

# Special Topics in Deep Learning

COMP 6211D & ELEC 6910T

Instructor: Qifeng Chen

# Course Website

<https://course.cse.ust.hk/comp6211d>

# Who we are

- Instructors: Qifeng Chen (cqf@ust.hk)
- TA: Hyukryul Yang (hyangbd@connect.ust.hk)  
Nayeon Lee (nayeon.lee@connect.ust.hk)

# Logistics

- In-class presentation
  - We will send out a list of papers in a couple of days
  - Send us three papers in the list you would like to present in a prioritized order
  - You may add a paper not in the list to your preference list
  - If you do not send us the preference list, we will assign a paper to you
  - Each student will present one paper for up to 12 minutes, followed by 3-minute Q&A
  - 5 students will present in each lecture
- Homework
  - First homework will be out in a week
- Attendance
  - Start after the add&drop period

# Machine Learning Basis

## Linear Regression

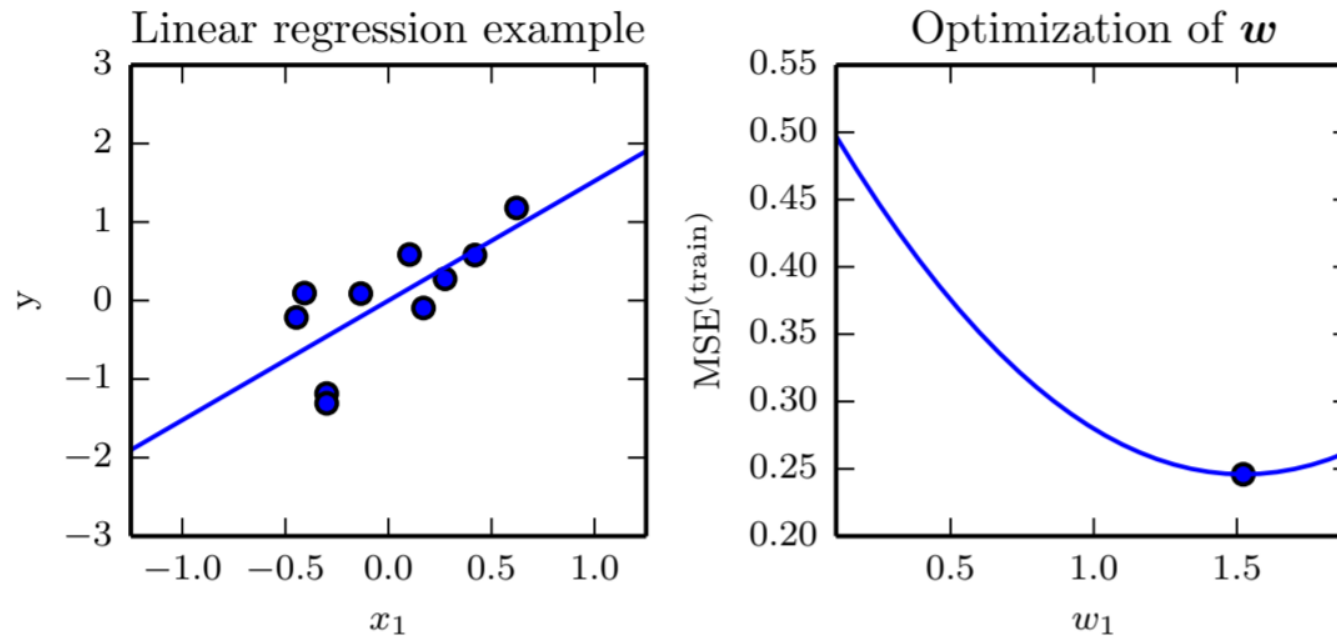


Figure 5.1

# Underfitting and Overfitting in Polynomial Estimation

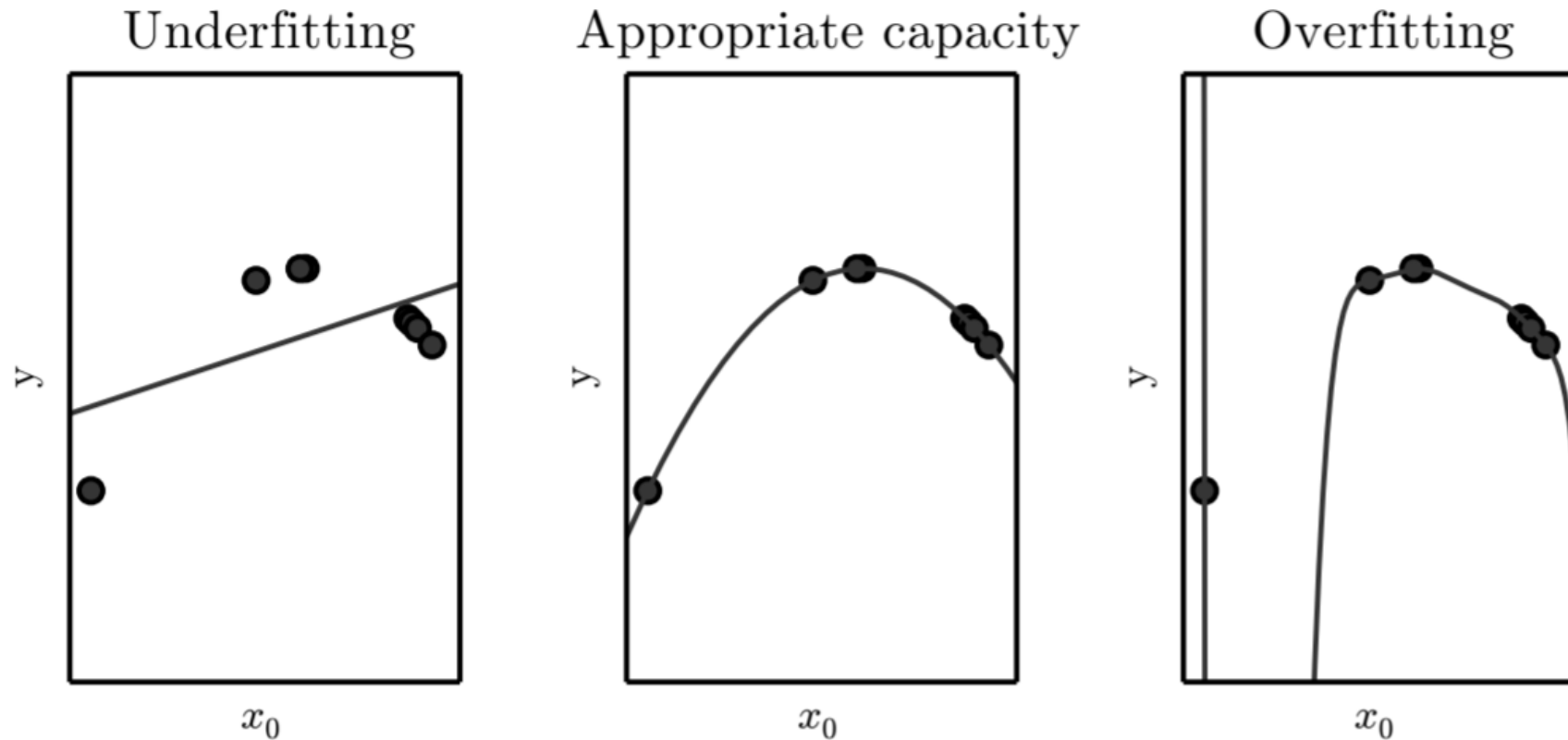


Figure 5.2

# Generalization and Capacity

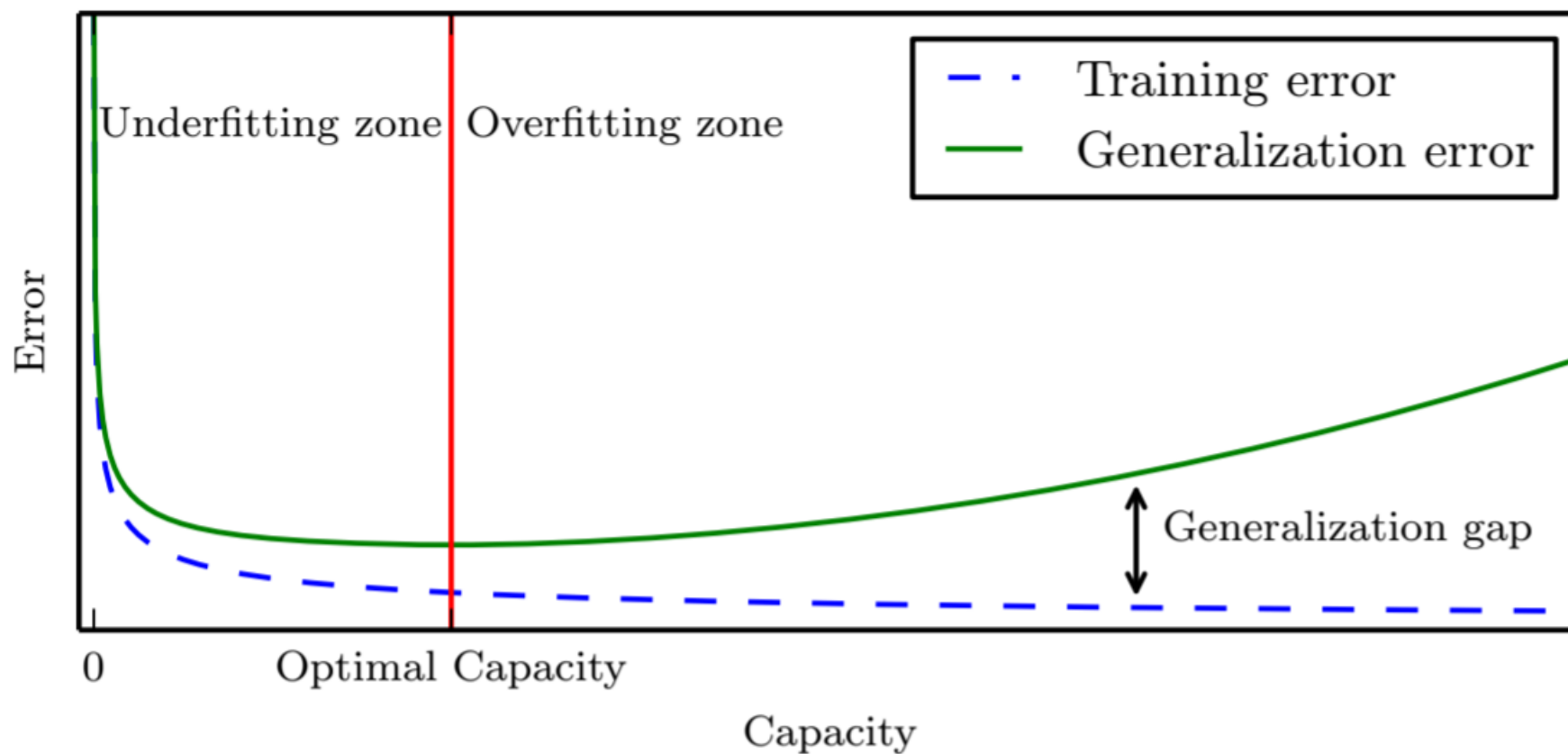


Figure 5.3

# Bias and Variance

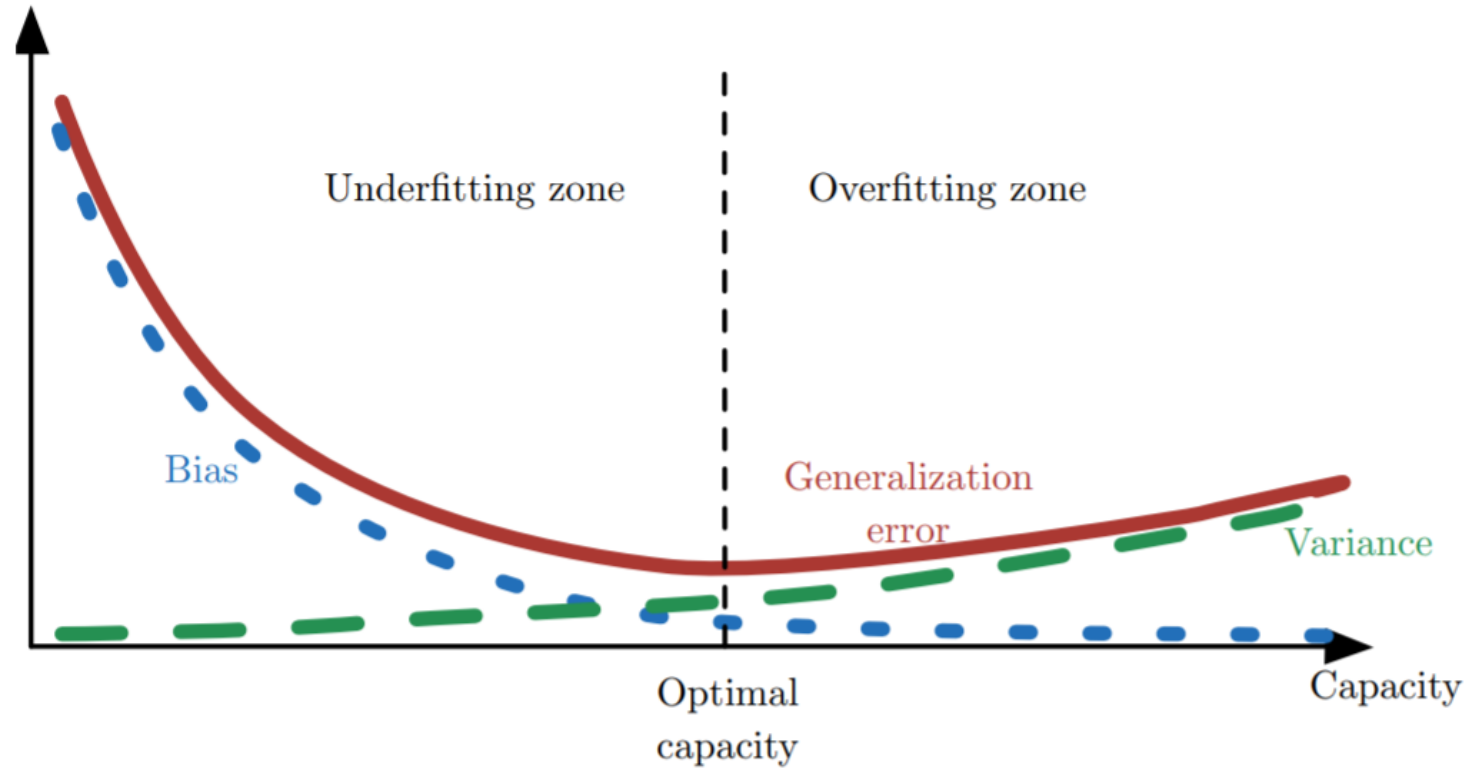


Figure 5.6



# The Rise of Deep Learning

## 'Deep Voice' Software Can Clone Anyone's Voice With Just 3.7 Seconds of Audio

Using snippets of voices, Baidu's 'Deep Voice' can generate new speech, accents, and tones.

Let There Be Sight: How Deep Learning Is Helping the Blind 'See'



## Technology outpacing security measures

Facial Recognition | Features and Interviews

## AI beats docs in cancer spotting

A new study provides a fresh example of machine learning as an important diagnostic tool. Paul Biegler reports.

## AI Can Help In Predicting Cryptocurrency Value



## DEEPMIND STARCRRAFT TRIUMPH



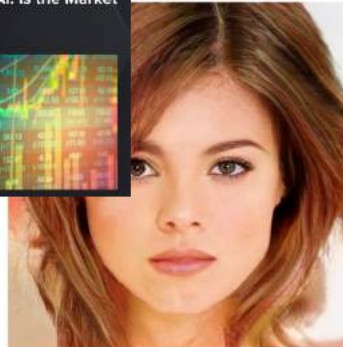
## 'Creative' AlphaZero leads way for chess computers and, maybe, science

Former chess world champion Garry Kasparov likes what he sees of computer that could be used to find cures for diseases



## How an A.I. 'Cat-and-Mouse Game' Generates Believable Fake Photos

By CADE METZ and KEITH COLLINS JAN 2, 2018



## Stock Predictions Based On AI: Is the Market Truly Predictable?



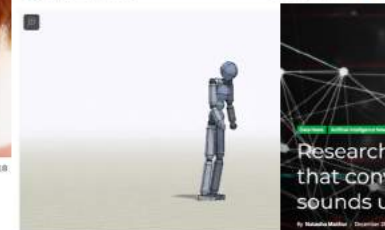
Complex of bacteria-infecting viral proteins modeled in CASP-13. The complex contained proteins that were modeled individually. PROTEIN DATA BANK

## Google's DeepMind acs protein folding

By Robert F. Service | Dec. 6, 2018, 12:05 PM

## After Millions of Trials, These Simulated Humans Learned to Do Perfect Backflips and Cartwheels

George Dornier 4/10/18 11:55am - Pinned to AI



## Neural networks everywhere

New chip reduces neural networks' power consumption by up to 95 percent, making them practical for battery-powered devices.

Wed, 01/16/2019 - 6:00am | Comment by Kenney Walker - Digital Reporter - @RandDMagazine



## AI faces show how far AI image generation has advanced in just four years

AI faces on the right aren't real; they're the product of machine learning



## Automation And Algorithms: De-Risking Manufacturing With Artificial Intelligence

Sarah Goehrkne Contributor Manufacturing 1 focus on the industrialization of additive manufacturing.

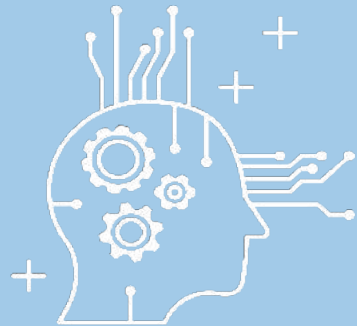
### TWEET THIS

The two key applications of AI in manufacturing are pricing and manufacturability feedback

# What is Deep Learning?

## ARTIFICIAL INTELLIGENCE

Any technique that enables computers to mimic human behavior



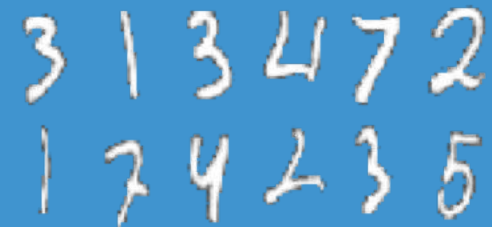
## MACHINE LEARNING

Ability to learn without explicitly being programmed



## DEEP LEARNING

Extract patterns from data using neural networks



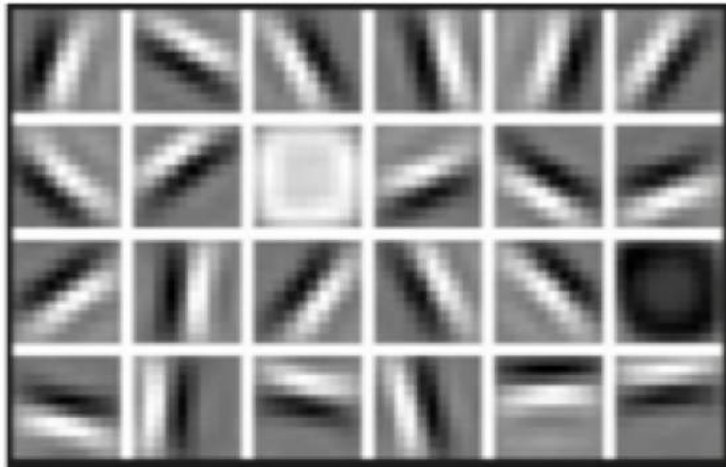
# Why Deep Learning and Why Now?

# Why Deep Learning?

Hand engineered features are time consuming, brittle and not scalable in practice

Can we learn the **underlying features** directly from data?

Low Level Features



Lines & Edges

Mid Level Features



Eyes & Nose & Ears

High Level Features

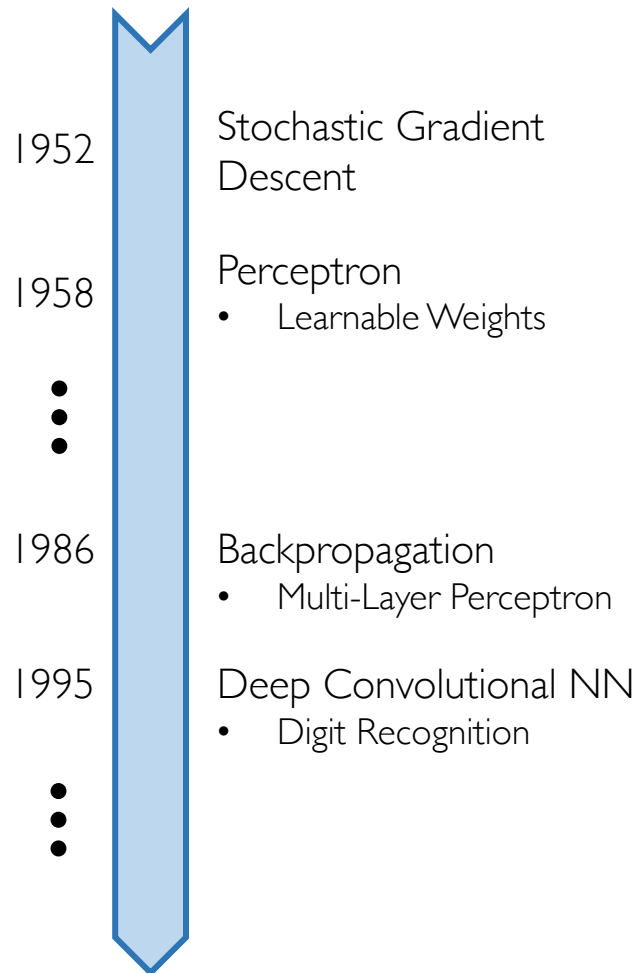


Facial Structure



# Why Now?

Neural Networks date back decades, so why the resurgence?



## 1. Big Data

- Larger Datasets
- Easier Collection & Storage

IMAGENET



## 2. Hardware

- Graphics Processing Units (GPUs)
- Massively Parallelizable



## 3. Software

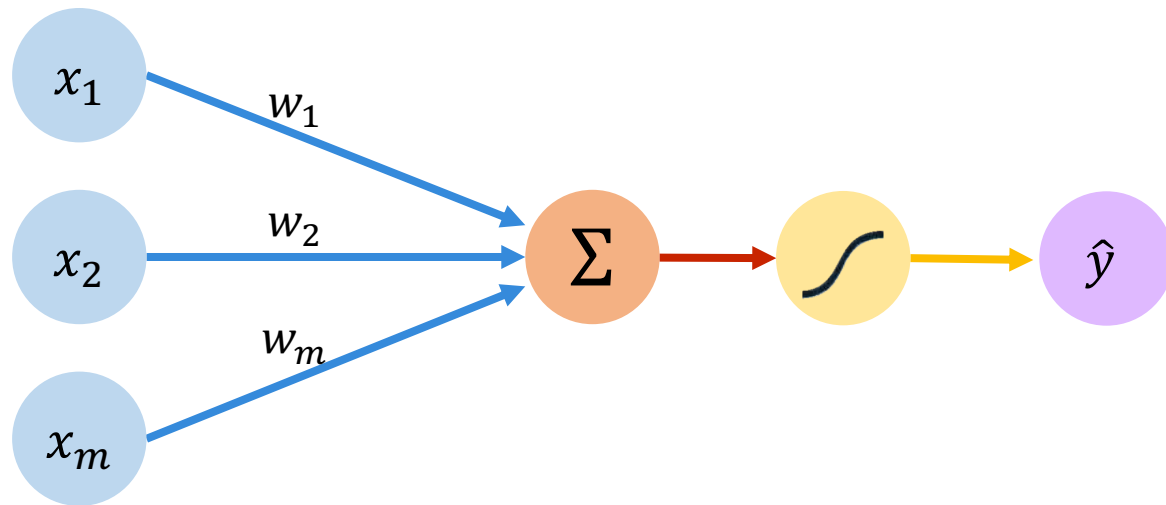
- Improved Techniques
- New Models
- Toolboxes



# The Perceptron

The structural building block of deep learning

# The Perceptron: Forward Propagation



Inputs      Weights      Sum      Non-Linearity      Output

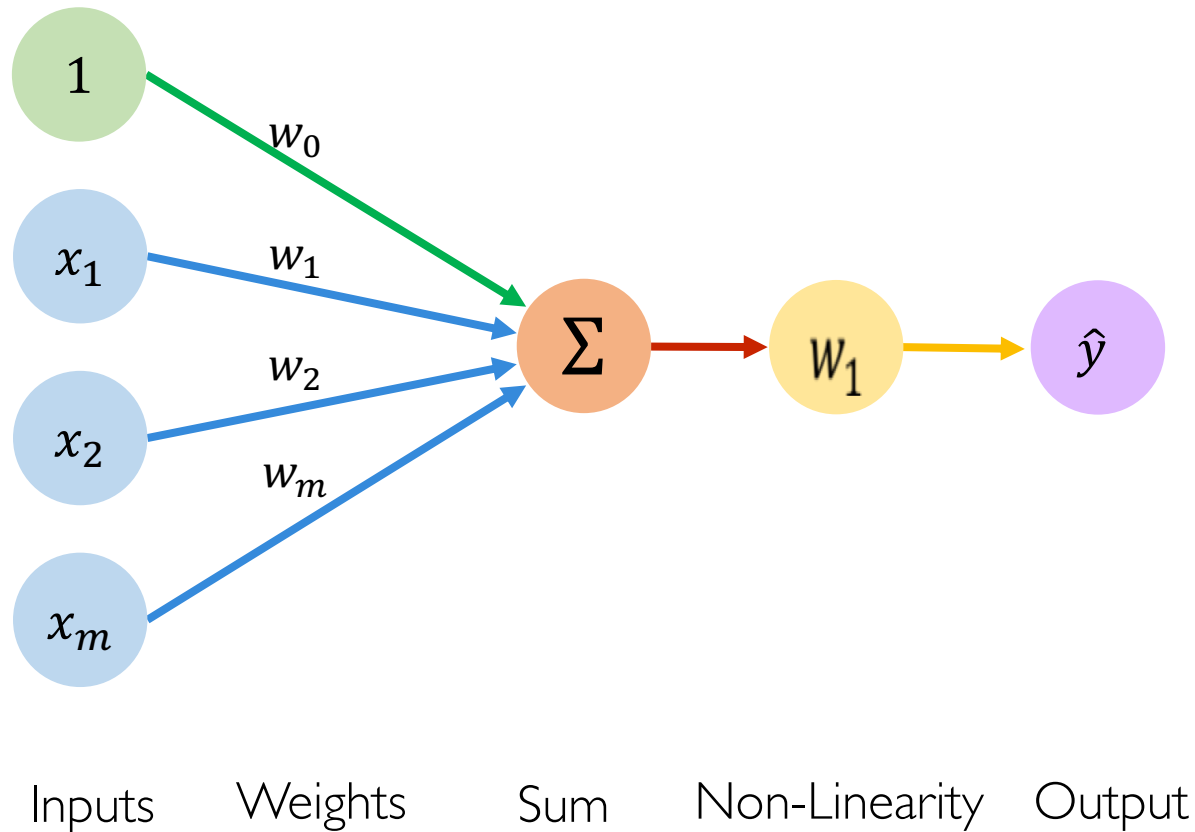
Output

Linear combination of inputs

$$\hat{y} = g \left( \sum_{i=1}^m x_i w_i \right)$$

Non-linear activation function

# The Perceptron: Forward Propagation



Output

Linear combination of inputs

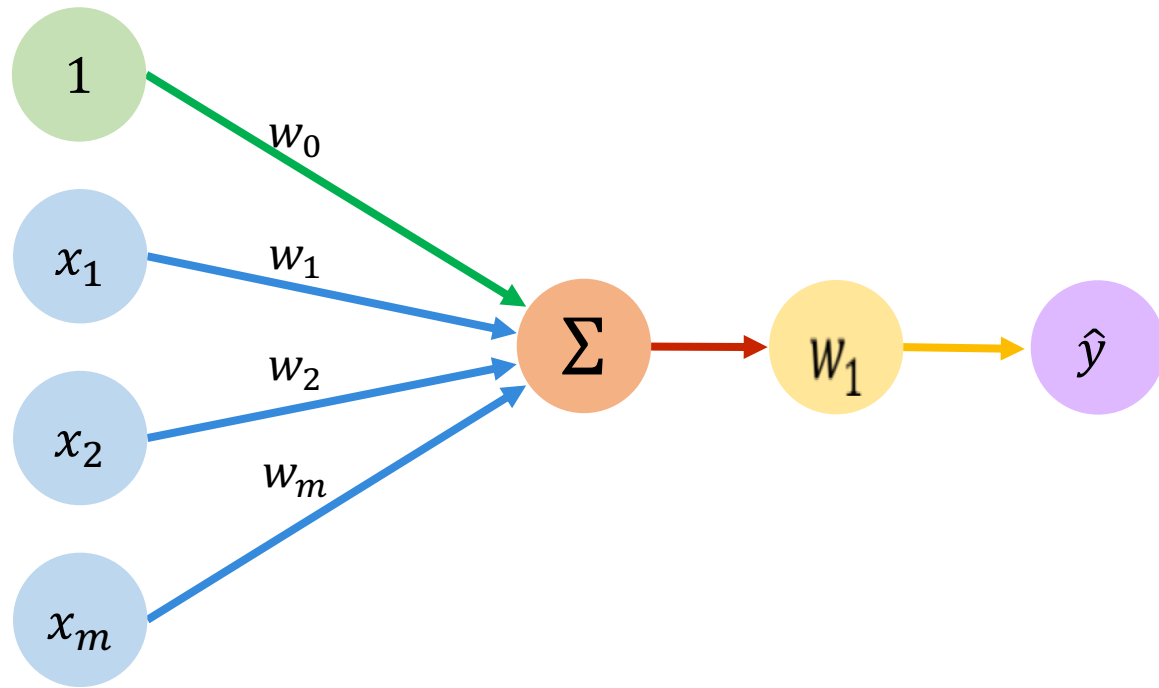
$$\hat{y} = g \left( w_0 + \sum_{i=1}^m x_i w_i \right)$$

Non-linear activation function

Bias



# The Perceptron: Forward Propagation



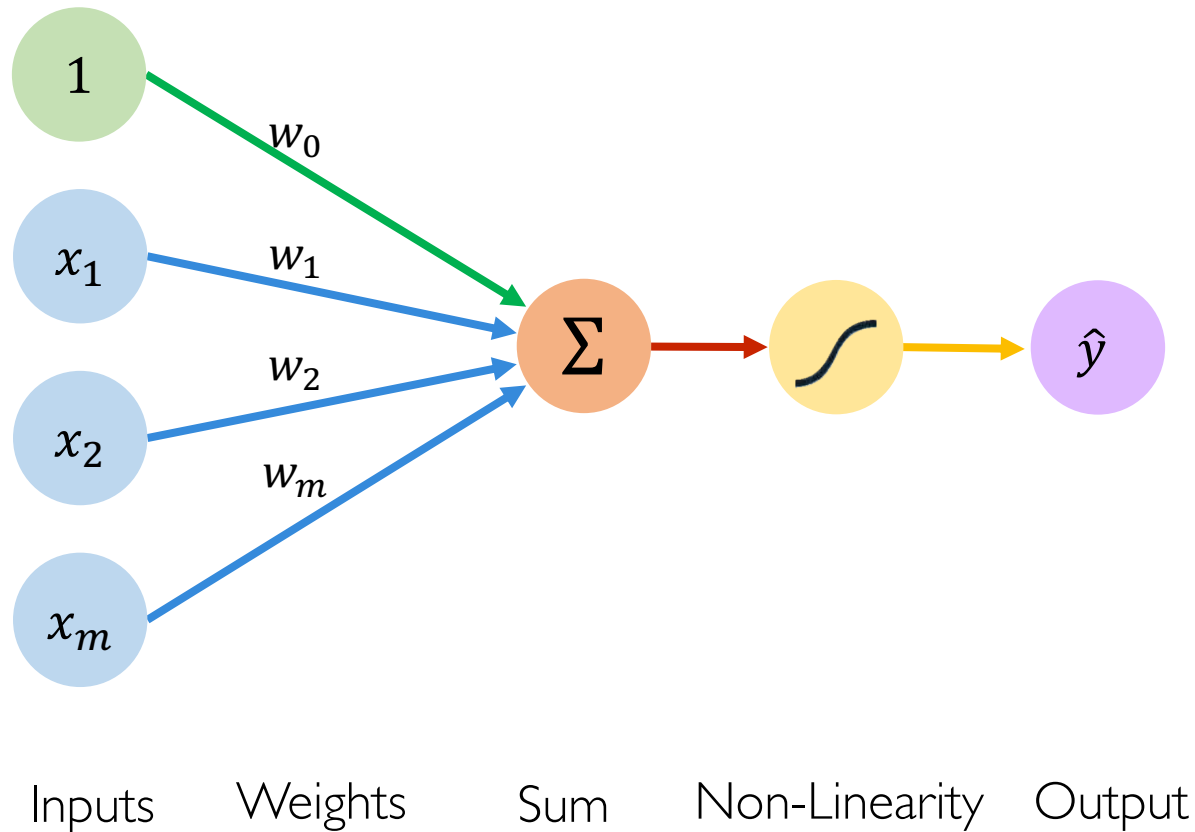
$$\hat{y} = g \left( w_0 + \sum_{i=1}^m x_i w_i \right)$$

$$\hat{y} = g ( w_0 + \mathbf{X}^T \mathbf{W} )$$

$$\text{where: } \mathbf{X} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} \text{ and } \mathbf{W} = \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix}$$

Inputs      Weights      Sum      Non-Linearity      Output

# The Perceptron: Forward Propagation

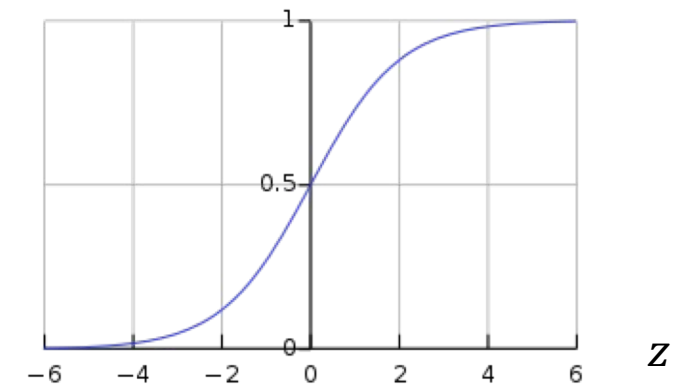


## Activation Functions

$$\hat{y} = g(w_0 + \mathbf{X}^T \mathbf{W})$$

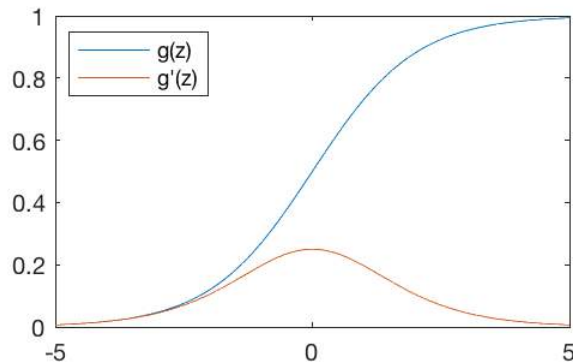
- Example: sigmoid function

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



# Common Activation Functions

Sigmoid Function



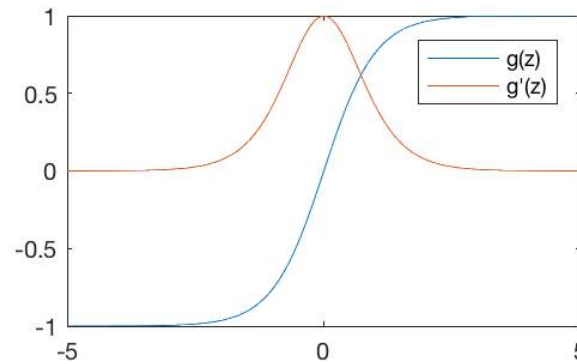
$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$



`tf.nn.sigmoid(z)`

Hyperbolic Tangent



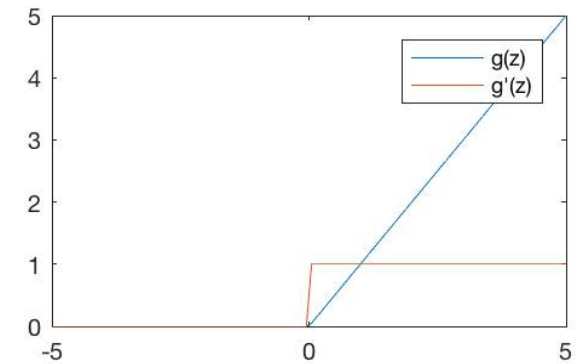
$$g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$



`tf.nn.tanh(z)`

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

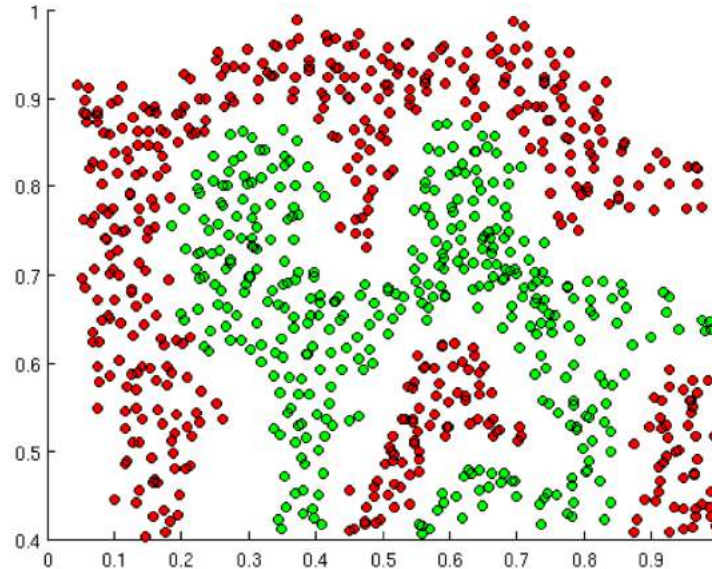


`tf.nn.relu(z)`

NOTE: All activation functions are non-linear

# Importance of Activation Functions

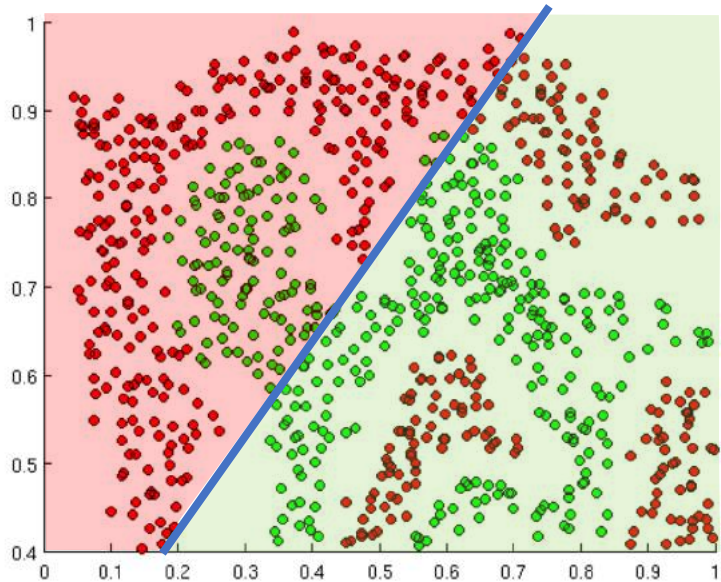
*The purpose of activation functions is to **introduce non-linearities** into the network*



What if we wanted to build a Neural Network to distinguish green vs red points?

# Importance of Activation Functions

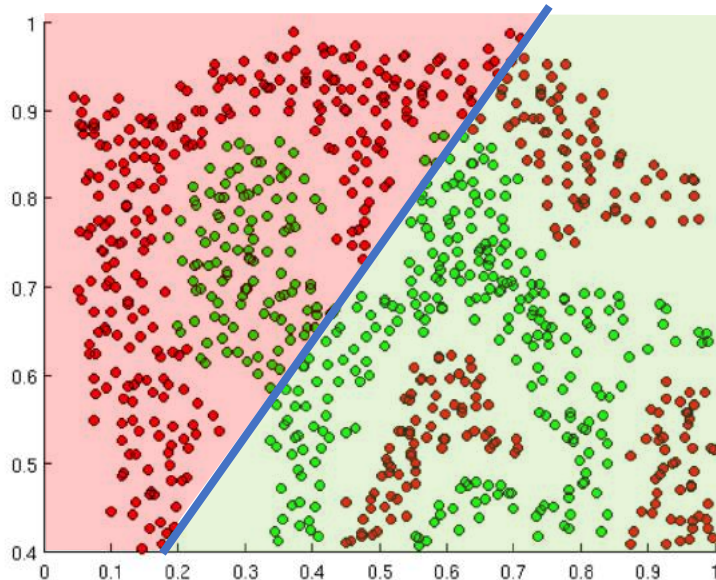
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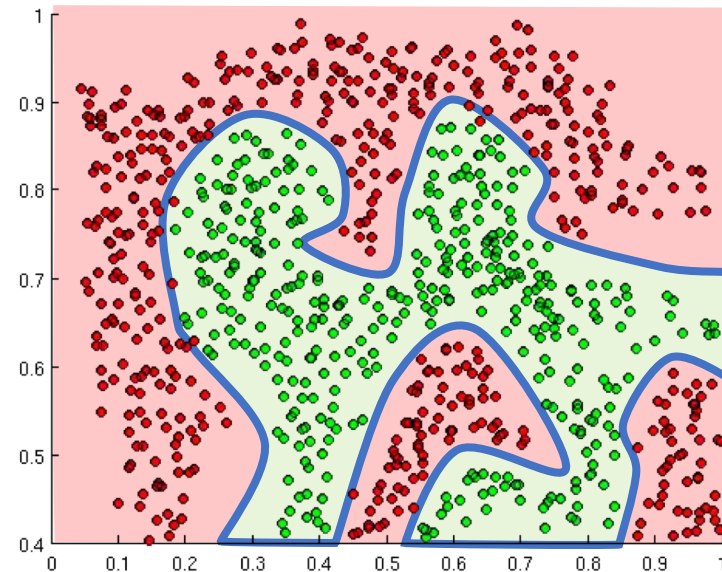
Linear Activation functions produce linear decisions no matter the network size

# Importance of Activation Functions

*The purpose of activation functions is to **introduce non-linearities** into the network*

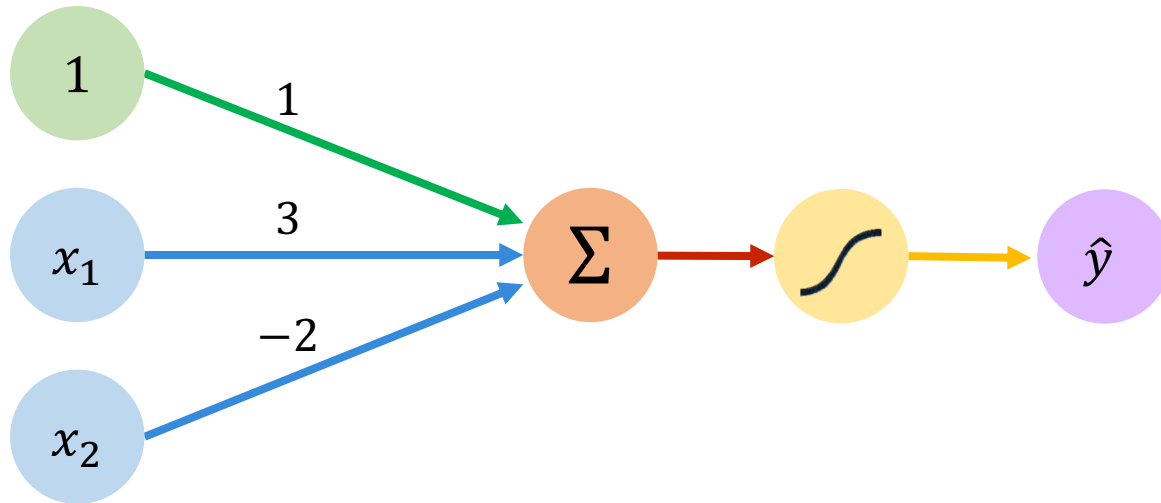


Linear Activation functions produce linear decisions no matter the network size



Non-linearities allow us to approximate arbitrarily complex functions

# The Perceptron: Example

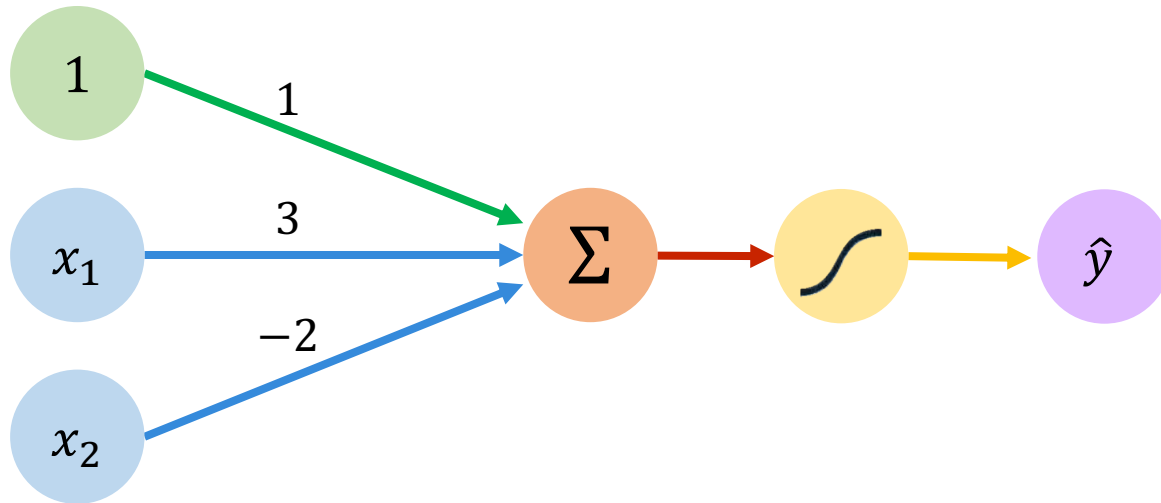


We have:  $w_0 = 1$  and  $\mathbf{W} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$

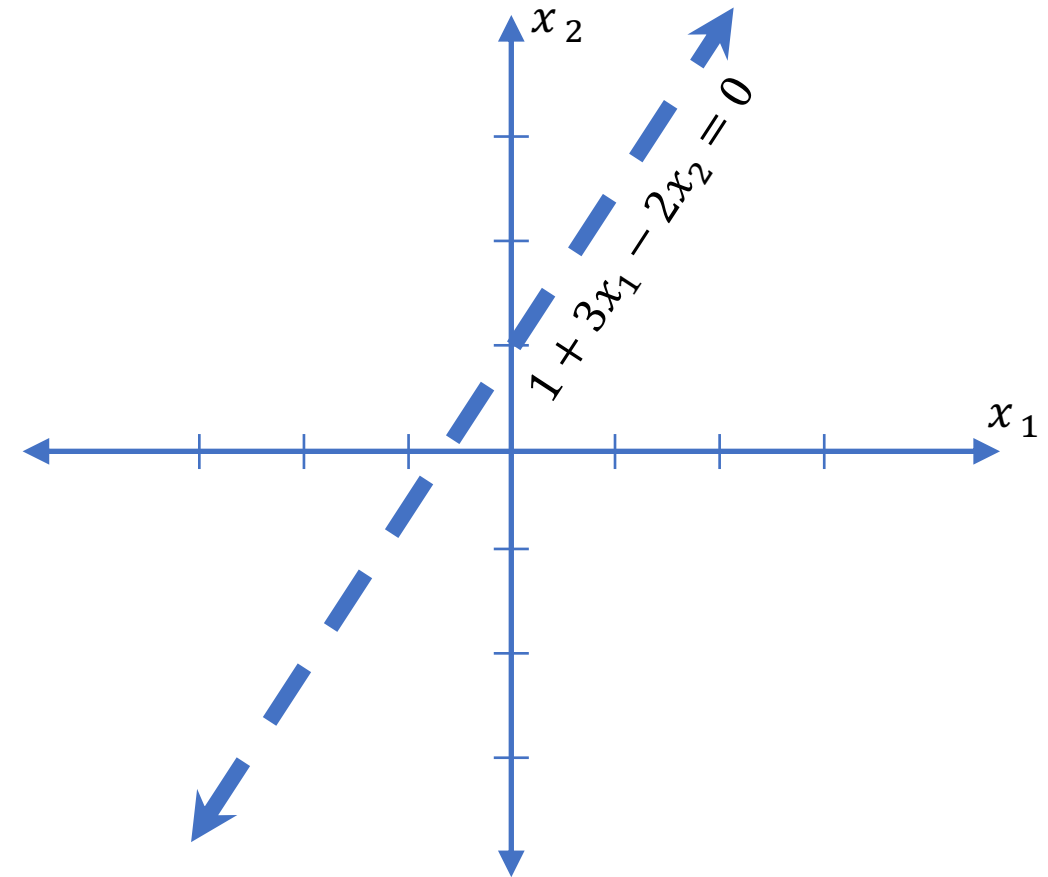
$$\begin{aligned}\hat{y} &= g(w_0 + \mathbf{X}^T \mathbf{W}) \\ &= g\left(1 + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 3 \\ -2 \end{bmatrix}\right) \\ \hat{y} &= g(1 + \underbrace{3x_1 - 2x_2})\end{aligned}$$

This is just a line in 2D!

# The Perceptron: Example

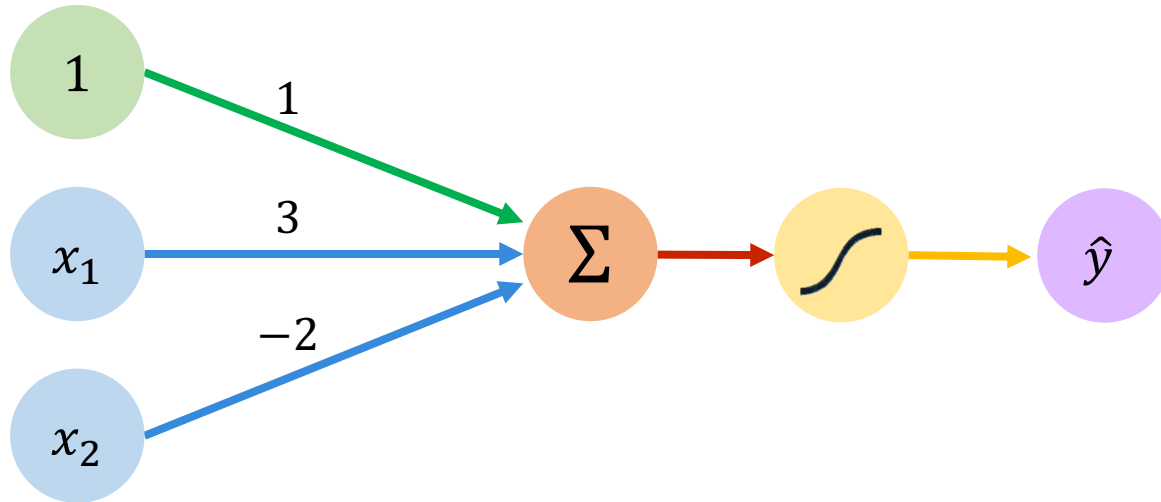


$$\hat{y} = g(1 + 3x_1 - 2x_2)$$





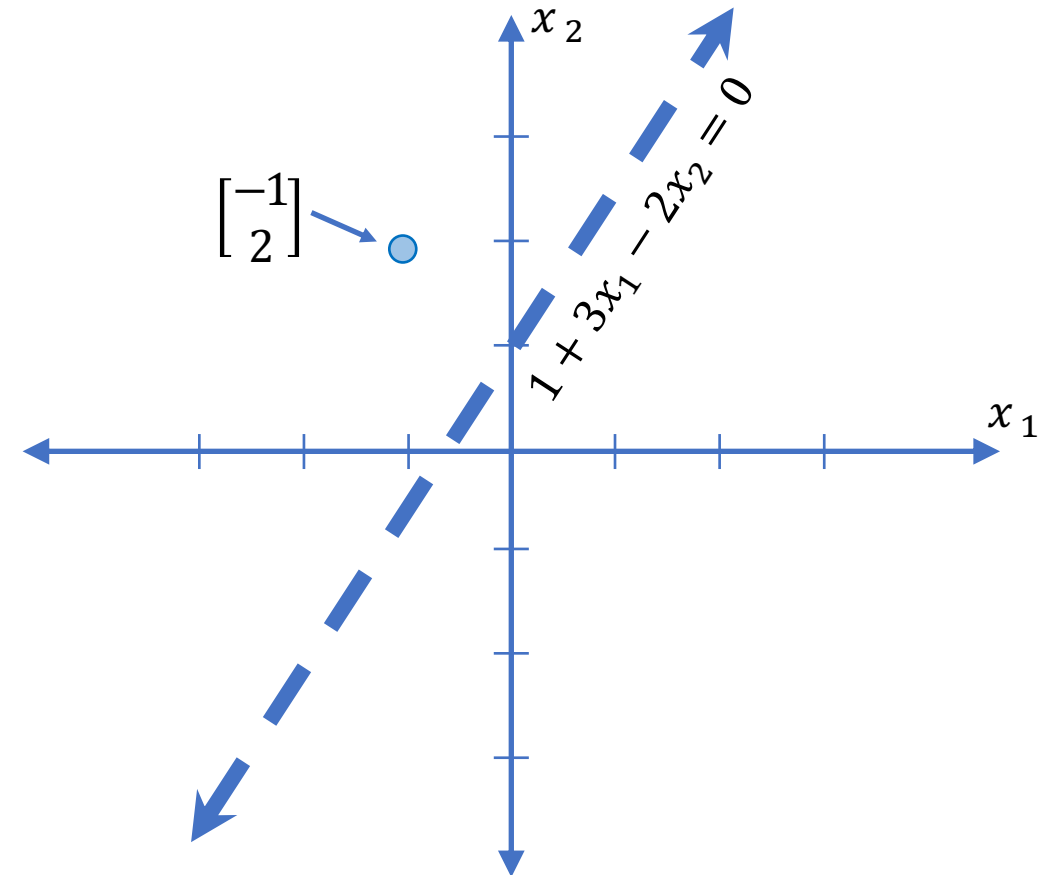
# The Perceptron: Example



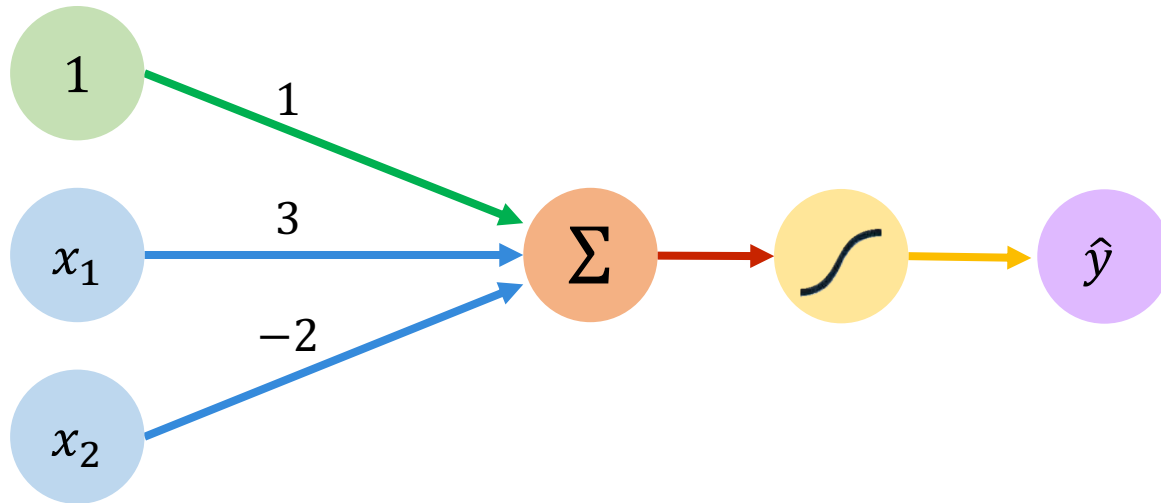
Assume we have input:  $\mathbf{X} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$

$$\begin{aligned}\hat{y} &= g(1 + (3 * -1) - (2 * 2)) \\ &= g(-6) \approx 0.002\end{aligned}$$

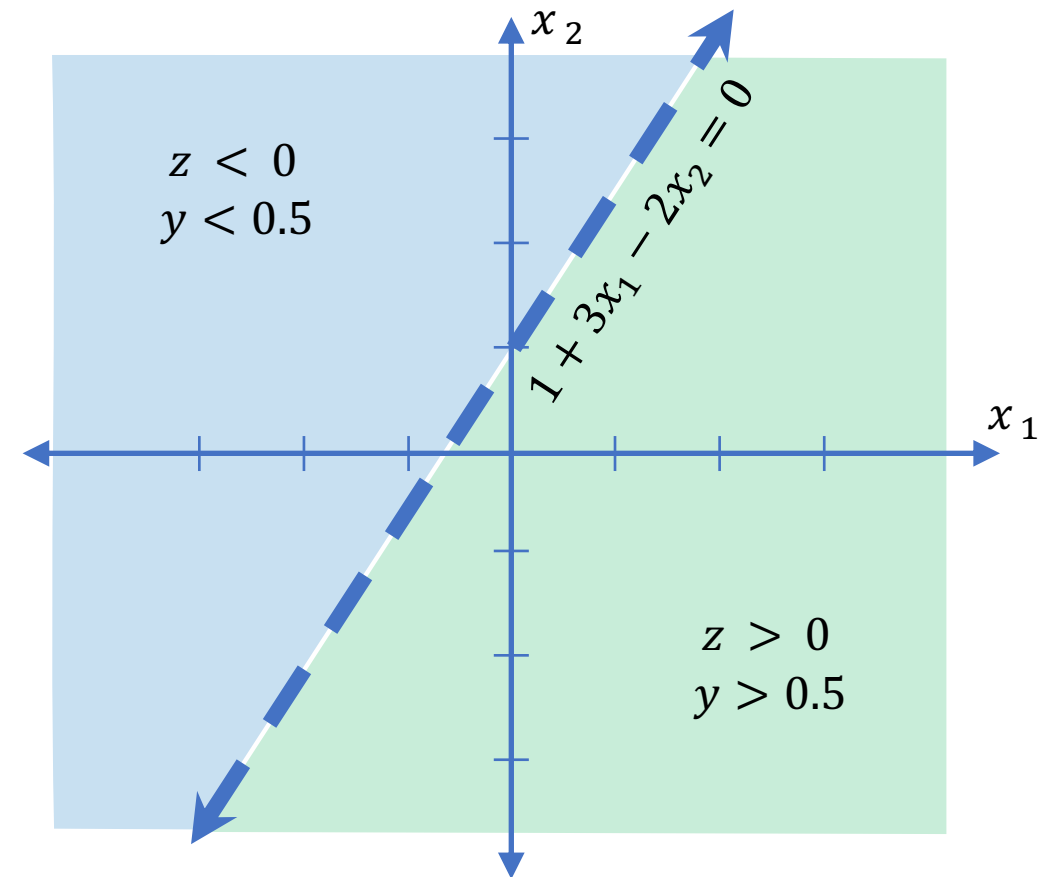
$$\hat{y} = g(1 + 3x_1 - 2x_2)$$



# The Perceptron: Example

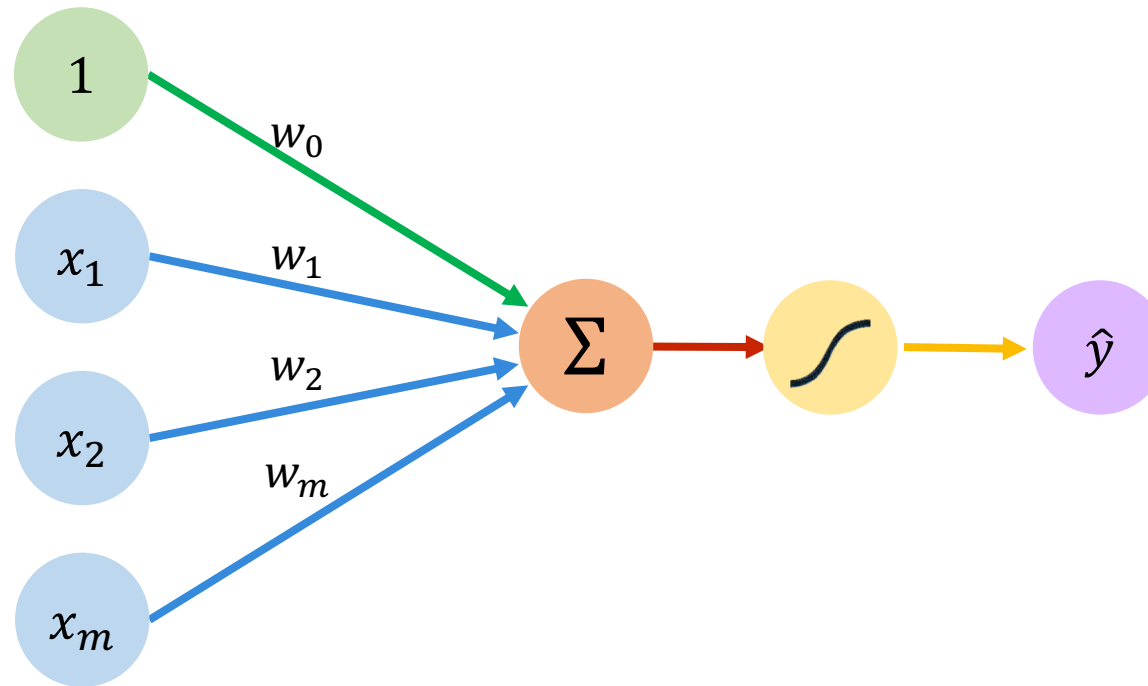


$$\hat{y} = g(1 + 3x_1 - 2x_2)$$



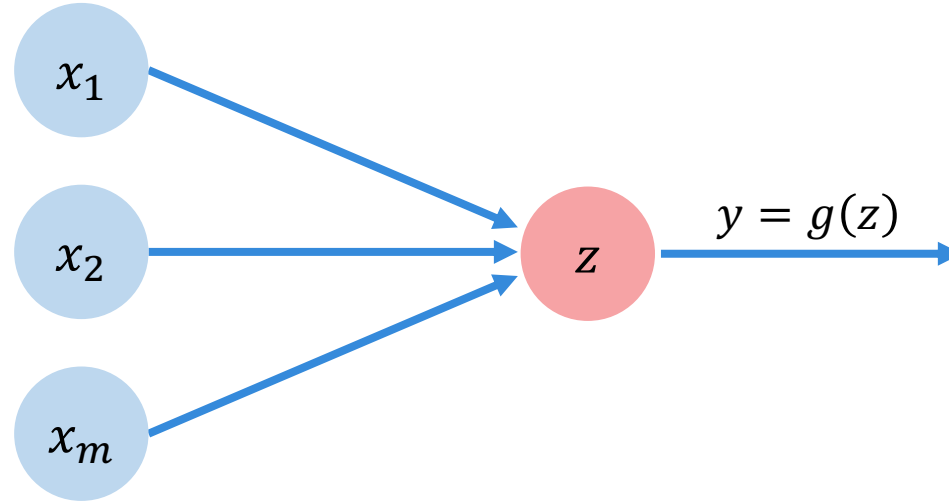
# Building Neural Networks with Perceptrons

# The Perceptron: Simplified



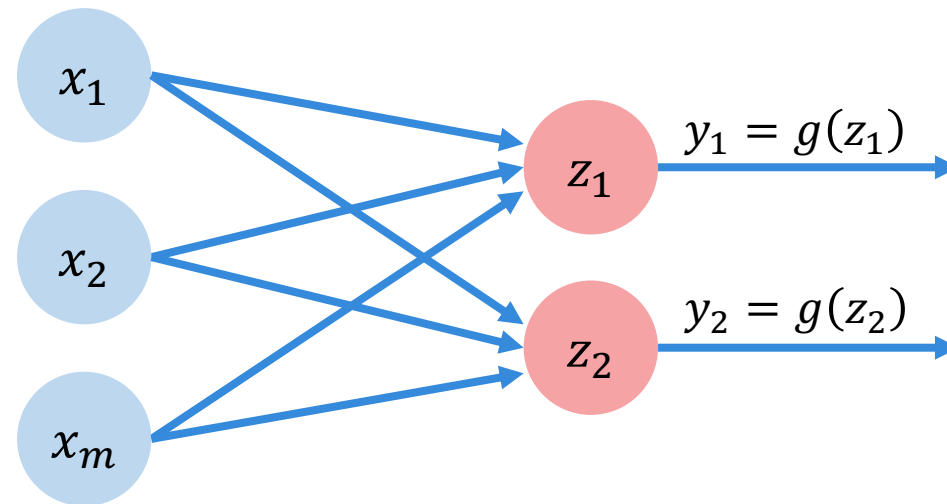
Inputs      Weights      Sum      Non-Linearity      Output

# The Perceptron: Simplified



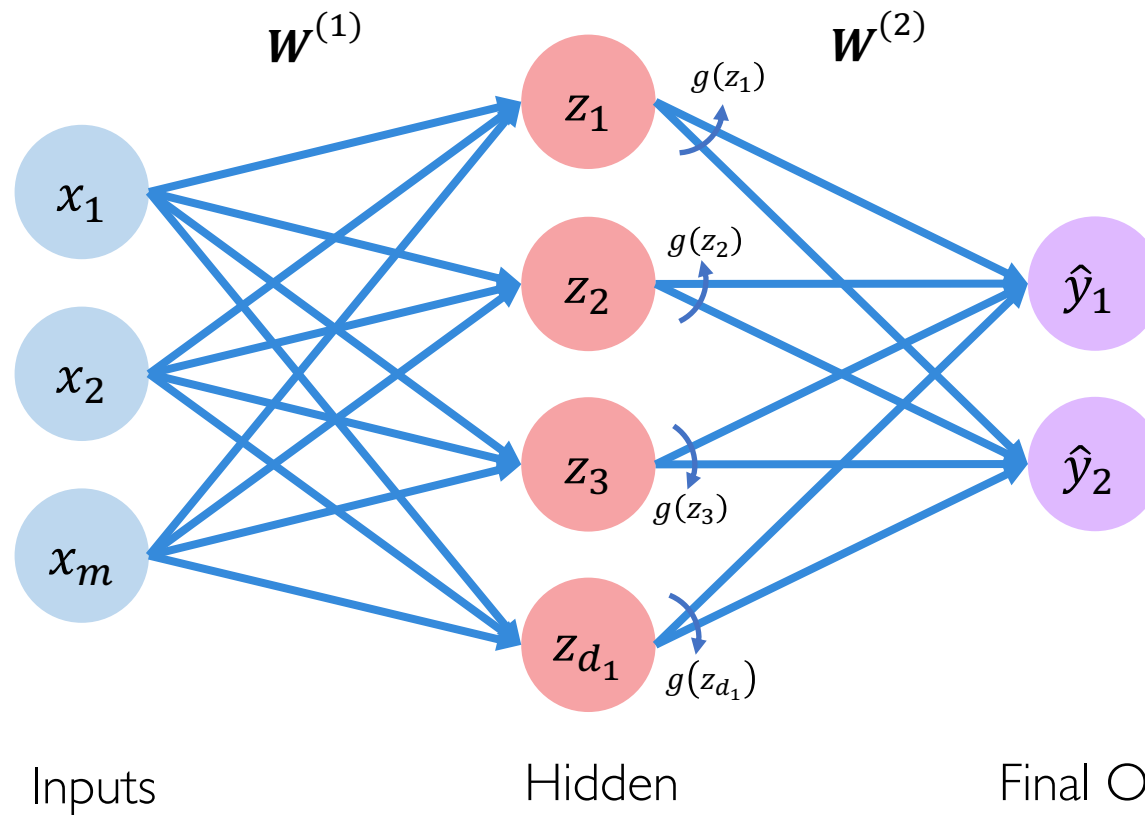
$$z = w_0 + \sum_{j=1}^m x_j w_j$$

# Multi Output Perceptron



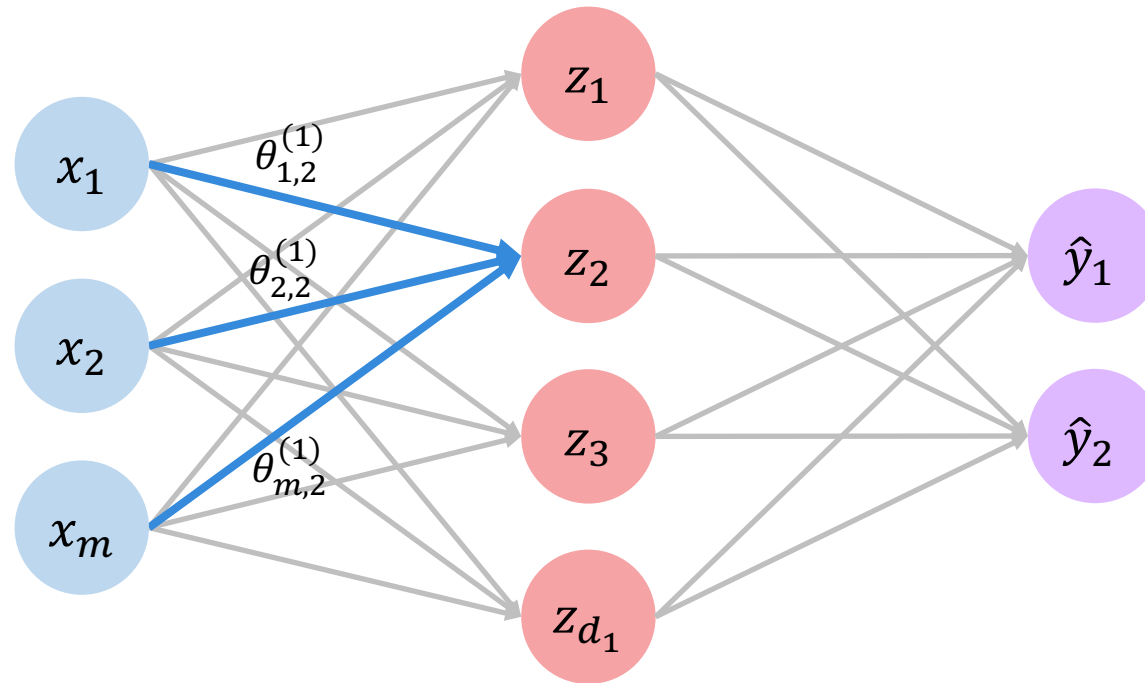
$$z_i = w_{0,i} + \sum_{j=1}^m x_j w_{j,i}$$

# Single Layer Neural Network



$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^m x_j w_{j,i}^{(1)} \quad \hat{y}_i = g \left( w_{0,i}^{(2)} + \sum_{j=1}^{d_1} z_j w_{j,i}^{(2)} \right)$$

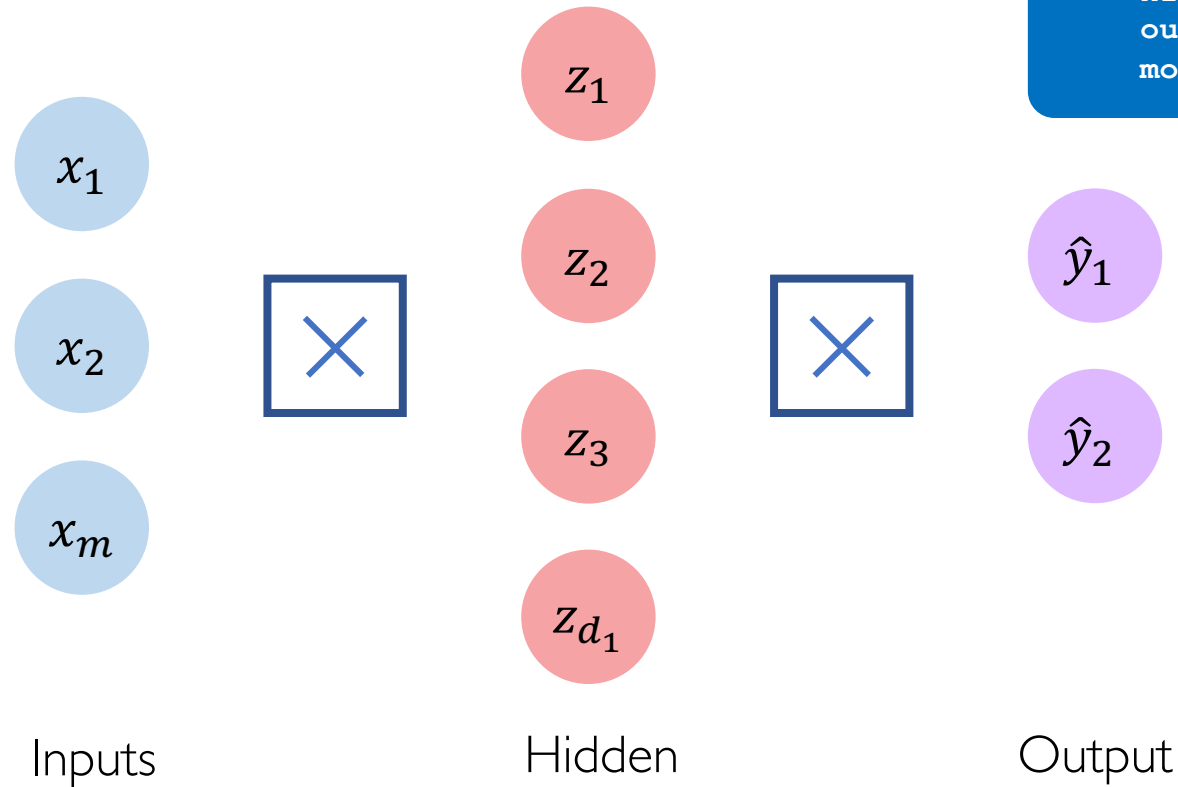
# Single Layer Neural Network



$$\begin{aligned} z_2 &= w_{0,2}^{(1)} + \sum_{j=1}^m x_j w_{j,2}^{(1)} \\ &= w_{0,2}^{(1)} + x_1 w_{1,2}^{(1)} + x_2 w_{2,2}^{(1)} + x_m w_{m,2}^{(1)} \end{aligned}$$

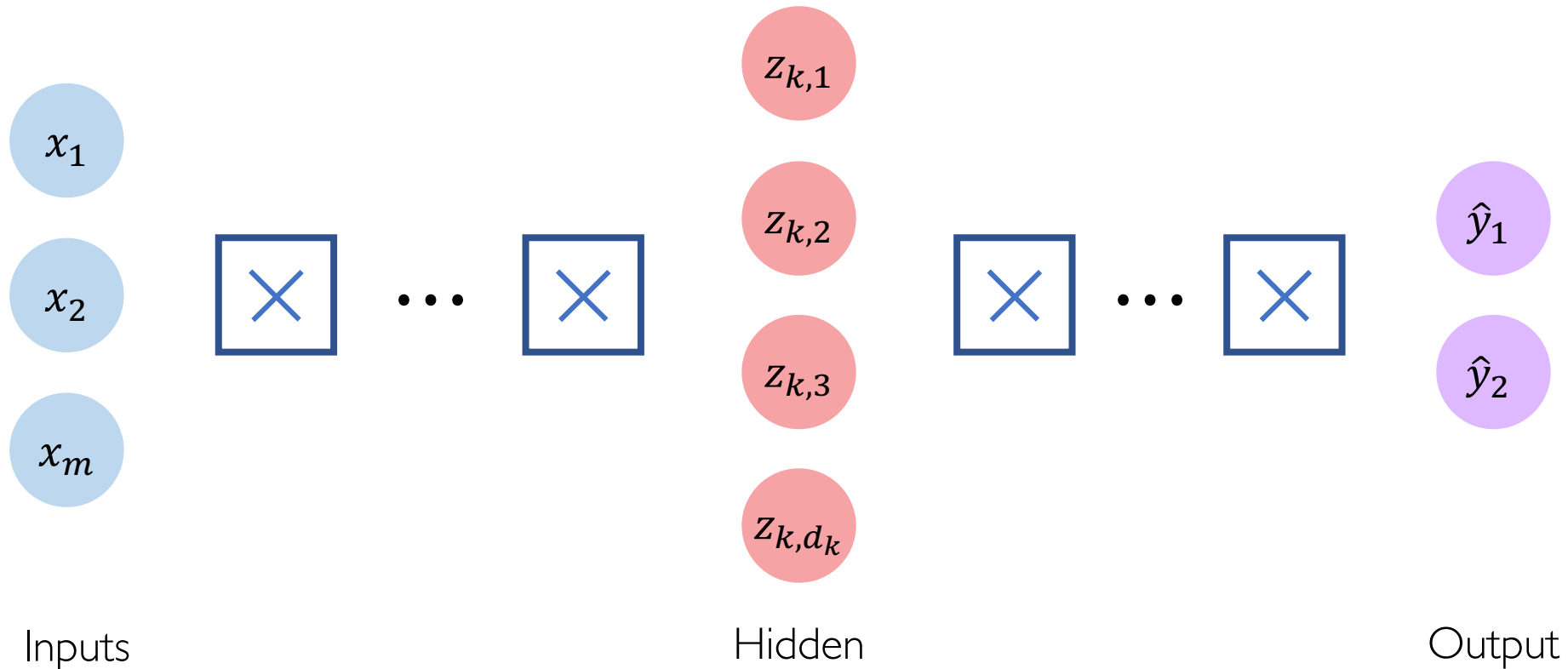


# Multi Output Perceptron



```
from tf.keras.layers import *  
  
inputs = Inputs(m)  
hidden = Dense(d1)(inputs)  
outputs = Dense(2)(hidden)  
model = Model(inputs, outputs)
```

# Deep Neural Network



$$z_{k,i} = w_{0,i}^{(k)} + \sum_{j=1}^{d_{k-1}} g(z_{k-1,j}) w_{j,i}^{(k)}$$

# Applying Neural Networks

# Example Problem

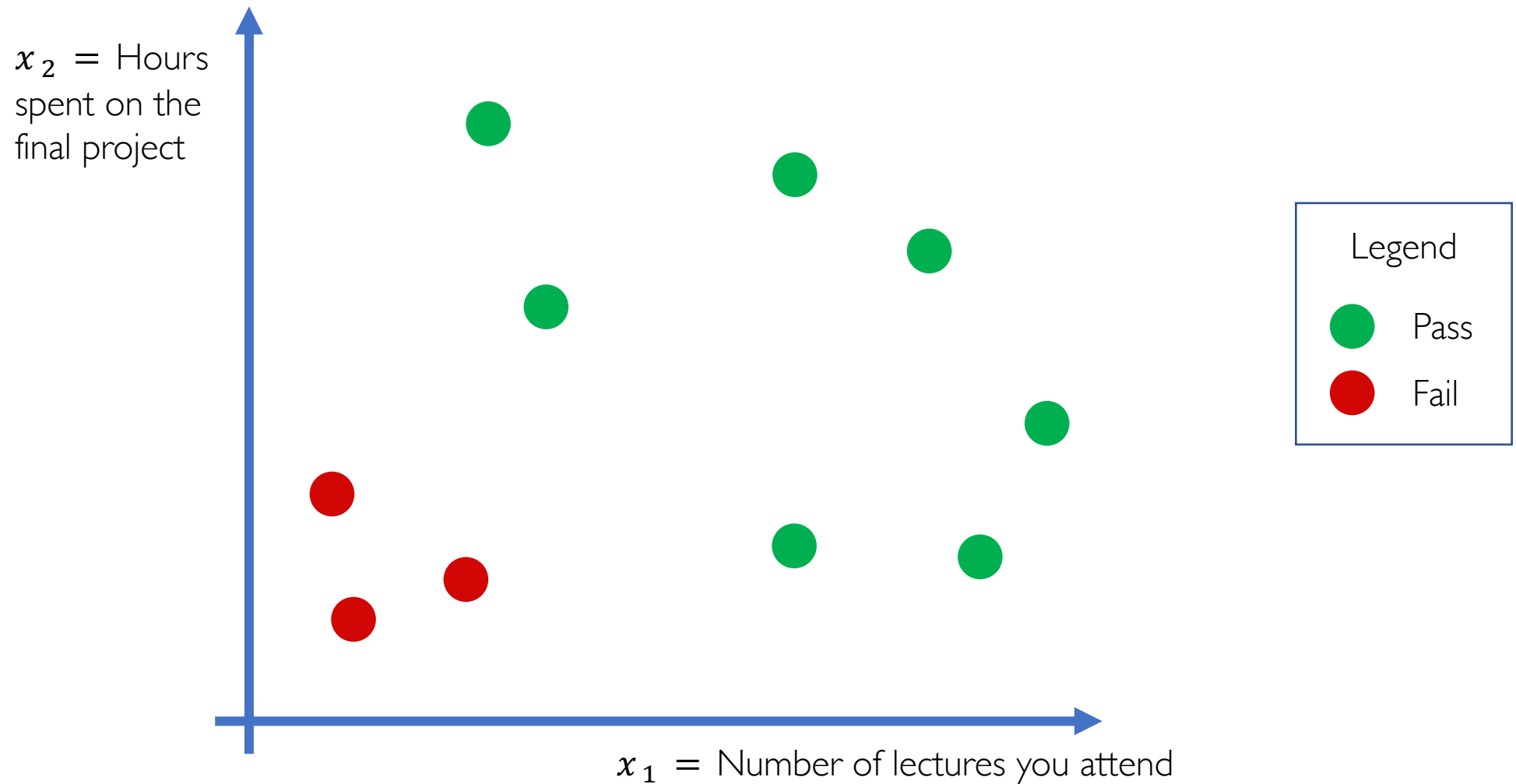
Will I pass this class?

Let's start with a simple two feature model

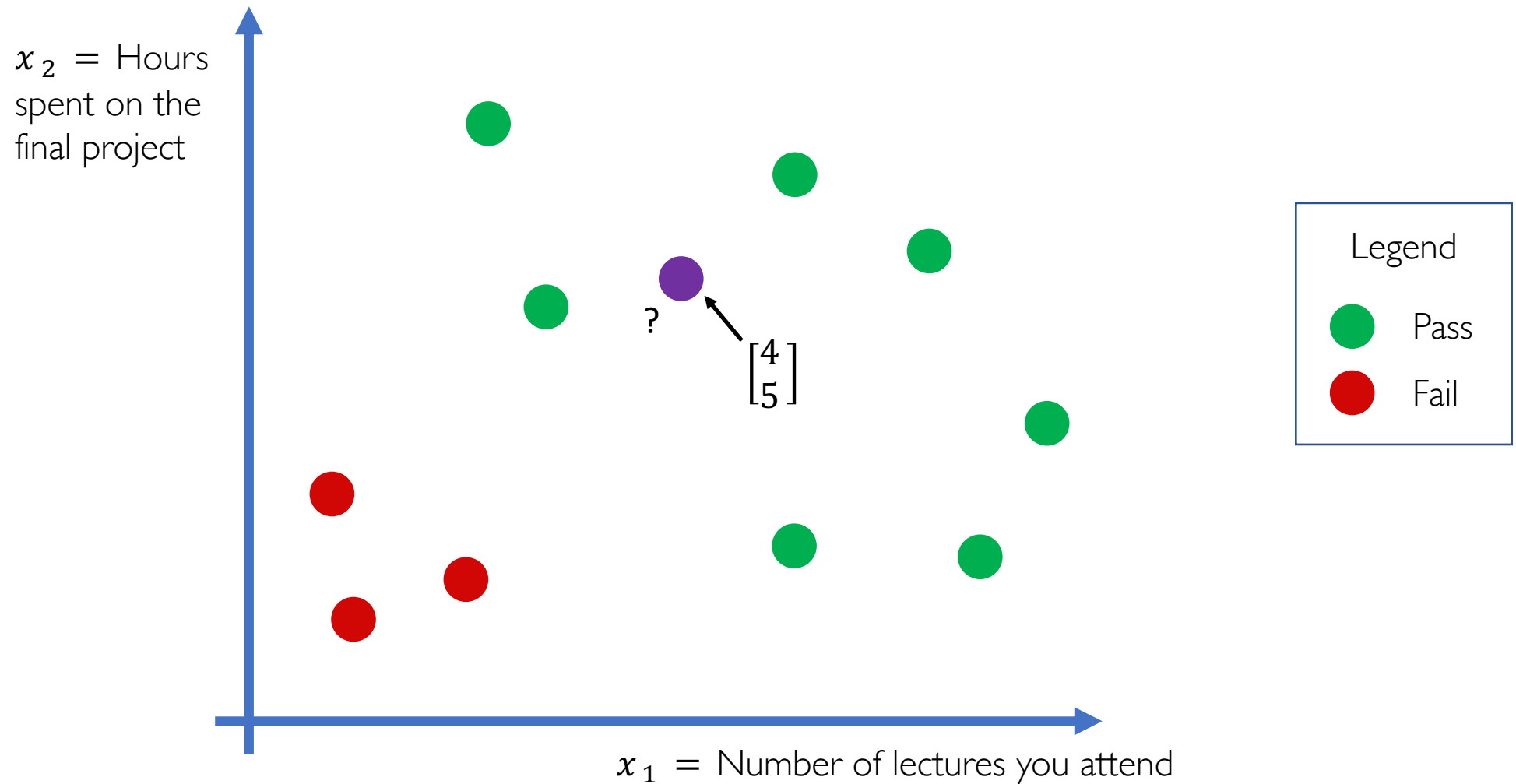
$x_1$  = Number of lectures you attend

$x_2$  = Hours spent on the final project

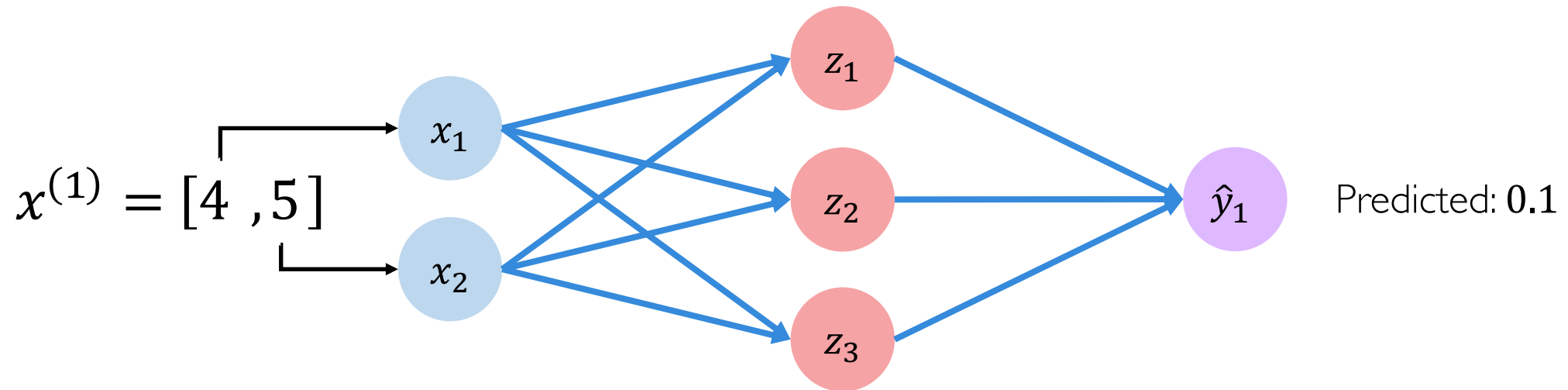
# Example Problem: Will I pass this class?



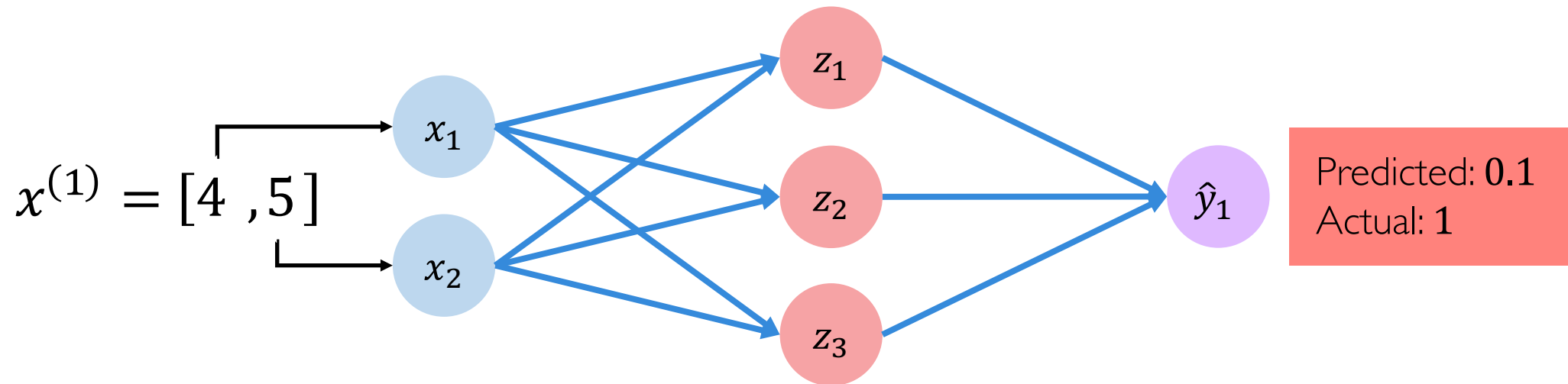
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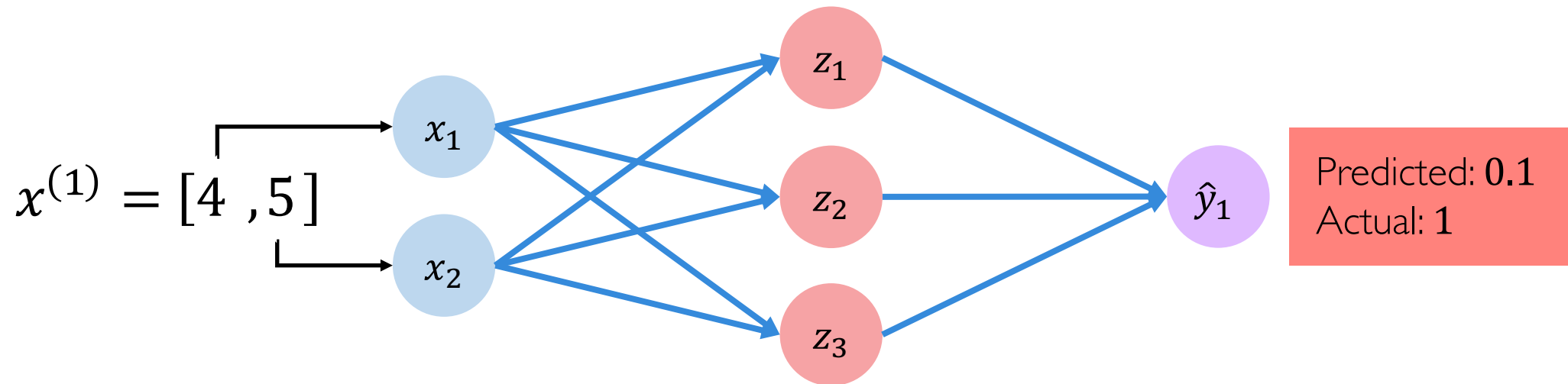
# Example Problem: Will I pass this class?





# Quantifying Loss

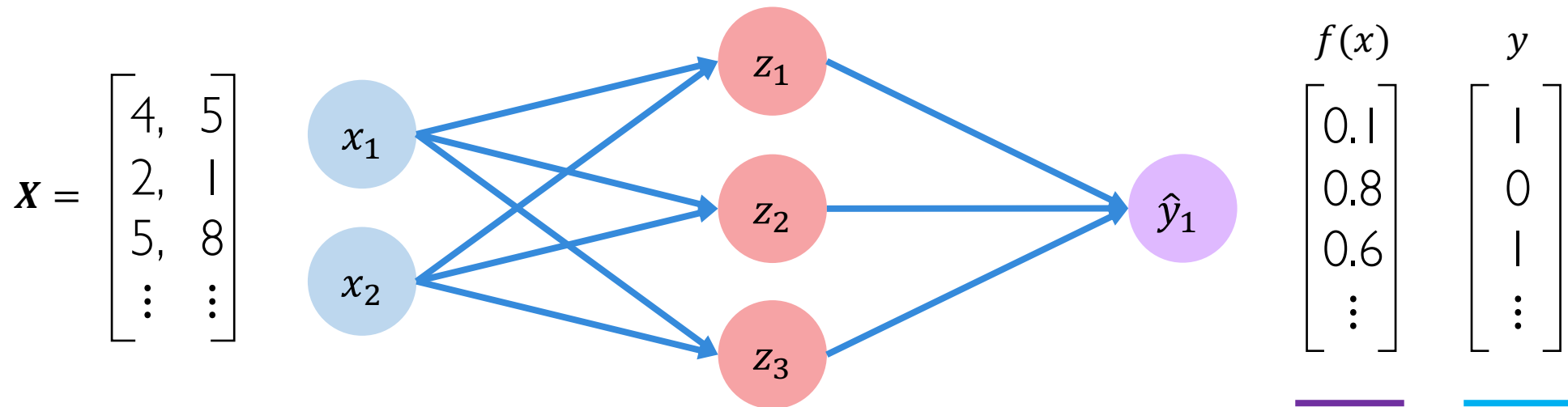
The **loss** of our network measures the cost incurred from incorrect predictions



$$\mathcal{L}(\underbrace{f(x^{(i)}; \mathbf{W})}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}})$$

# Empirical Loss

The **empirical loss** measures the total loss over our entire dataset



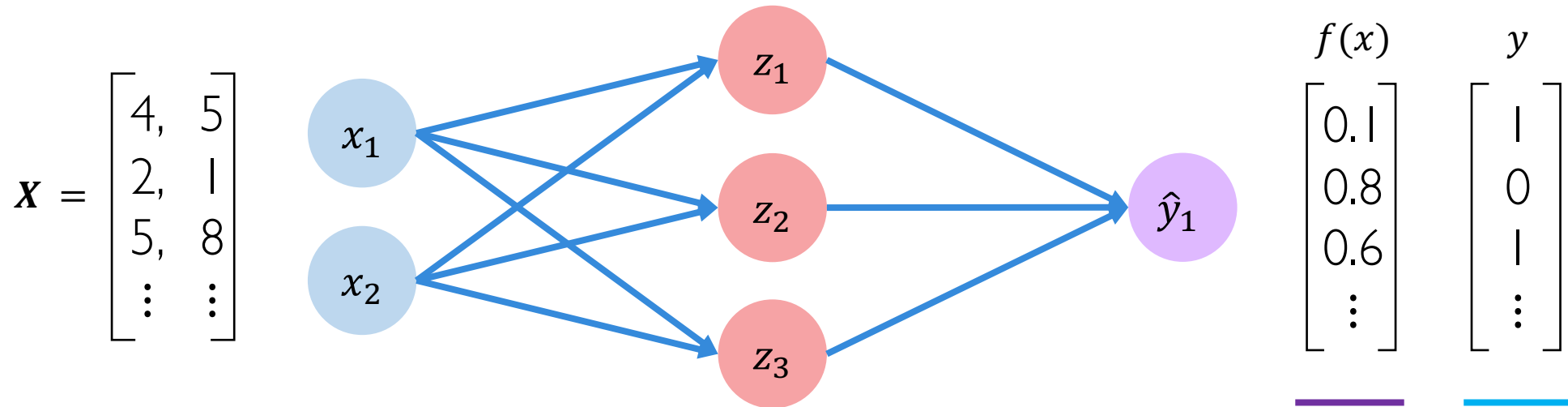
Also known as:

- Objective function
- Cost function
- Empirical Risk

$$J(\mathbf{W}) = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(\underbrace{f(x^{(i)}; \mathbf{W})}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}})$$

# Binary Cross Entropy Loss

*Cross entropy loss* can be used with models that output a probability between 0 and 1



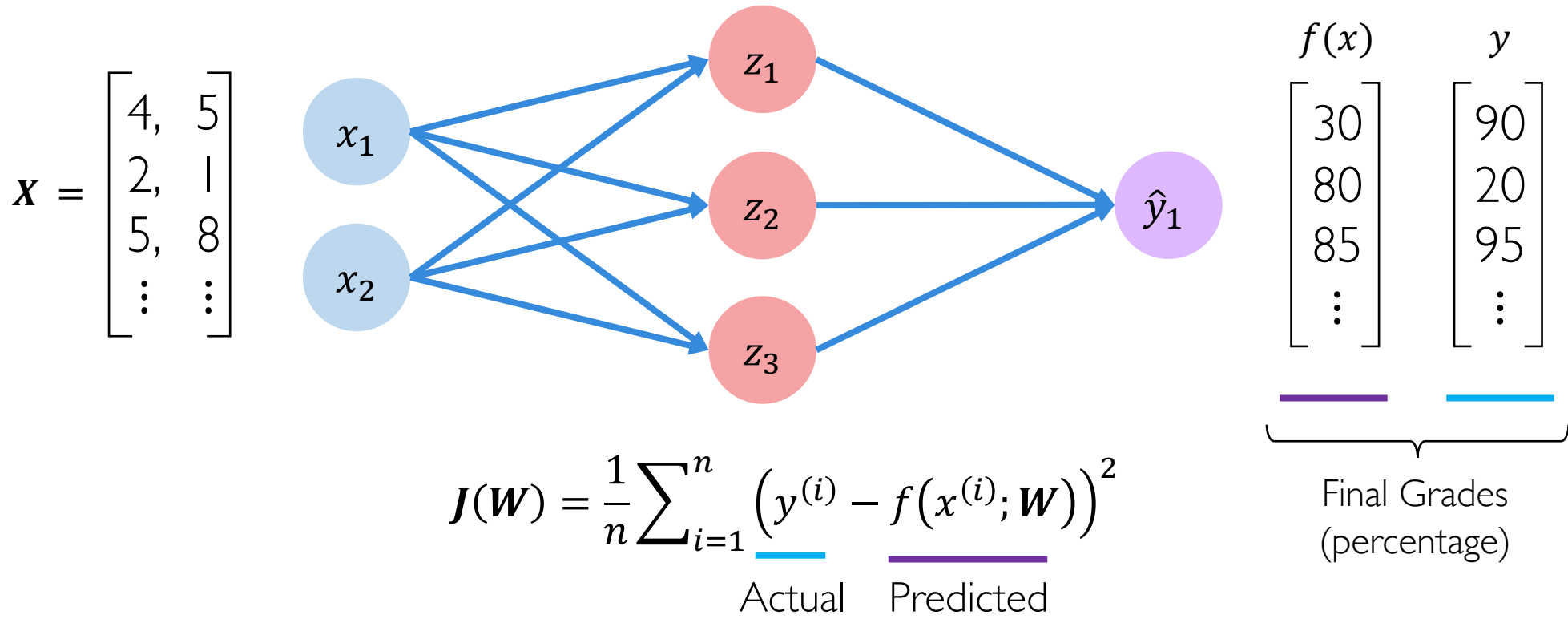
$$J(W) = \frac{1}{n} \sum_{i=1}^n \underbrace{y^{(i)}}_{\text{Actual}} \log \left( \underbrace{f(x^{(i)}; W)}_{\text{Predicted}} \right) + (1 - \underbrace{y^{(i)}}_{\text{Actual}}) \log \left( 1 - \underbrace{f(x^{(i)}; W)}_{\text{Predicted}} \right)$$



```
loss = tf.reduce_mean( tf.nn.softmax_cross_entropy_with_logits(model.y, model.pred) )
```

# Mean Squared Error Loss

*Mean squared error loss* can be used with regression models that output continuous real numbers



```
loss = tf.reduce_mean( tf.square( tf.subtract( model.y, model.pred ) ) )
```

# Training Neural Networks

# Loss Optimization

We want to find the network weights that *achieve the lowest loss*

$$\mathbf{W}^* = \operatorname{argmin}_{\mathbf{W}} \frac{1}{n} \sum_{i=1}^n \mathcal{L}(f(x^{(i)}; \mathbf{W}), y^{(i)})$$

$$\mathbf{W}^* = \operatorname{argmin}_{\mathbf{W}} J(\mathbf{W})$$

# Loss Optimization

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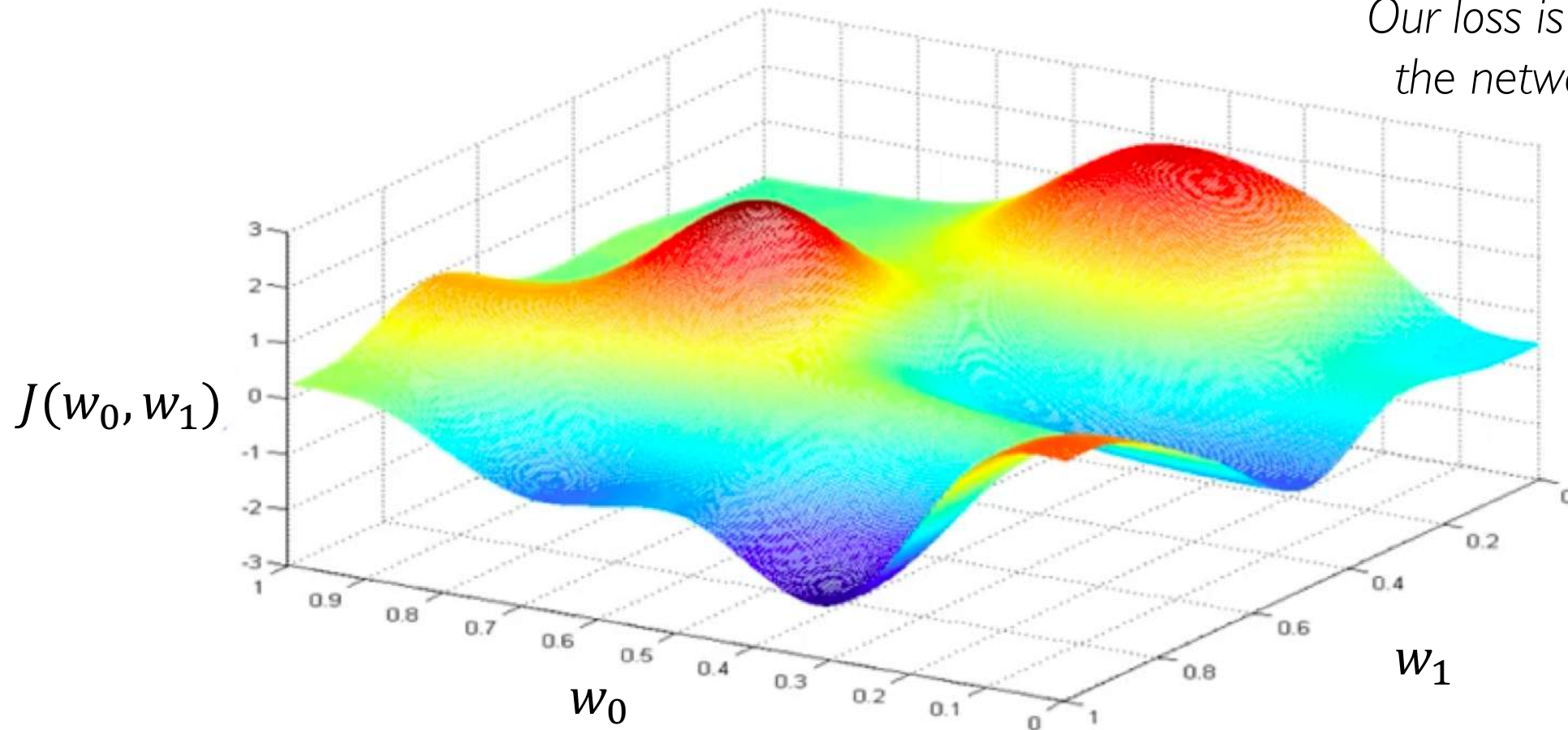
Remember:

$$\mathbf{W} = \{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \dots\}$$

# Loss Optimization

$$W^* = \underset{W}{\operatorname{argmin}} J(W)$$

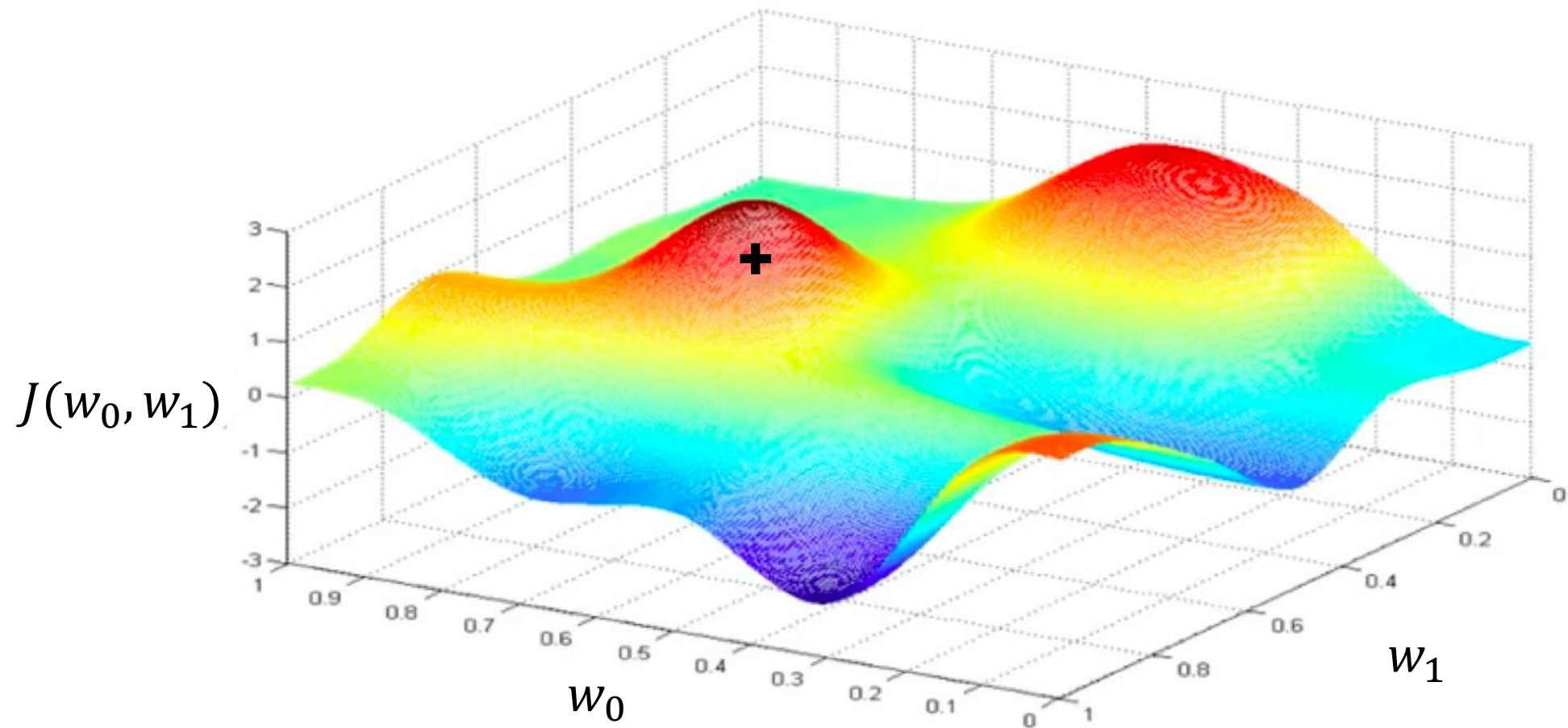
Remember:  
*Our loss is a function of  
the network weights!*





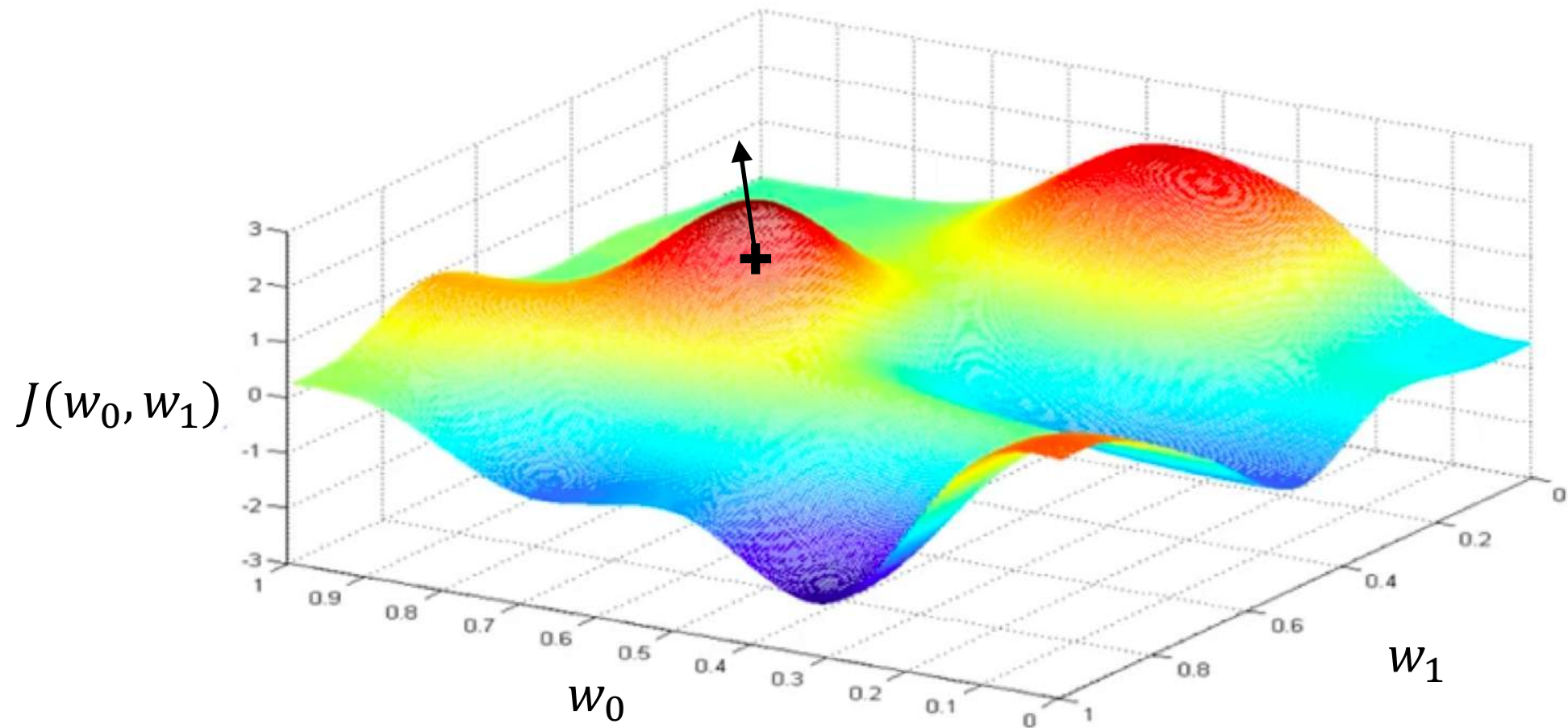
# Loss Optimization

Randomly pick an initial  $(w_0, w_1)$



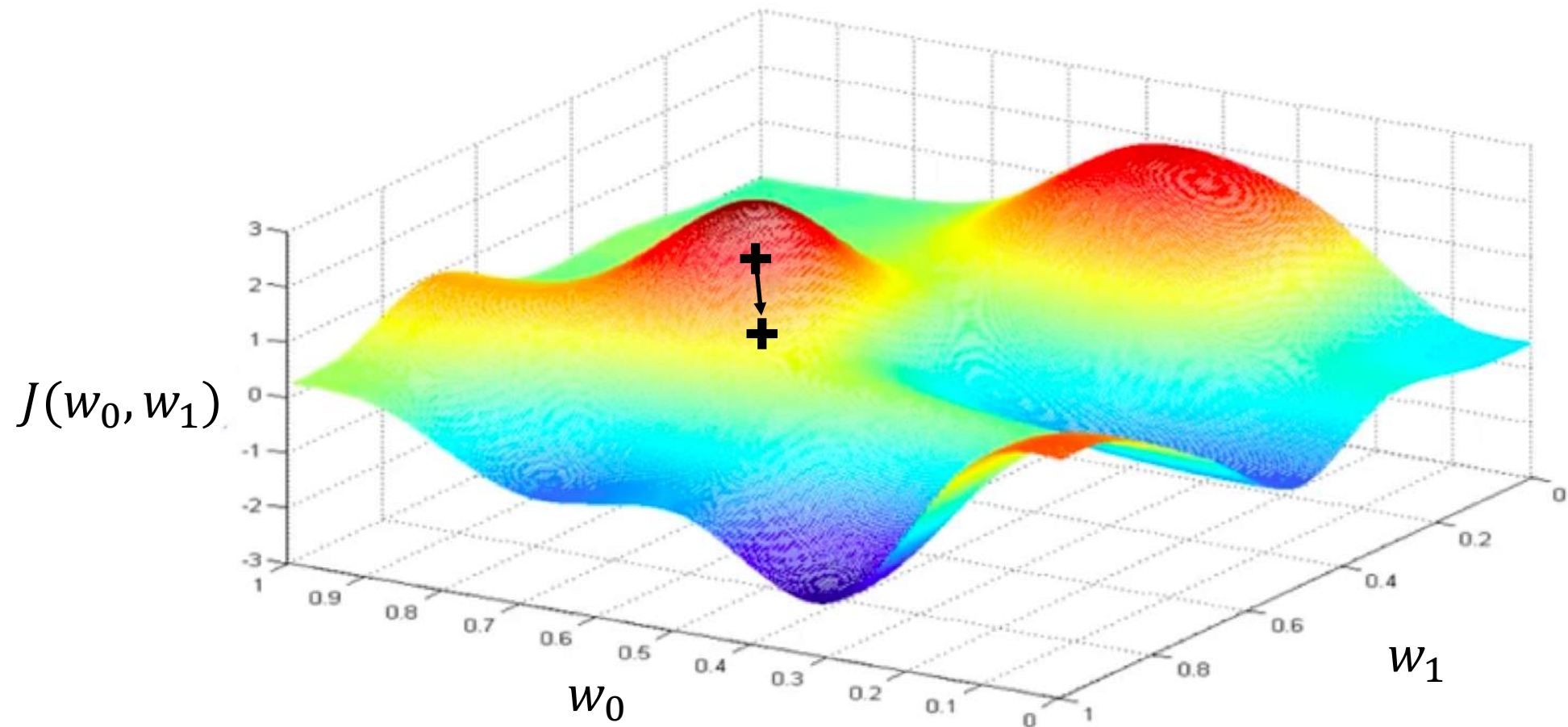
# Loss Optimization

Compute gradient,  $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$



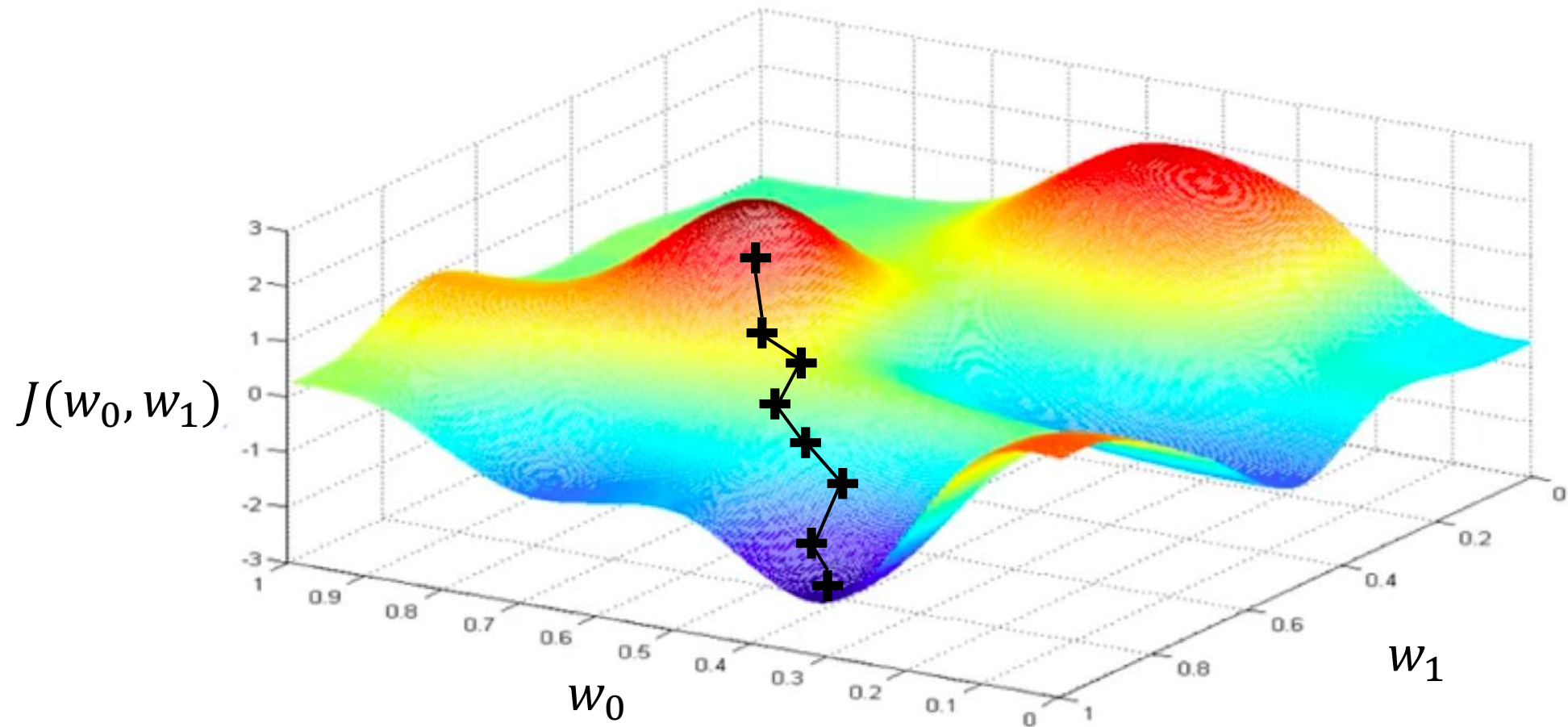
# Loss Optimization

Take small step in opposite direction of gradient



# Gradient Descent

Repeat until convergence



# Gradient Descent

## Algorithm

1. Initialize weights randomly  $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3.     Compute gradient,  $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$
4.     Update weights,  $\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$
5. Return weights

 `weights = tf.random_normal(shape, stddev=sigma)`

 `grads = tf.gradients(ys=loss, xs=weights)`

 `weights_new = weights.assign(weights - lr * grads)`



# Gradient Descent

## Algorithm

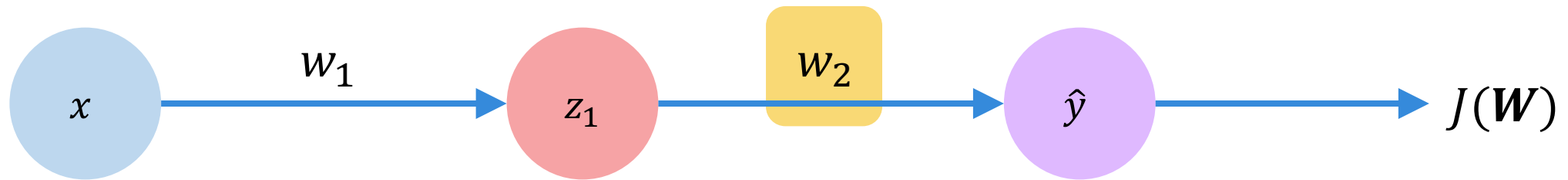
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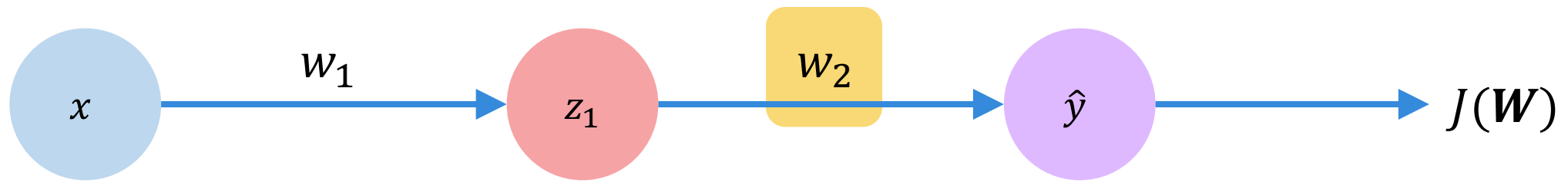
 `weights_new = weights.assign(weights - lr * grads)`

# Computing Gradients: Backpropagation



*How does a small change in one weight (ex.  $w_2$ ) affect the final loss  $J(\mathbf{W})$ ?*

# Computing Gradients: Backpropagation

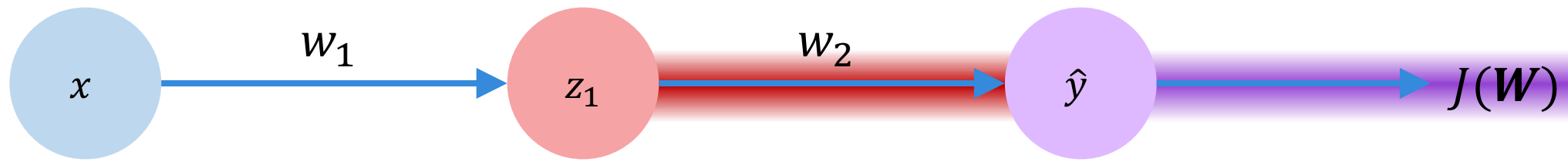


$$\frac{\partial J(W)}{\partial w_2} =$$

Let's use the chain rule!

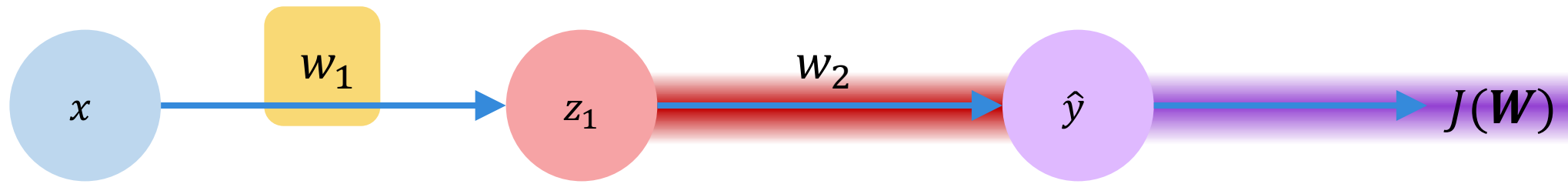


# Computing Gradients: Backpropagation



$$\frac{\partial J(W)}{\partial w_2} = \underbrace{\frac{\partial J(W)}{\partial \hat{y}}}_{\text{purple}} * \underbrace{\frac{\partial \hat{y}}{\partial w_2}}_{\text{red}}$$

# Computing Gradients: Backpropagation

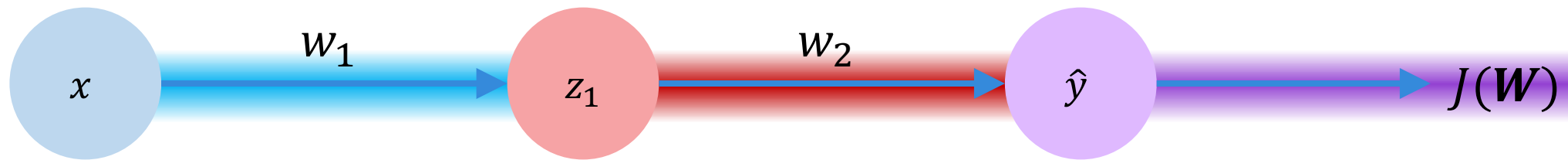


$$\frac{\partial J(W)}{\partial w_1} = \frac{\partial J(W)}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_1}$$

Apply chain rule!

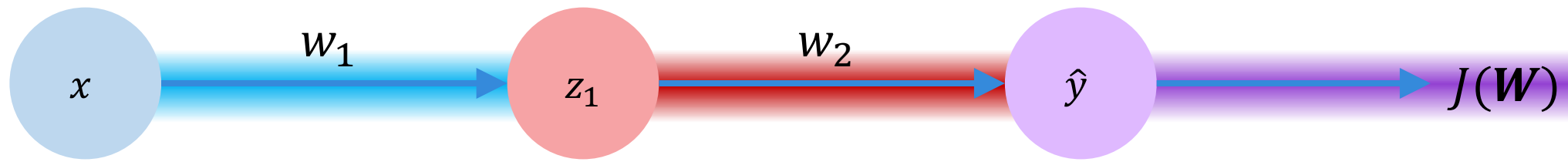
Apply chain rule!

# Computing Gradients: Backpropagation



$$\frac{\partial J(W)}{\partial w_1} = \underbrace{\frac{\partial J(W)}{\partial \hat{y}}}_{\text{purple}} * \underbrace{\frac{\partial \hat{y}}{\partial z_1}}_{\text{red}} * \underbrace{\frac{\partial z_1}{\partial w_1}}_{\text{blue}}$$

# Computing Gradients: Backpropagation

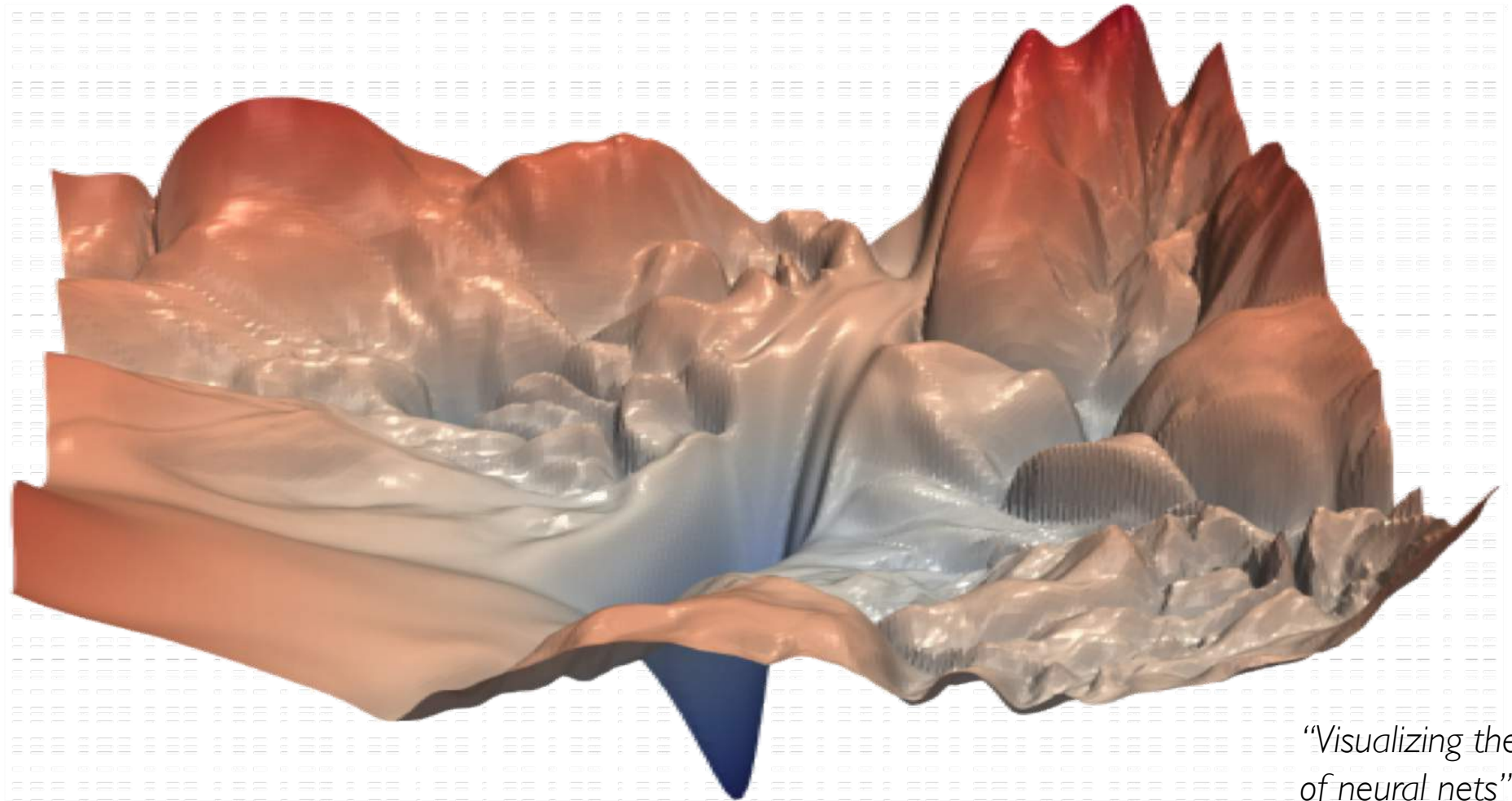


$$\frac{\partial J(W)}{\partial w_1} = \underbrace{\frac{\partial J(W)}{\partial \hat{y}}}_{\text{purple}} * \underbrace{\frac{\partial \hat{y}}{\partial z_1}}_{\text{red}} * \underbrace{\frac{\partial z_1}{\partial w_1}}_{\text{blue}}$$

Repeat this for **every weight in the network** using gradients from later layers

# Neural Networks in Practice: Optimization

# Training Neural Networks is Difficult



*“Visualizing the loss landscape of neural nets”. Dec 2017.*

# Loss Functions Can Be Difficult to Optimize

**Remember:**

Optimization through gradient descent

$$\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$$

# Loss Functions Can Be Difficult to Optimize

**Remember:**

Optimization through gradient descent

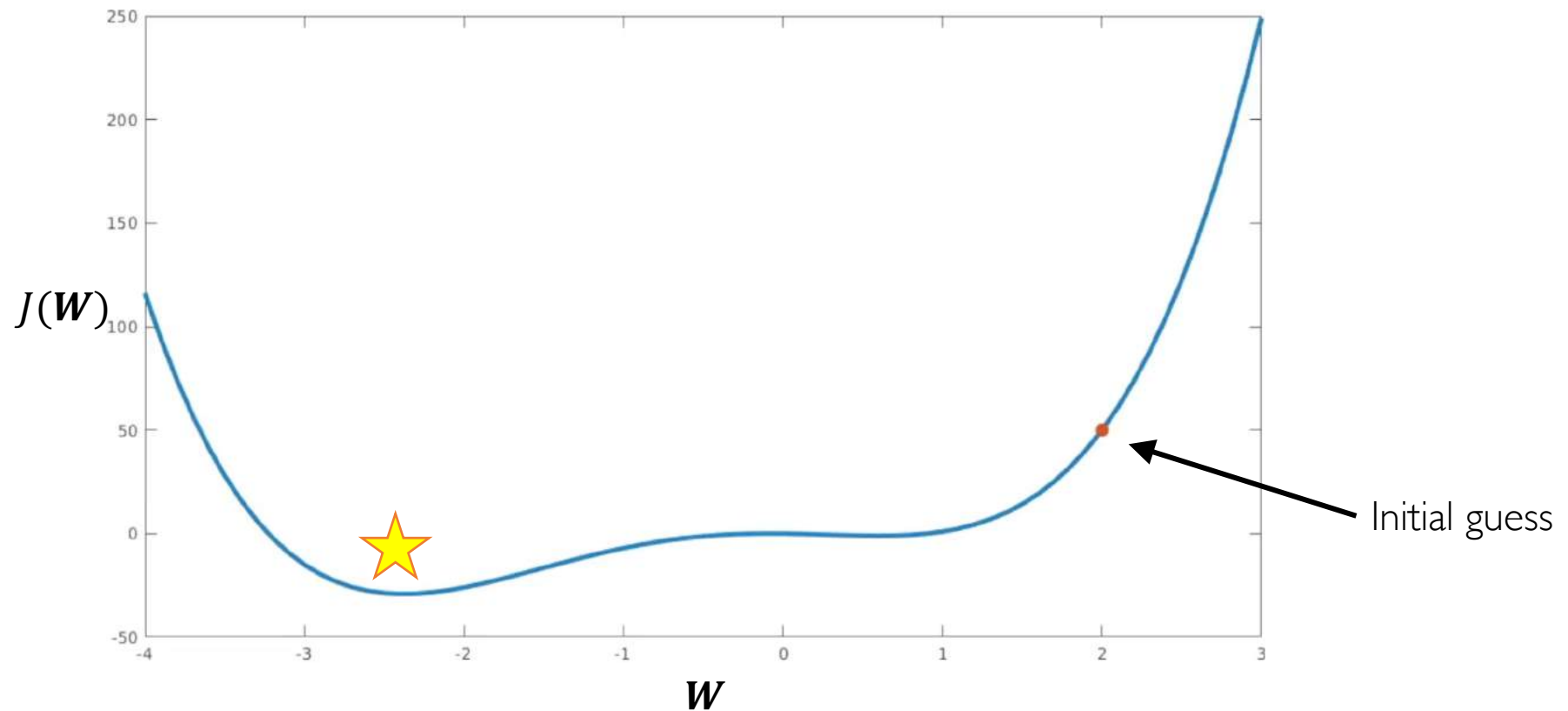
$$\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$$

How can we set the  
learning rate?



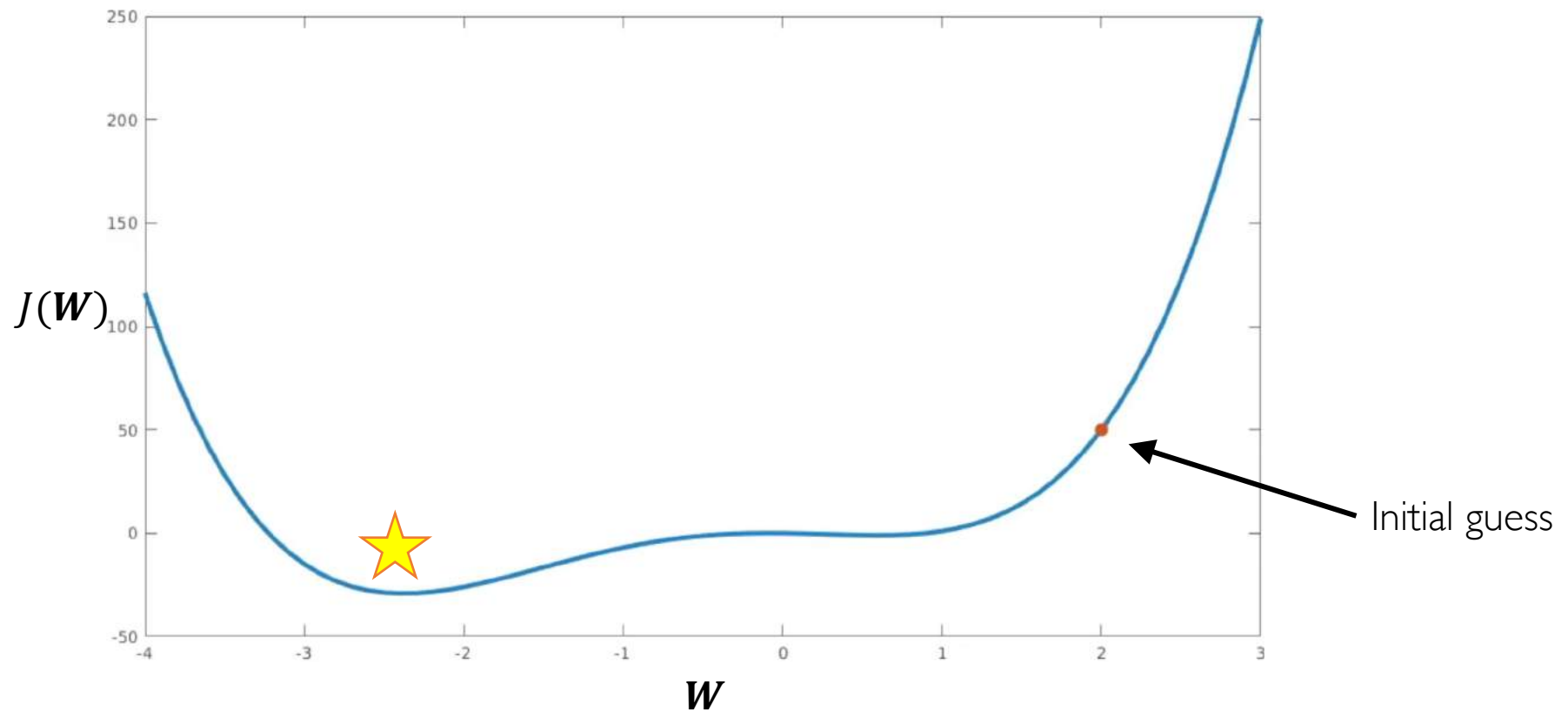
# Setting the Learning Rate

*Small learning rate* converges slowly and gets stuck in false local minima



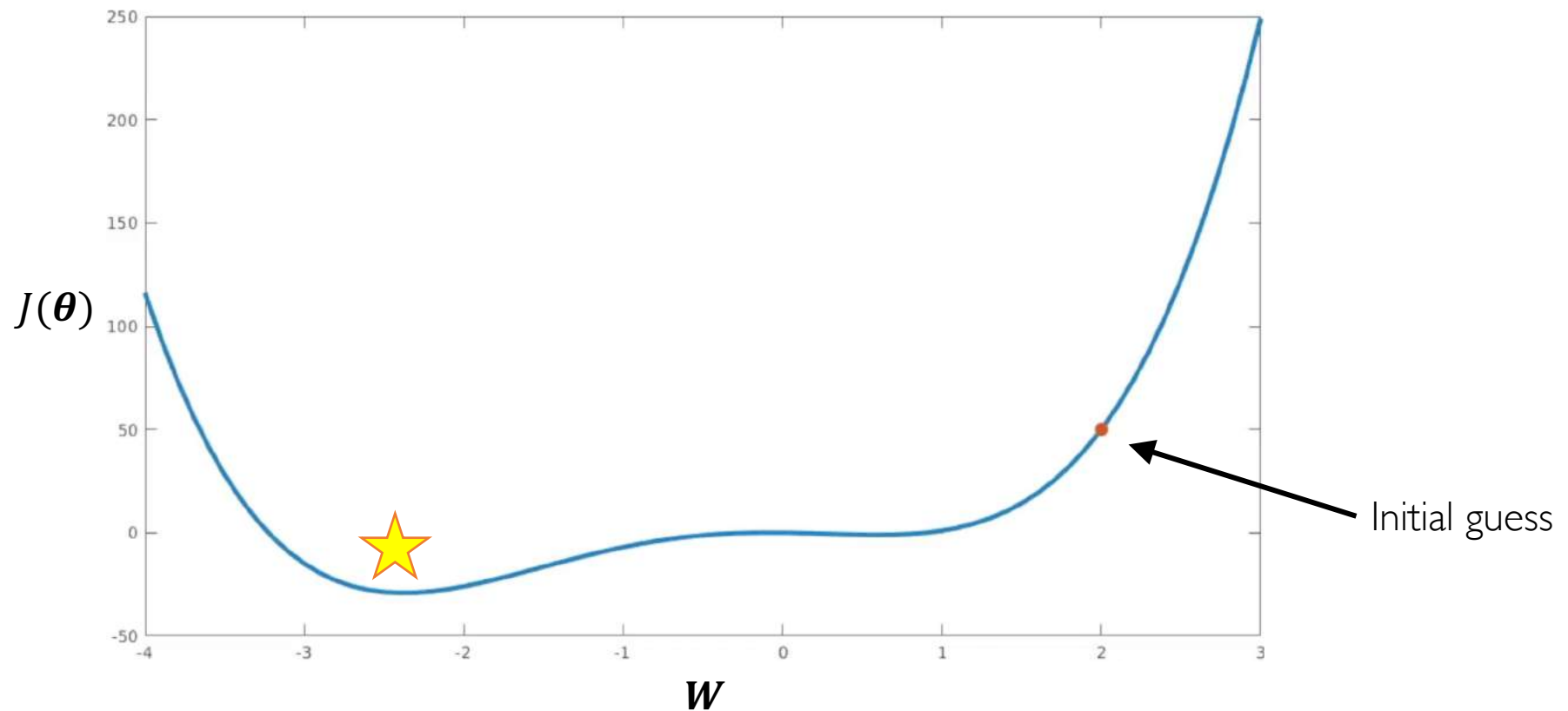
# Setting the Learning Rate

*Large learning rates overshoot, become unstable and diverge*



# Setting the Learning Rate

*Stable learning rates converge smoothly and avoid local minima*



# How to deal with this?

## Idea 1:

Try lots of different learning rates and see what works “just right”

# How to deal with this?

## Idea 1:

Try lots of different learning rates and see what works “just right”

## Idea 2:

Do something smarter!

Design an adaptive learning rate that “adapts” to the landscape

# Adaptive Learning Rates

- Learning rates are no longer fixed
- Can be made larger or smaller depending on:
  - how large gradient is
  - how fast learning is happening
  - size of particular weights
  - etc...

# Adaptive Learning Rate Algorithms

- Momentum



`tf.train.MomentumOptimizer`

Qian et al. "On the momentum term in gradient descent learning algorithms." 1999.

- Adagrad



`tf.train.AdagradOptimizer`

Duchi et al. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." 2011.

- Adadelata



`tf.train.AdadeltaOptimizer`

Zeiler et al. "ADADELTA: An Adaptive Learning Rate Method." 2012.

- Adam



`tf.train.AdamOptimizer`

Kingma et al. "Adam: A Method for Stochastic Optimization." 2014.

- RMSProp



`tf.train.RMSPropOptimizer`

Additional details: <http://runderio/optimizing-gradient-descent/>

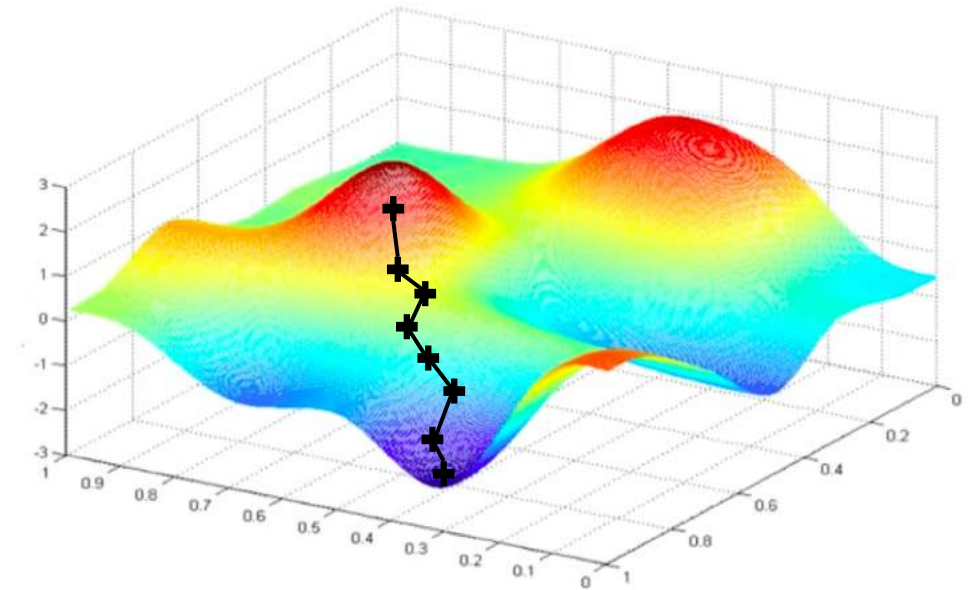
# Neural Networks in Practice: Mini-batches



# Gradient Descent

## Algorithm

1. Initialize weights randomly  $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3.     Compute gradient,  $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$
4.     Update weights,  $\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$
5. Return weights

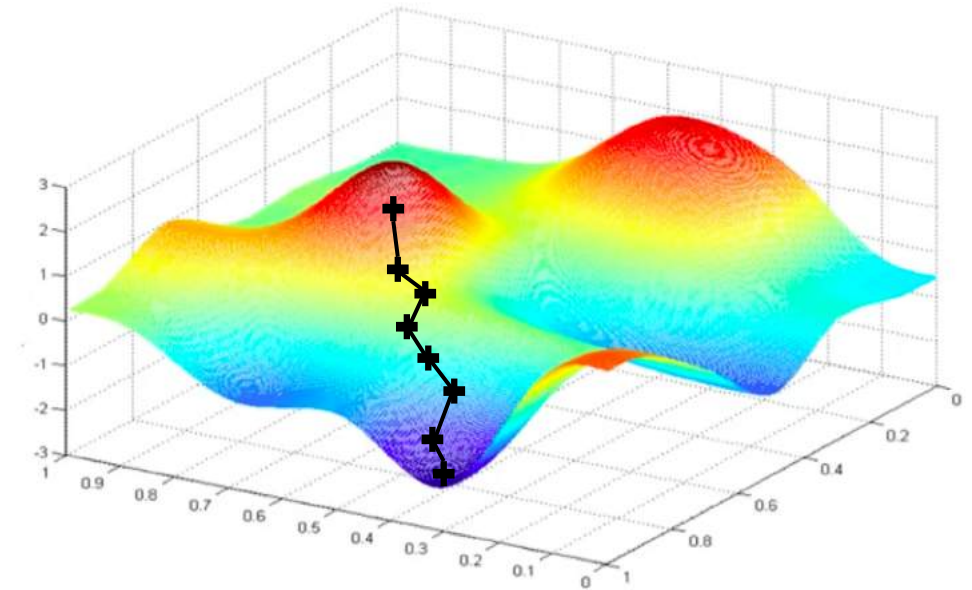


# Gradient Descent

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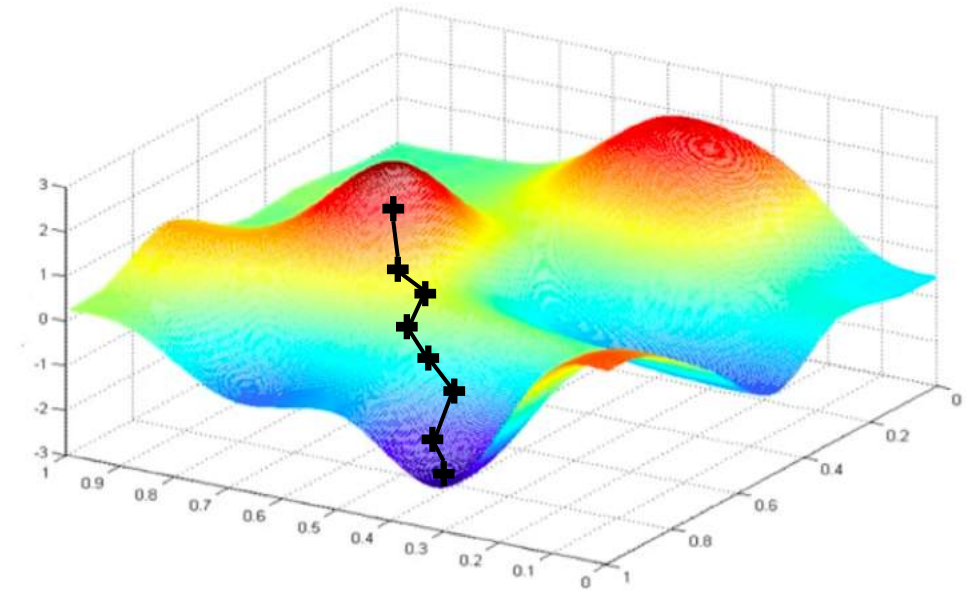
Can be very  
computational to  
compute!



# Stochastic Gradient Descent

## Algorithm

1. Initialize weights randomly  $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3.     Pick single data point  $i$
4.     Compute gradient,  $\frac{\partial J_i(\mathbf{W})}{\partial \mathbf{W}}$
5.     Update weights,  $\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$
6. Return weights

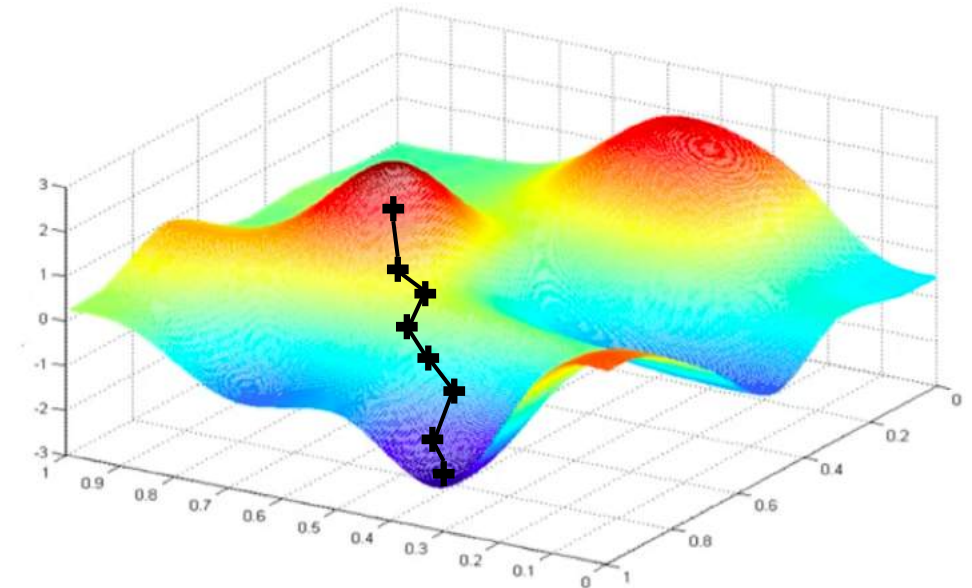


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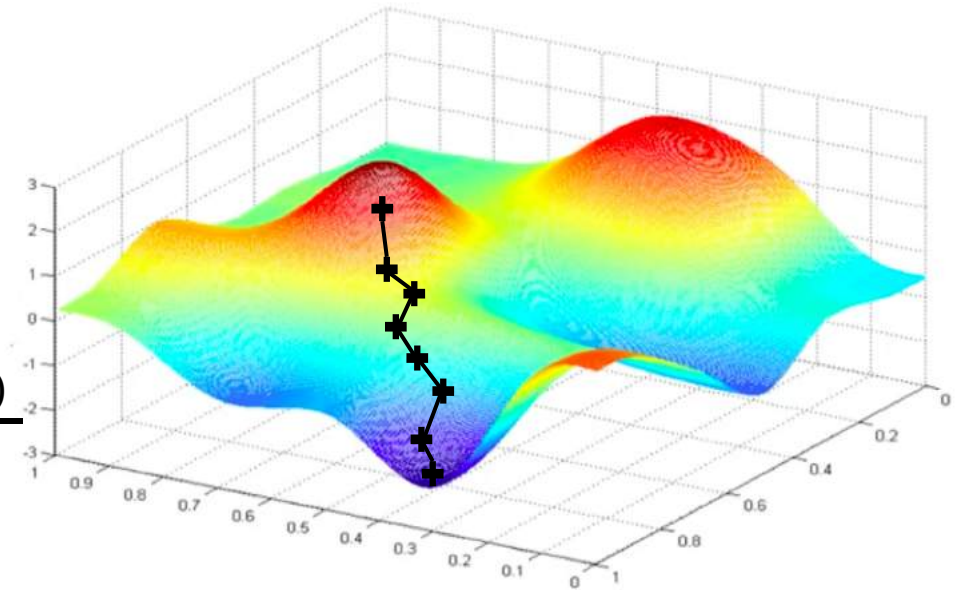
Easy to compute but  
**very noisy**  
(stochastic)!



# Stochastic Gradient Descent

## Algorithm

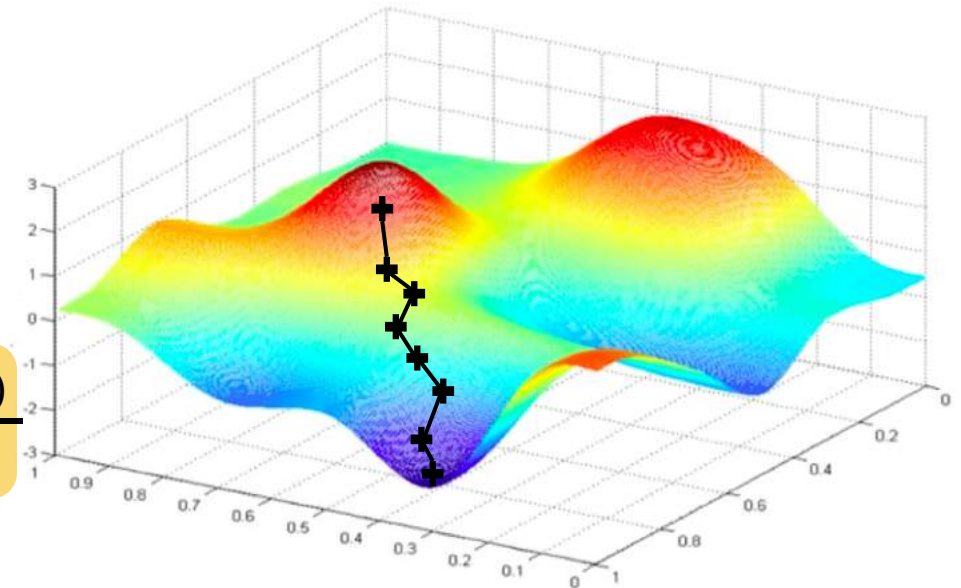
1. Initialize weights randomly  $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3.     Pick batch of  $B$  data points
4.     Compute gradient,  $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}} = \frac{1}{B} \sum_{k=1}^B \frac{\partial J_k(\mathbf{W})}{\partial \mathbf{W}}$
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Fast to compute and a much better  
estimate of the true gradient!

# Mini-batches while training

## More accurate estimation of gradient

Smoother convergence  
Allows for larger learning rates

# Mini-batches while training

More accurate estimation of gradient

Smoother convergence

Allows for larger learning rates

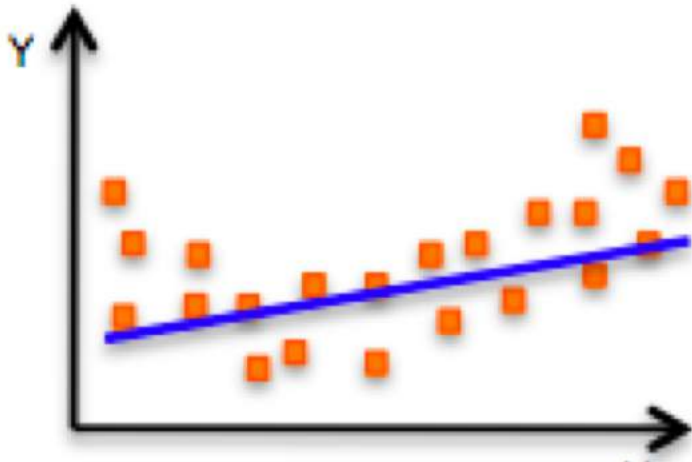
**Mini-batches lead to fast training!**

Can parallelize computation + achieve significant speed increases on GPU's



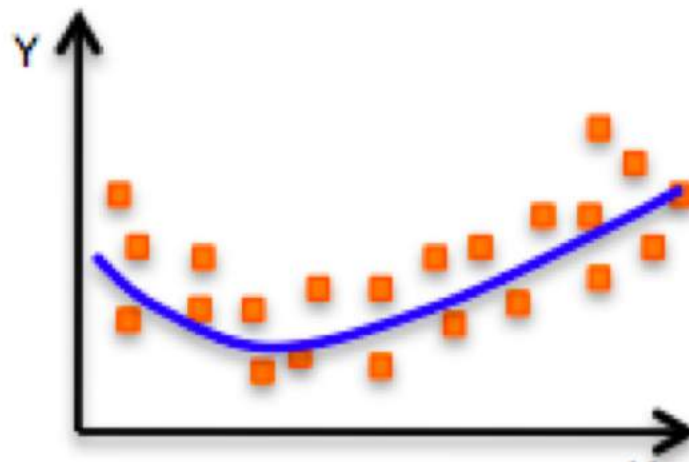
# Neural Networks in Practice: Overfitting

# The Problem of Overfitting

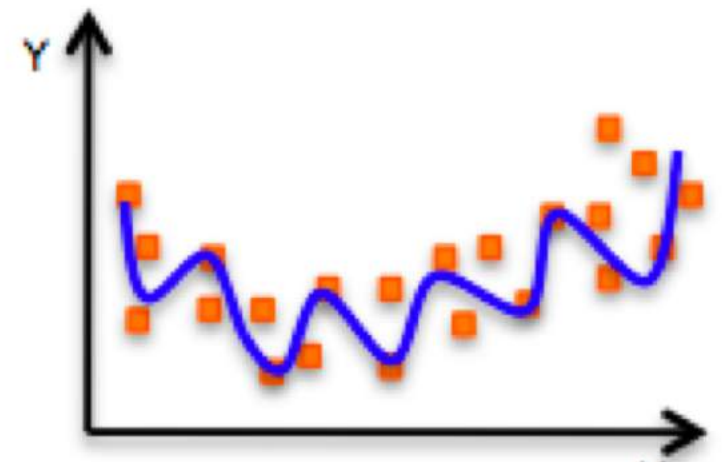


## Underfitting

Model does not have capacity to fully learn the data



## Ideal fit



## Overfitting

Too complex, extra parameters, does not generalize well

# Regularization

## *What is it?*

*Technique that constrains our optimization problem to discourage complex models*

# Regularization

## *What is it?*

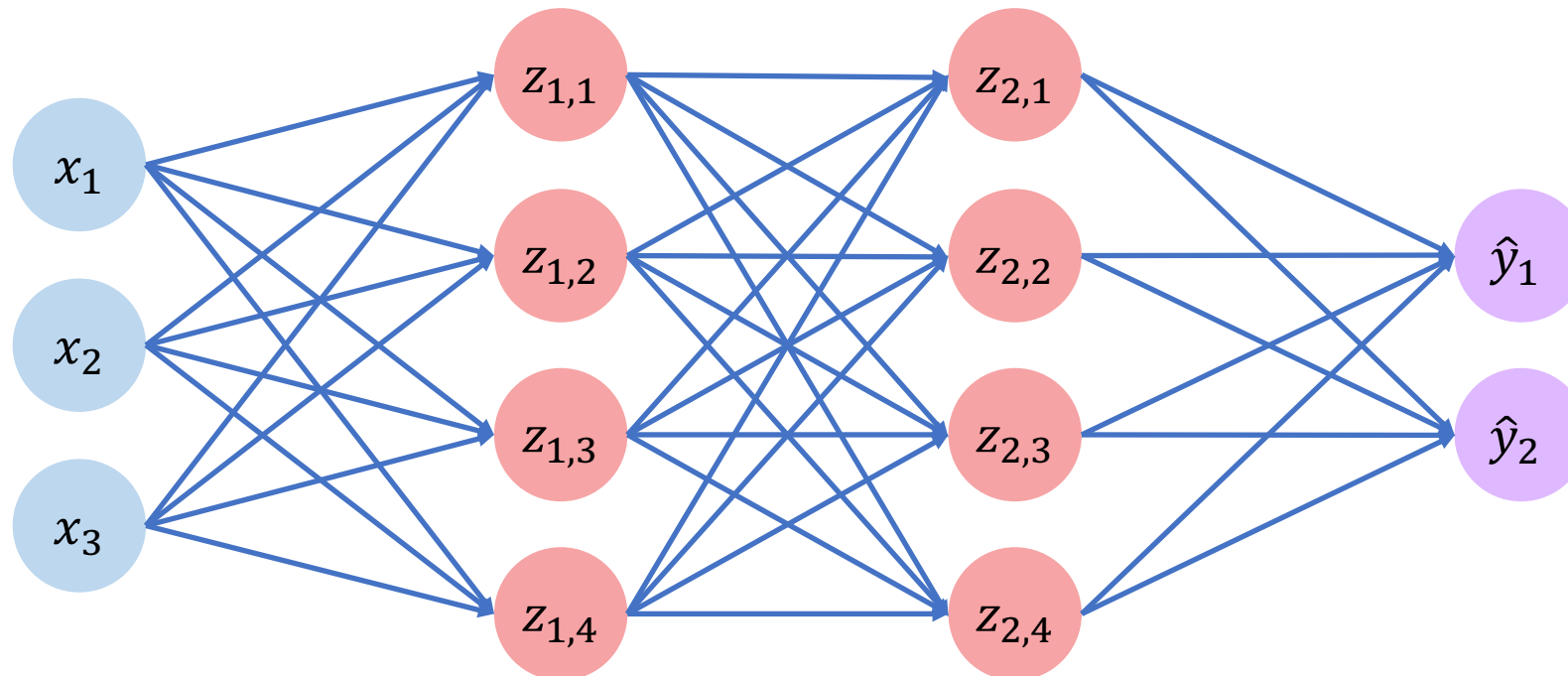
*Technique that constrains our optimization problem to discourage complex models*

## **Why do we need it?**

*Improve generalization of our model on unseen data*

# Regularization I: Dropout

- During training, randomly set some activations to 0

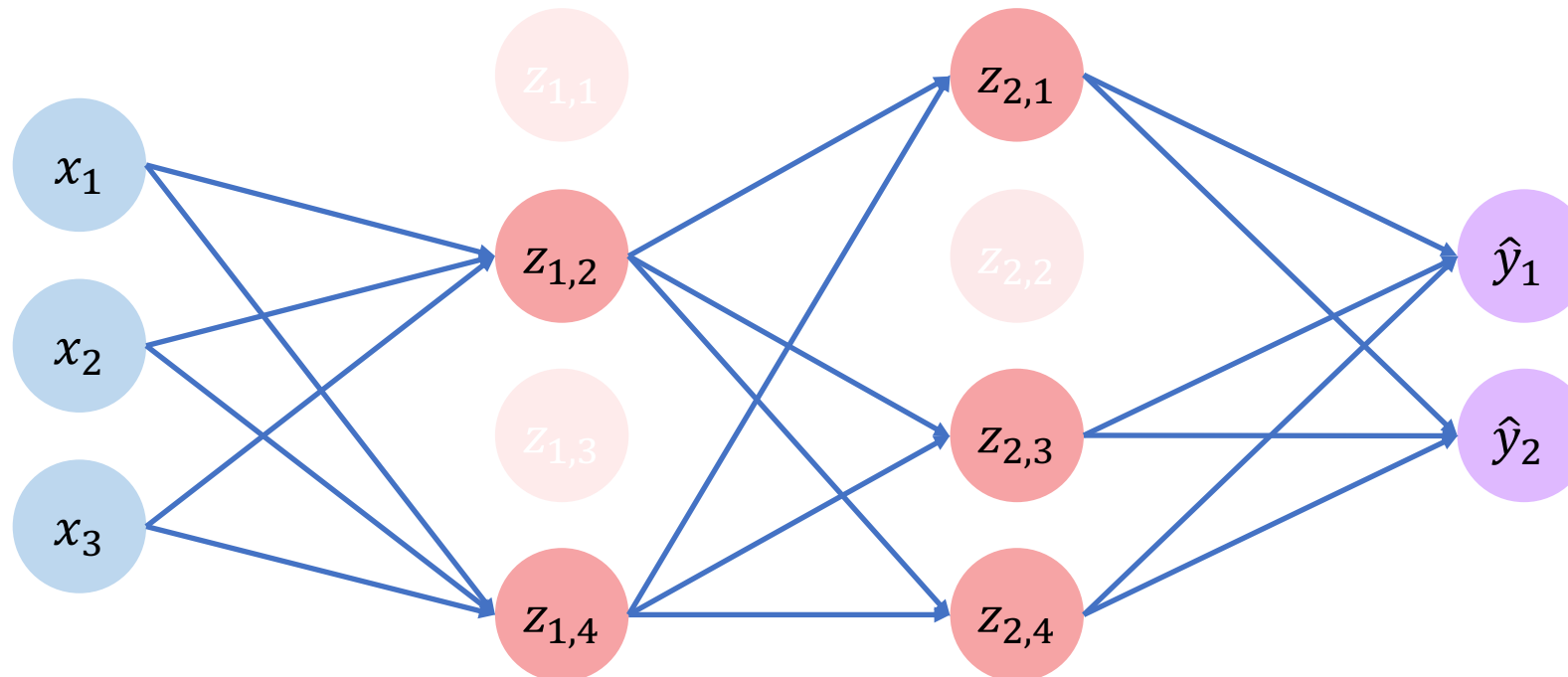


# Regularization I: Dropout

- During training, randomly set some activations to 0
  - Typically 'drop' 50% of activations in layer
  - Forces network to not rely on any 1 node



`tf.keras.layers.Dropout (p=0.5)`

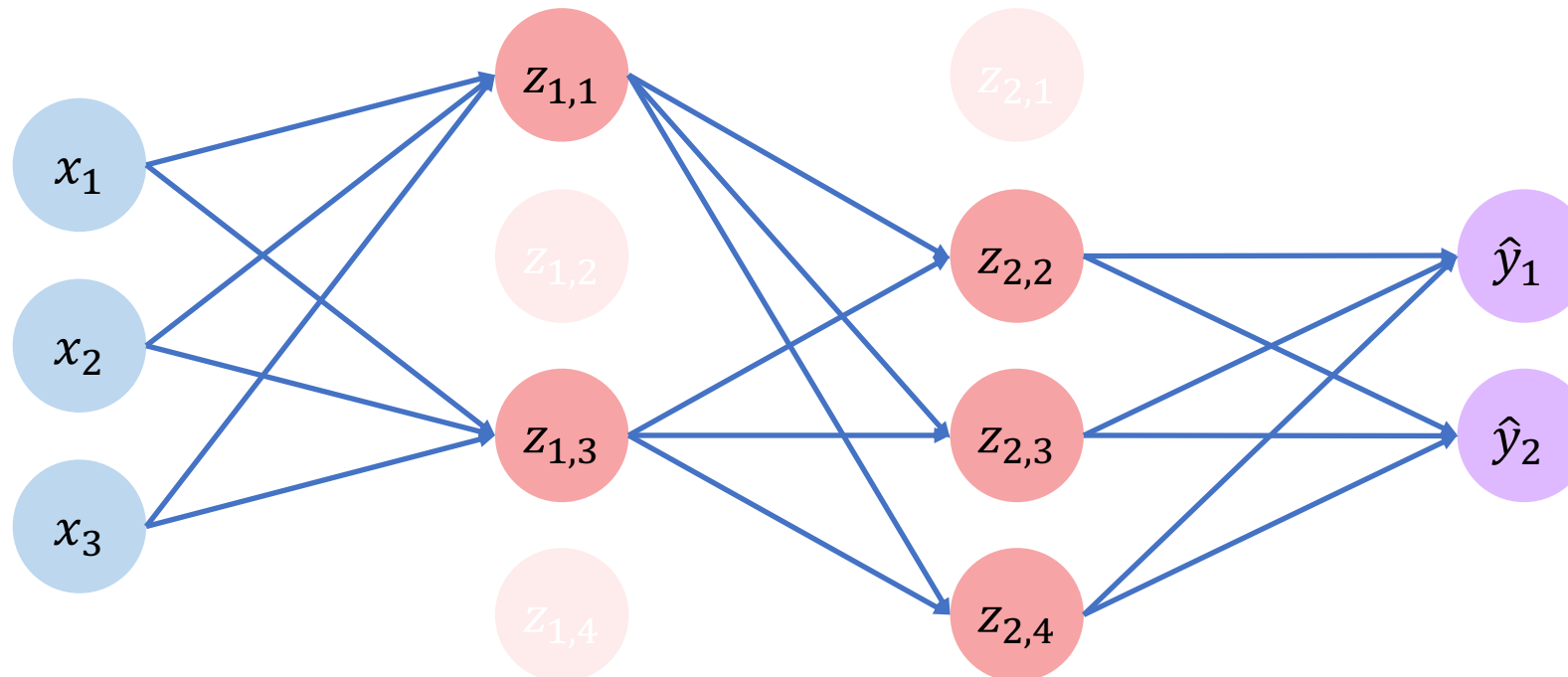


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- Stop training before we have a chance to overfit





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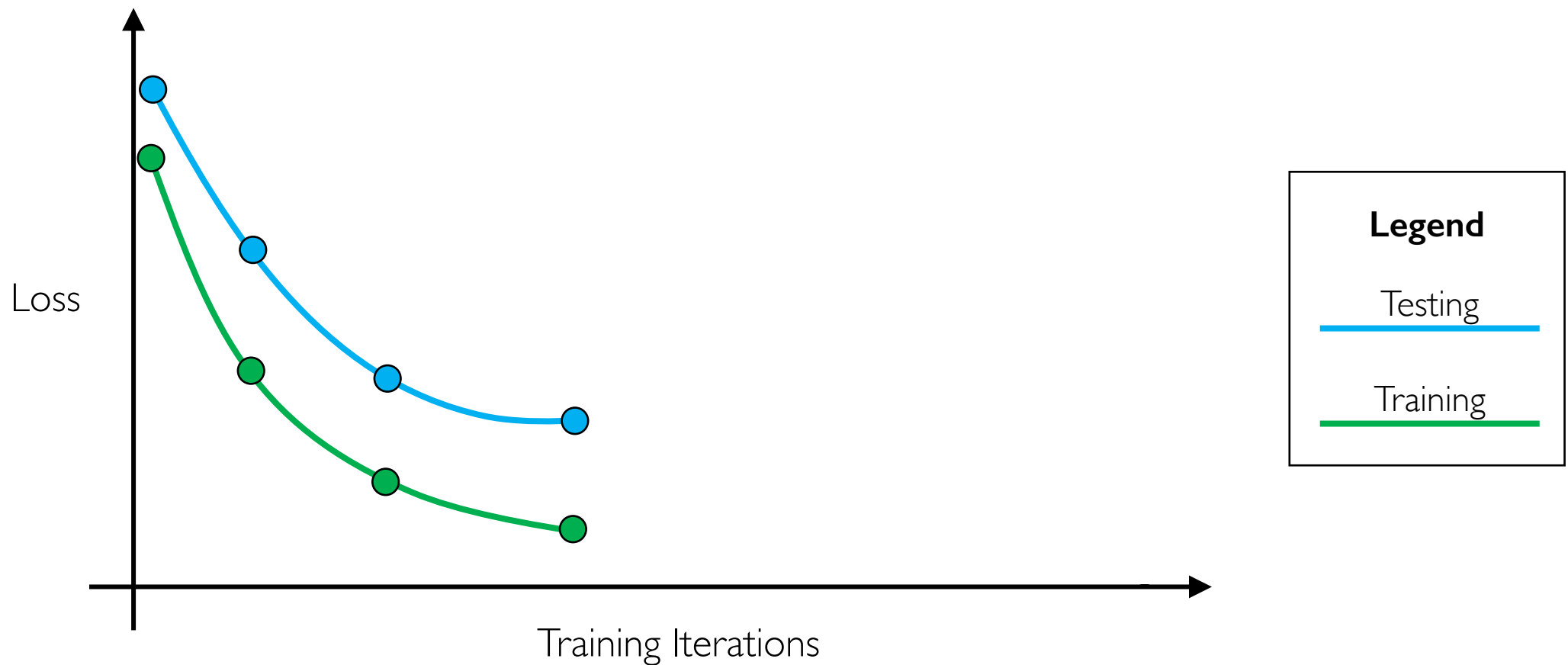
# Regularization 2: Early Stopping

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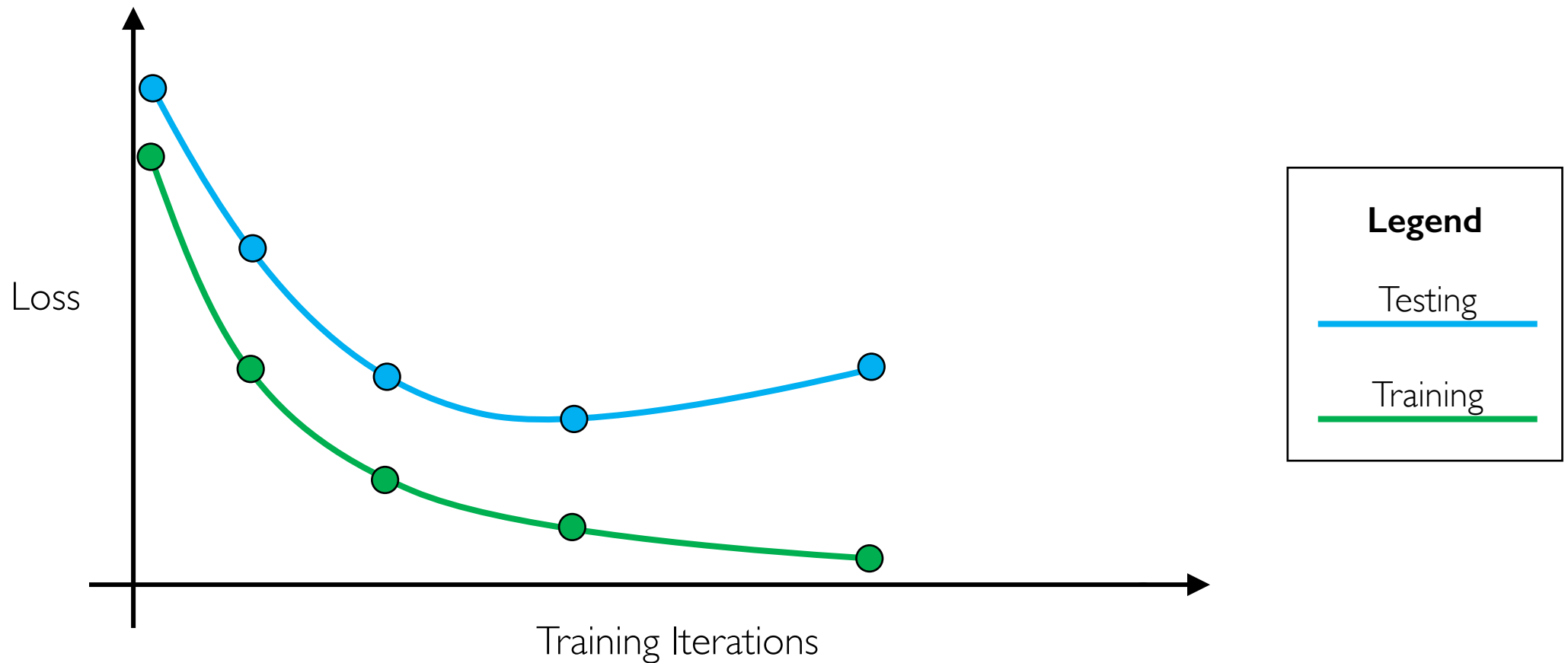
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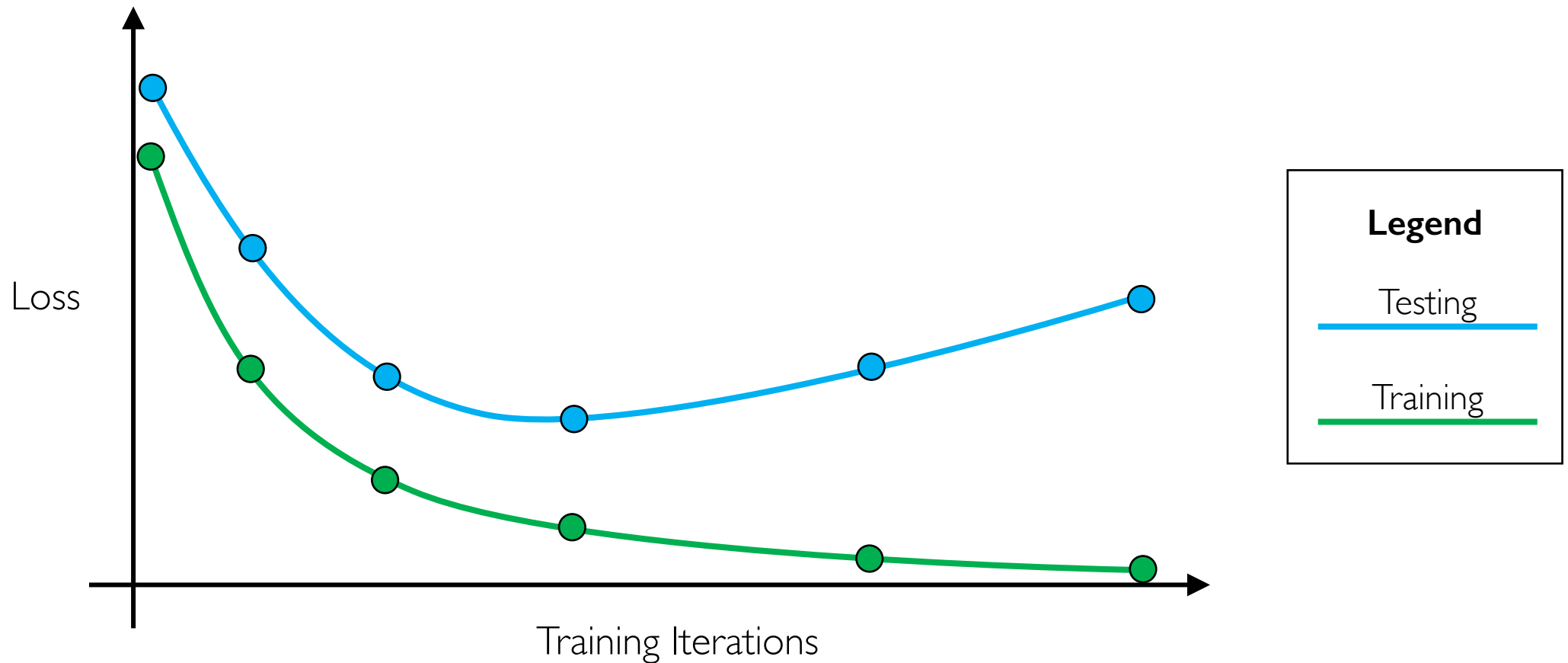
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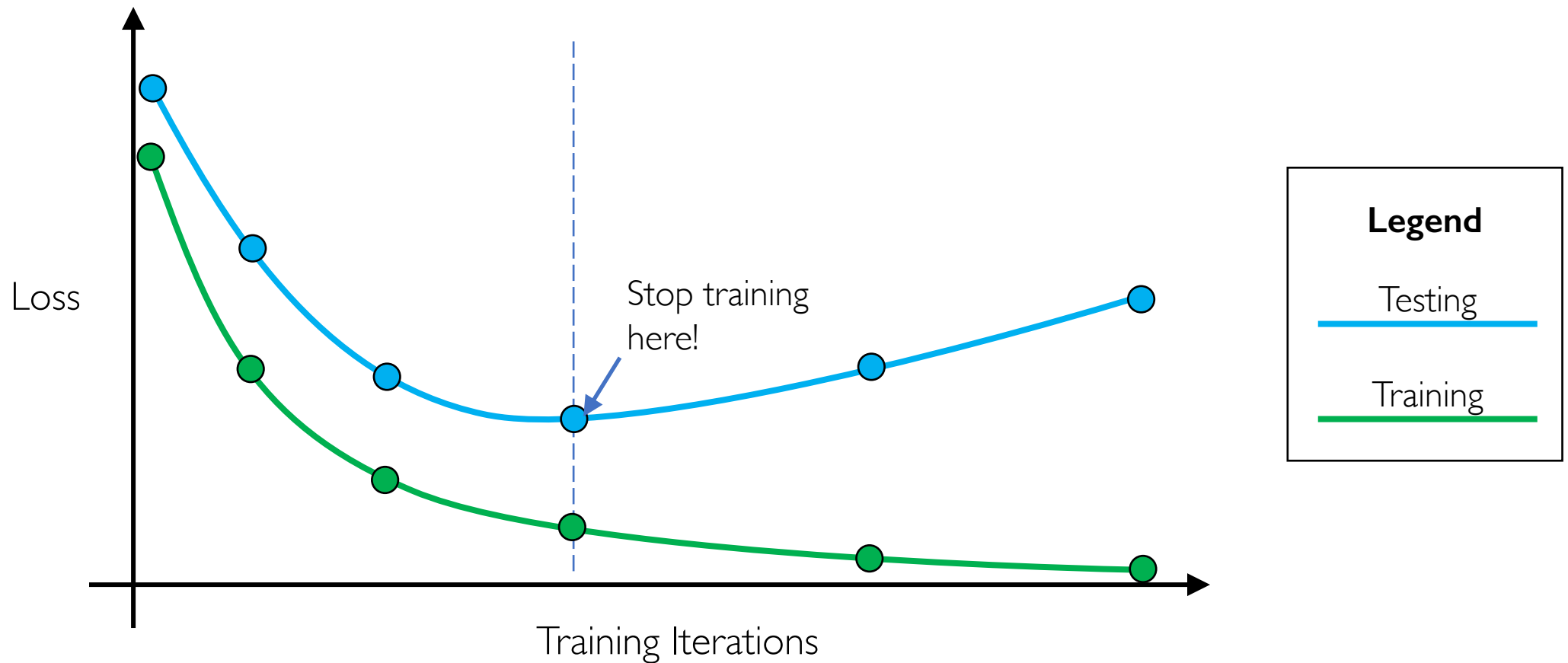
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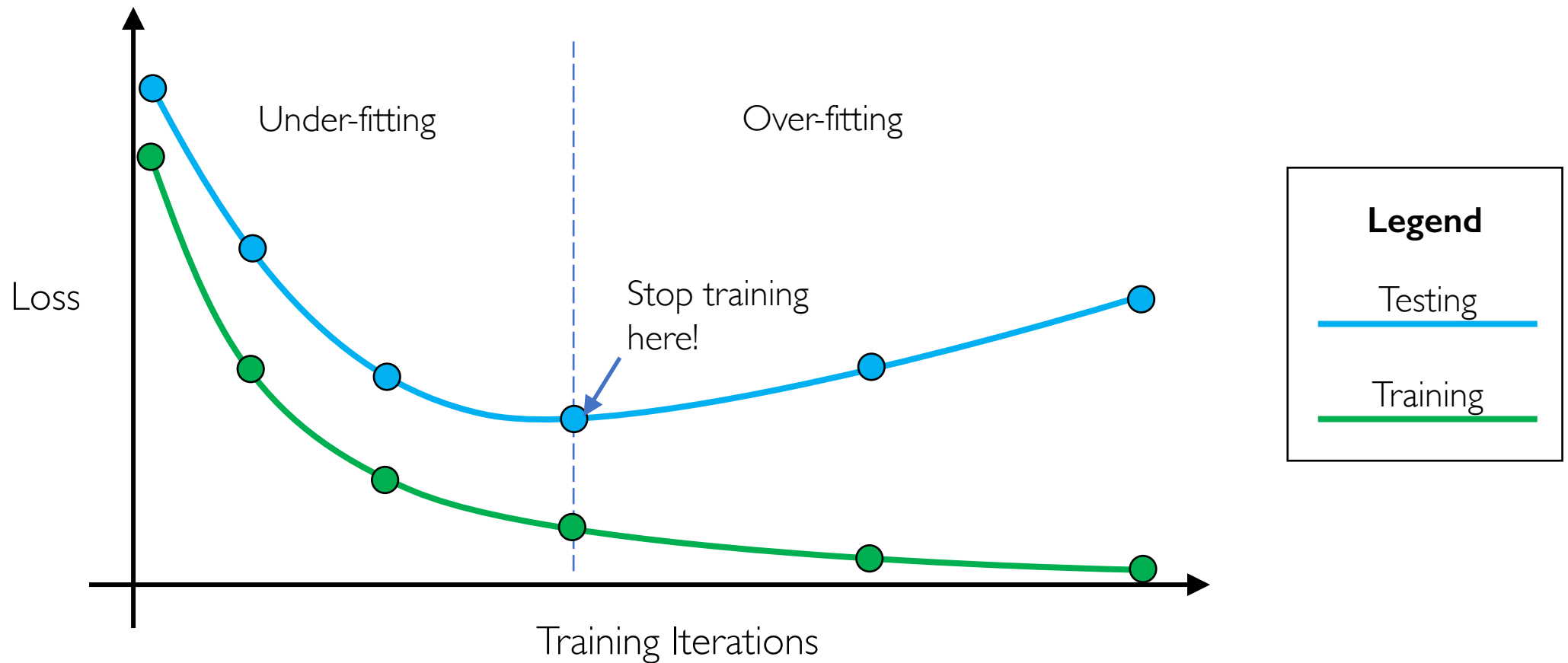
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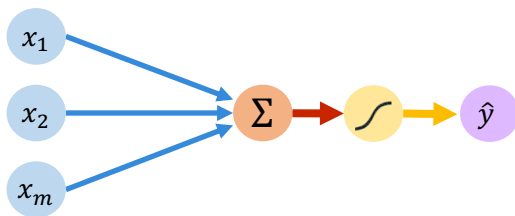
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# Core Foundation Review

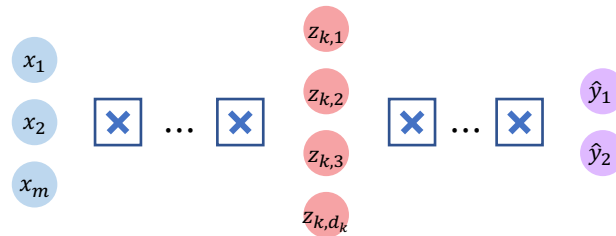
## The Perceptron

- Structural building blocks
- Nonlinear activation functions



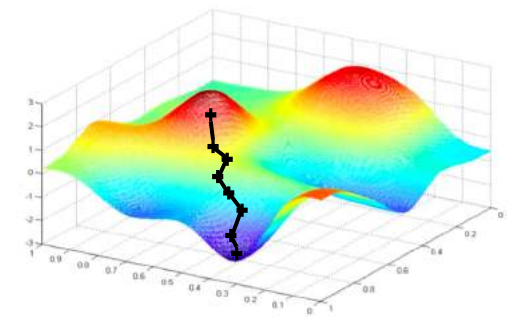
## Neural Networks

- Stacking Perceptrons to form neural networks
- Optimization through backpropagation



## Training in Practice

- Adaptive learning
- Batching
- Regularization





Questions?