss function was quadratic with one minima



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Question: How many minima does this function have?

Answer: We do not know

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

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Activation functions make the neural network powerful

Linear regression: analytical solution for $oldsymbol{ heta}$

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Neural network: no analytical solution for heta

Lecture 1: Introduction

Linear regression: analytical solution for heta

Neural network: no analytical solution for heta

So how to find θ for a neural network?

Lecture 1: Introduction

To find θ for a neural network, we use **gradient descent**

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Gradient descent optimizes differentiable functions

We must be able to take the derivative or gradient of the loss function to use gradient descent

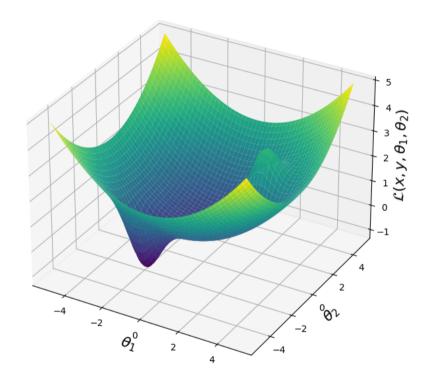
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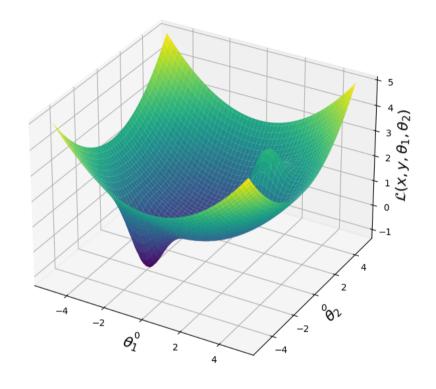
We must be able to take the derivative or gradient of the loss function to use gradient descent

How does gradient descent work?

A differentiable loss function produces a manifold

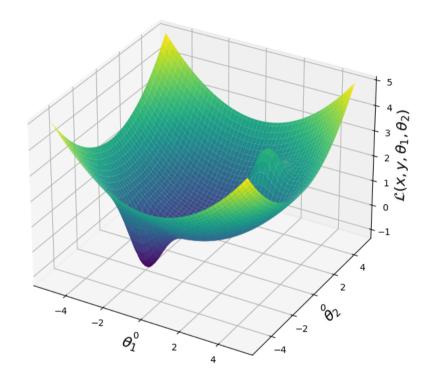


A differentiable loss function produces a manifold



Our goal is to find the lowest point on this manifold

A differentiable loss function produces a manifold

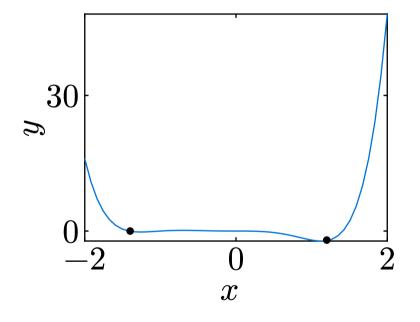


Our goal is to find the lowest point on this manifold The lowest point solves arg $\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$

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

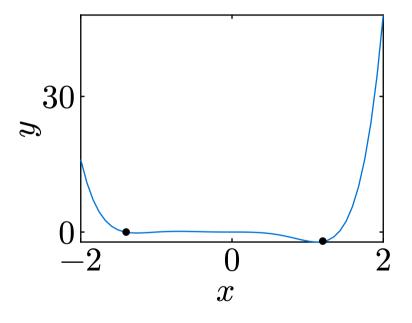
Lecture 1: Introduction

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



Lecture 1: Introduction

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



In practice, a local optima provides a good enough model

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

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



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!



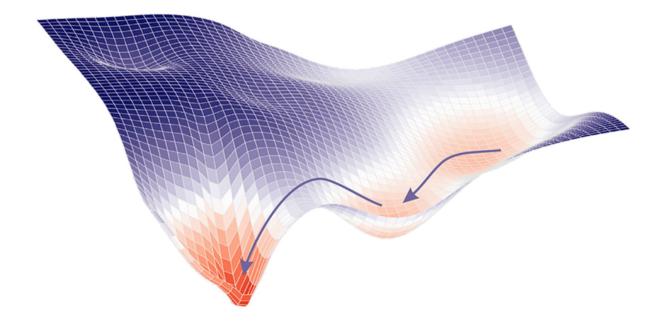
You see this, which way do you walk next?



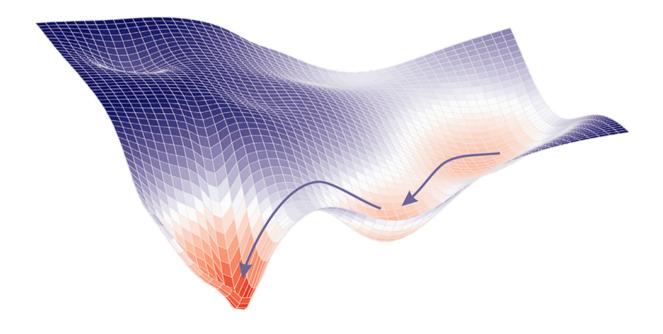
This is gradient descent

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

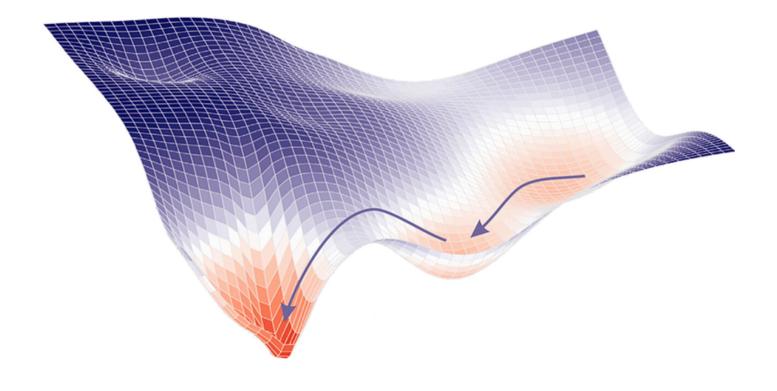
In gradient descent, we look at the **slope** of the loss function And we walk in the steepest direction In gradient descent, we look at the **slope** of the loss function And we walk in the steepest direction

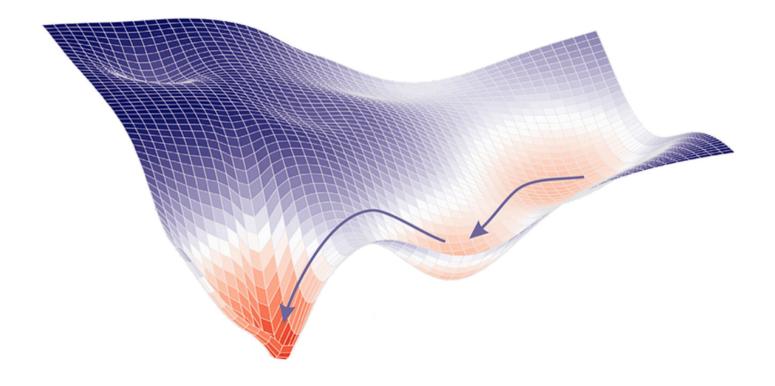


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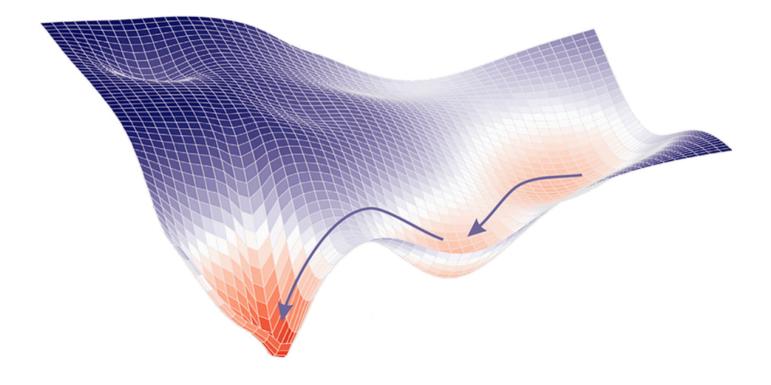


And then we repeat



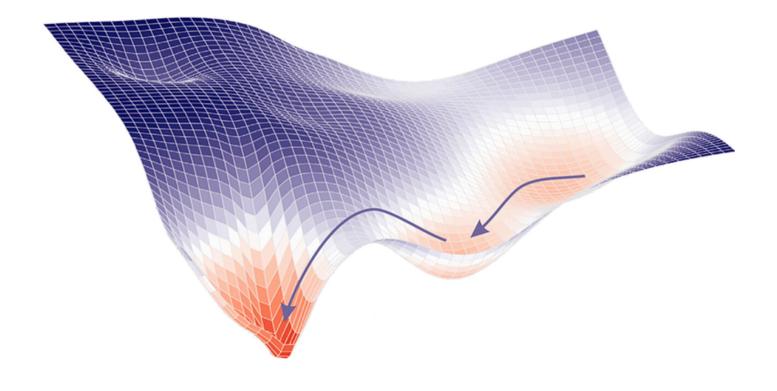


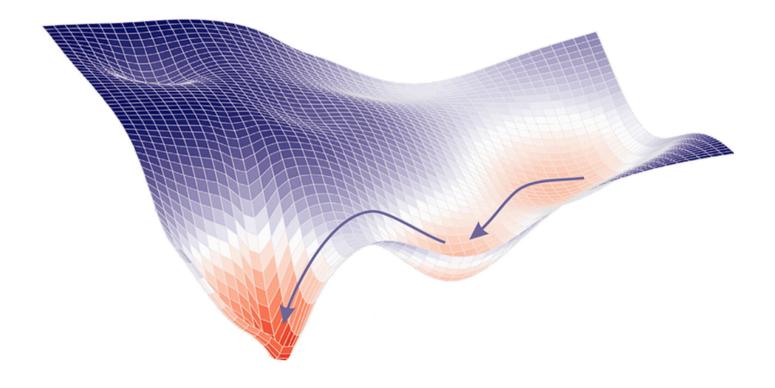
We find the gradient $abla_{m{ heta}}\mathcal{L}(m{X},m{Y},m{ heta})$



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

And update θ in the steepest direction





Eventually, we arrive at the bottom

With gradient descent, the loss function must be differentiable

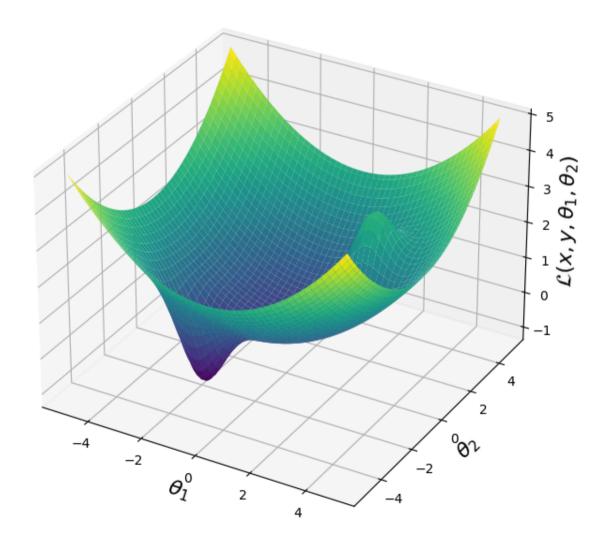
With gradient descent, the loss function must be differentiable

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

The gradient descent algorithm:

1:**function** Gradient Descent($X, Y, \mathcal{L}, t, \alpha$)

- 2: > Randomly initialize parameters
- 3: $\theta \leftarrow \mathcal{N}(0,1)$
- 4: **for** $i \in 1...t$ **do**
- 5: Compute the gradient of the loss
- 6: $\boldsymbol{J} \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
- 7: b Update the parameters using the negative gradient
- 8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \alpha \boldsymbol{J}$
- 9: return θ



Step 1: Compute the gradient of the loss

Step 1: Compute the gradient of the loss

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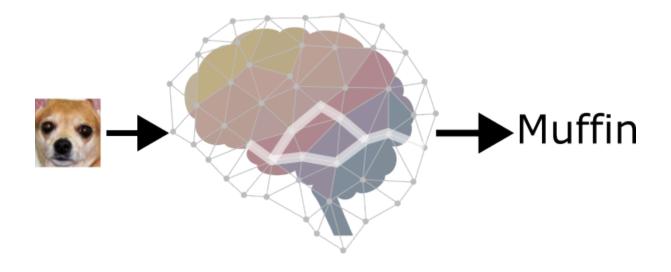
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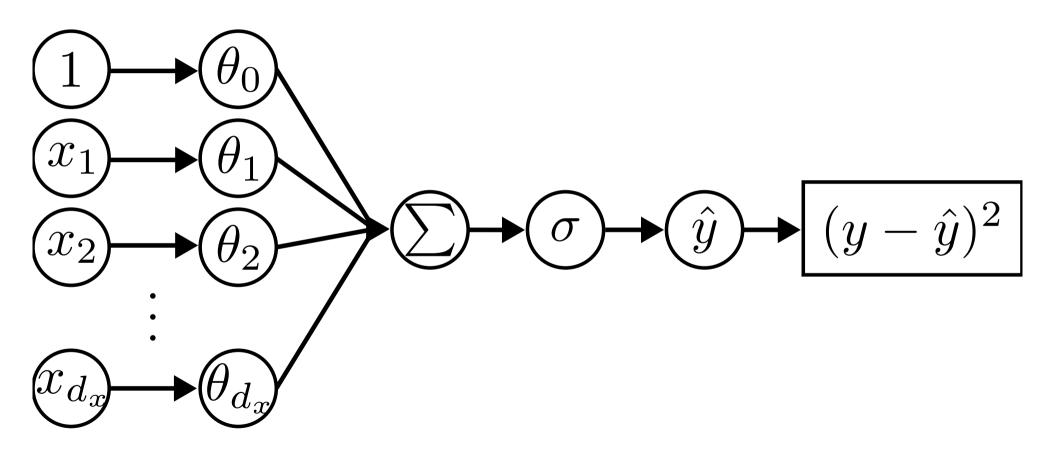
We propagate errors from the loss function **backward** through each layer of the neural network

We call this process **backpropagation**

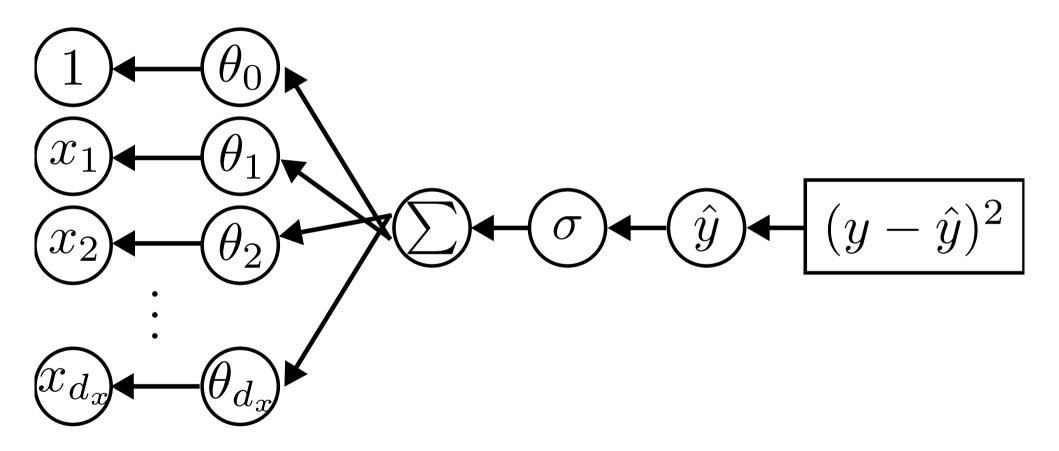
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Forward propagation



Backward propagation



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

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

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

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

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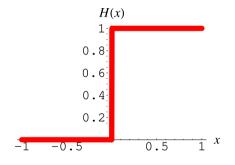
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$$\begin{split} \nabla_{\boldsymbol{\theta}} f(\boldsymbol{x}, \boldsymbol{\theta}) &= \nabla_{\boldsymbol{\theta}} [\sigma] (\boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}) \cdot \nabla_{\boldsymbol{\theta}} (\boldsymbol{\theta}^{\top} \overline{\boldsymbol{x}}) \\ \text{What is } \nabla_{\boldsymbol{\theta}} \sigma? \end{split}$$

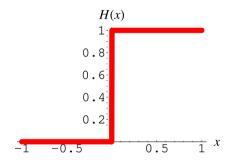
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What is $\nabla_{\theta} \sigma$?



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



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

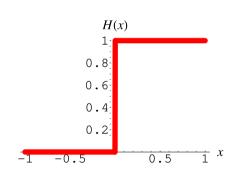
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

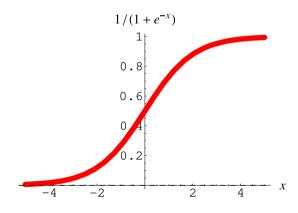
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We call this approximation the **sigmoid function**

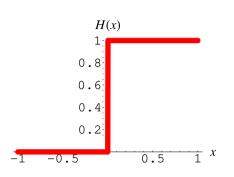
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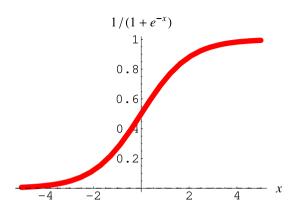
We call this approximation the **sigmoid function**





The sigmoid function has finite and nonzero derivative everywhere

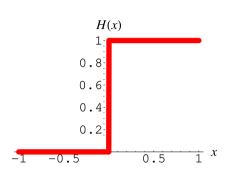


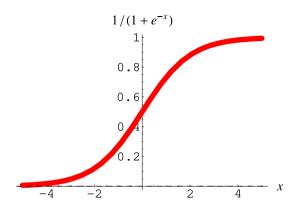


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The derivative of the sigmoid function is

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





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$$\nabla_{\boldsymbol{z}} \sigma(\boldsymbol{z}) = \sigma(\boldsymbol{z}) \odot (1 - \sigma(\boldsymbol{z}))$$

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

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

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

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

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

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Recall the deep neural network has many layers

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

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And that we call them in series

$$egin{aligned} oldsymbol{z}_1 &= f_1(oldsymbol{x}, oldsymbol{arphi}) \ oldsymbol{z}_2 &= f_2(oldsymbol{z}_1, oldsymbol{\psi}) \ &drawpsilon \ oldsymbol{z}_\ell &= f_\ell(oldsymbol{z}_{\ell-1}, oldsymbol{\xi}) \end{aligned}$$

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Take the gradient of both sides

$$egin{aligned}
abla_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} egin{aligned}
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abla_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} f_2(oldsymbol{z}_1,oldsymbol{\psi}) \\ & arphi \\
abla_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} egin{aligned} z_2 &=
abla_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} f_\ell(oldsymbol{z}_{\ell-1},oldsymbol{\xi}) \end{aligned}$$

Take the gradient of both sides

$$egin{aligned}
abla_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} oldsymbol{z}_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} oldsymbol{z}_1 &=
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Each layer only uses one set of parameters

$$egin{aligned}
abla_{oldsymbol{arphi}} oldsymbol{z}_1 &=
abla_{oldsymbol{arphi}} f_1(oldsymbol{x}, oldsymbol{arphi}) \
abla_{oldsymbol{\psi}} oldsymbol{z}_2 &=
abla_{oldsymbol{\psi}} f_2(oldsymbol{z}_1, oldsymbol{\psi}) \ &dots \
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abla_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} oldsymbol{z}_{oldsymbol{arphi},oldsymbol{\psi},...,oldsymbol{\xi}} oldsymbol{z}_1 &=
abla_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} f_1(oldsymbol{x},oldsymbol{arphi}) \ &arphi_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\psi},oldsymbol{\xi}} oldsymbol{z}_2 &=
abla_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} f_2(oldsymbol{z}_1,oldsymbol{\psi}) \ &arepsilon & arphi_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} oldsymbol{z}_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}} oldsymbol{z}_{oldsymbol{arphi},oldsymbol{\xi},oldsymbol{\xi}_{oldsymbol{arphi},oldsymbol{\psi},oldsymbol{\xi}_{oldsymbol{arphi},oldsymbol{\xi}_{oldsymbol{\zeta},oldsymbol{\xi}_{oldsymbol{\zeta},oldsymbol{\xi}_{oldsymbol{$$

Each layer only uses one set of parameters

$$egin{aligned}
abla_{oldsymbol{arphi}} oldsymbol{z}_1 &=
abla_{oldsymbol{arphi}} f_1(oldsymbol{x}, oldsymbol{arphi}) \
abla_{oldsymbol{\psi}} oldsymbol{z}_2 &=
abla_{oldsymbol{\psi}} f_2(oldsymbol{z}_1, oldsymbol{\psi}) \ &dots \
abla_{oldsymbol{arphi}} oldsymbol{z}_{oldsymbol{\psi}} =
abla_{oldsymbol{\psi}} f_2(oldsymbol{z}_1, oldsymbol{\psi}) \end{aligned}$$

The gradient of a deep neural network is

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

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Where each layer gradient is

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

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$$\mathcal{L}(oldsymbol{X},oldsymbol{Y},oldsymbol{ heta}) = \sum_{i=1}^n \left(fig(oldsymbol{x}_{[i]},oldsymbol{ heta}ig) - oldsymbol{y}_{[i]}
ight)^2$$

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$$abla_{m{ heta}} \mathcal{L}(m{X},m{Y},m{ heta}) =
abla_{m{ heta}} \sum_{i=1}^n \left(fig(m{x}_{[i]},m{ heta}ig) - m{y}_{[i]}
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abla_{m{ heta}} ig(fig(m{x}_{[i]},m{ heta}ig) - m{y}_{[i]}ig)^2$$

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

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$$abla_{m{ heta}}\mathcal{L}(m{X},m{Y},m{ heta}) = \sum_{i=1}^n 2ig(fig(m{x}_{[i]},m{ heta}ig) - m{y}_{[i]}ig)ar{
abla}_{m{ heta}}fig(m{x}_{[i]},m{ heta}ig)$$

$$egin{aligned} oldsymbol{
abla}_{oldsymbol{ heta}}f(oldsymbol{x},[oldsymbol{\phi}\ \psi\ ...\ oldsymbol{\xi}]^{ op}) = egin{bmatrix}
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abla_{oldsymbol{\psi}}f_2(oldsymbol{z}_1,oldsymbol{\psi}) \
& arphi \
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abla_{m{ heta}} fig(m{x}_{[i]},m{ heta}ig)$$

$$egin{aligned} oldsymbol{
abla}_{oldsymbol{ heta}}f(oldsymbol{x}, [oldsymbol{\phi} \ oldsymbol{\psi} \ oldsymbol{...} \ oldsymbol{\xi}f(oldsymbol{z}, [oldsymbol{\phi} \ oldsymbol{\psi} \ oldsymbol{...} \ oldsymbol{\xi} \ oldsymbol{\xi} \ oldsymbol{\xi}f(oldsymbol{z}, oldsymbol{\psi}, oldsymbol{\omega}, oldsymbol{\psi}) \end{bmatrix}$$

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

Answer: The gradient is necessary for gradient descent

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- 1:for $i \in 1...t$ do
- > Compute the gradient of the loss 2:
- $J \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$ 3:
- > Update the parameters using the negative gradient 4:
- $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \alpha \boldsymbol{J}$ 5:

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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

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

```
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
J = gradient L(X, Y, theta)
# Update parameters
alpha = 0.0001
theta = theta - alpha * J
```

```
import torch
optimizer = torch.optim.SGD(lr=0.0001)
def L(X, Y, model):
# Pytorch will record a graph of all operations
loss = L(X, Y, model) # compute gradient
# Traverse the graph and compute the full gradient
loss.backward()
optimizer.step() # Update the parameters
optimizer.zero grad() # Always remember to do this
```

Time for some interactive coding

https://colab.research.google.com/drive/1W8WVZ8n_9yJCcOqkPVURp_ wJUx3EQc5w