Deep Learning

CSCI 1470

Day 5: MLPs and Optimization

Eric Ewing

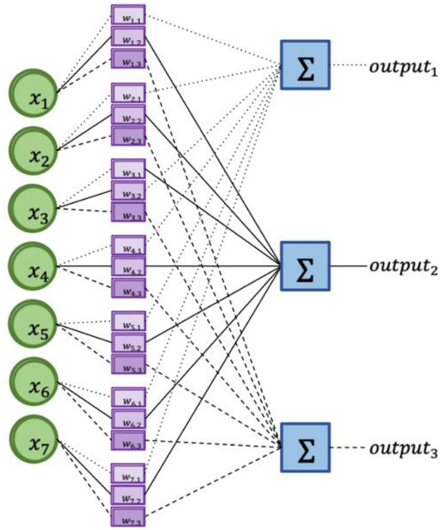
Friday, 1/31/25

Review

Perceptrons used for binary classification.

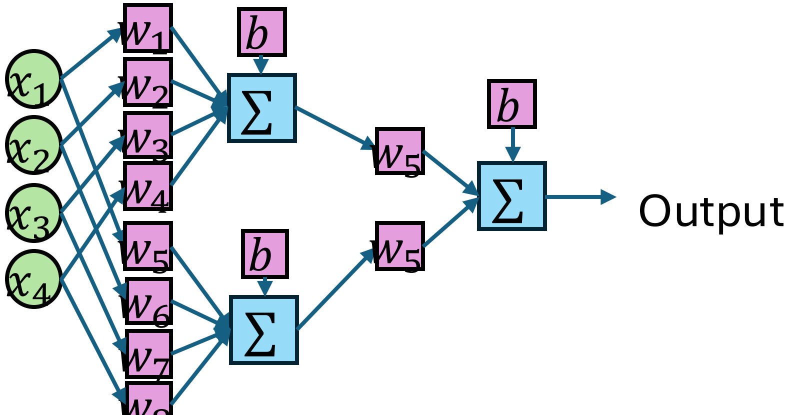
Want to perform multi-class classification?

Multiple Perceptrons sharing inputs



Want to learn more complex functions?

Multiple Layers



Today's Goals

Introduction to the theory of neural networks

(1) Universal Approximation Theory

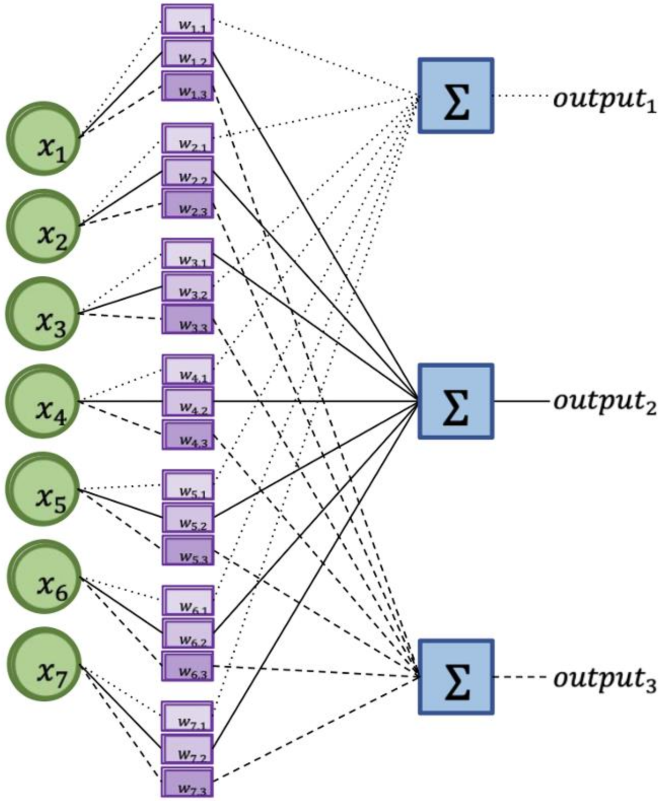
(2) How do we train Neural Networks?

Multi-Class Classification

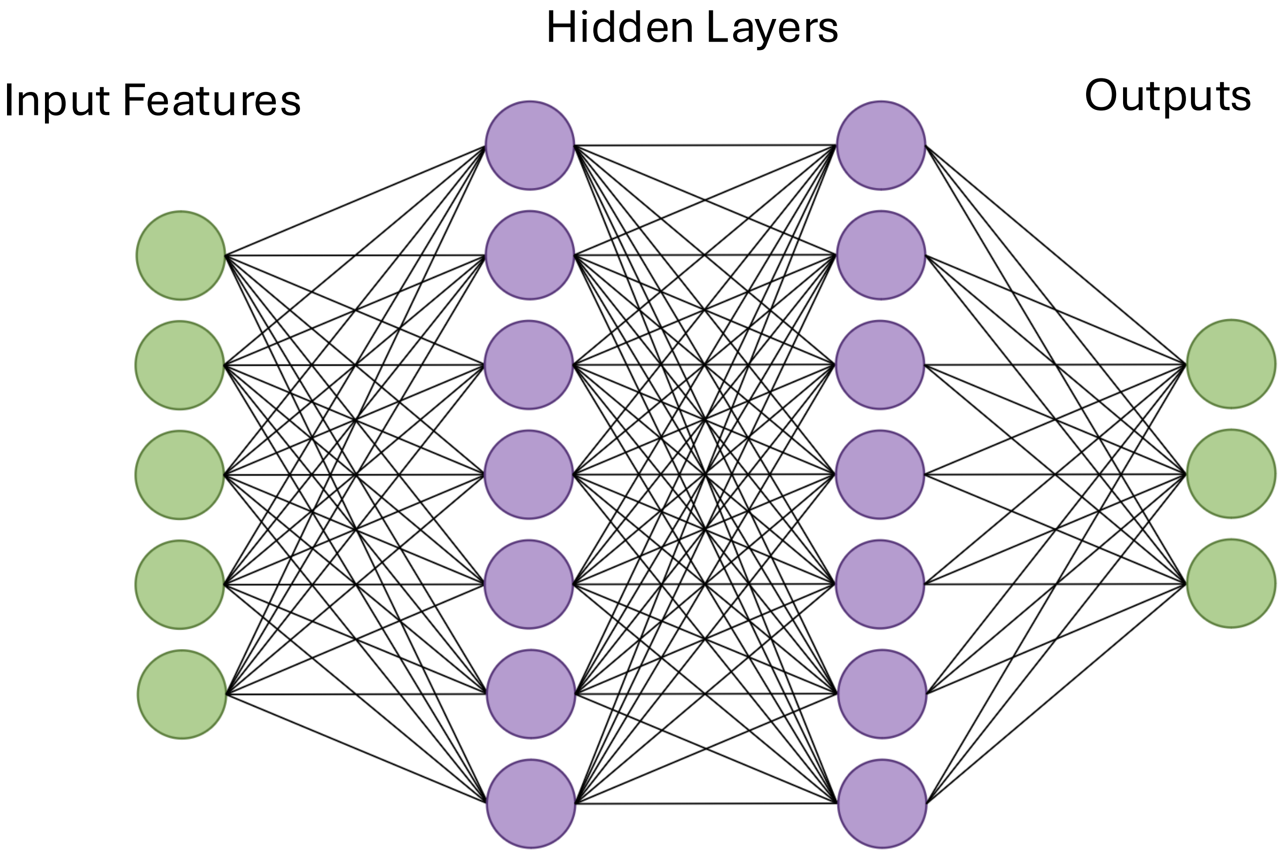
Multi-class classification with "perceptrons"

Need to remove threshold function from outputs

Why?



MLPs

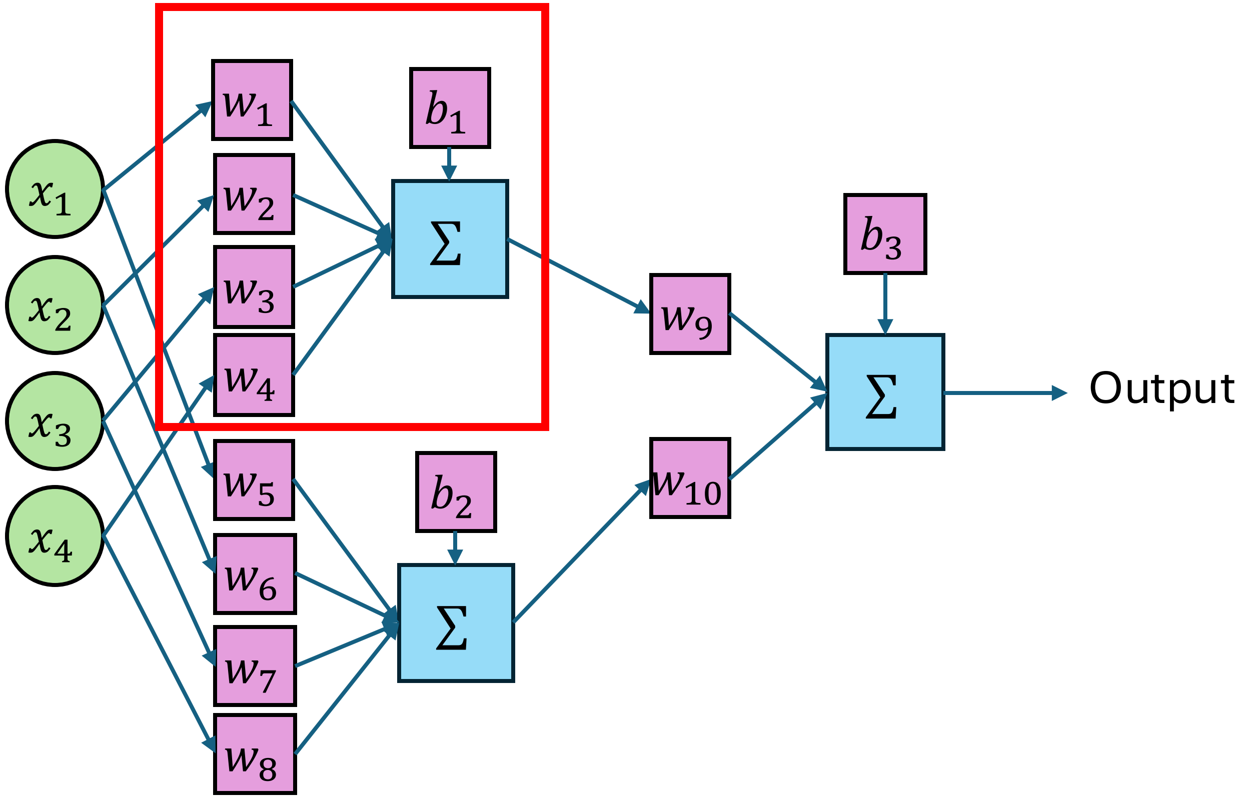


A Multi-Layered Neural Net

Multi-Layer Perceptrons

What happens if we remove the threshold activations from a multi-layer perceptron?

Let $\mathrm{w}^{(1)} = [w_1, w_2, w_3, w_4]$
Perceptron #1: $\mathrm{z}_1 = x^T w^{(1)} + b_1$



Multi-Layer Perceptrons

What happens if we remove the activations from a multi-layer perceptron?

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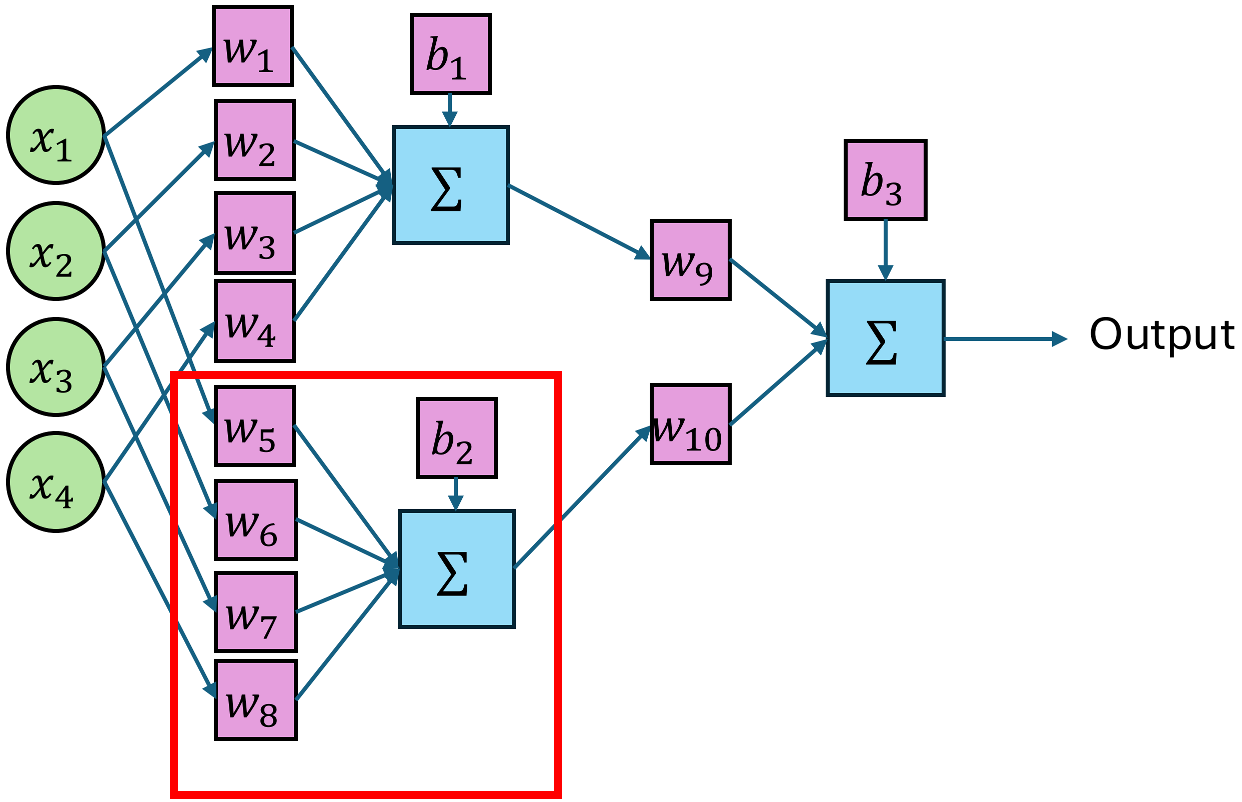

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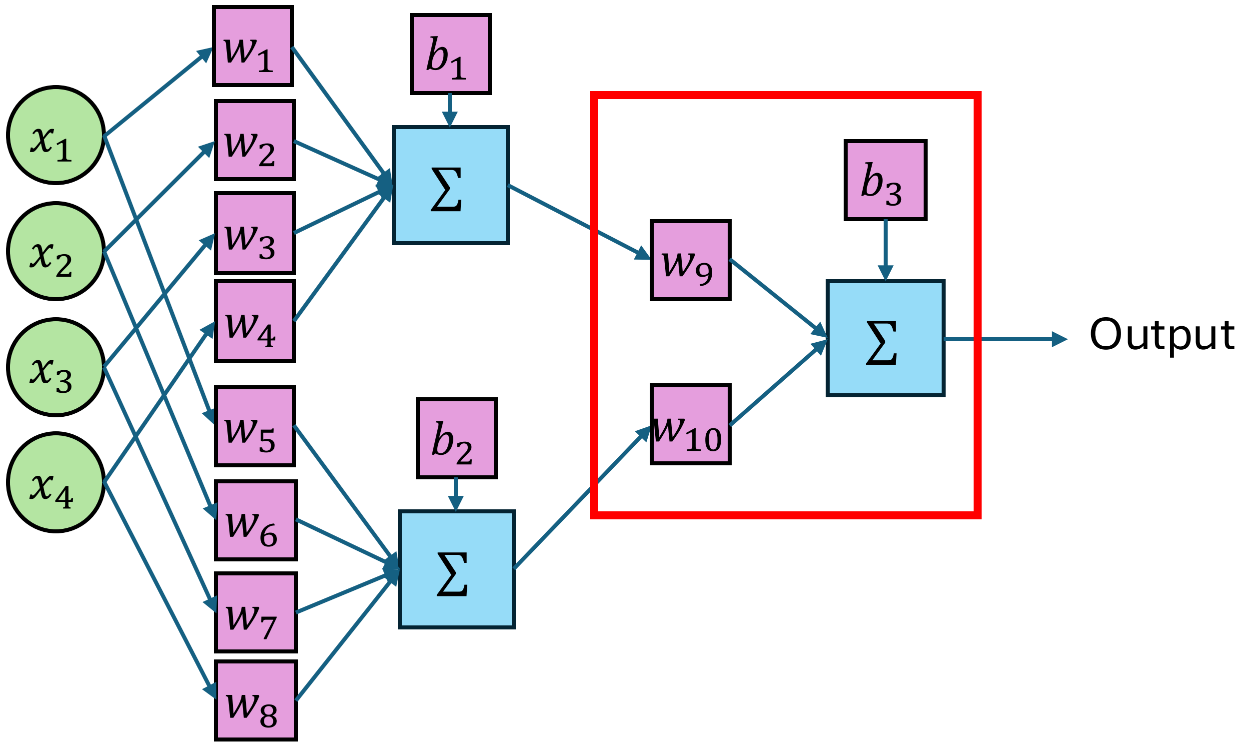

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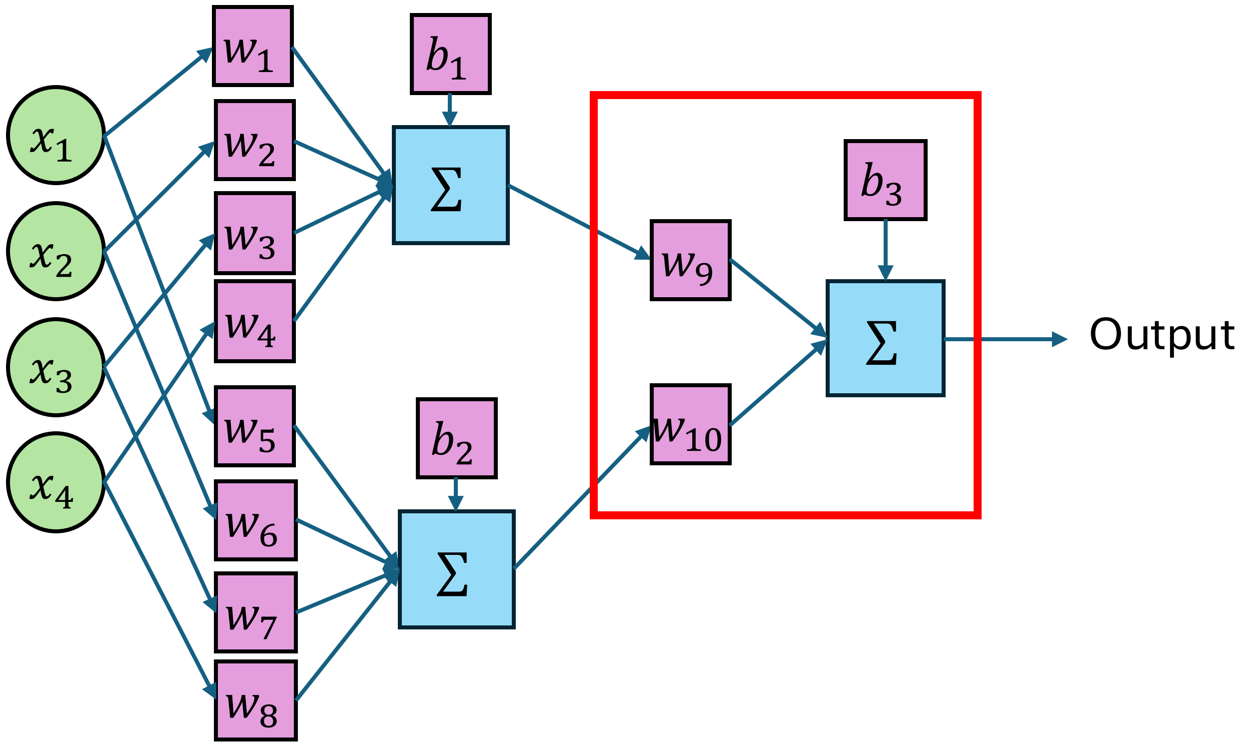
Entire Network:
$w_9\left(x^T w^{(1)} + b_1\right) + w_{10}\left(x^T w^{(2)} + b_2\right) + b_3$



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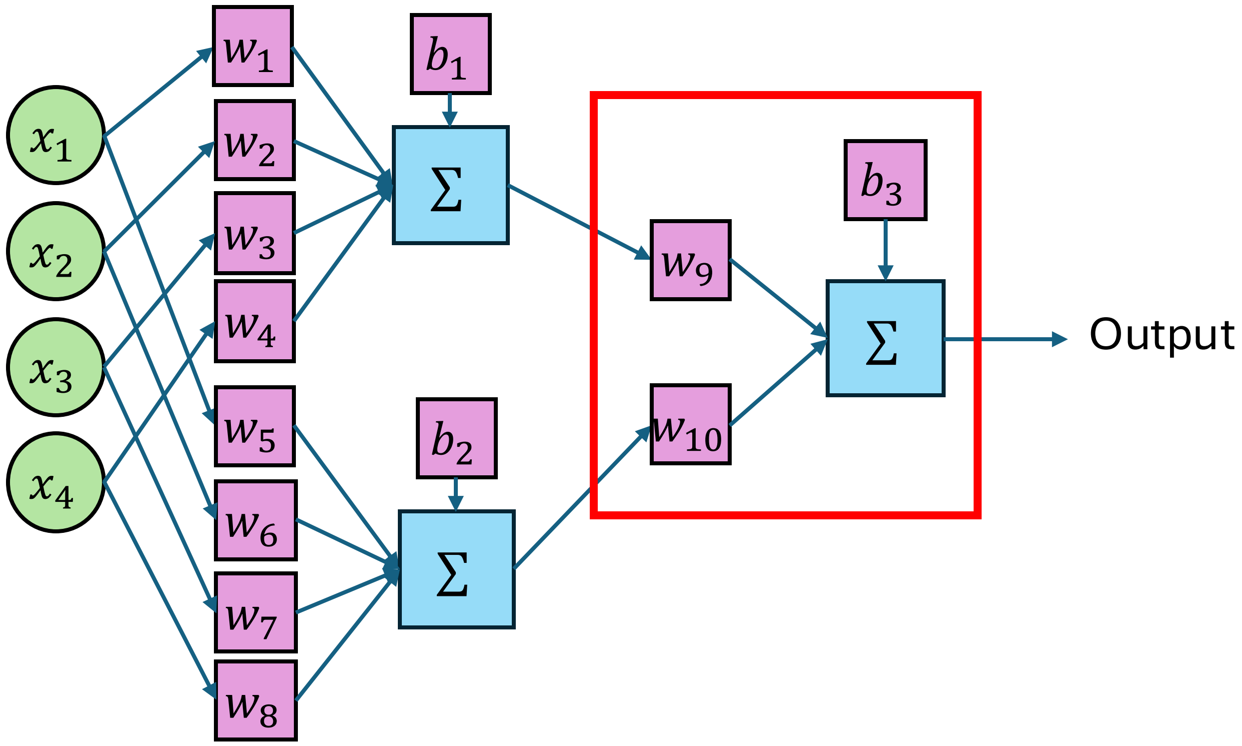

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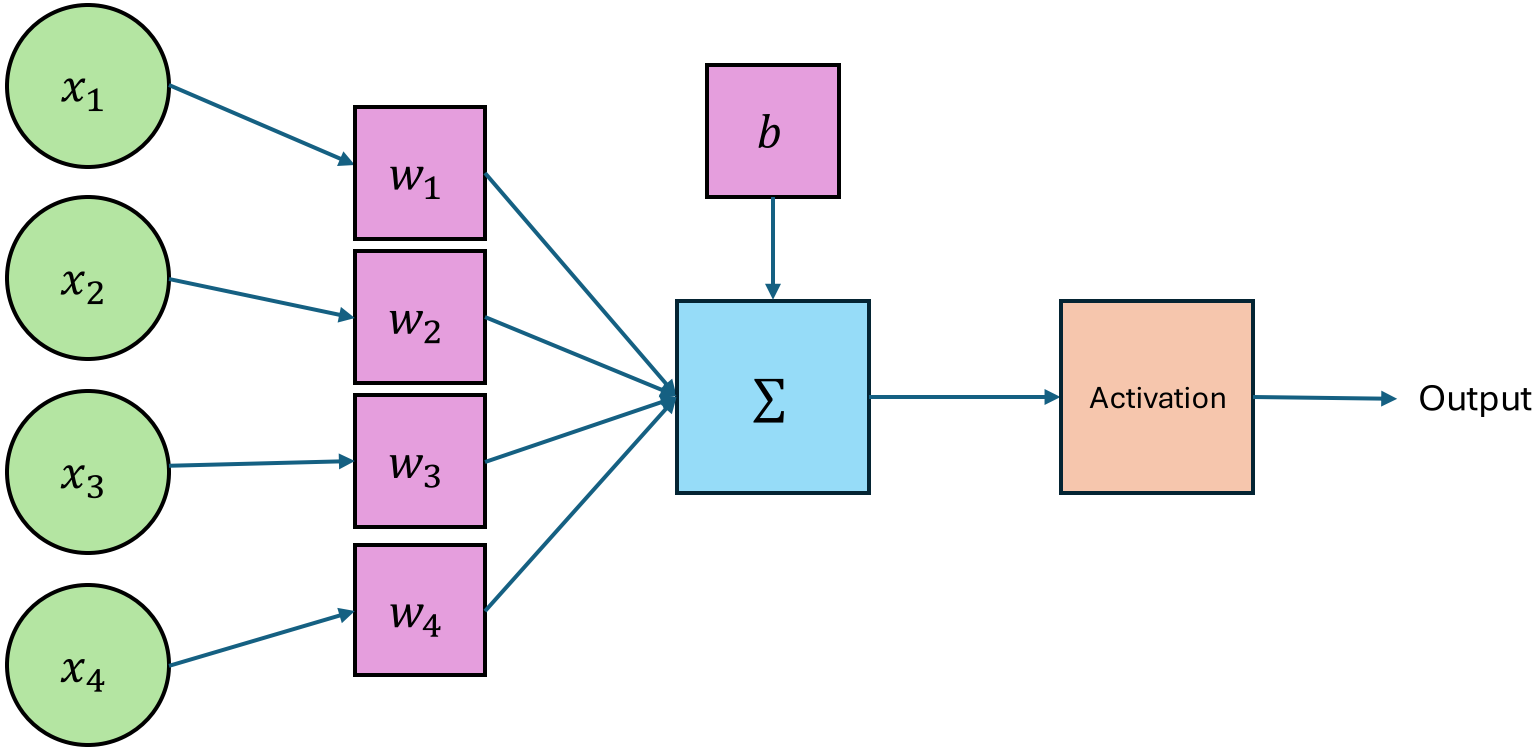
Multi-Layer Perceptrons without non-linear activation functions are linear functions

Activation Functions

Non-linear functions applied to output of neuron



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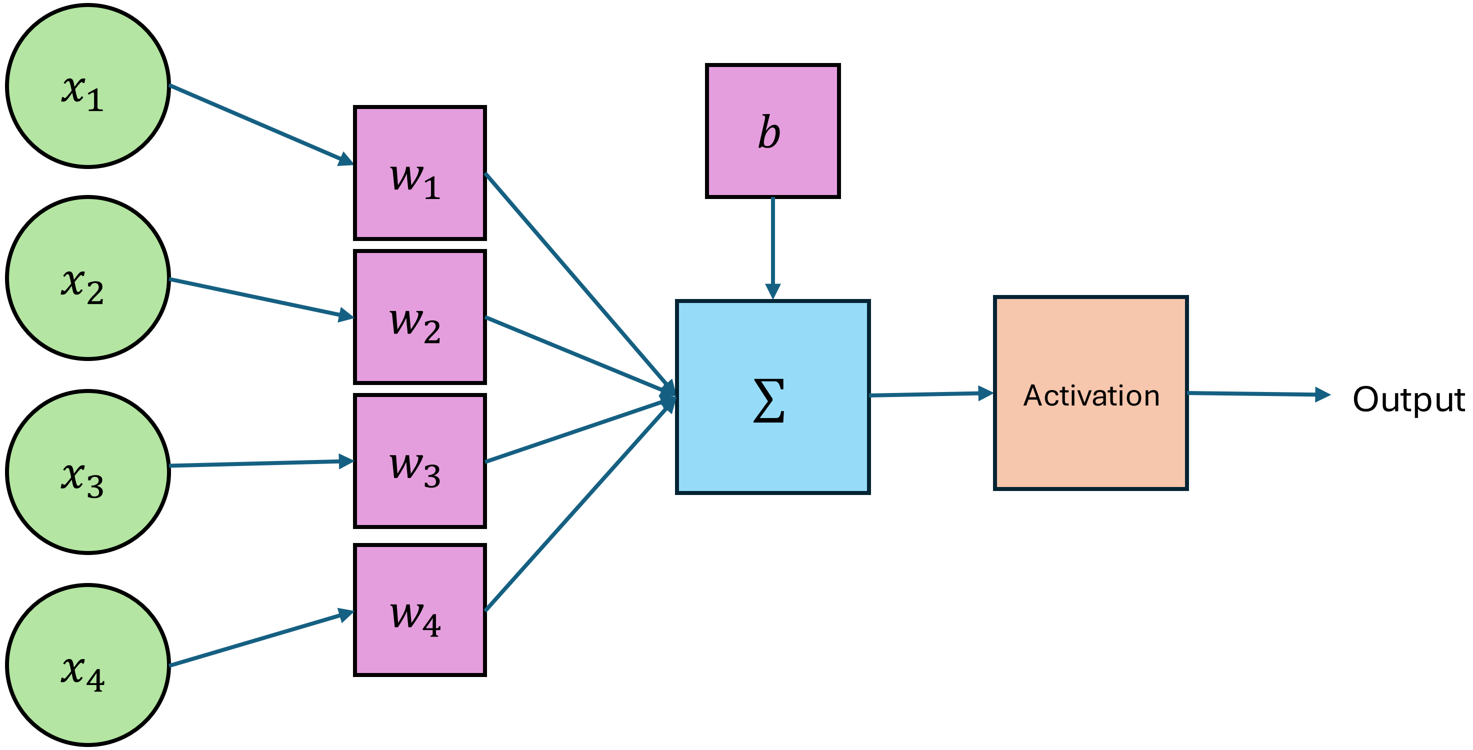
In the perceptron case, the activation function is the threshold



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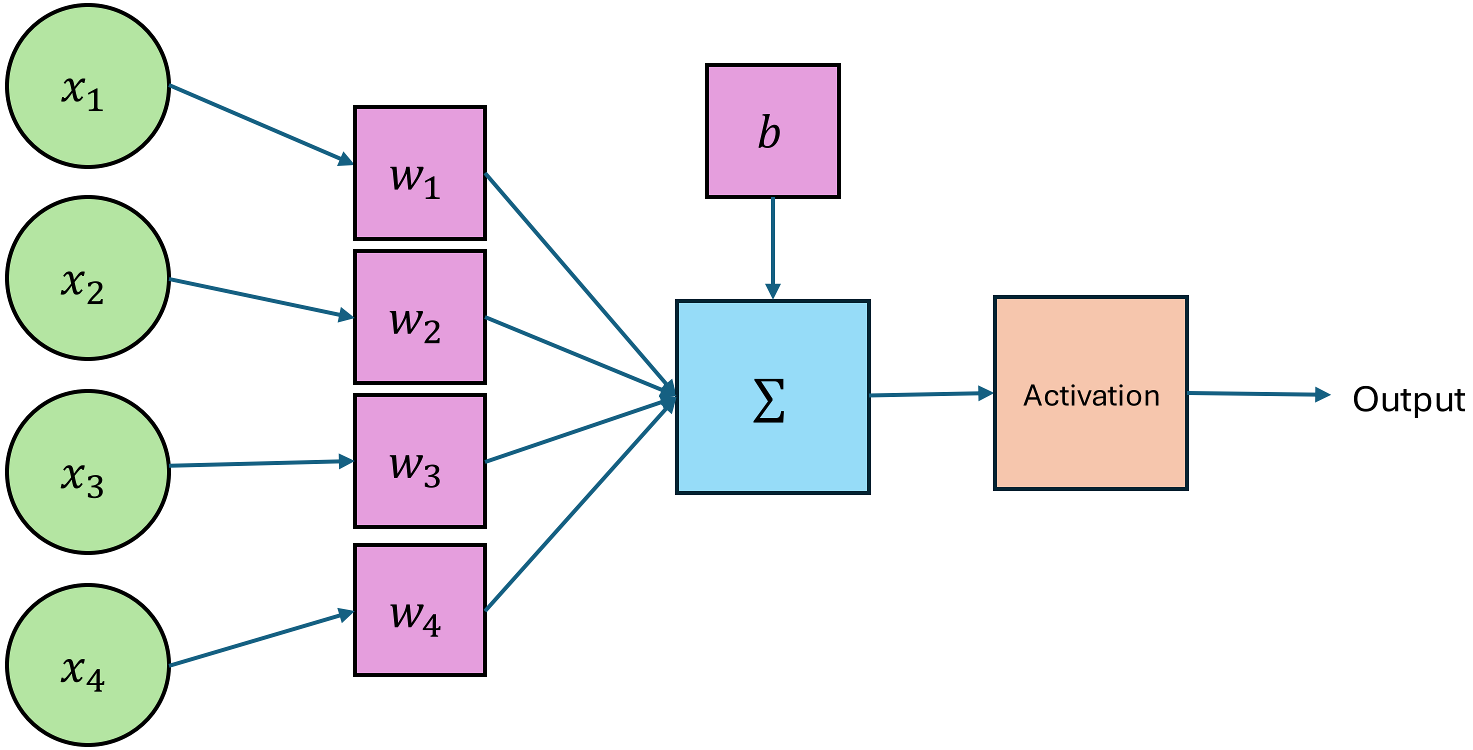
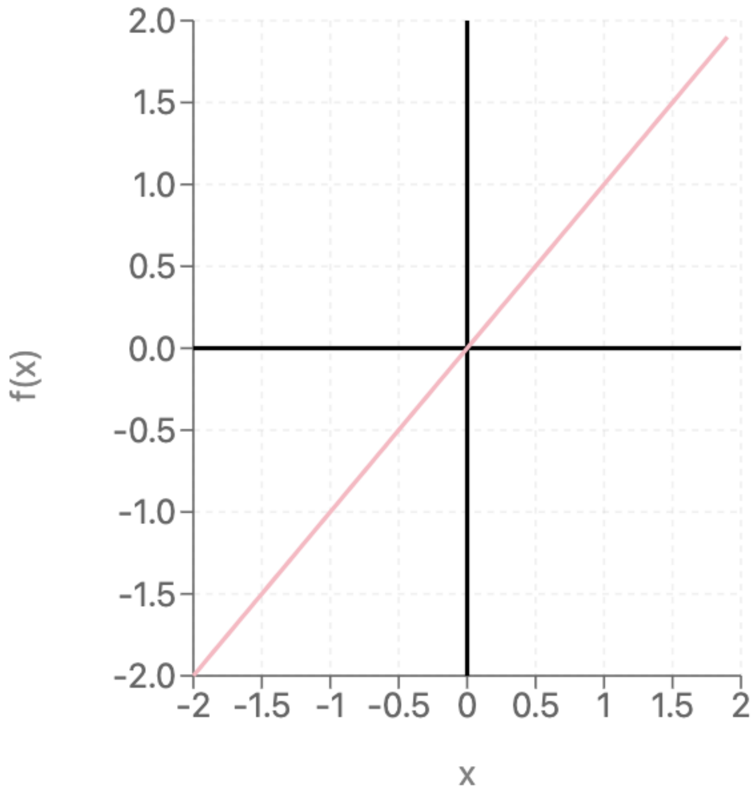


Common Activation Functions

Linear (No Activation)

f(x) = x



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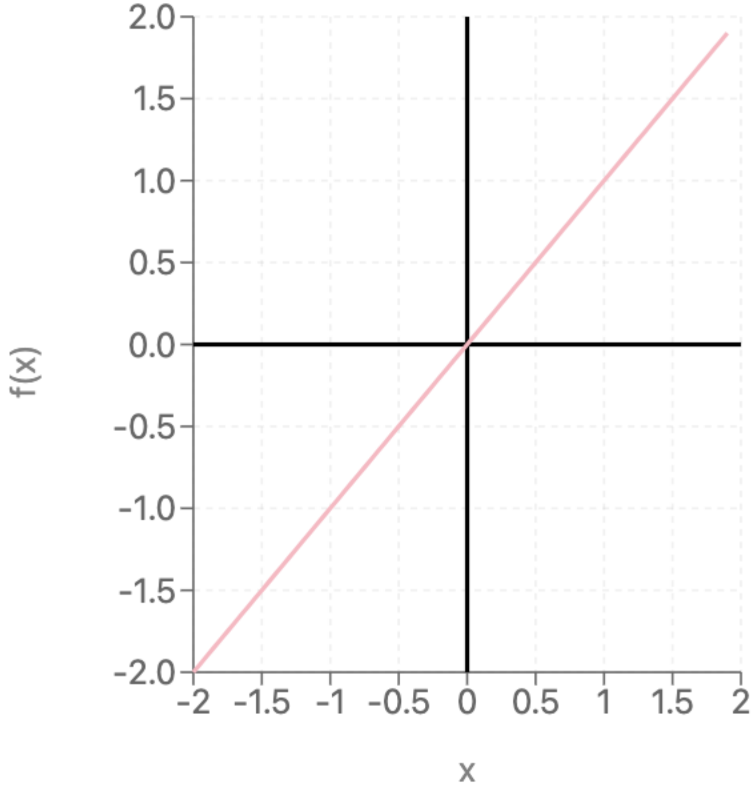
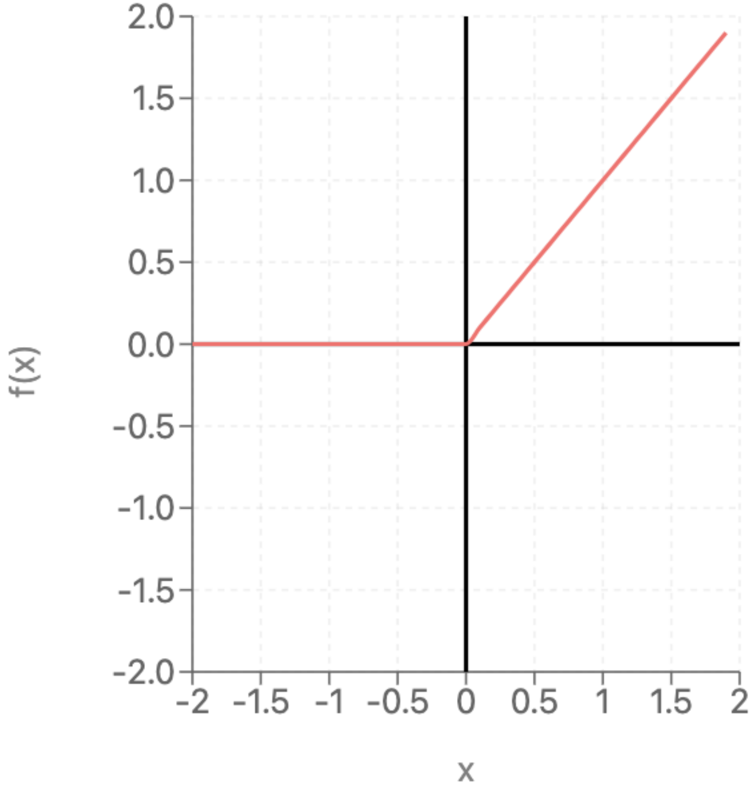


ReLU

f(x) = max(0, x)



Common Activation Functions

Rectified Linear Unit (ReLU):
One of the most common Activation Functions
Advantages: Simple, easy to compute gradients

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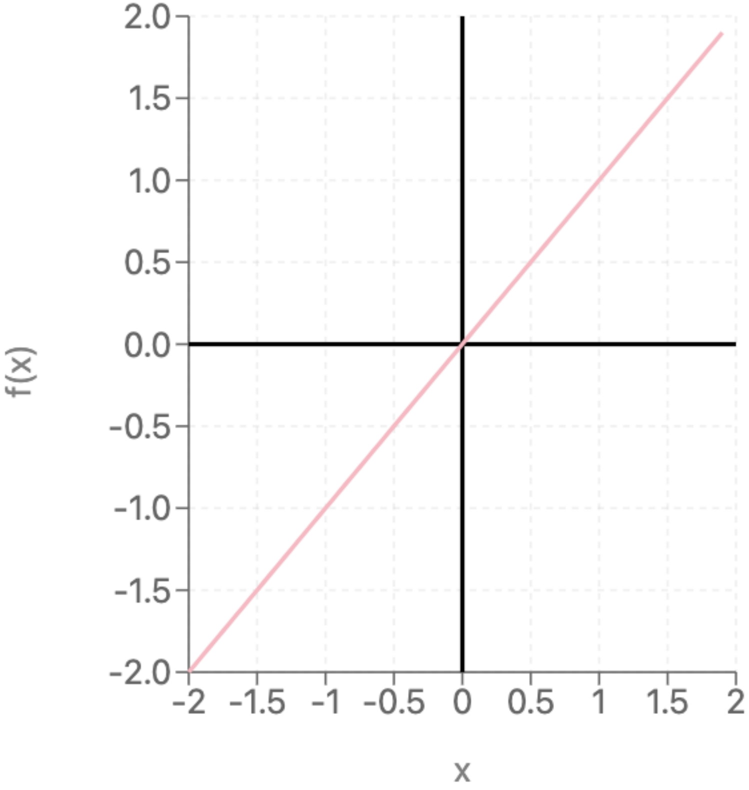

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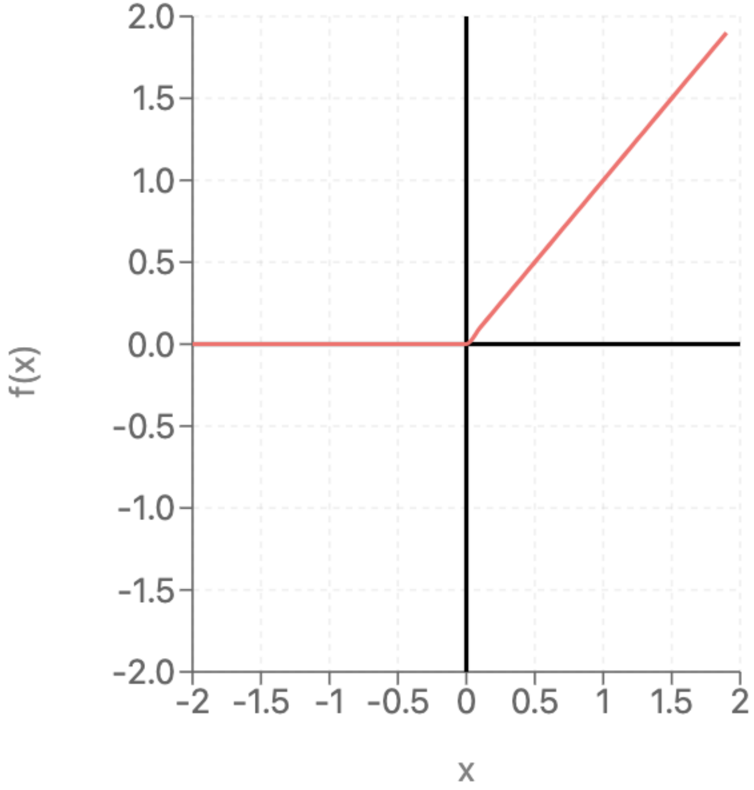

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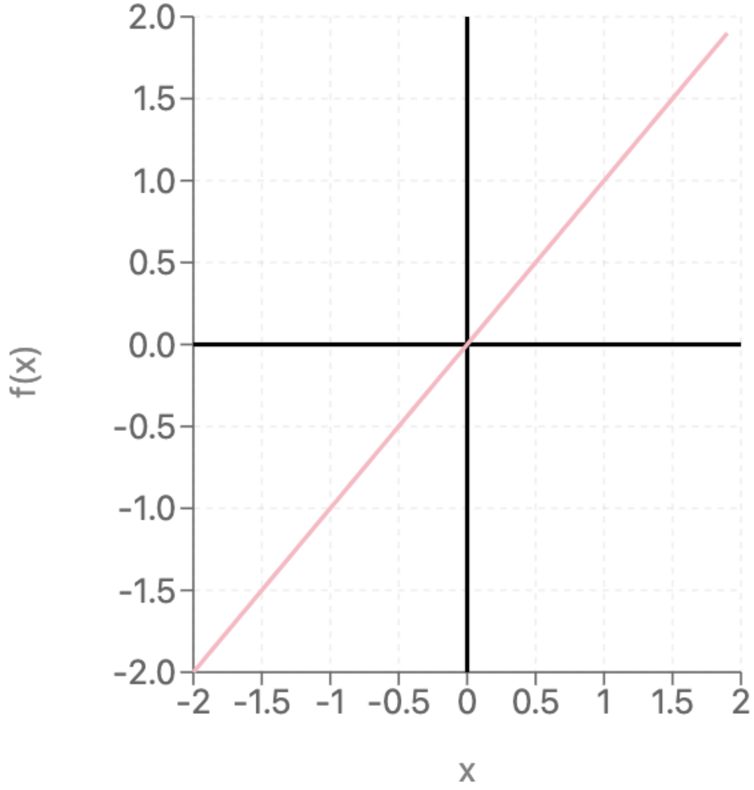

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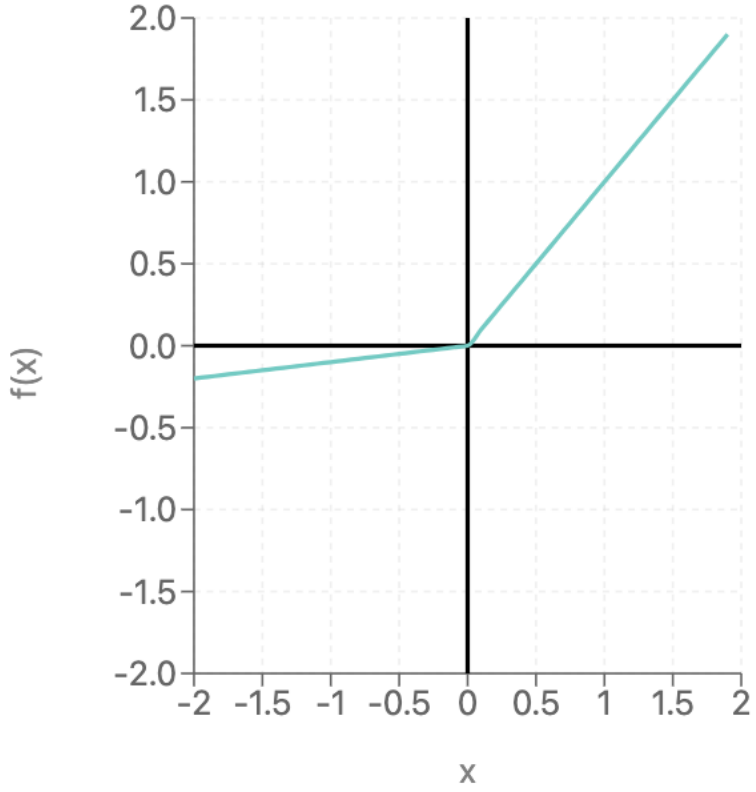
f(x) = x if x > 0 else 0.1x



Common Activation Functions

Leaky ReLU:
Common substitute for ReLU, often has better performance
Advantages: Fixes “dying neurons” issue with ReLU.

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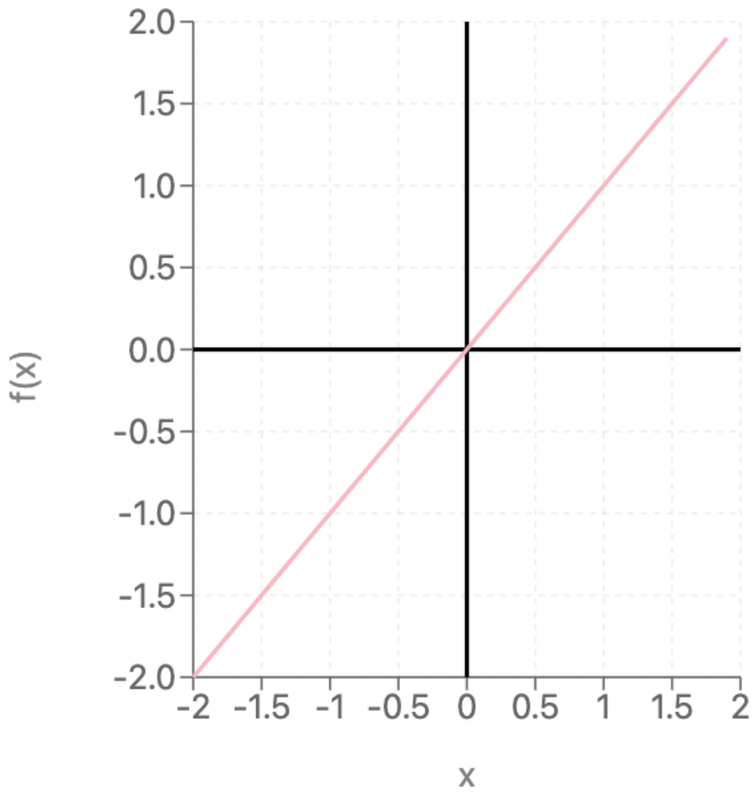

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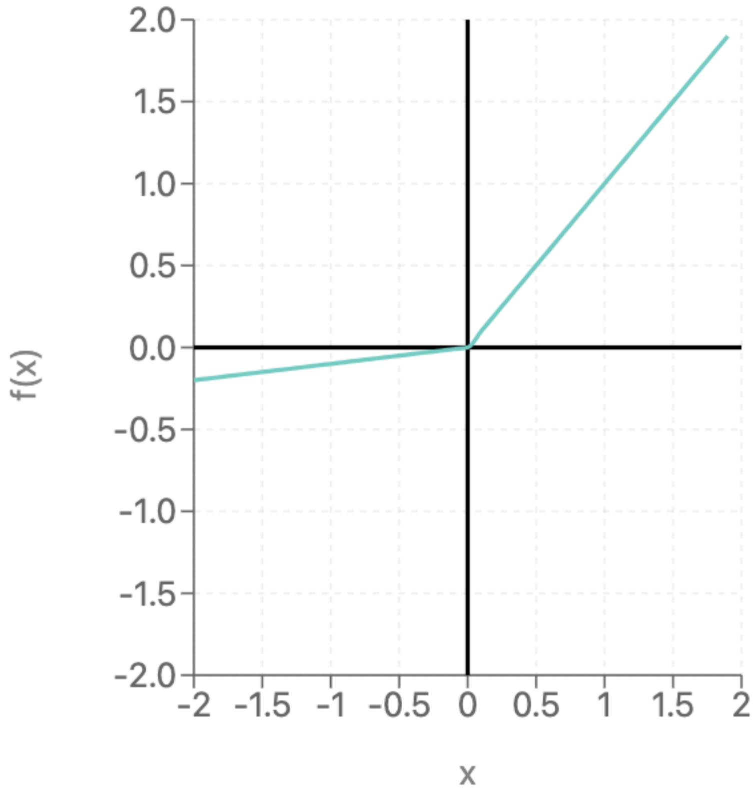
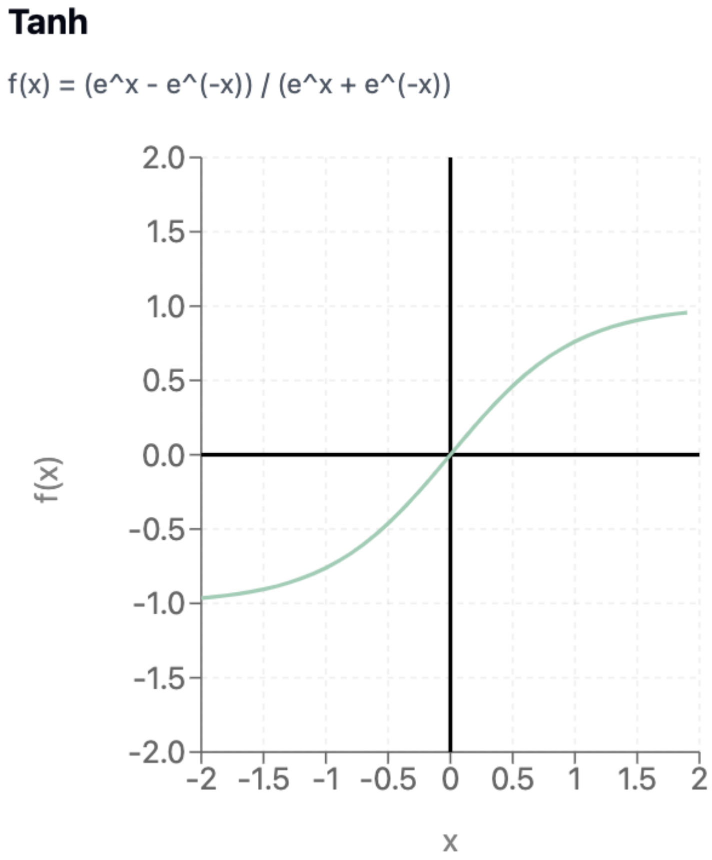


Tanh



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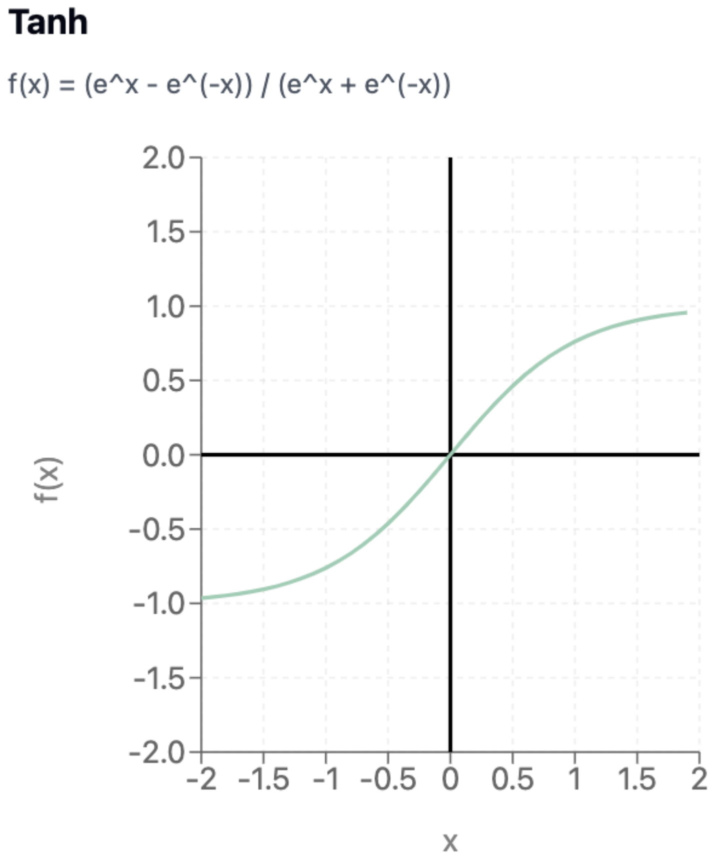
Tanh:
Advantages:
- Always maps output between -1 and 1 (learning is easier when input is normalized and this holds for intermediate layers as well)
- Continuously differentiable

Disadvantages:
- Slower to compute
- Extreme differences in input to activation can get squashed (i.e., z=100 will be very close to z=10000)



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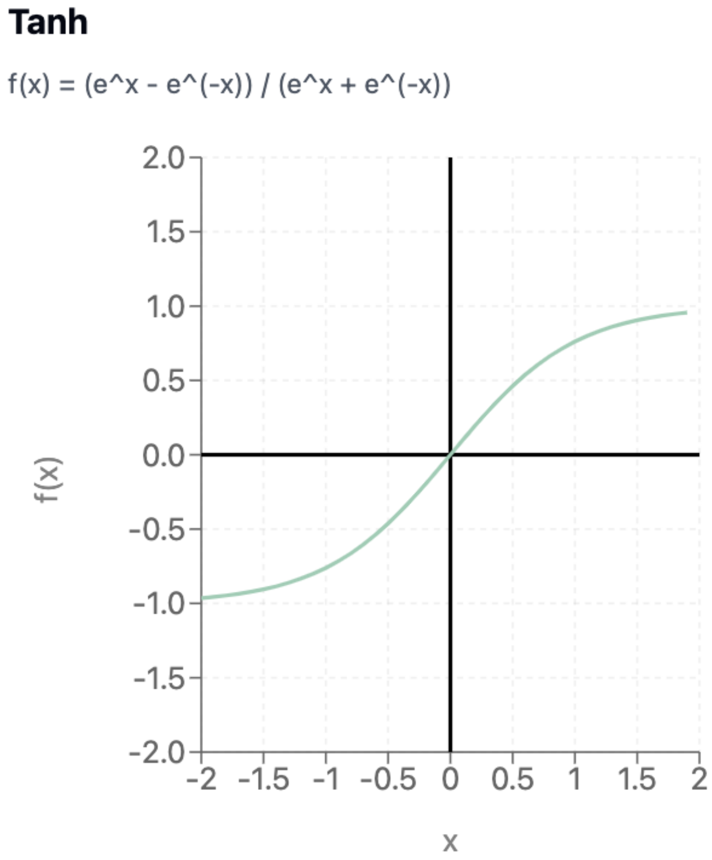
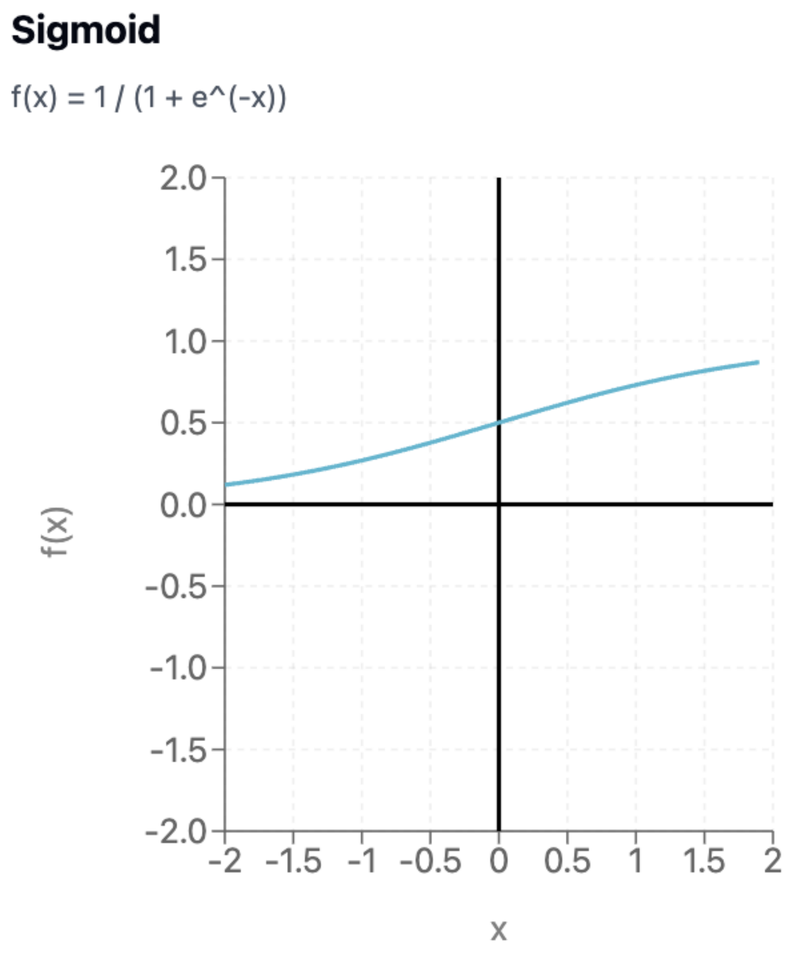
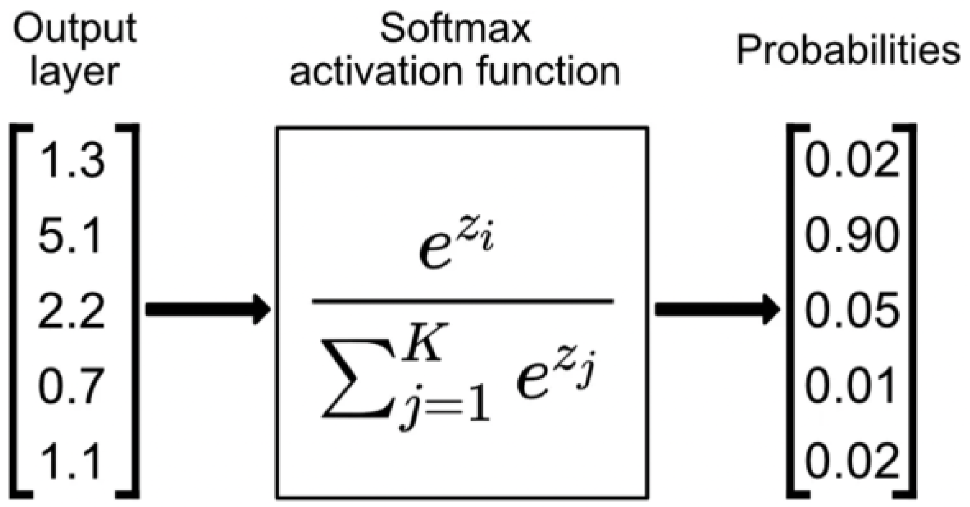


Special Activation Functions for Output





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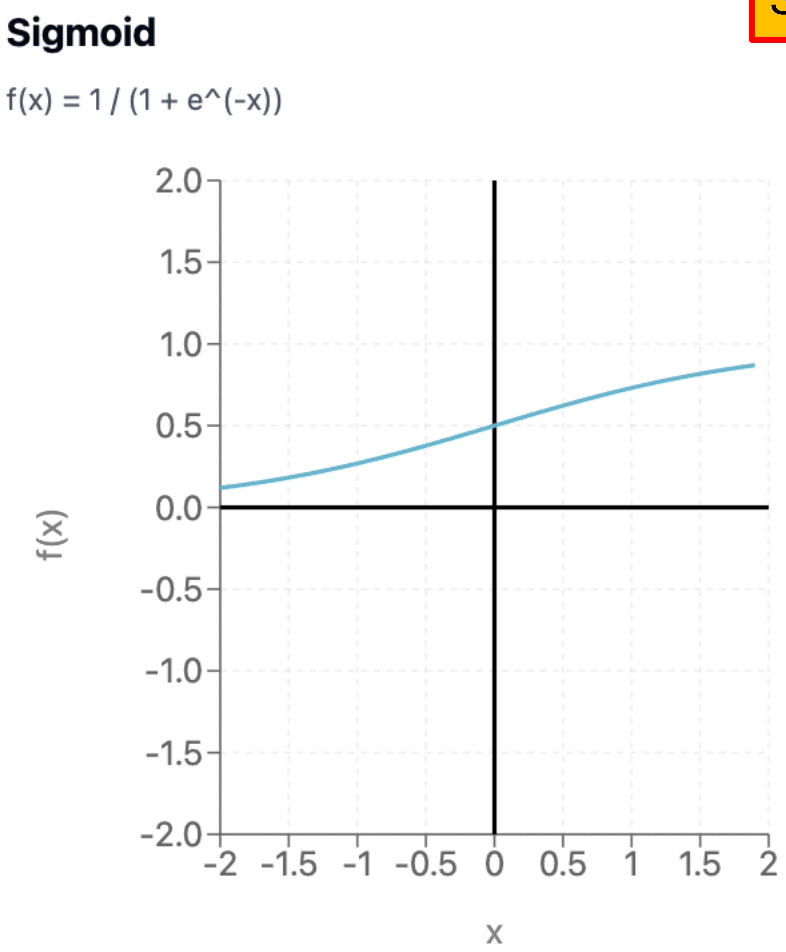
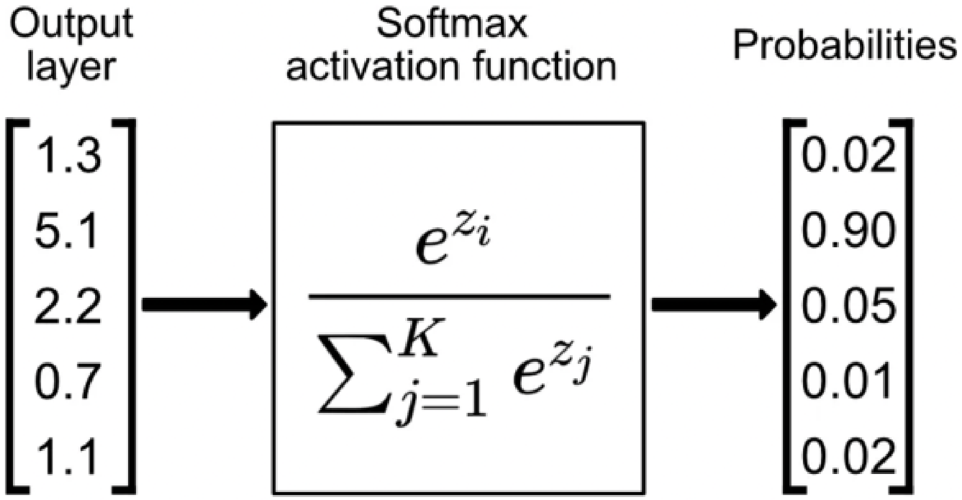
Sigmoid maps input to [0, 1]
Softmax maps vector of inputs to probabilities (outputs sum to 1)





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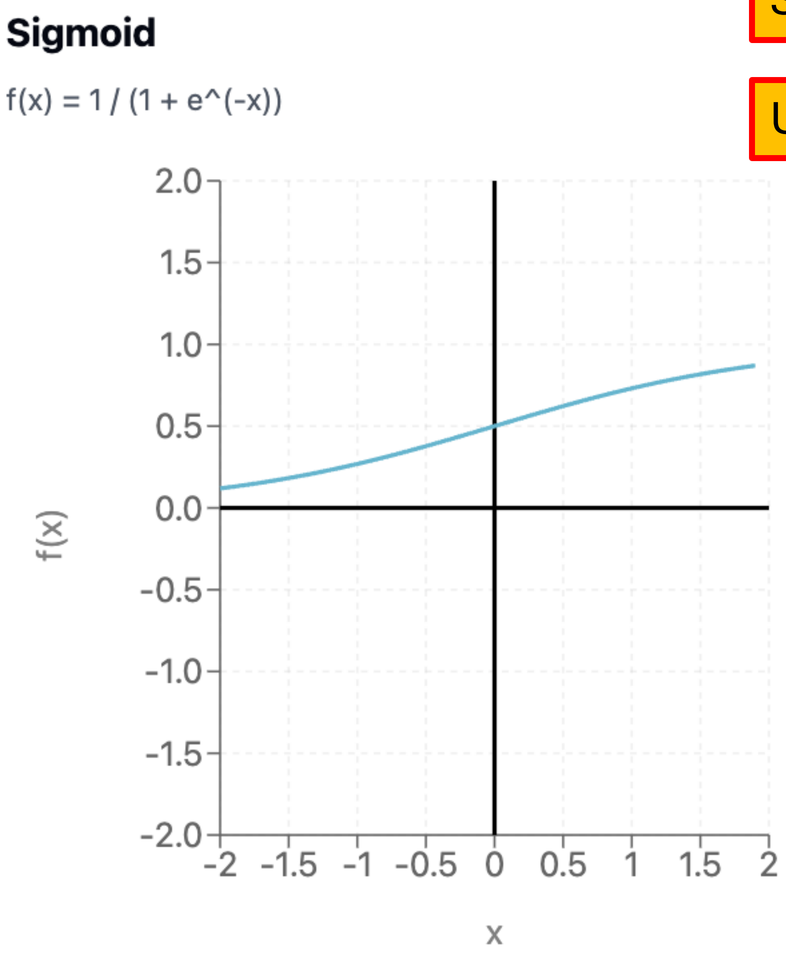
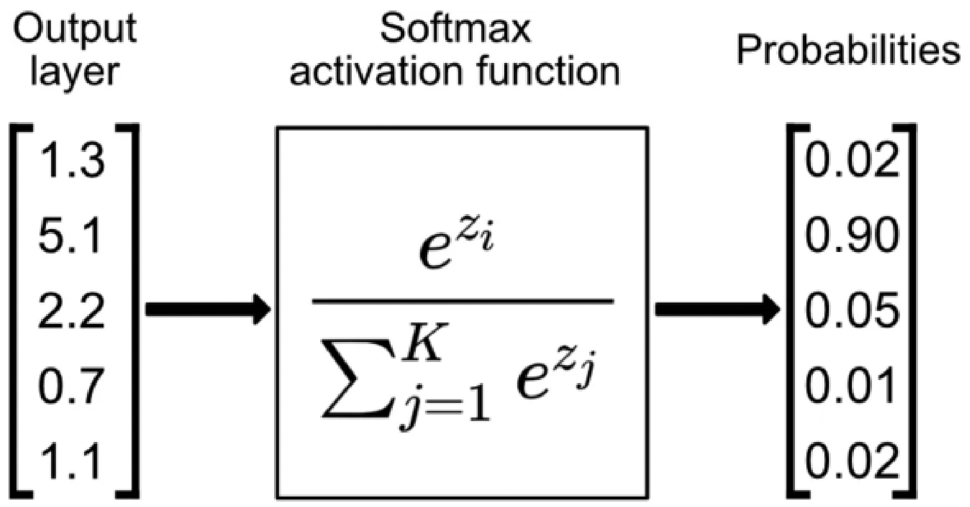
Used for classification tasks

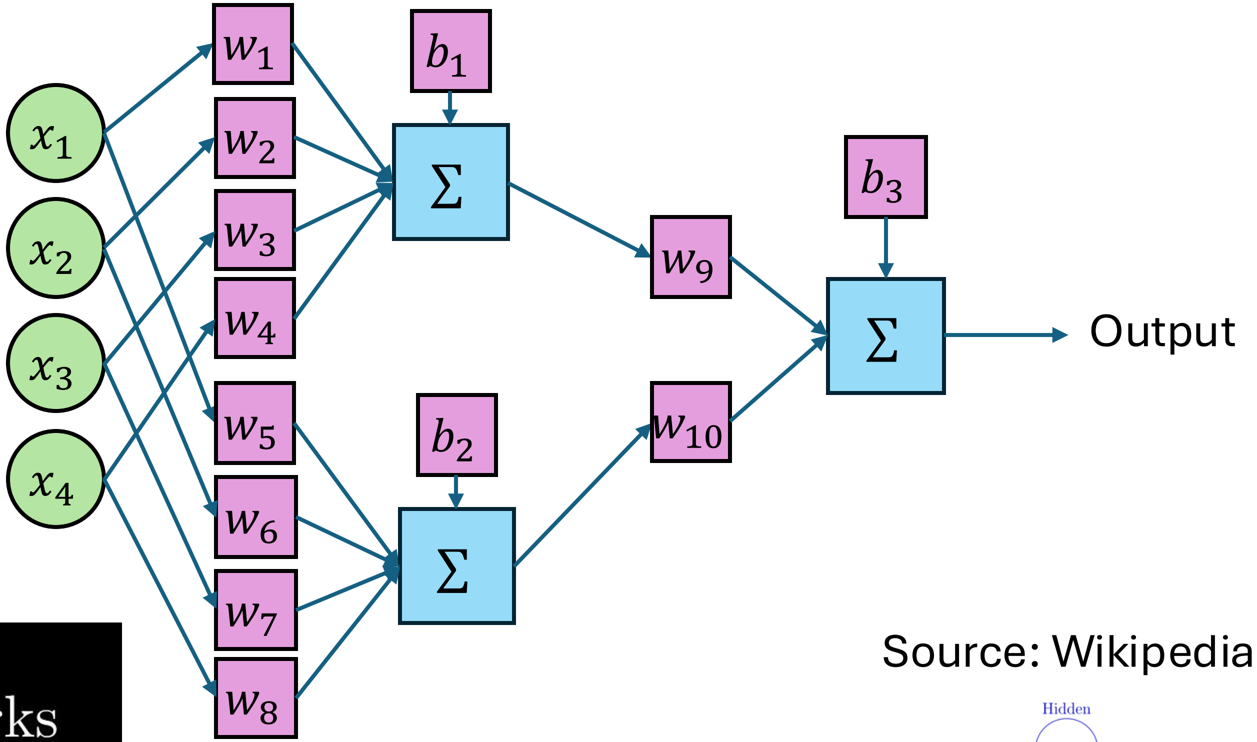




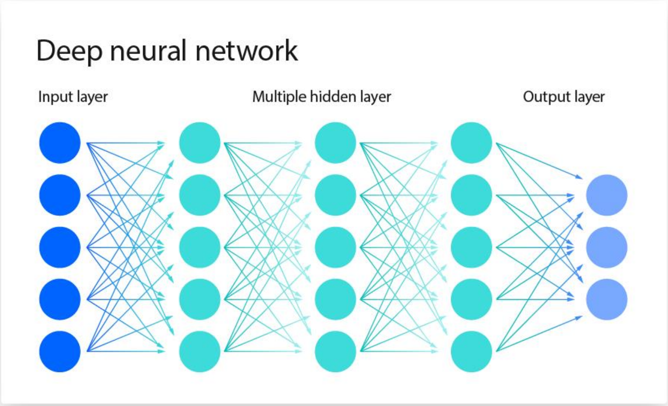
MLPs With Activation Functions

We almost never draw activation functions in our neural network diagrams, but they must always be there!

Source: Me



Source: IBM



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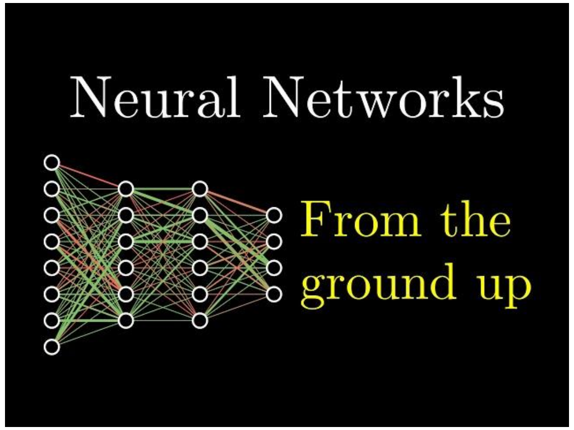
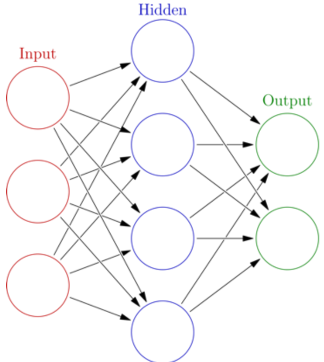


Source: Wikipedia



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    - If $\epsilon = 0$, i.e., we want a perfect approximation, we may need an infinitely wide network.
    - This is an **existence** theorem, meaning it tells you that a neural network exists with these properties. It does not tell you how to find the weights of this network.

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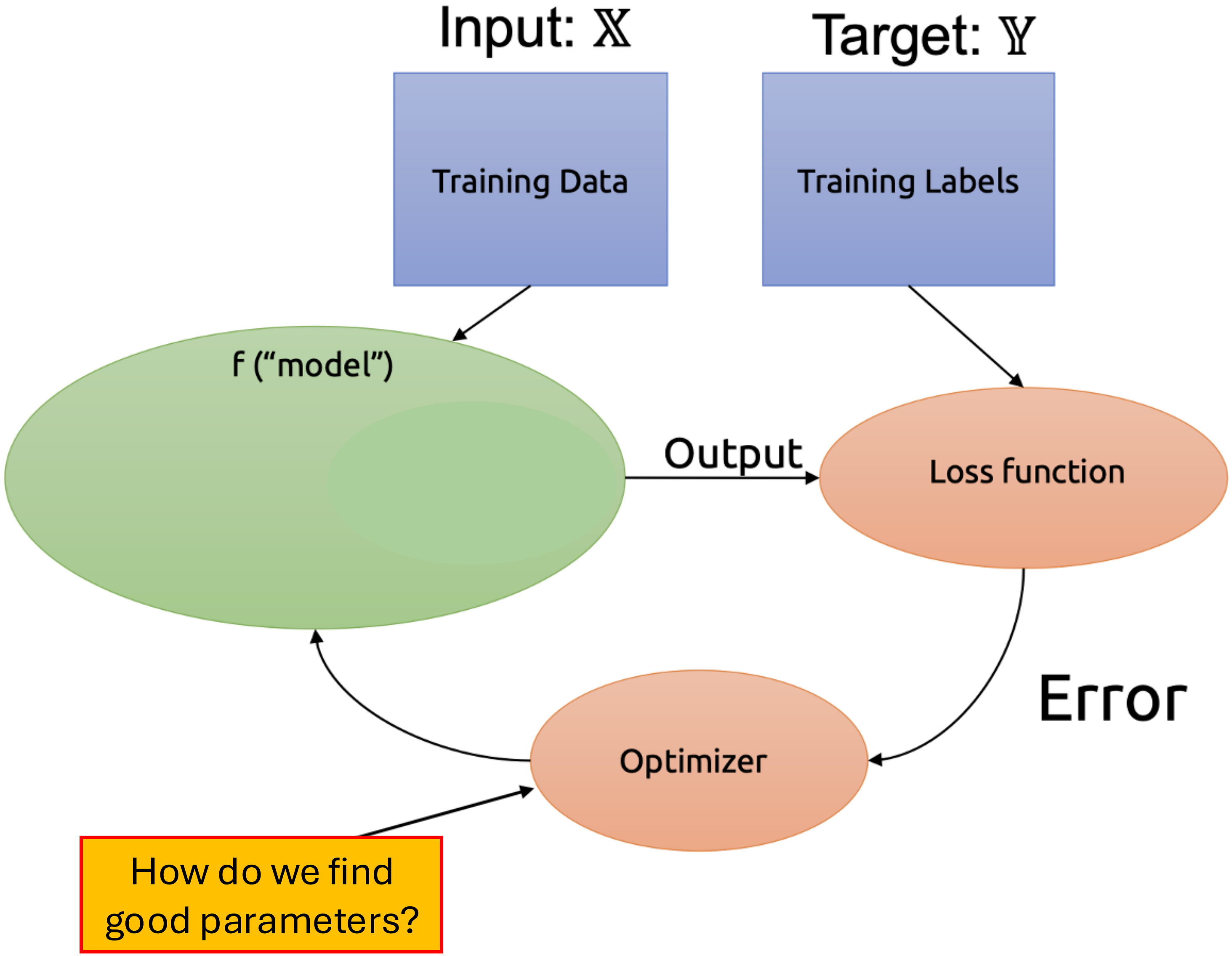
This theorem explains why neural networks are good at fitting the training dataset, not why they perform well on the test dataset.

Optimization

Learning Network Parameters



Option 1: Closed Form Solution

Goal: Minimize *Loss* function

Process:

- Find derivative (or gradient) of loss function
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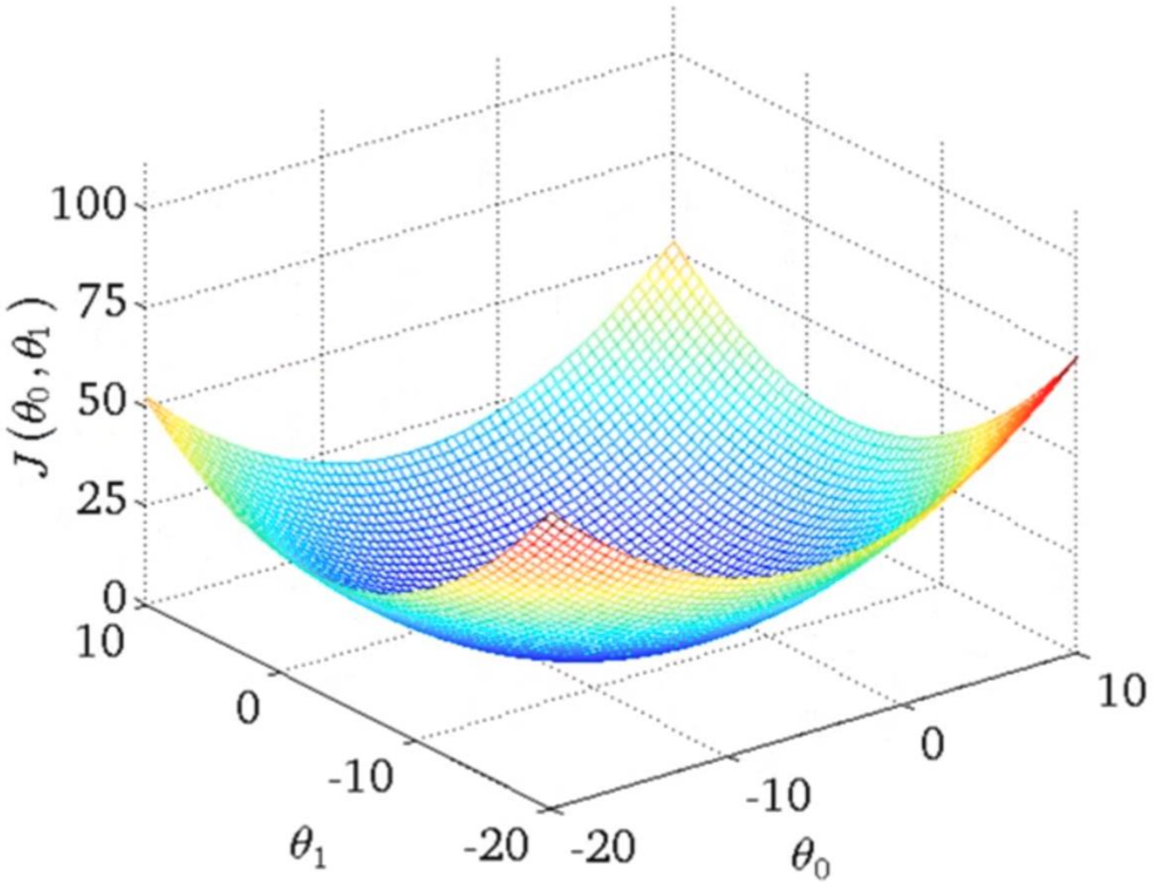
MSE is *convex* with respect to the parameters of the linear Regression

Convexity



Formally:

- For any two points x_1, x_2 and $\lambda \in [0, 1]$
- $\lambda f(x_1) + (1 - \lambda) f(x_2) \leq \lambda x_1 + (1 - \lambda) x_2$

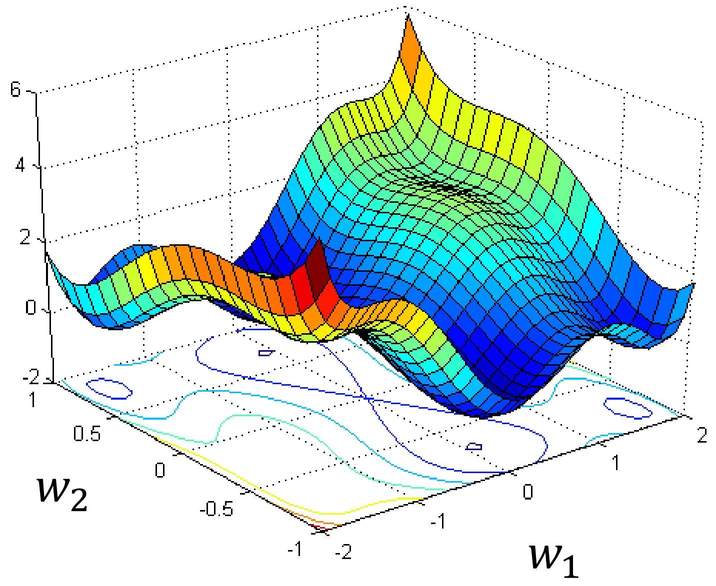
The line connecting any two points on the graph will always be above the function.

For convex functions, finding a point with $\nabla f = 0$ is **sufficient** for knowing the point is a **global** minimum

Picture Source: Andrew Ng

Non-Convex Functions

MSE is **not** convex with respect to network parameters when non-linear activations are involved.



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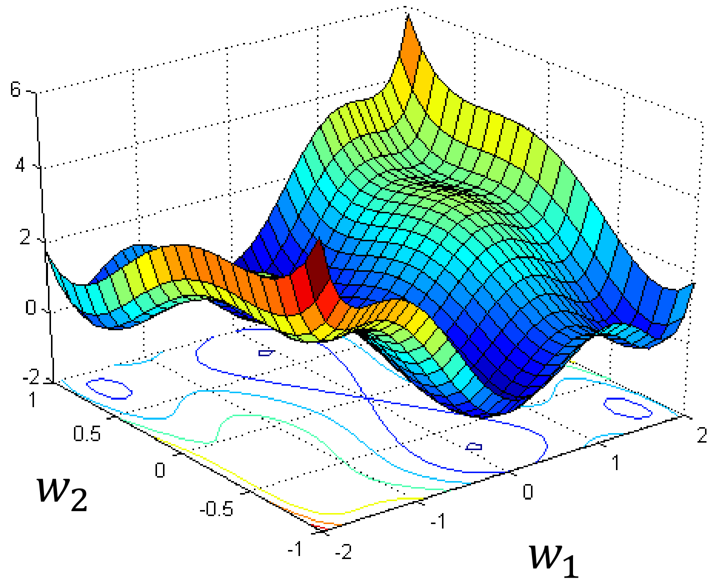

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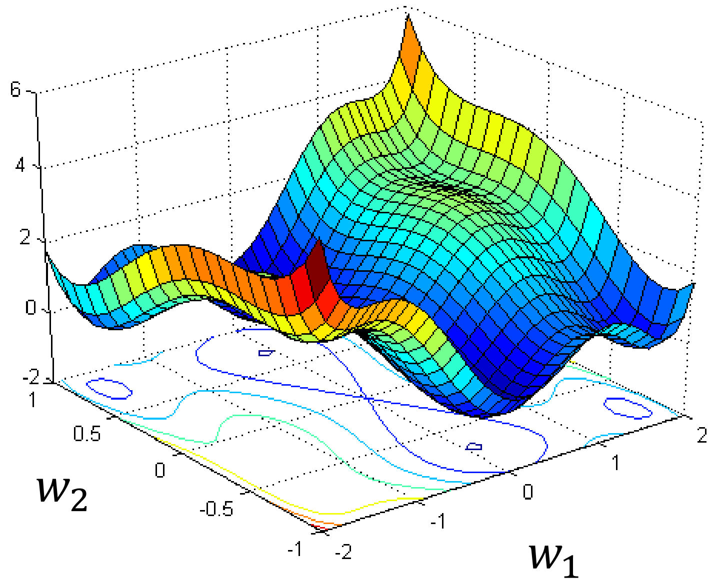

Local maxima

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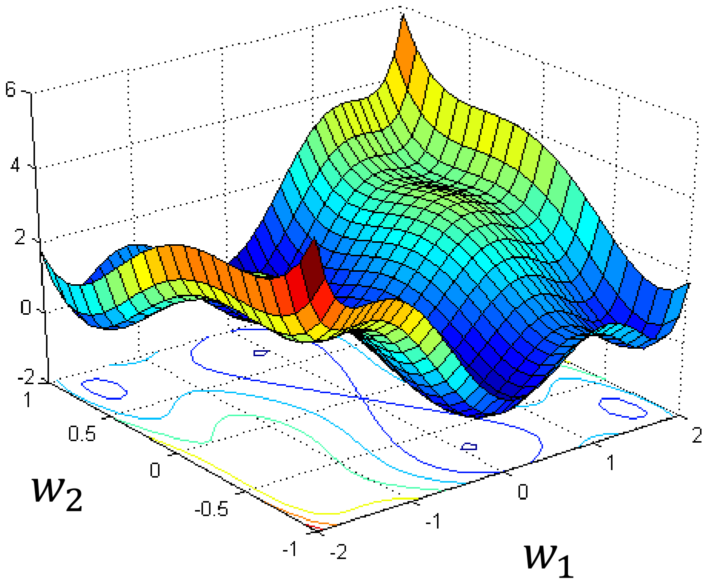

Saddle points

Local maxima

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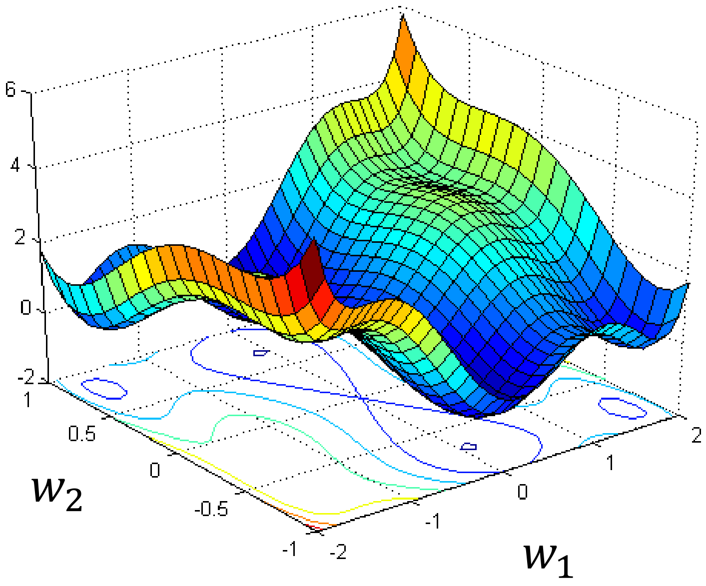
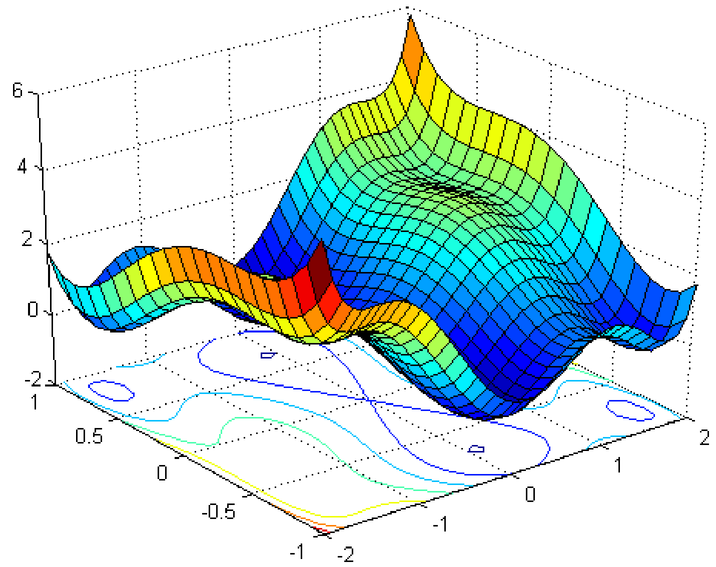


Local maxima

If ReLU or other piecewise activation function is used, may need 2^n piecewise functions to write out ∇f_θ...

Option 2: Gradient Descent

1. Start with some initial set of parameters
2. Take small step in the direction of the negative gradient
3. Repeat 2 until convergence



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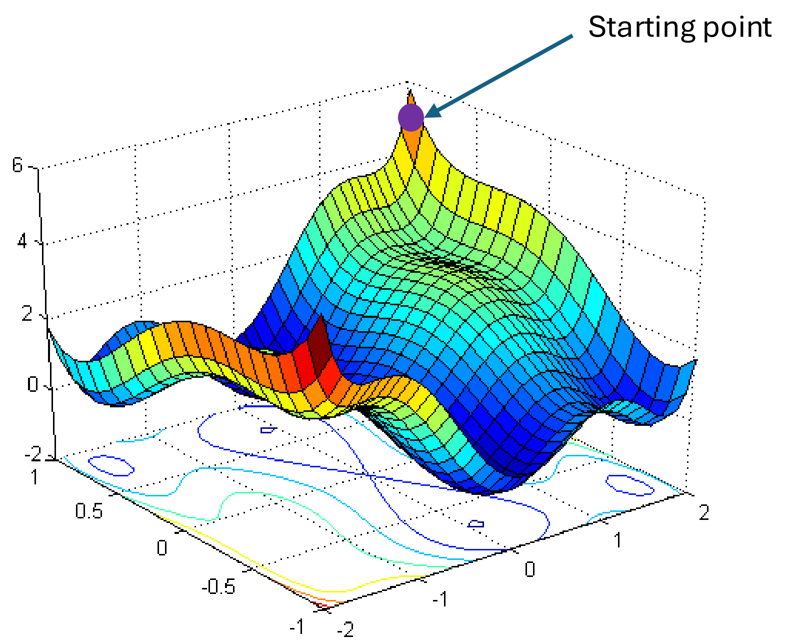

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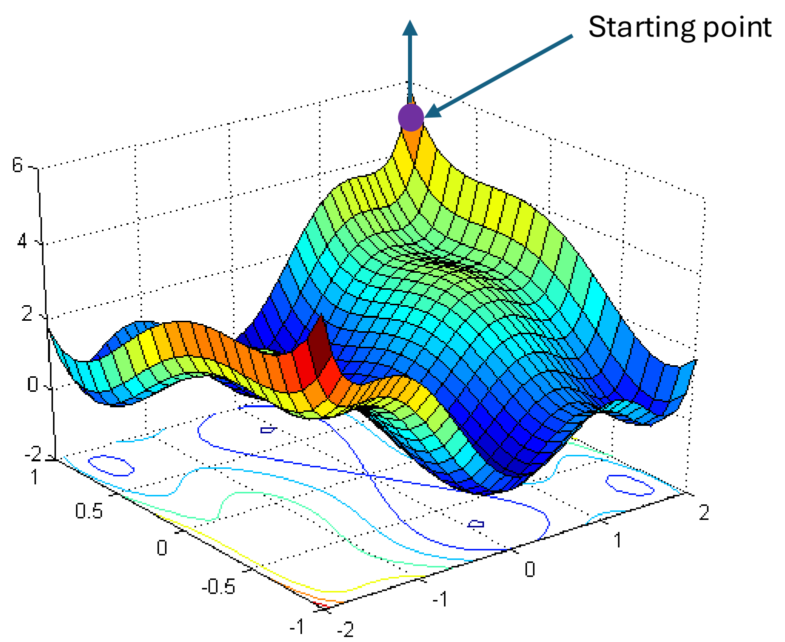
Gradient points in direction of increasing loss



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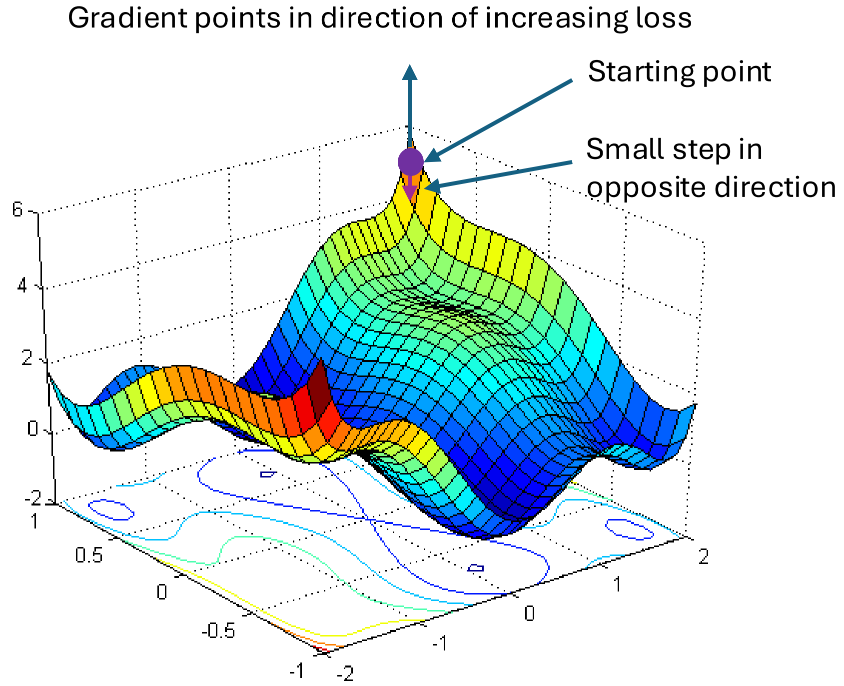

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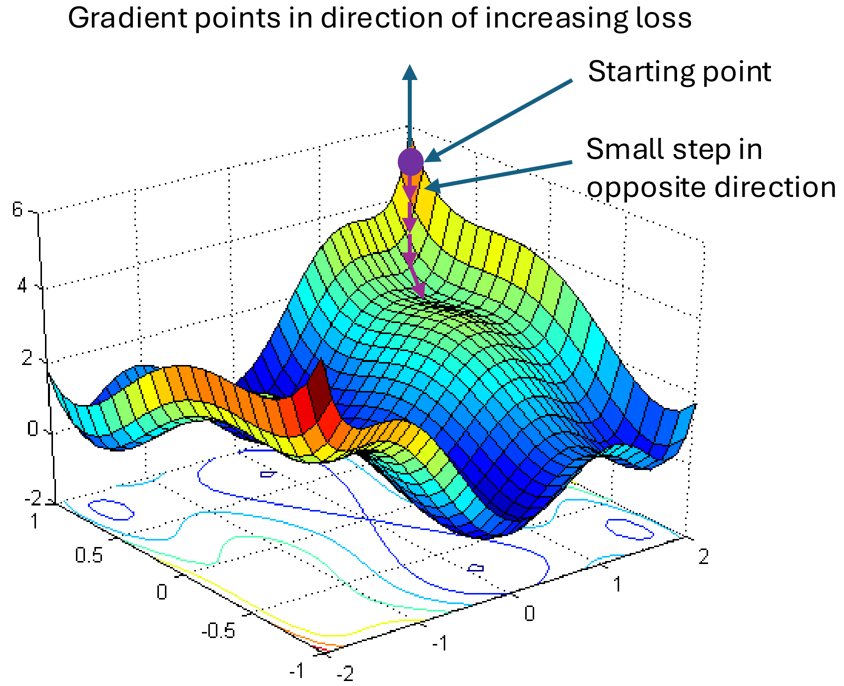

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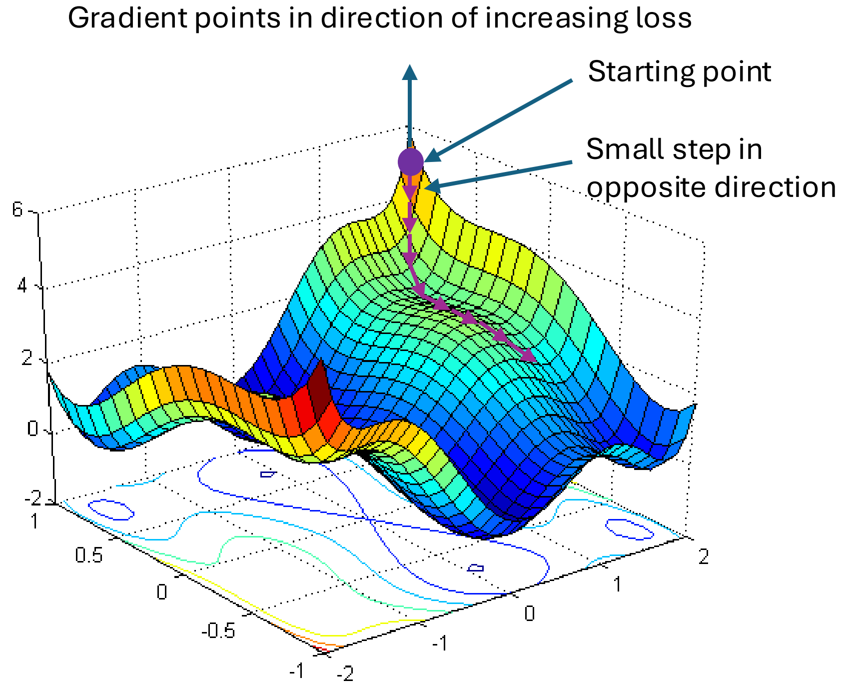

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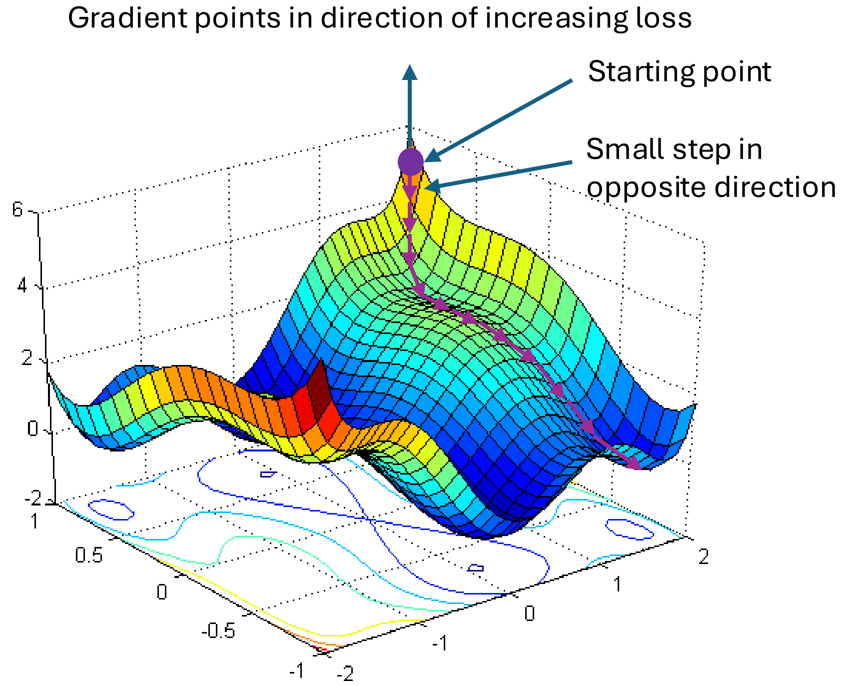

Vector Calculus

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Vector Calculus

- Partial Derivative: the derivative of a multi-variable function with respect to one of its inputs
- Example: $f(x, w, b) = wx + b$
- The partial derivative with respect to w is $\frac{\partial f}{\partial w}$
- How to compute: Treat all other variables as constants and differentiate with respect to that variable

$$\frac{\partial f}{\partial w} = \frac{\partial}{\partial w}(wx + b) = \frac{\partial}{\partial w}(wx) + \frac{\partial}{\partial w}(b) = x$$

Gradients

Gradient: the vector of partial derivatives

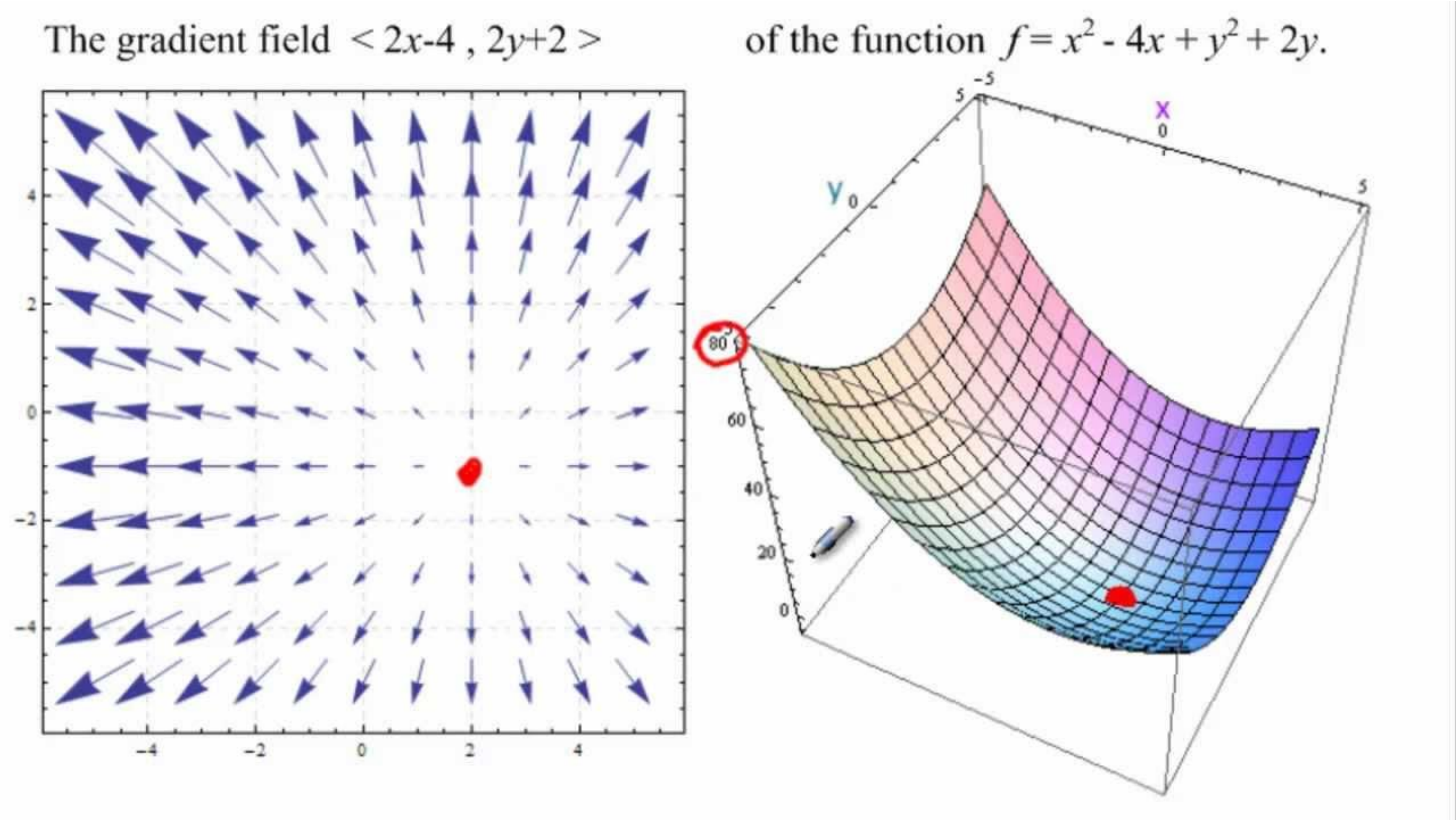
Vector “points” in direction of increasing f values.

$$\nabla f = [\frac{\partial f}{\partial w}, \frac{\partial f}{\partial b}, \ldots]$$

$$f(x, w, b) = wx + b$$

$$\nabla f_\theta = [\frac{\partial f}{\partial w}, \frac{\partial f}{\partial b}, \frac{\partial f}{\partial x}]$$

Gradients



The gradient field < 2x-4 , 2y+2 > of the function f = x² - 4x + y² + 2y.
x
y
80
60
40
20
0

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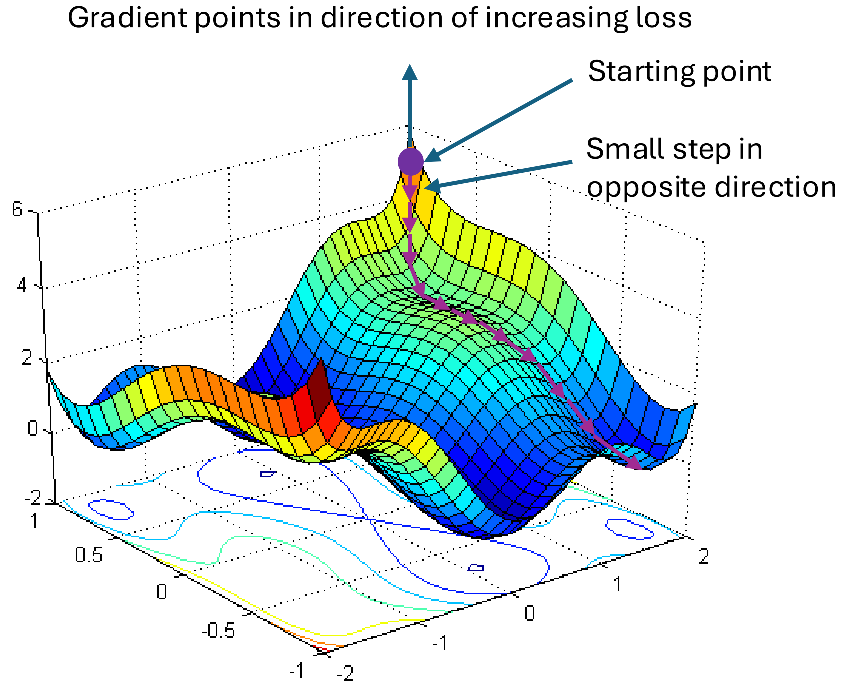

For N iterations or until $\Delta\theta < \epsilon$:

$$\vec{\theta} \leftarrow \theta - \alpha \nabla f_\theta$$

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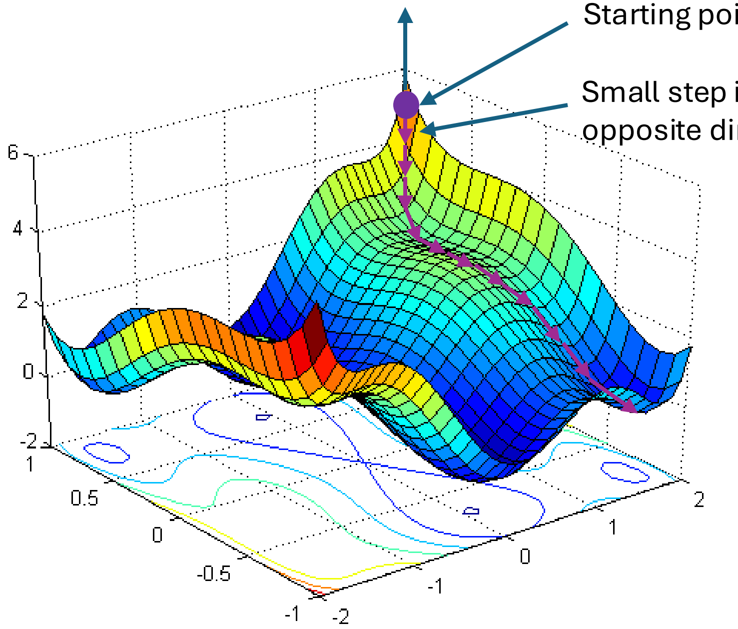
Gradient of what?

Gradient points in direction of increasing loss

Starting point

Small step in opposite direction



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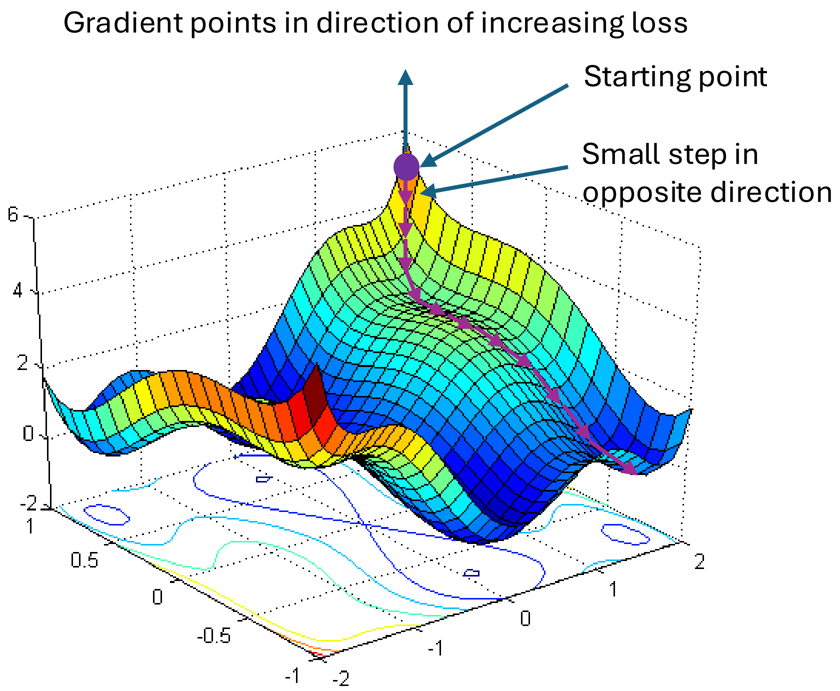

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Gradient of what?

Why is this negative?

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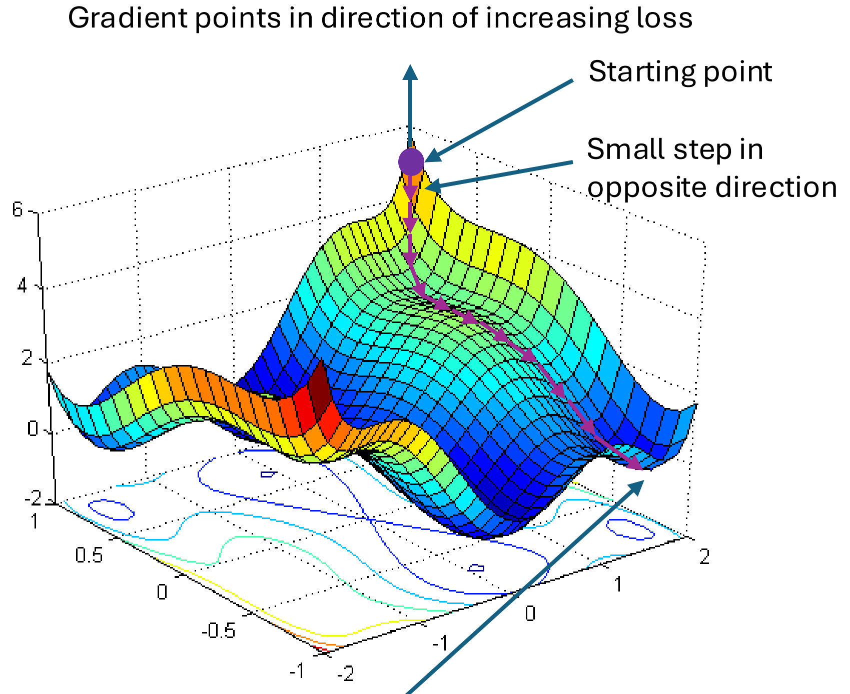

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Gradient of what?

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Wait, this isn't even the best θ

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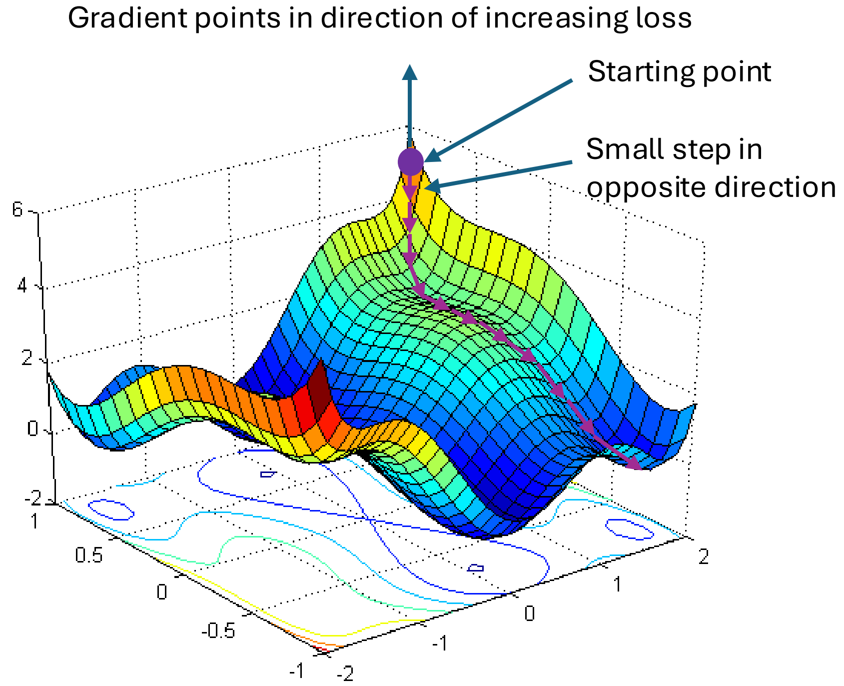

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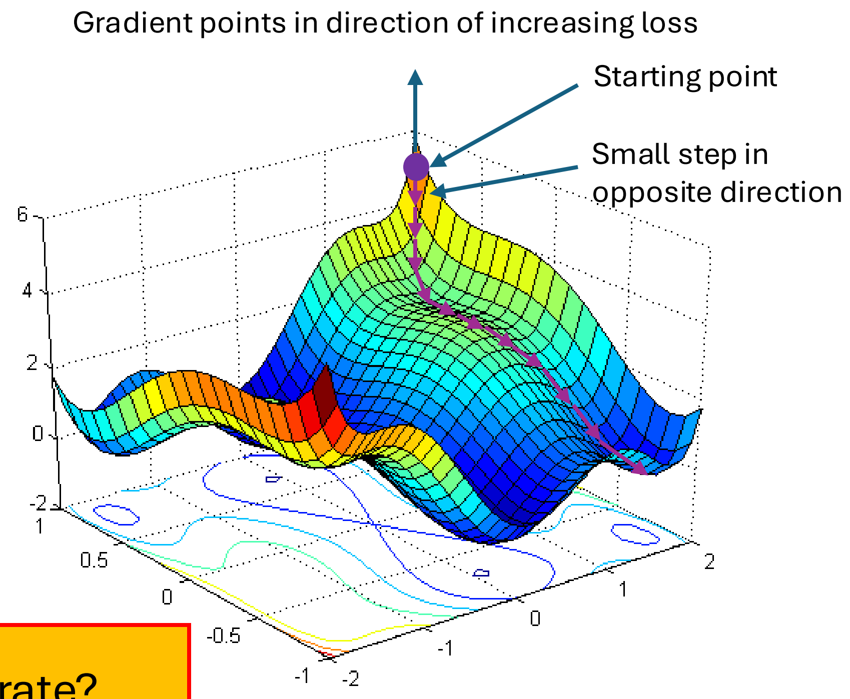

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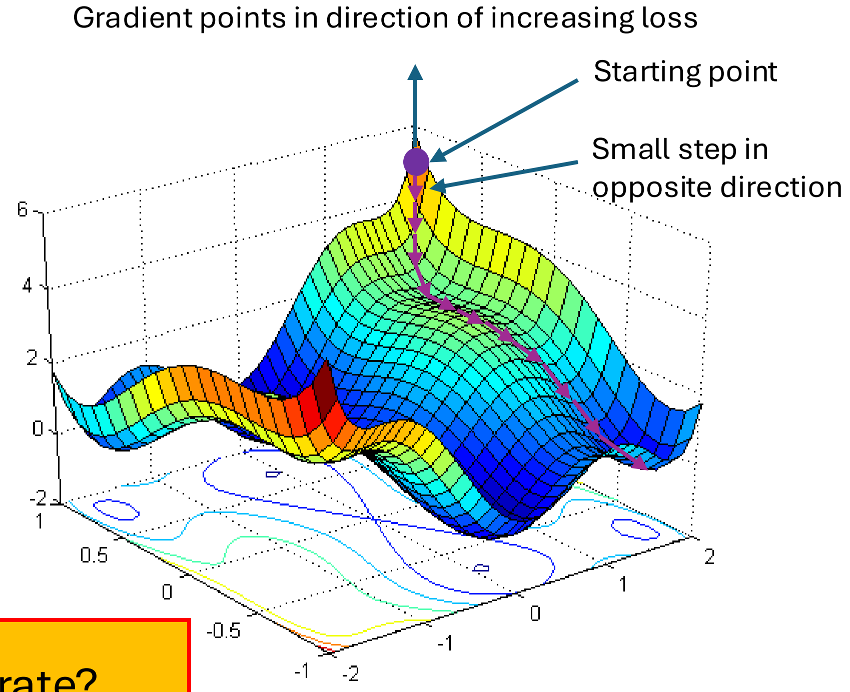

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Derivatives/Gradients only hold locally

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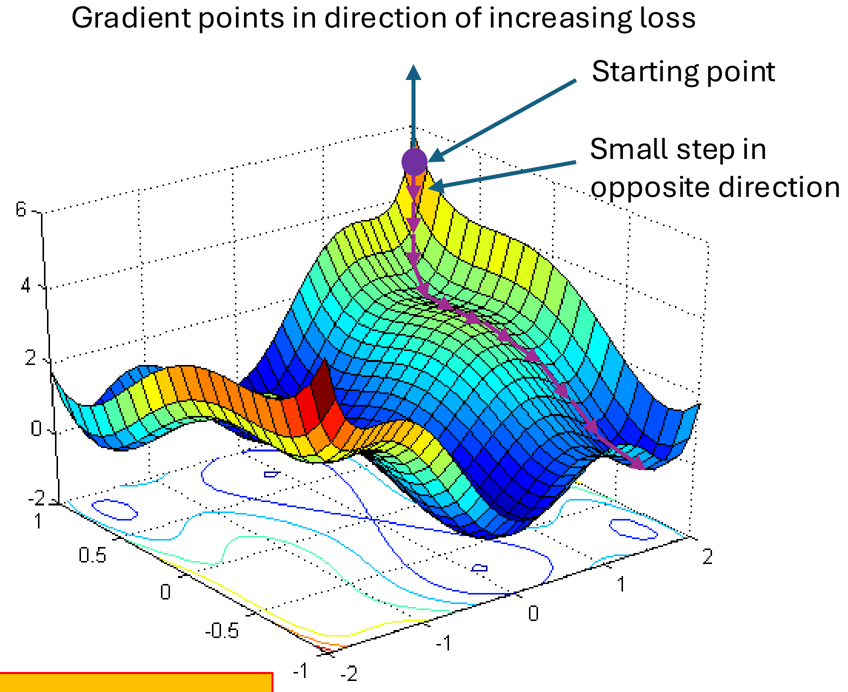

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Gradient Descent does not converge to the global minimum.
It can (and pretty much always does) get stuck in local minima.

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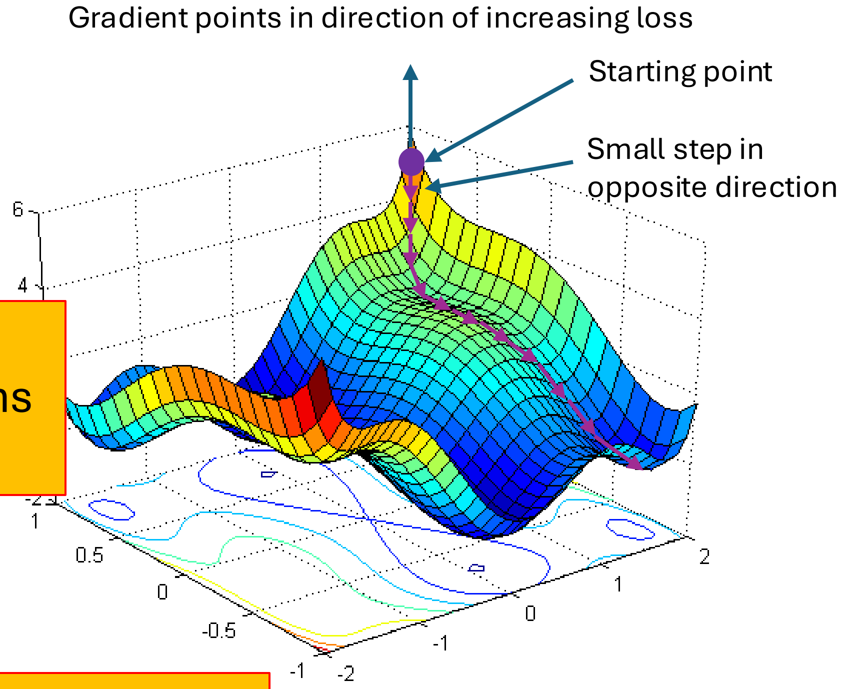
Understanding gradient descent is the single most important concept in all of Deep Learning. Most decisions in DL are made for reasons related to gradients.

For N iterations or until $\Delta\theta < \epsilon$:

$$\vec{\theta} \leftarrow \theta - \alpha \nabla f_{\theta}$$



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Review: Mean Squared Error

Used previously for linear regression:

Model with parameters θ

$$MSE = \frac{\sum_i^n (y_i - f_\theta(\vec{x}))\hat{}2}{n}$$

Used for regression tasks (prediction of continuous variable)

Gradients

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Gradient descent needs gradients, how do we actually calculate them?

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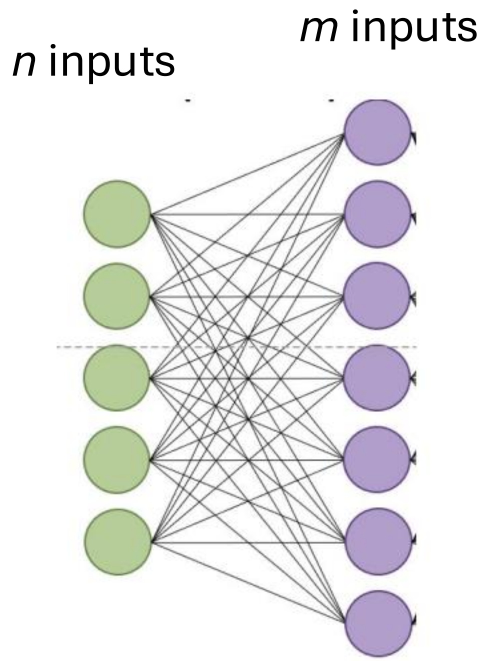
But what is this?

$f_\theta = wx + b$
For a single output

Weight Matrix

- We have an input of size *n* and we want an output vector of size *m*.
- We will represent our weights as a matrix.
  - What should the dimensions of our matrix be?



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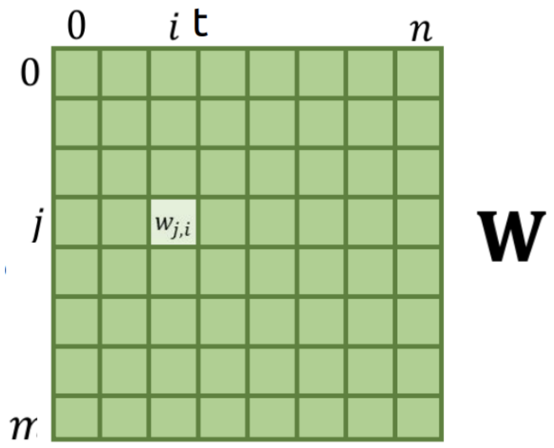
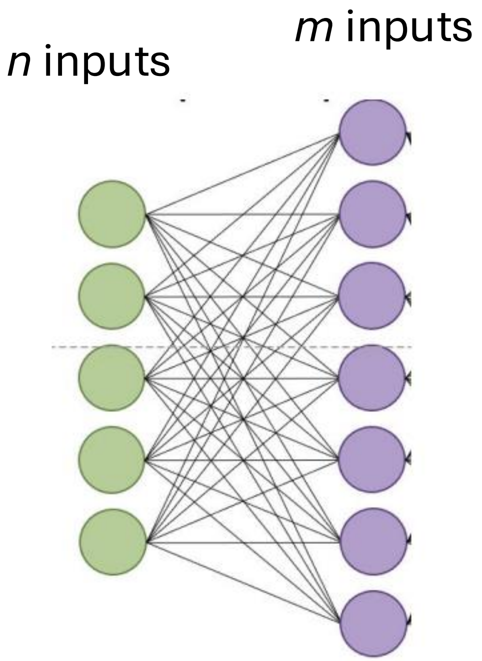
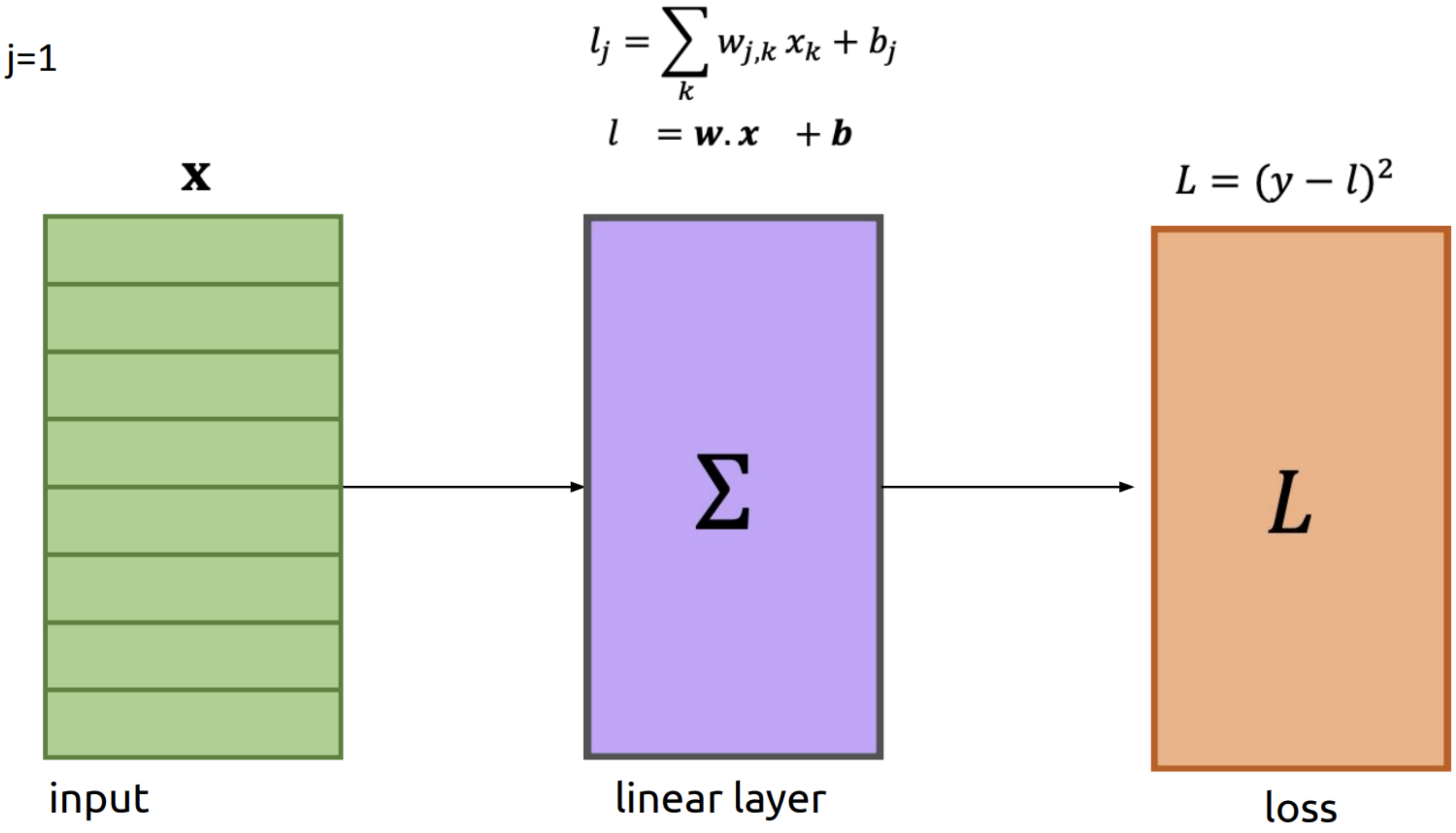
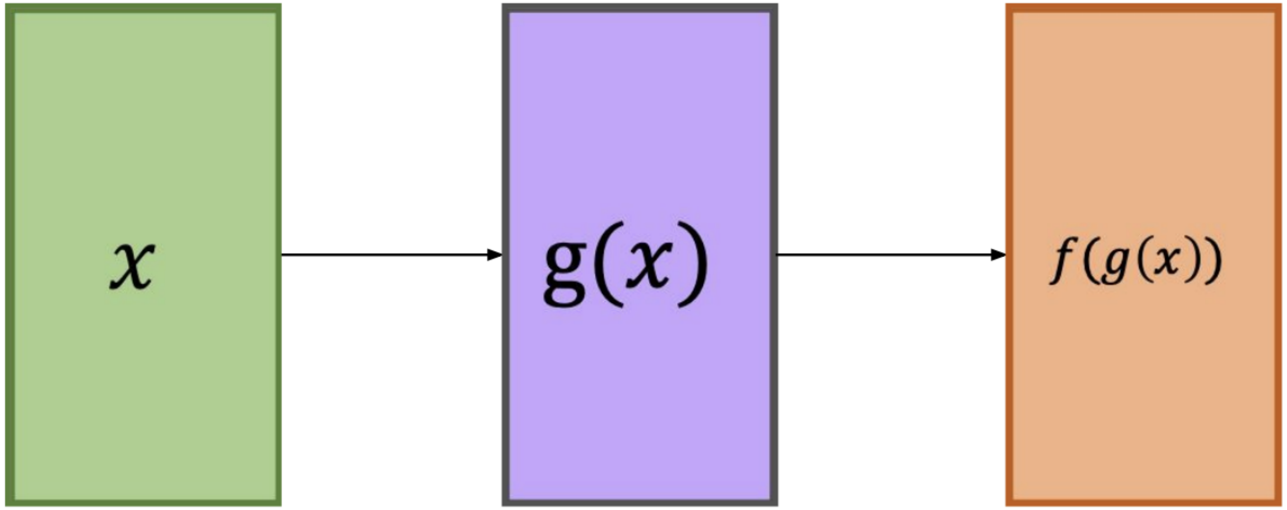
$w_{j,i}$ is the j^{th} row and the i^{th} column of our matrix, or the weight multiplied by the i^{th} index of the input which is used to create the j^{th} index in the output






j=1
$l_j = \sum_k w_{j,k} x_k + b_j$
$l = \boldsymbol{w}.\boldsymbol{x} + \boldsymbol{b}$
$\mathbf{x}$
$L = (y - l)^2$
Σ
L
input
linear layer
loss

Looking at composite function!



Chain rule

If f and g are both differentiable and $F(x)$ is the composite function defined by $F(x) = f(g(x))$ then F is differentiable and F' is given by the product

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

Differentiate outer function

Differentiate inner function

Courtesy: https://www.onlinemathlearning.com/chain-rule.html

Applying Chain rule [Example]

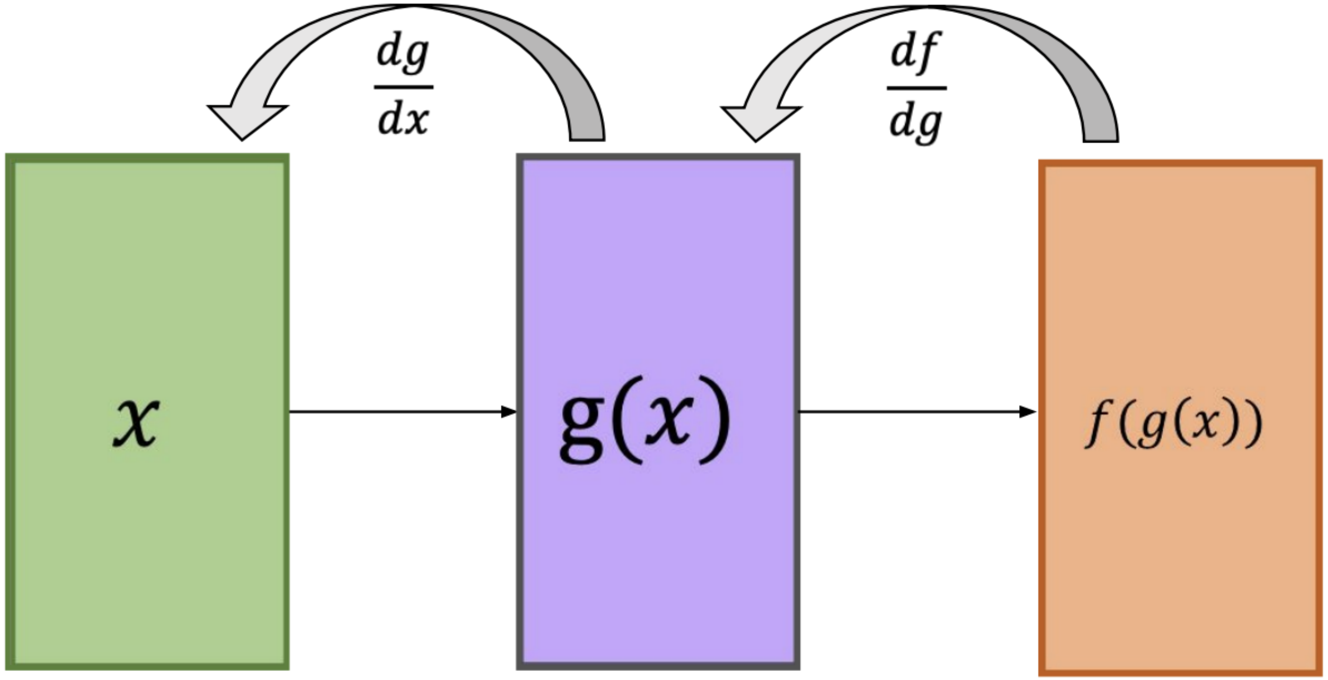
$$f(x) = x^2 \qquad \mathrm{g}(x) = (2x^2 + 1)$$

$$F(x) = f(g(x))$$

$$F(x) = (2x^2 + 1)^2$$

The Chain Rule (for Differentiation)

- Given arbitrary function: $f\big(g(x)\big) \Rightarrow \frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}$



Each layer computes the gradients with respect to it's variables and passes the result backwards

Backpropagation

(or backward pass)

Classification

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In general, we'd like to optimize the accuracy of our model (#correct/#total)

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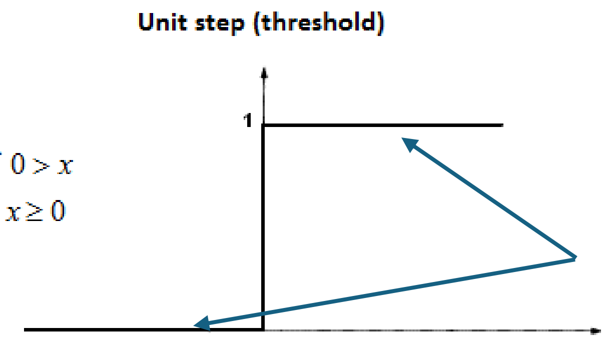
Gradient is only non-zero when changing a θ has an impact on output predictions

$$f(x) = \begin{cases} 0 \text{ if } 0 > x \\ 1 \text{ if } x \geq 0 \end{cases}$$



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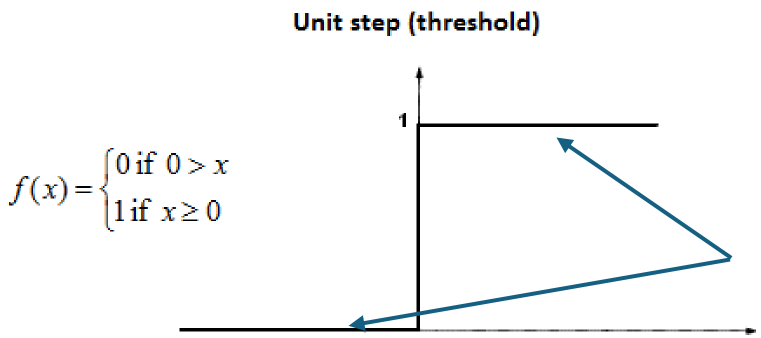
We cannot use classification as a loss function because it is **incompatible with gradient descent**



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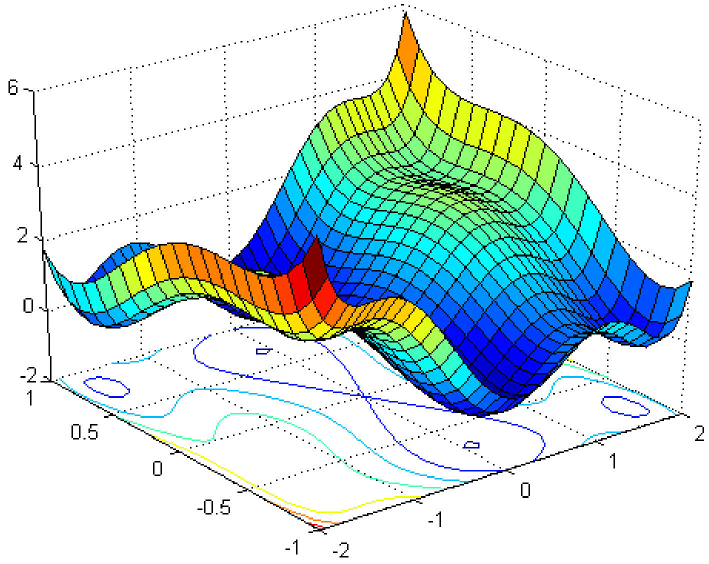
Remaining Questions for next week:

1) What loss function can we use for classification?
2) How do we actually calculate the gradient of a network?
    1) If the loss function is applied to the whole dataset, shouldn't we be concerned about the size of the dataset?
    2) Gradient descent is an iterative approach. If each iteration is slow, the whole algorithm will take too long to finish.
3) Gradient descent can get stuck in local minima.

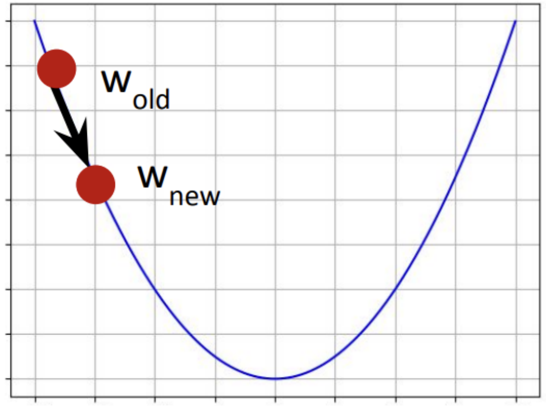
Can we do better?



Recap

Optimization

- Calculating gradients
- Gradient Descent for MSE Loss
- Convex and Non convex functions



Building a Neural Network

- Non-linear Activation Functions
- Hidden layers of neurons
- Loss Function
- Chain rule for backprop