Deep Neural Network

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

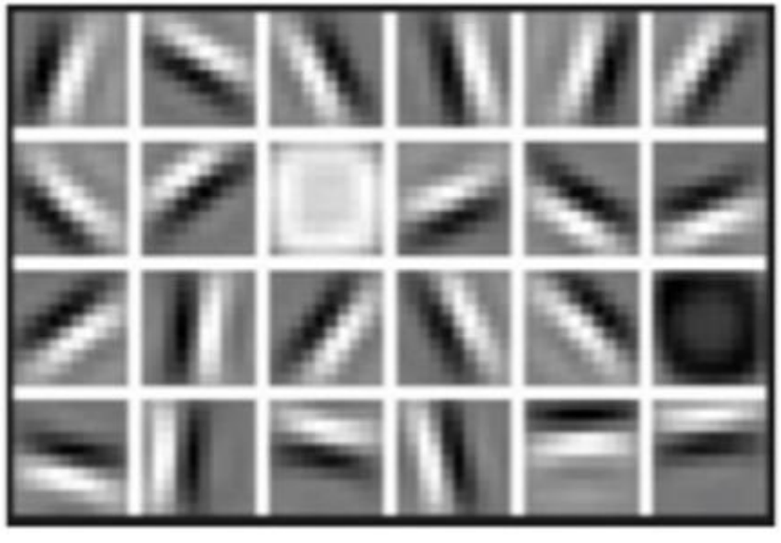
Extract patterns from data using neural networks

Why Deep Learning?

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?

1952 Stochastic Gradient Descent

1958 Perceptron
- Learnable Weights

1986 Backpropagation
- Multi-Layer Perceptron

1995 Deep Convolutional NN
- Digit Recognition

1. Big Data

- Larger Datasets
- Easier Collection & Storage

IMAGENET

WIKIPEDIA
The Free Encyclopedia

2. Hardware

- Graphics Processing Units (GPUs)
- Massively Parallelizable

3. Software

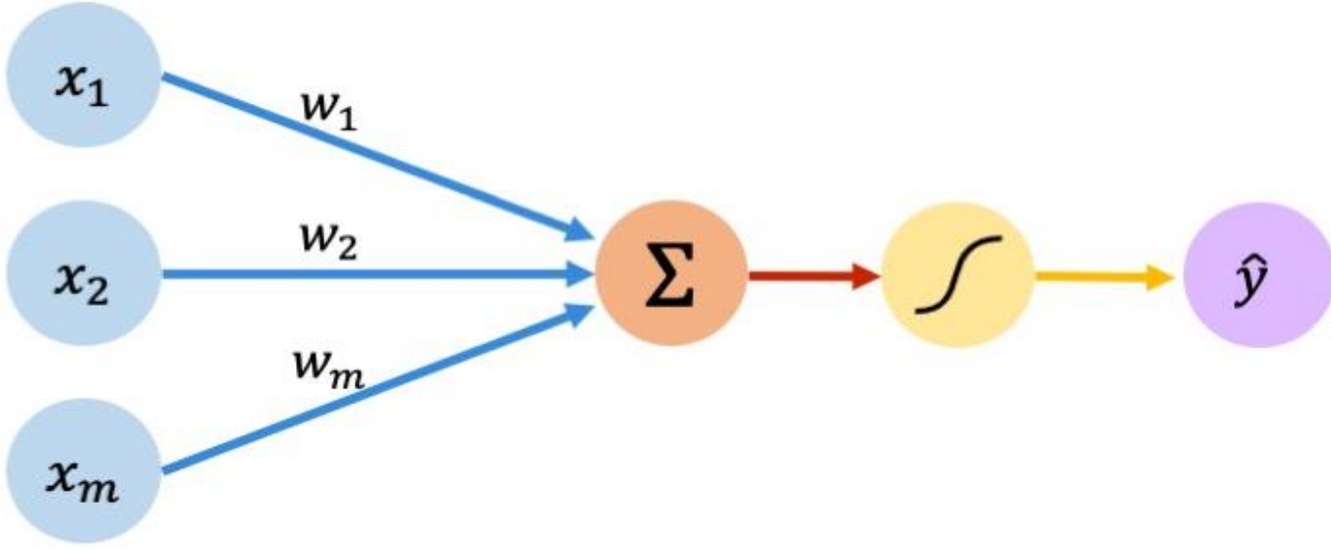
- Improved Techniques
- New Models
- Toolboxes

TensorFlow

The Perceptron

The structural building block of deep learning

The Perceptron: Forward Propagation



Inputs Weights Sum Non-Linearity Output

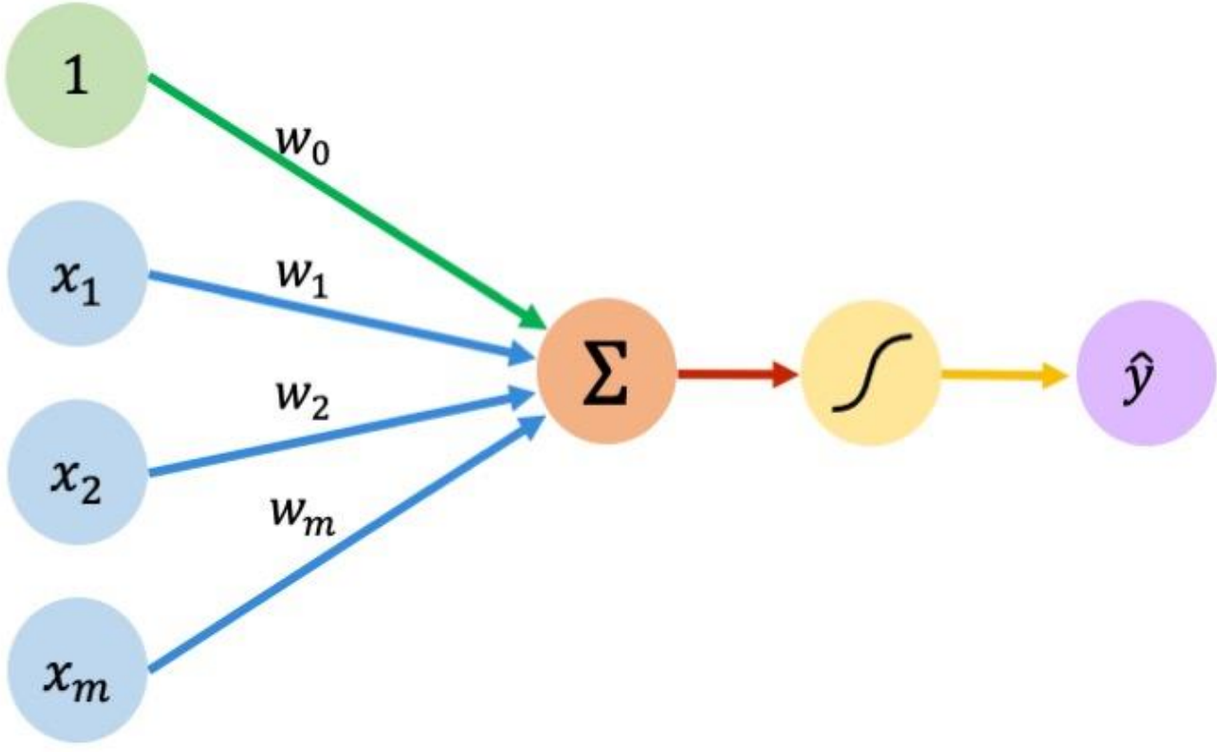
Output

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



Inputs Weights Sum Non-Linearity Output

Output

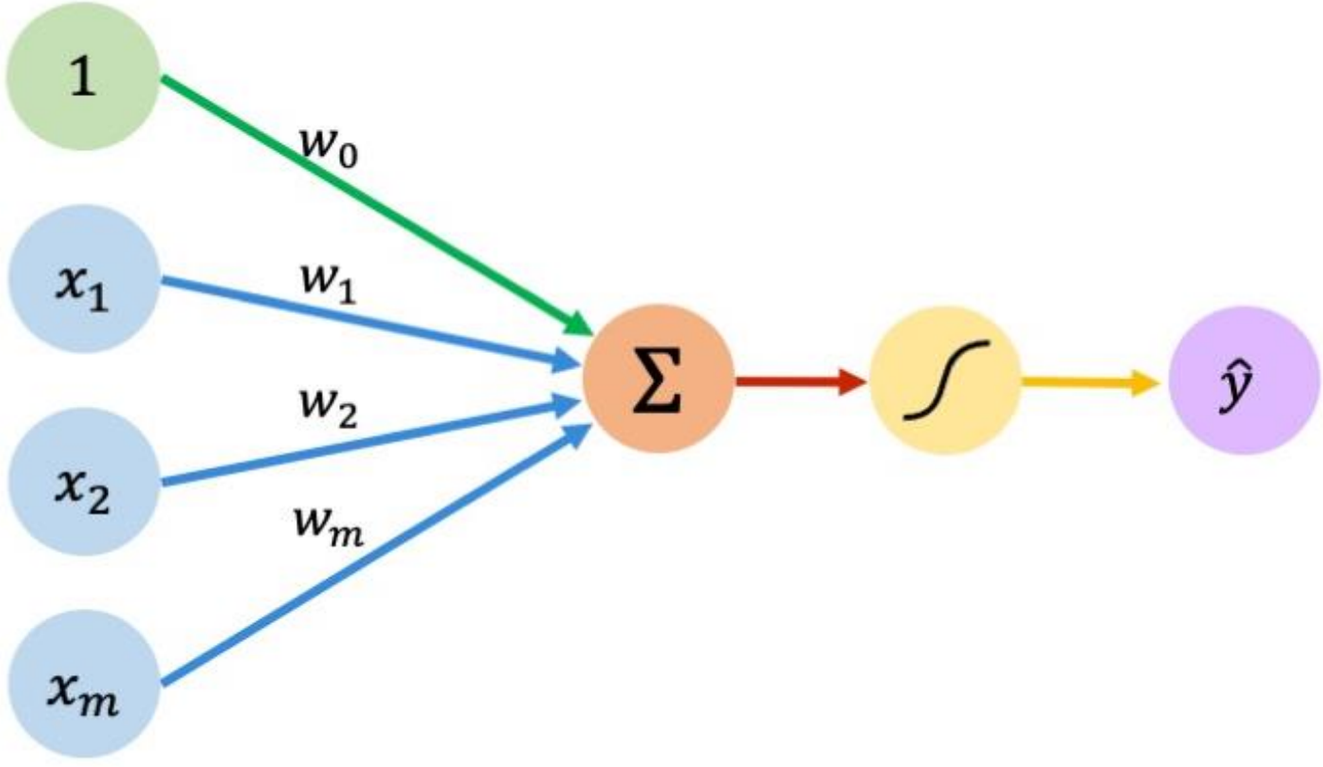
Linear combination of inputs

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

Non-linear activation function

Bias

The Perceptron: Forward Propagation



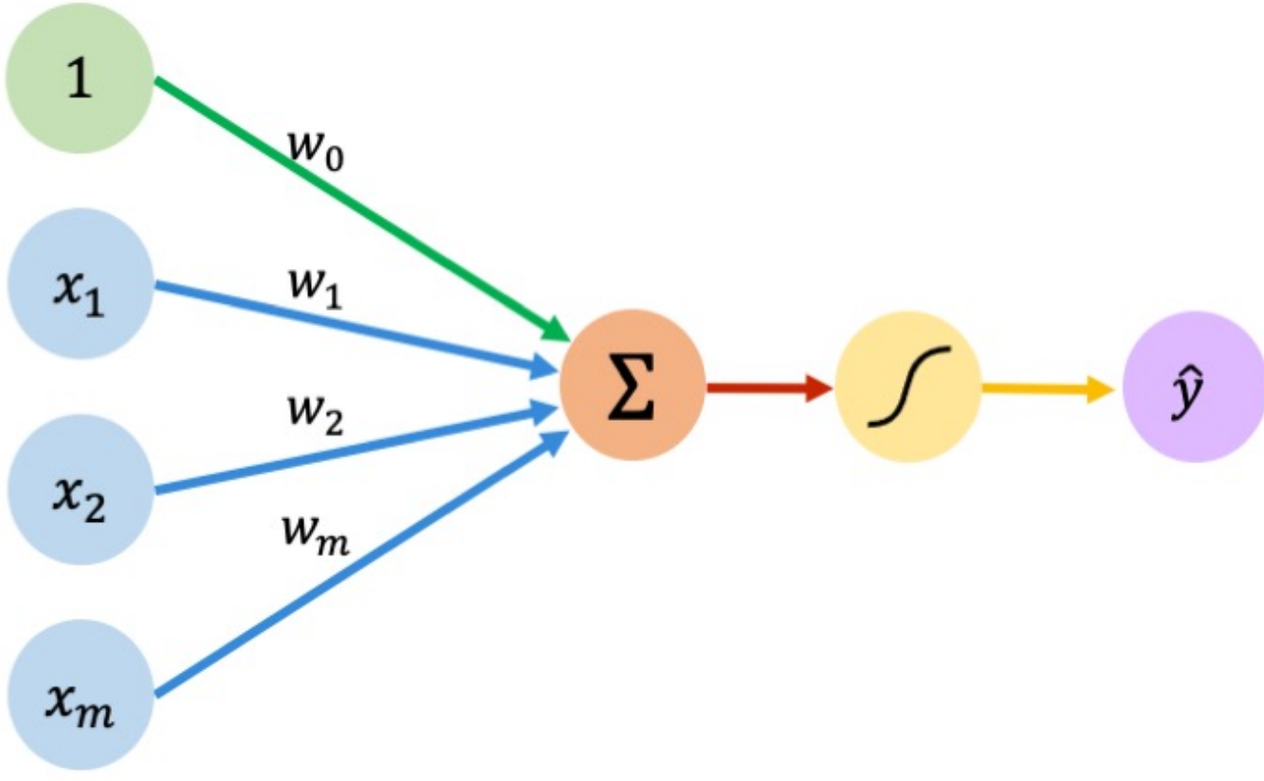
Inputs Weights Sum Non-Linearity Output

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

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

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

The Perceptron: Forward Propagation



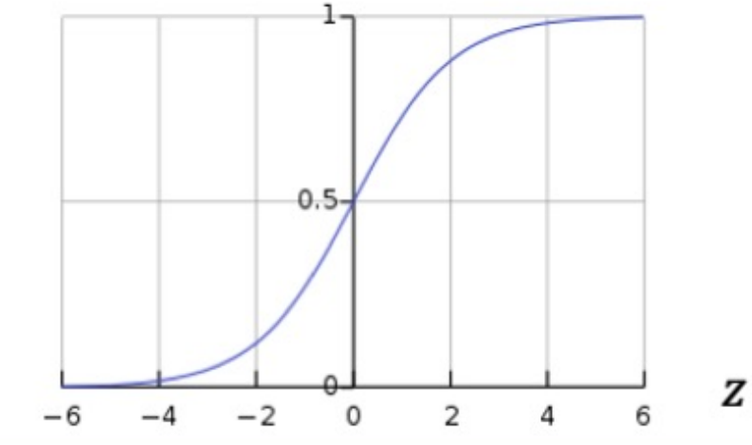
Inputs Weights Sum Non-Linearity Output

Activation Functions

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

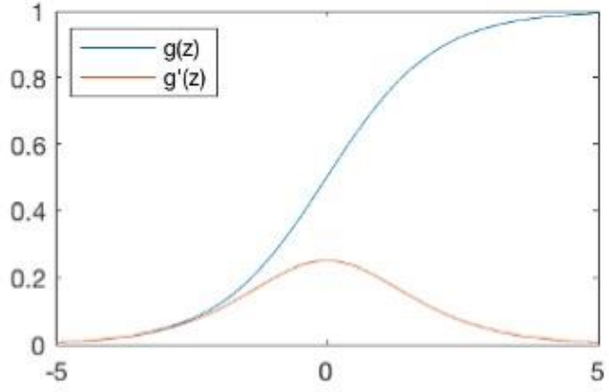
- Example: sigmoid function

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



Common Activation Functions

Sigmoid Function

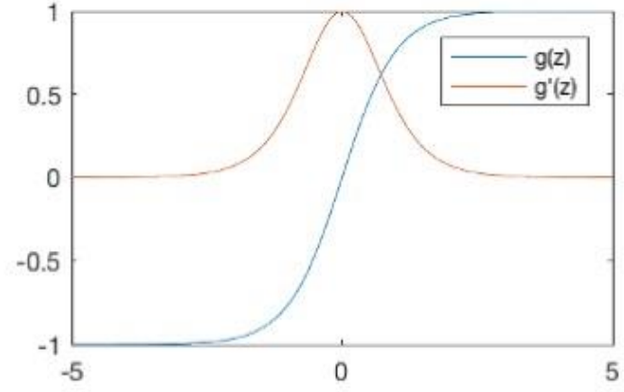


$$g(z) = \frac{1}{1 + e^{-z}}$$

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

`tf.math.sigmoid(z)`

Hyperbolic Tangent

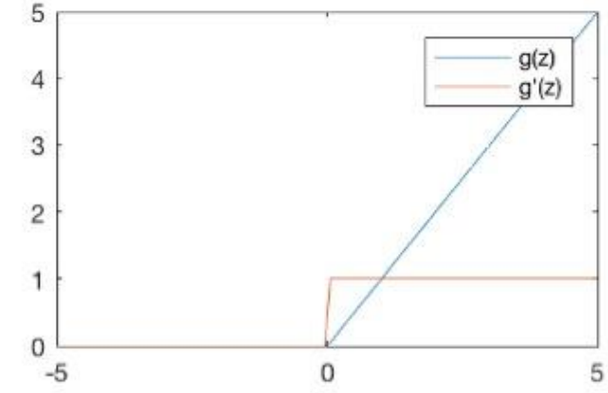


$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

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

`tf.math.tanh(z)`

Rectified Linear Unit (ReLU)



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

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

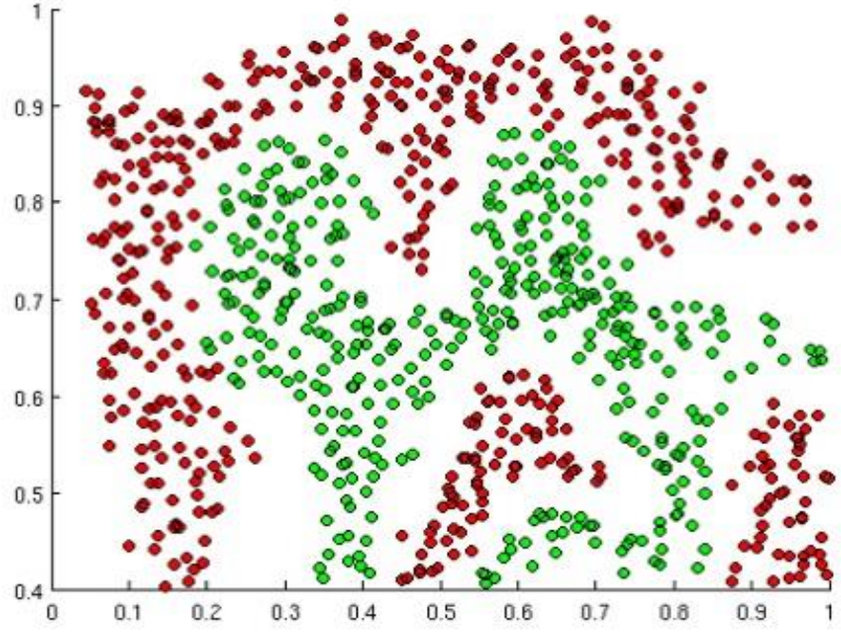
`tf.nn.relu(z)`

TensorFlow code blocks

NOTE: All activation functions are non-linear

Importance of Activation Functions

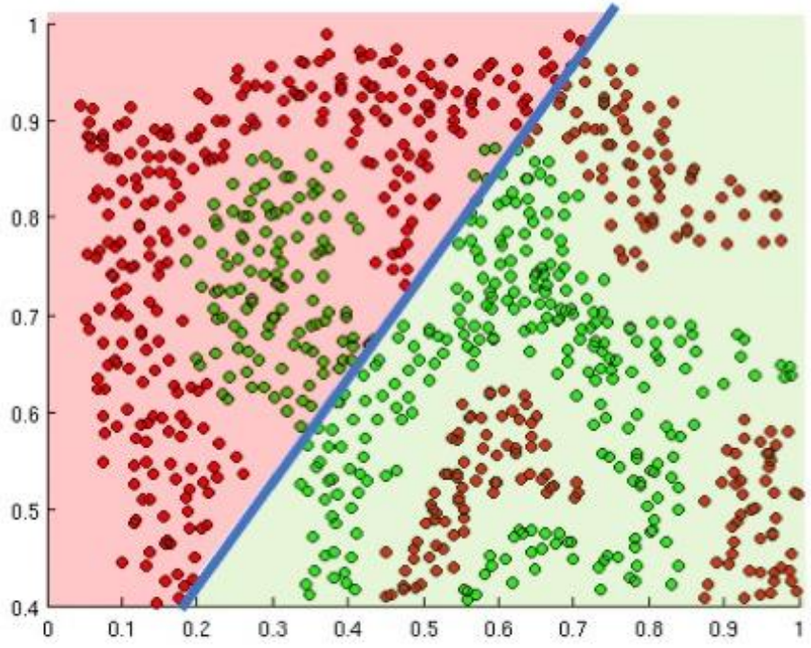
*The purpose of activation functions is to **introduce non-linearities** into the network*



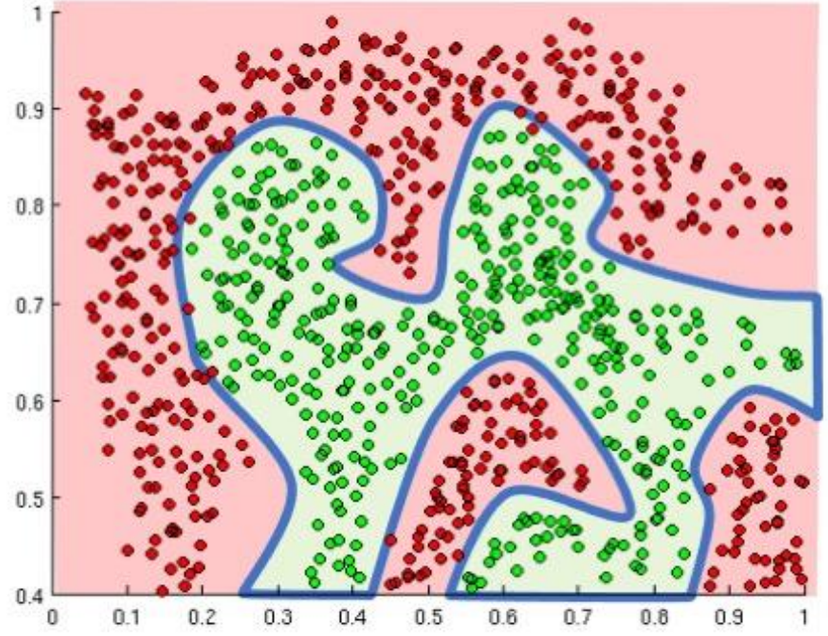
What if we wanted to build a neural network to distinguish green vs red points?

Importance of Activation Functions

*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

Applying Neural Networks

Example Problem

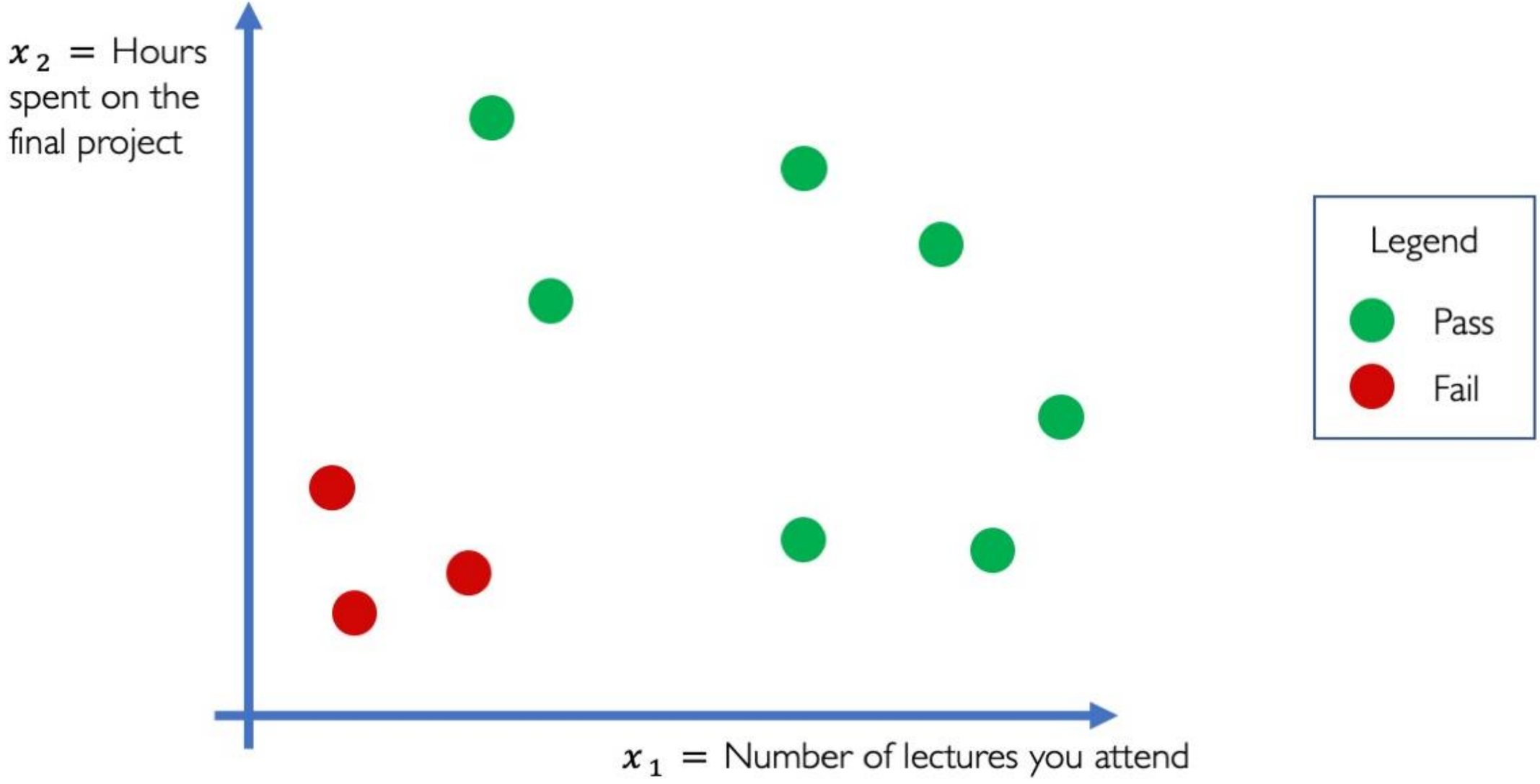
Will I pass this class?

Let's start with a simple two feature model

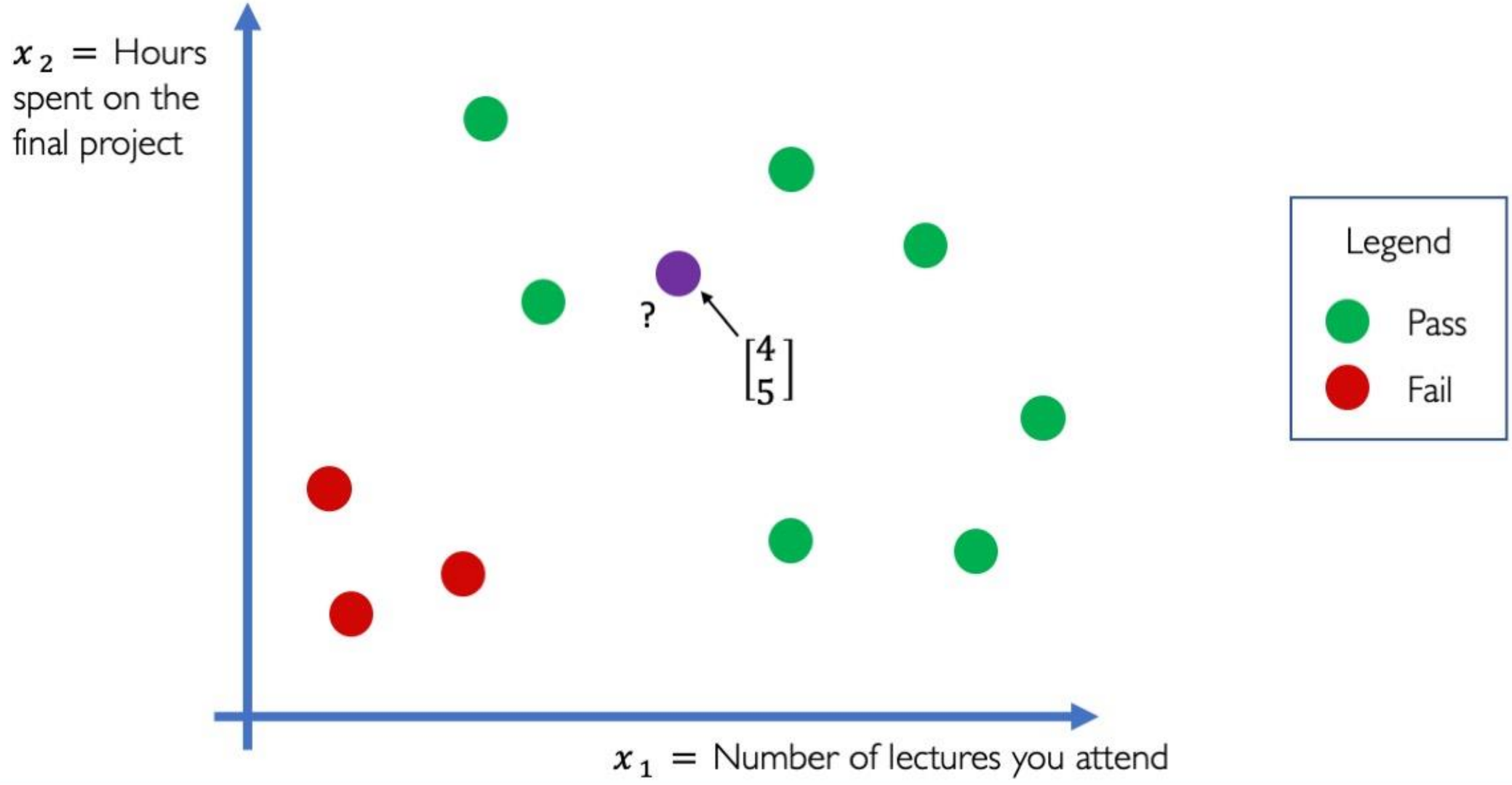
x_1 = Number of lectures you attend

x_2 = Hours spent on the final project

Example Problem: Will I pass this class?



Example Problem: Will I pass this class?



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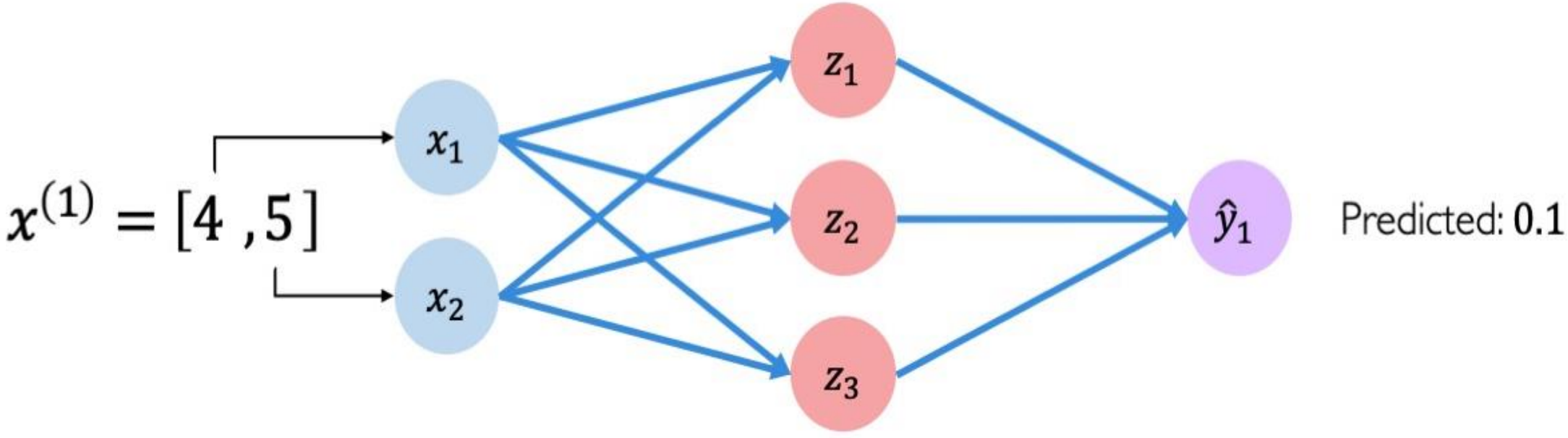
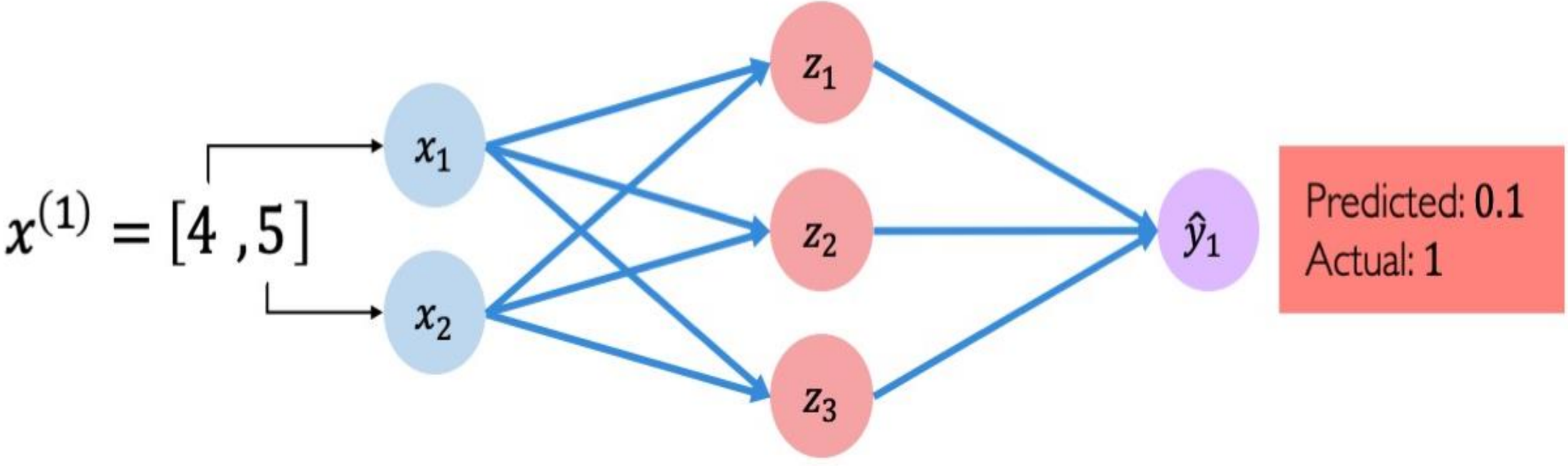
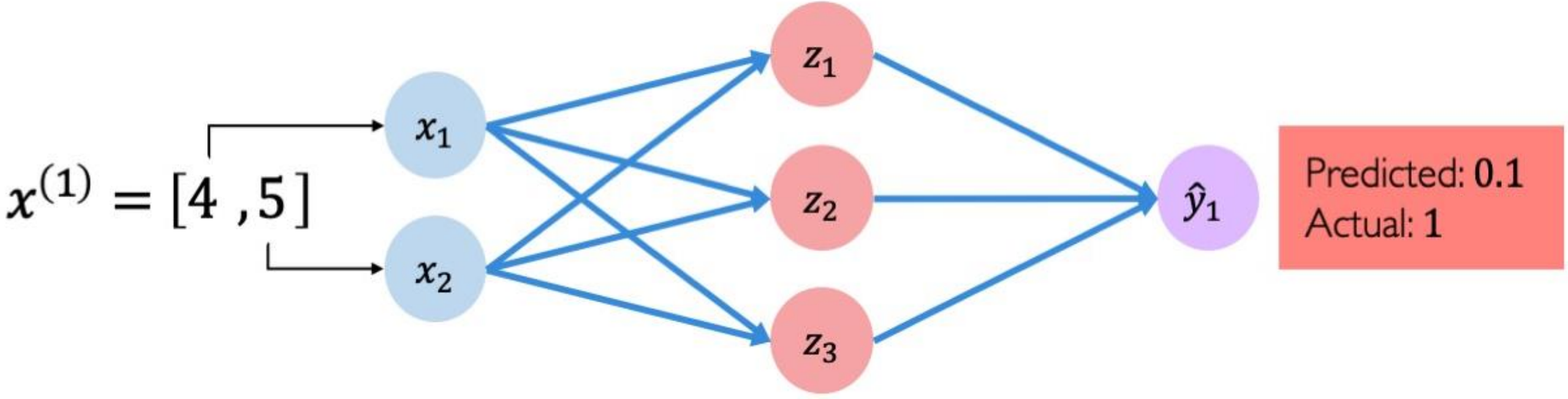


Example Problem: Will I pass this class?



Quantifying Loss

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



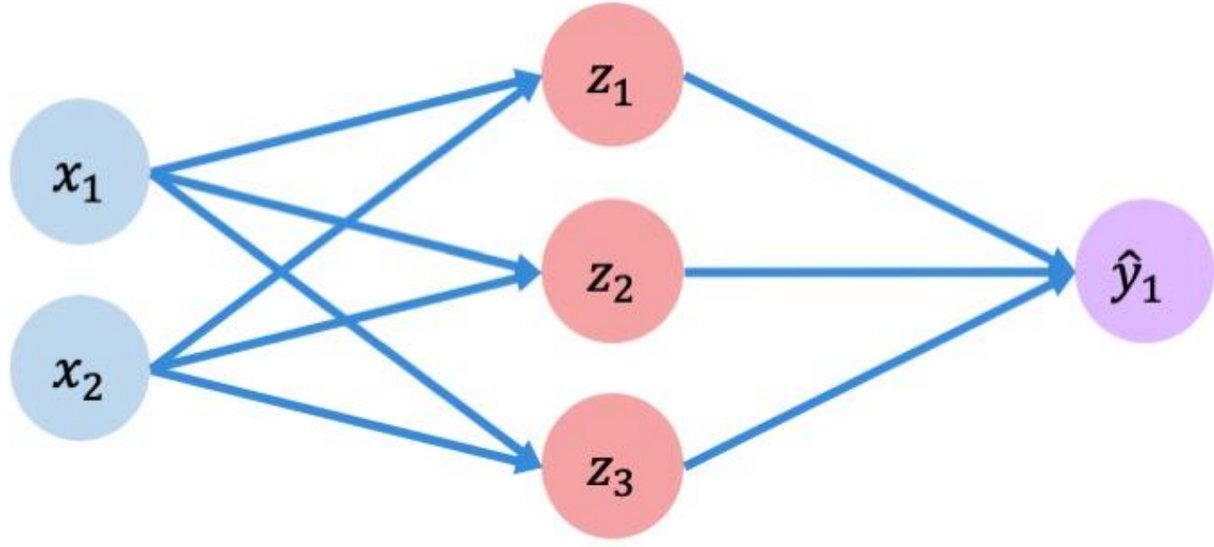
$$\mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

Predicted Actual

Empirical Loss

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

$$\boldsymbol{X} = \begin{bmatrix} 4, & 5 \\ 2, & 1 \\ 5, & 8 \\ \vdots & \vdots \end{bmatrix}$$



$f(x)$ y

$$\begin{bmatrix} 0.1 \\ 0.8 \\ 0.6 \\ \vdots \end{bmatrix} \begin{matrix} \times \\ \times \\ \checkmark \\ \end{matrix} \begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}$$

Also known as:
- Objective function
- Cost function
- Empirical Risk

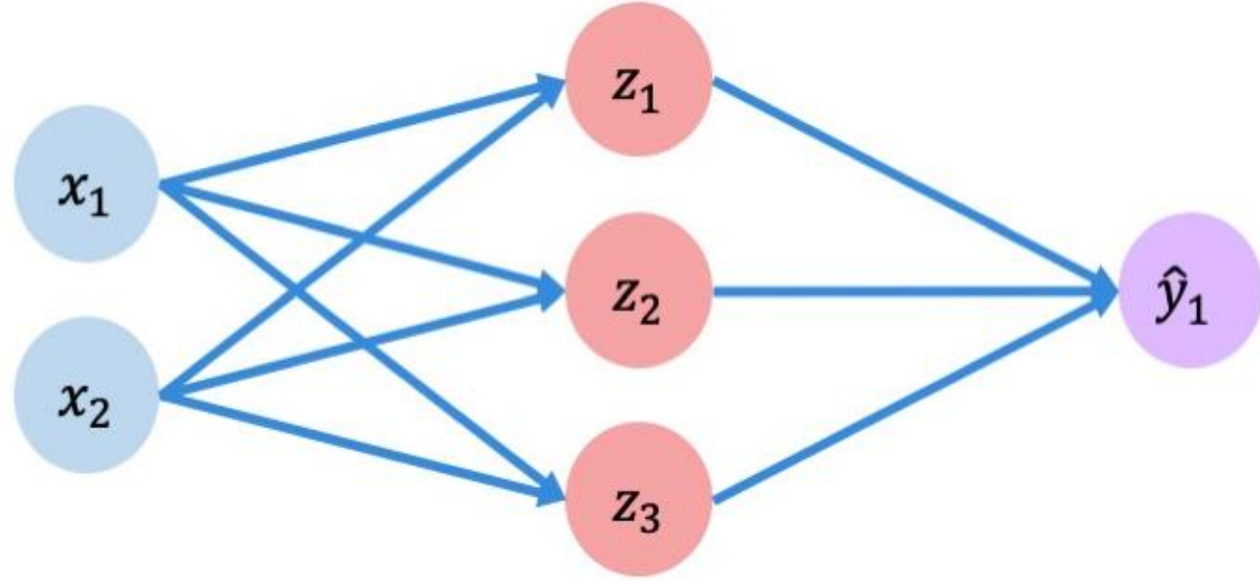
$$\boldsymbol{J(W)} = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

Predicted Actual

Binary Cross Entropy Loss

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

$$\boldsymbol{X} = \begin{bmatrix} 4, & 5 \\ 2, & 1 \\ 5, & 8 \\ \vdots & \vdots \end{bmatrix}$$



$f(x)$ y

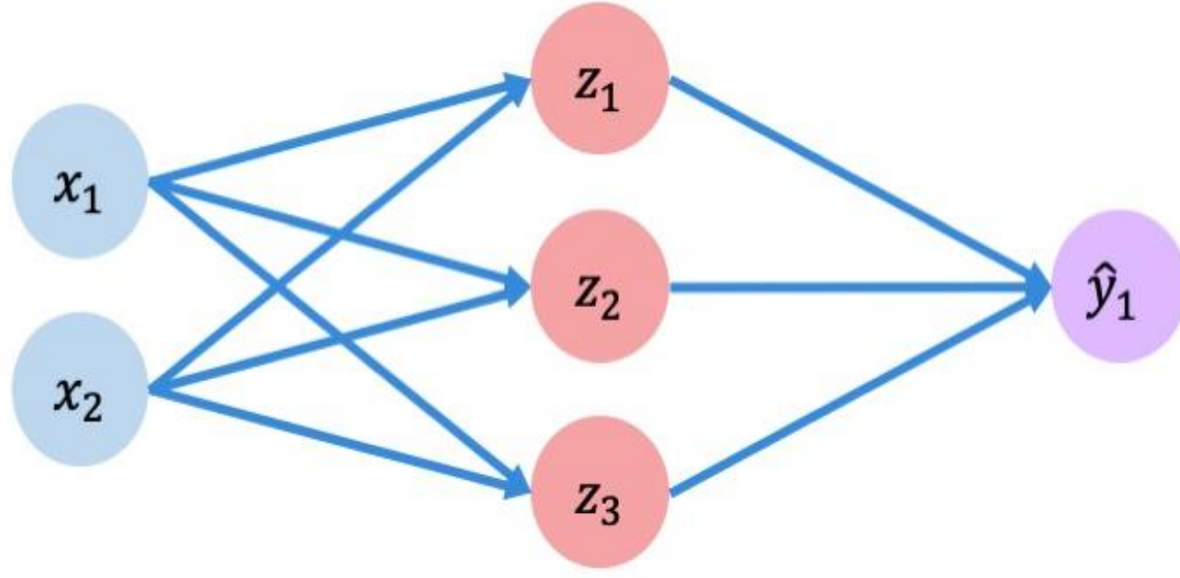
$$\begin{bmatrix} 0.1 \\ 0.8 \\ 0.6 \\ \vdots \end{bmatrix} \begin{matrix} \times \\ \times \\ \checkmark \\ \end{matrix} \begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}$$

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

Mean Squared Error Loss

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

$$\boldsymbol{X} = \begin{bmatrix} 4, & 5 \\ 2, & 1 \\ 5, & 8 \\ \vdots & \vdots \end{bmatrix}$$



$$J(\boldsymbol{W}) = \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - f\left(x^{(i)}; \boldsymbol{W}\right)\right)^2$$

Actual Predicted

$f(x)$ y

$$\begin{bmatrix} 30 \\ 80 \\ 85 \\ \vdots \end{bmatrix} \begin{matrix} \times \\ \times \\ \checkmark \\ \end{matrix} \begin{bmatrix} 90 \\ 20 \\ 95 \\ \vdots \end{bmatrix}$$

Final Grades (percentage)

Training Neural Networks

Loss Optimization

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

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

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

Loss Optimization

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

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

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

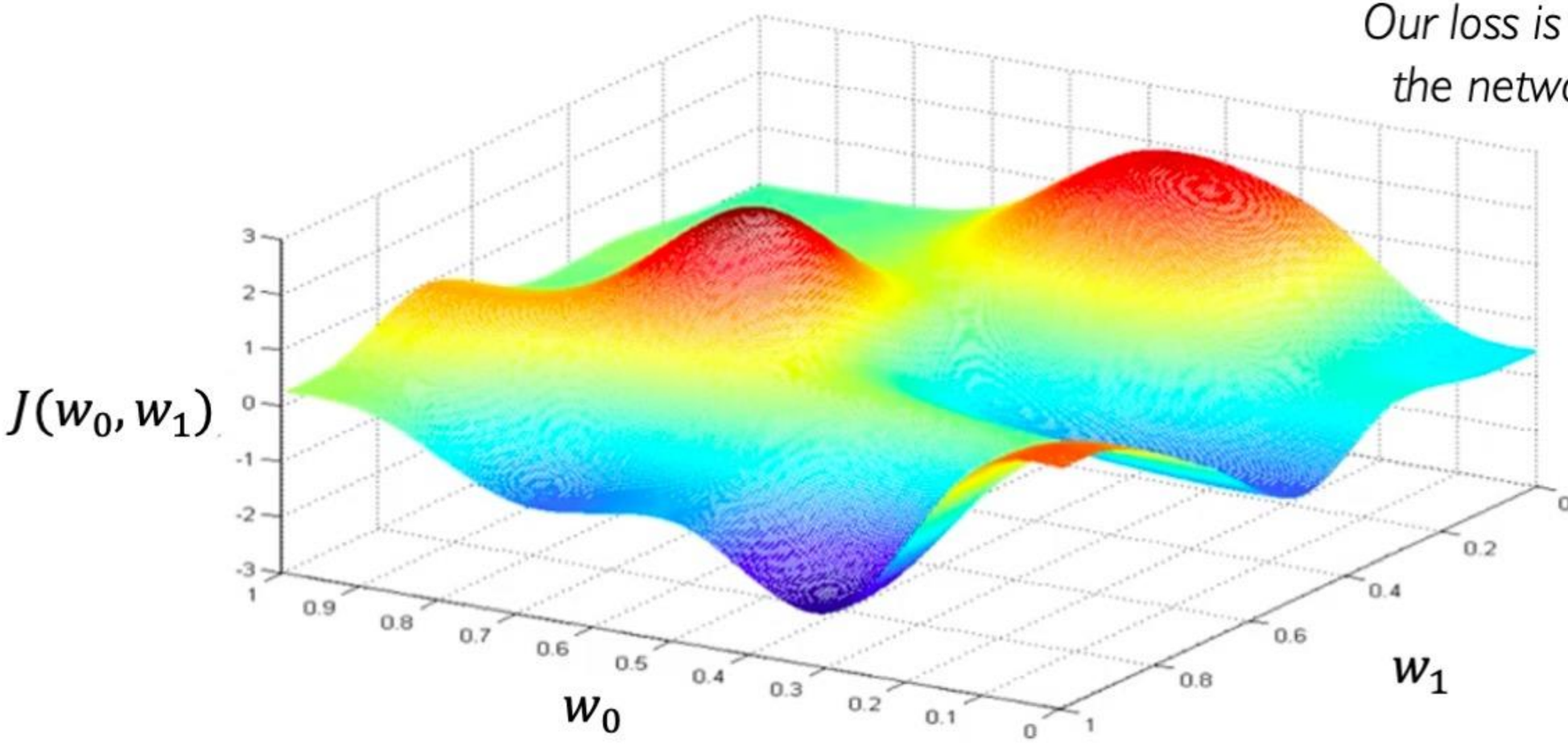
Remember:
$\boldsymbol{W} = \{\boldsymbol{W}^{(0)}, \boldsymbol{W}^{(1)}, \dots\}$

Loss Optimization

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

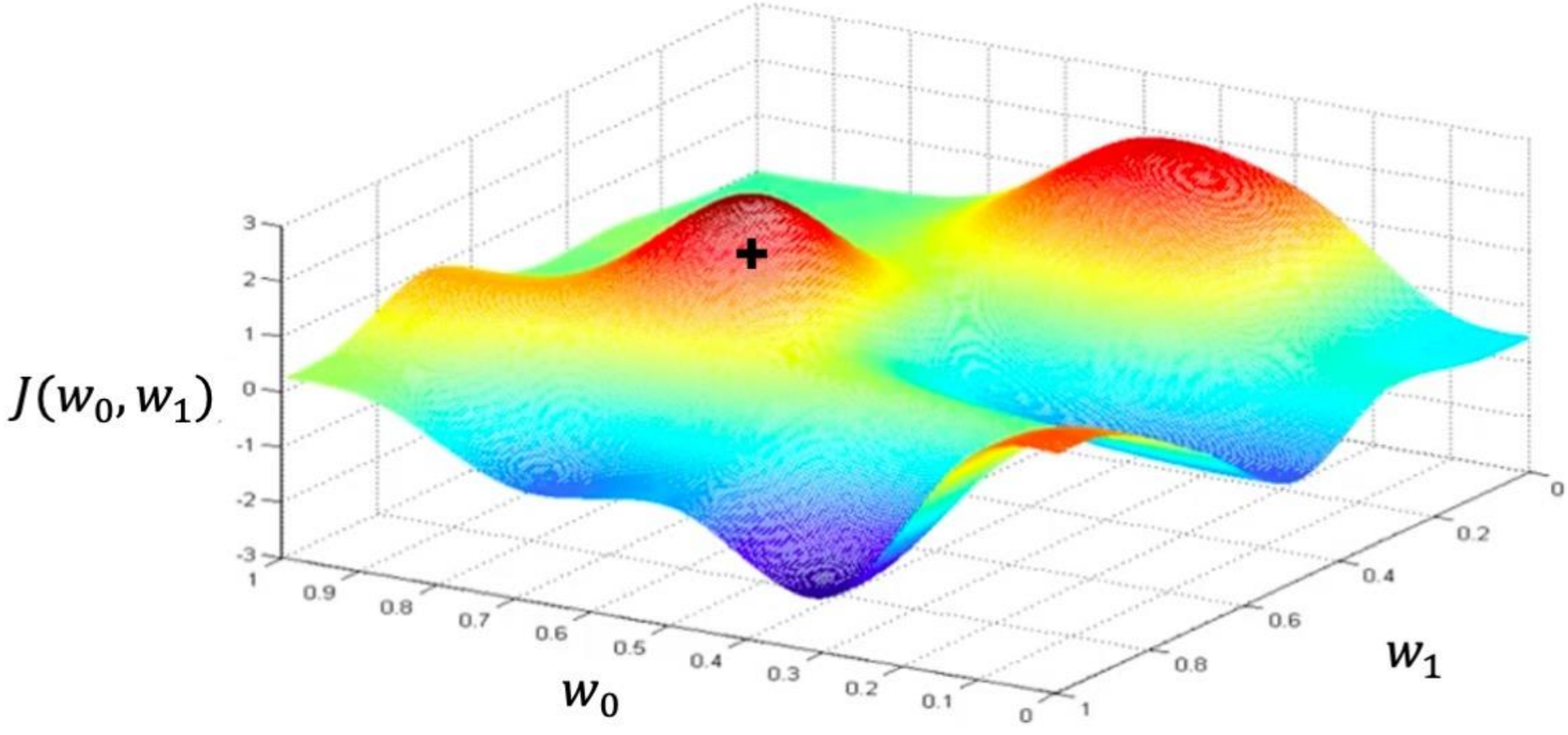
Remember:

Our loss is a function of the network weights!



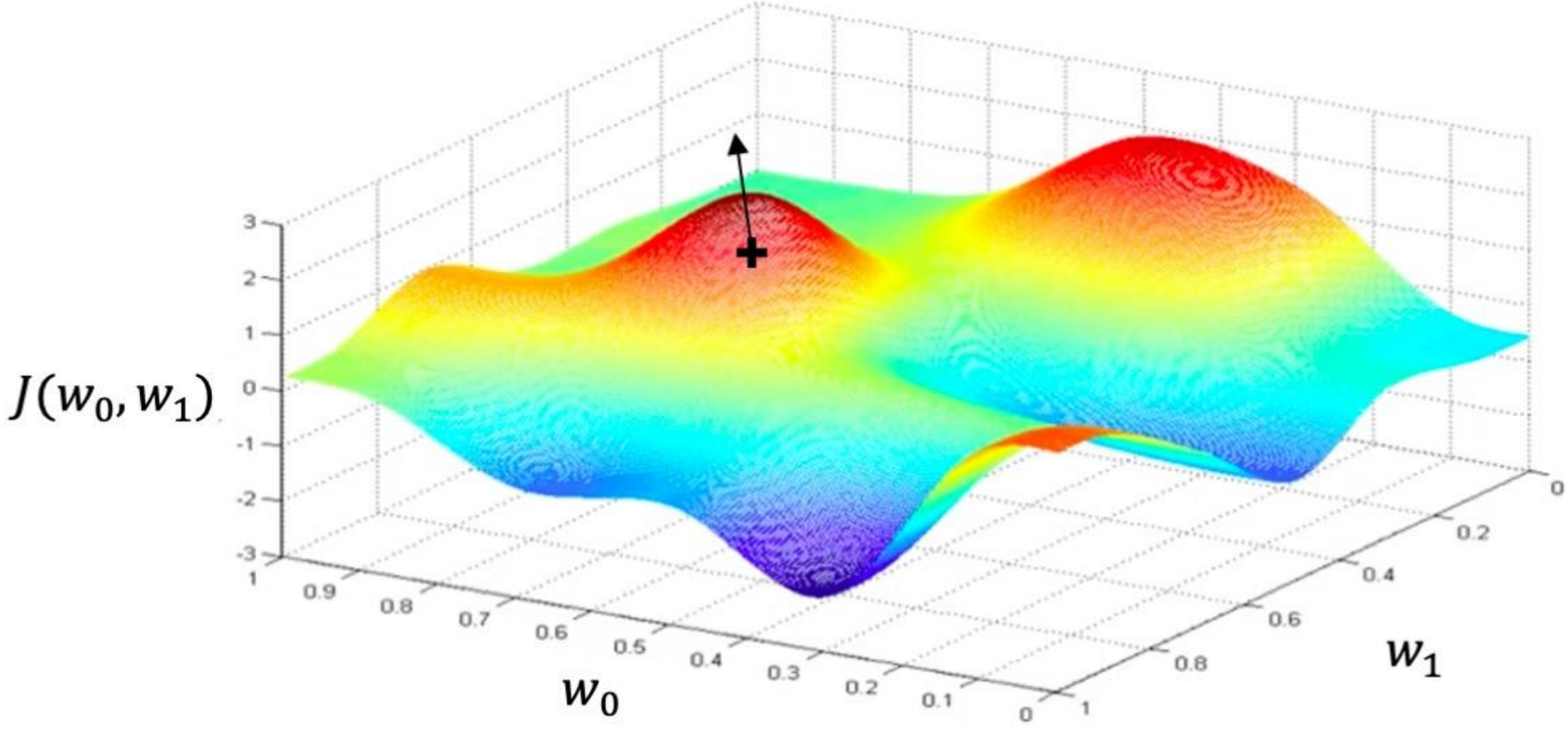
Loss Optimization

Randomly pick an initial (w_0, w_1)



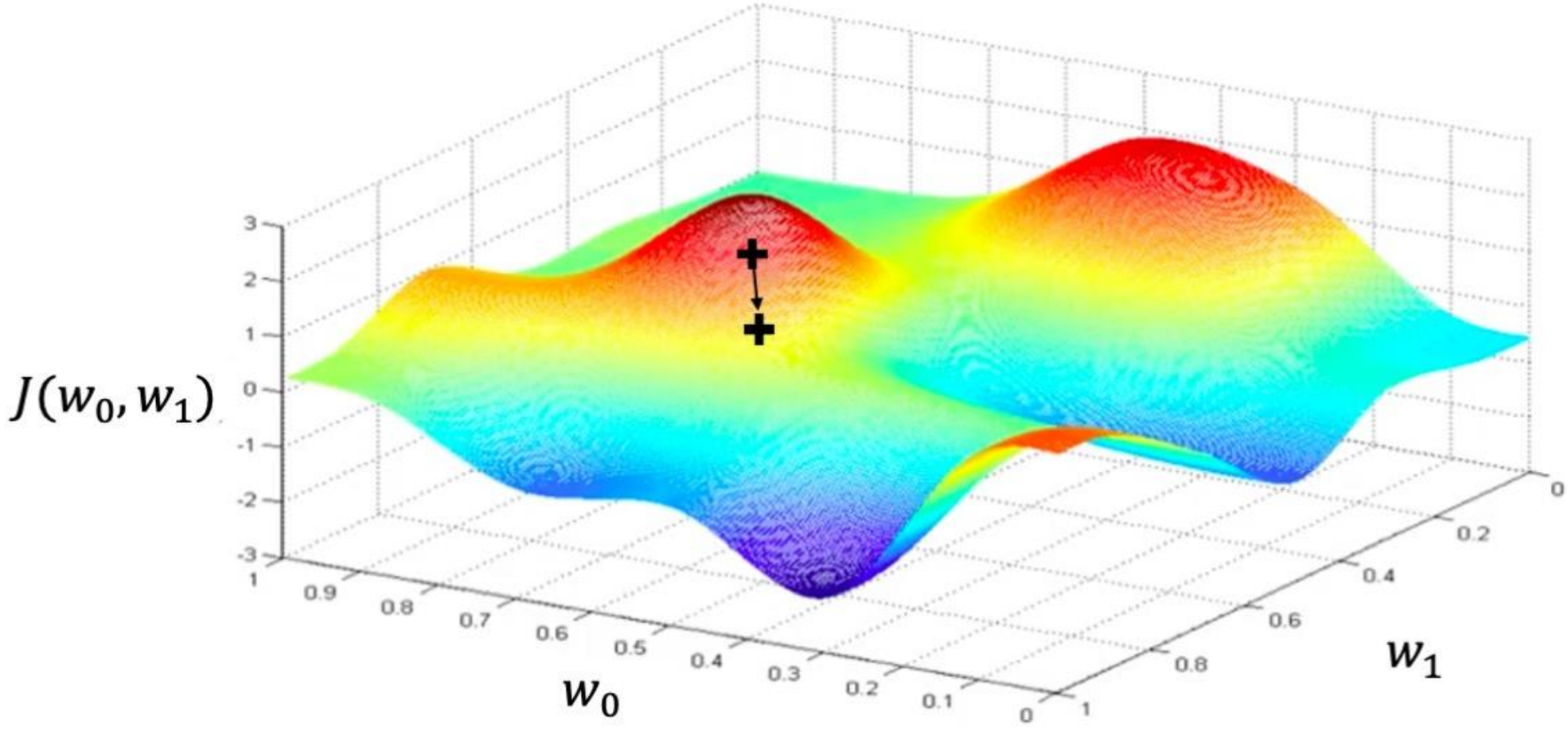
Loss Optimization

Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$



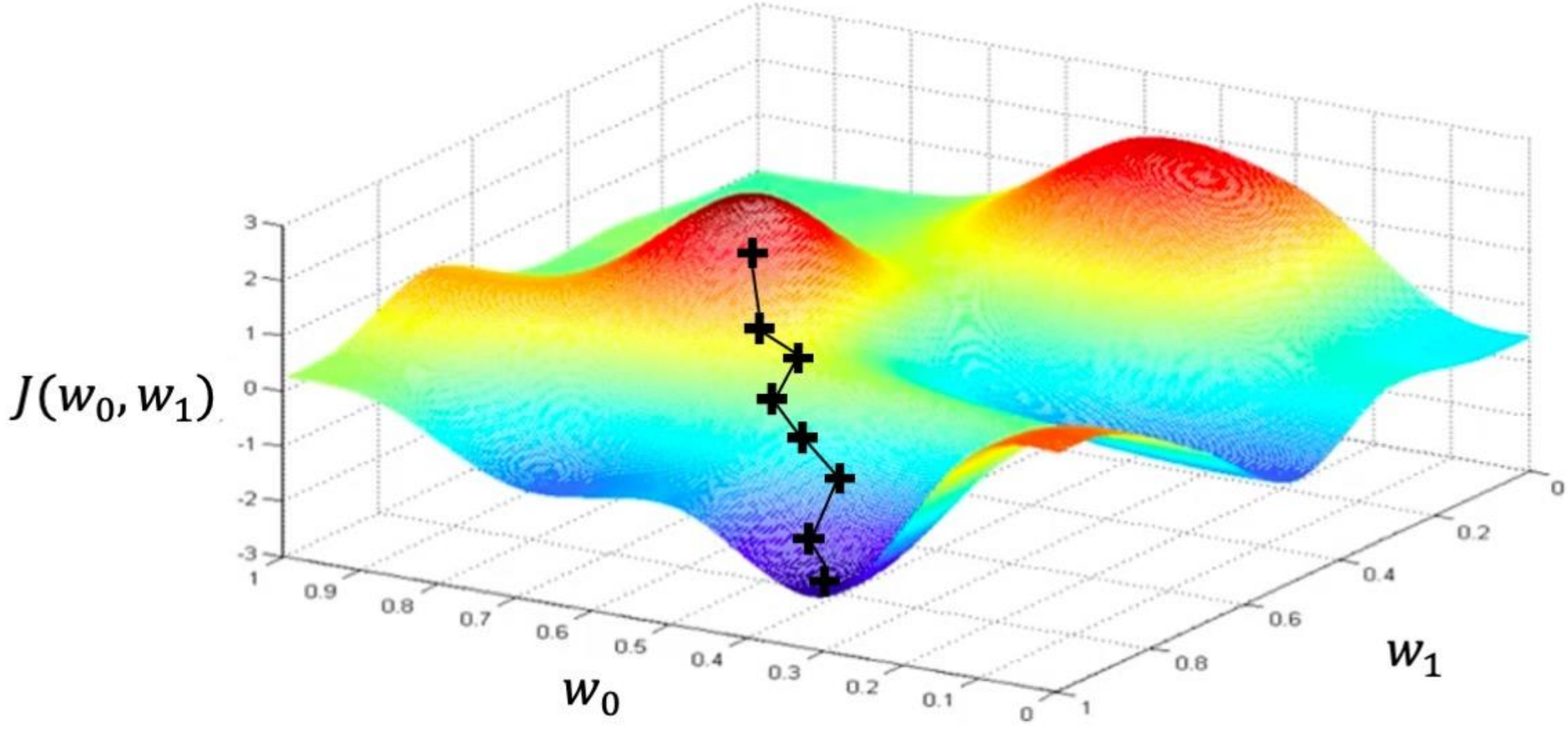
Loss Optimization

Take small step in opposite direction of gradient



Gradient Descent

Repeat until convergence

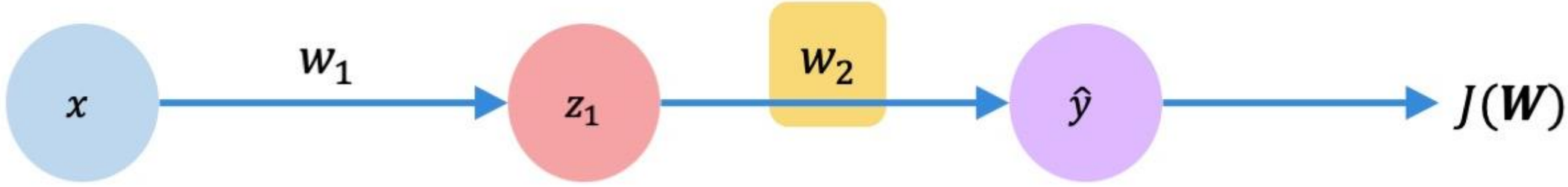


Gradient Descent

Algorithm

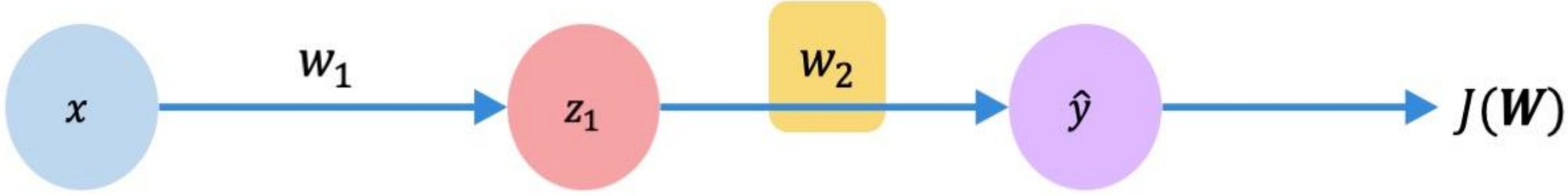
1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5.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

Computing Gradients: Backpropagation



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

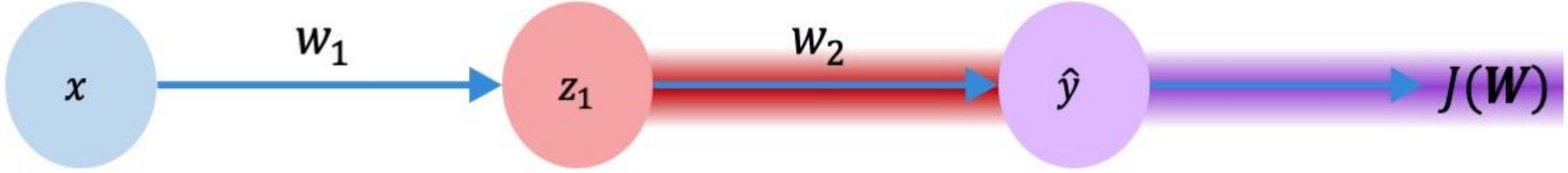
Computing Gradients: Backpropagation



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

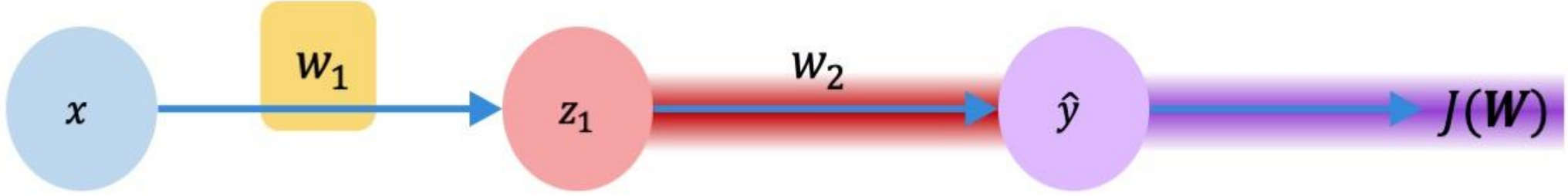
Let's use the chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\boldsymbol{W})}{\partial w_2} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_2}$$

Computing Gradients: Backpropagation

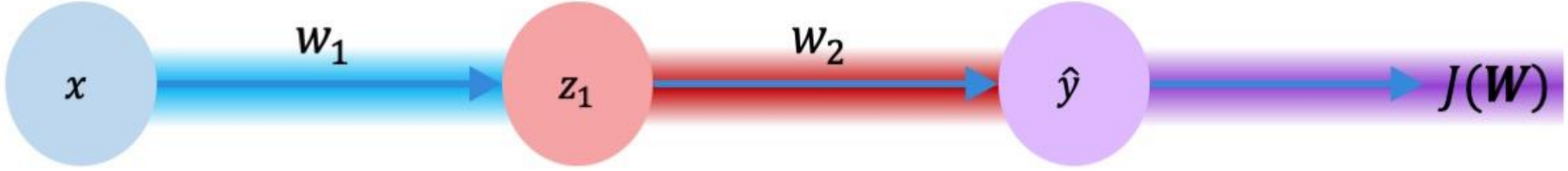


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_1}$$

Apply chain rule!

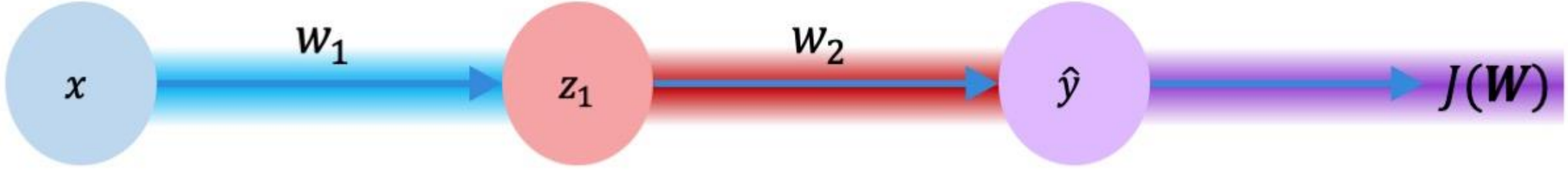
Apply chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

Computing Gradients: Backpropagation

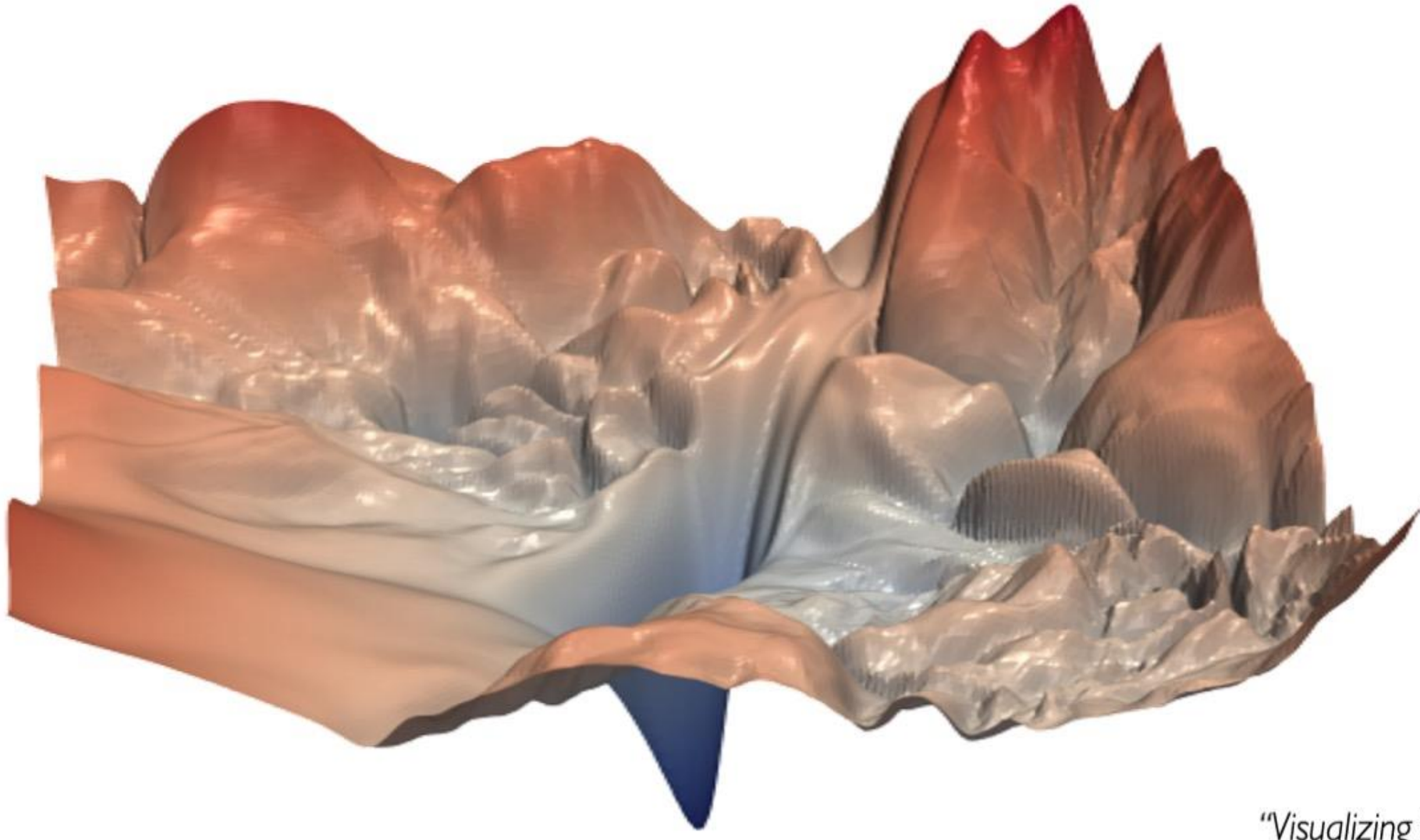


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

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

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

Loss Functions Can Be Difficult to Optimize

Remember:

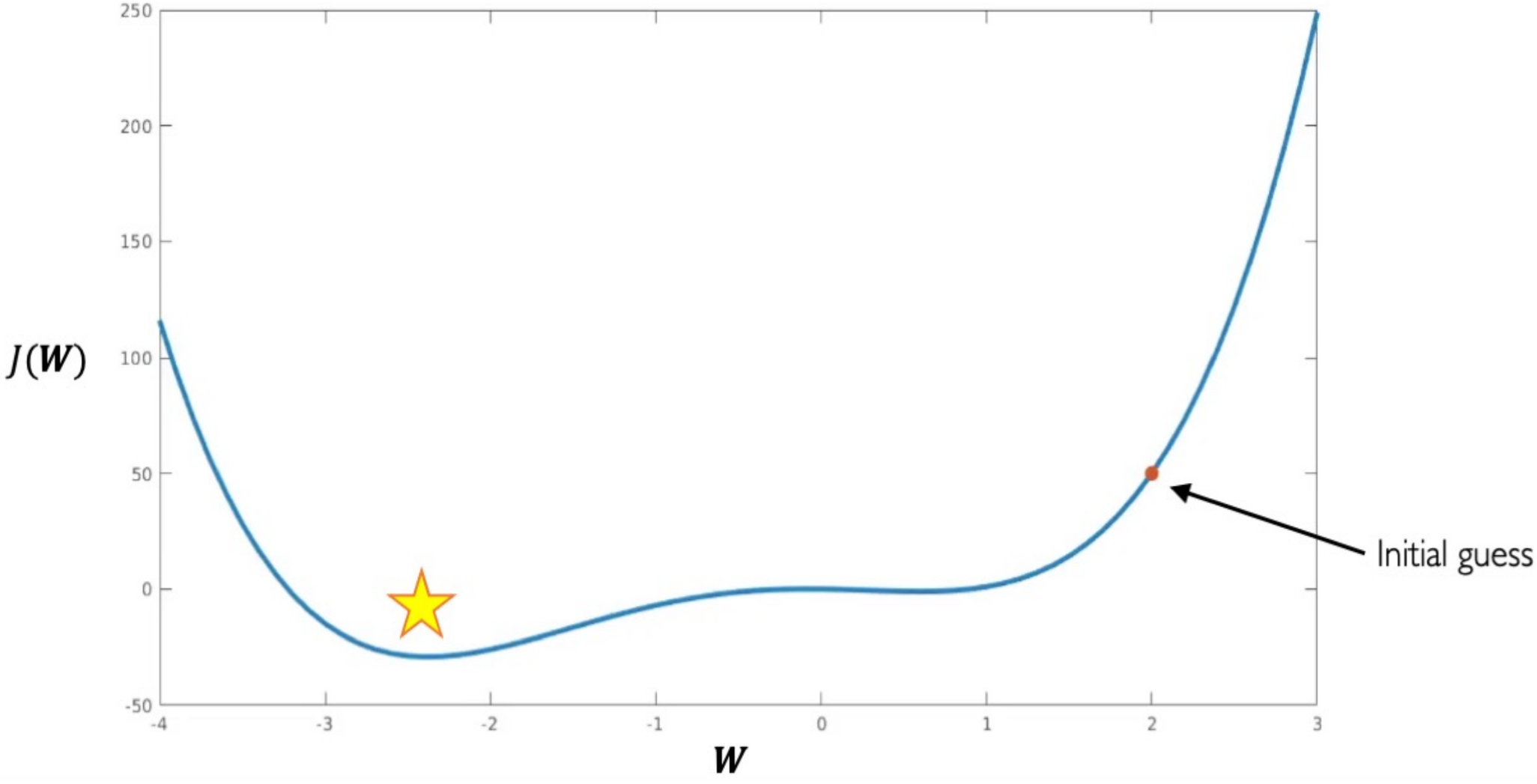
Optimization through gradient descent

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

How can we set the learning rate?

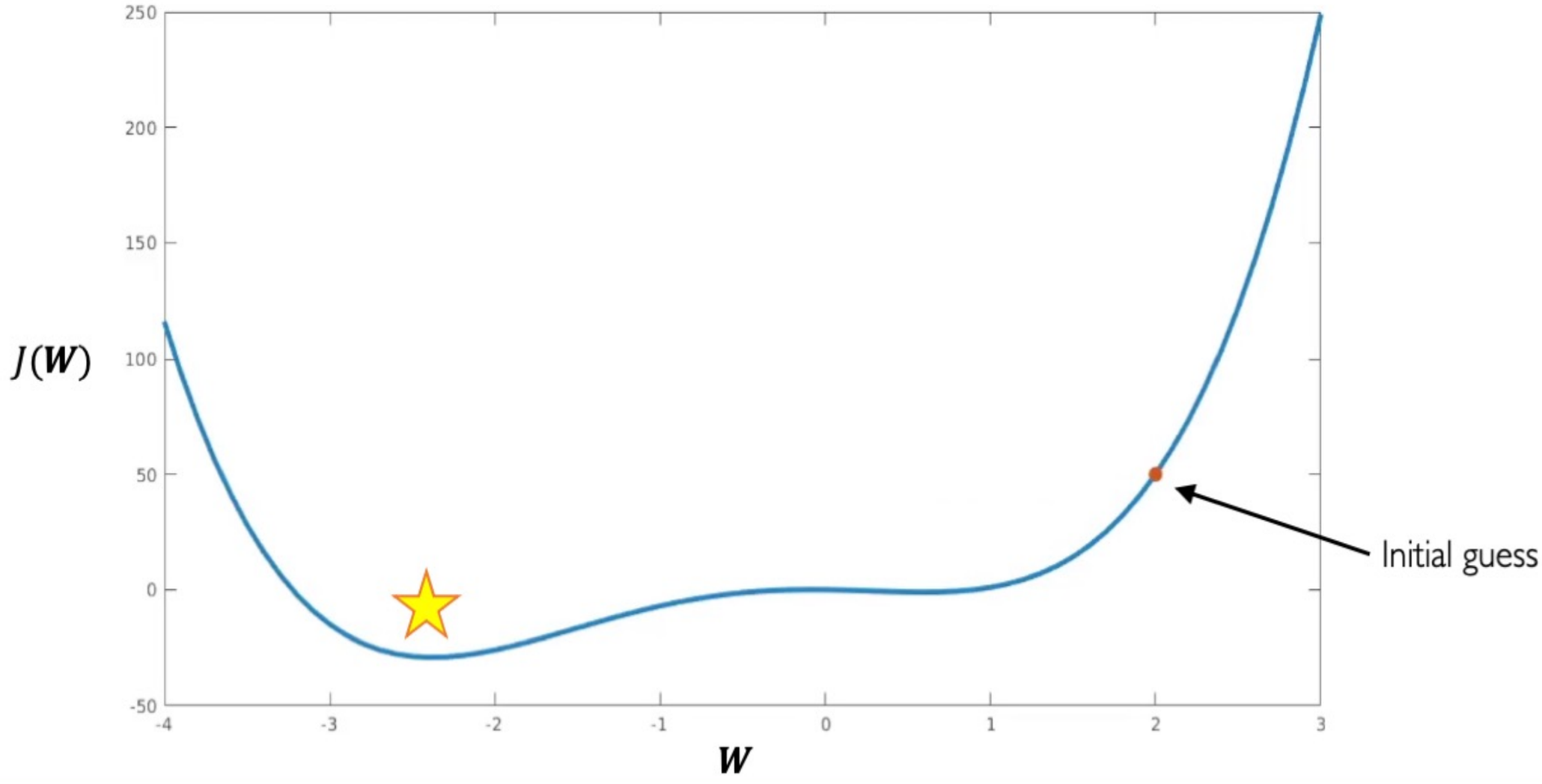
Setting the Learning Rate

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



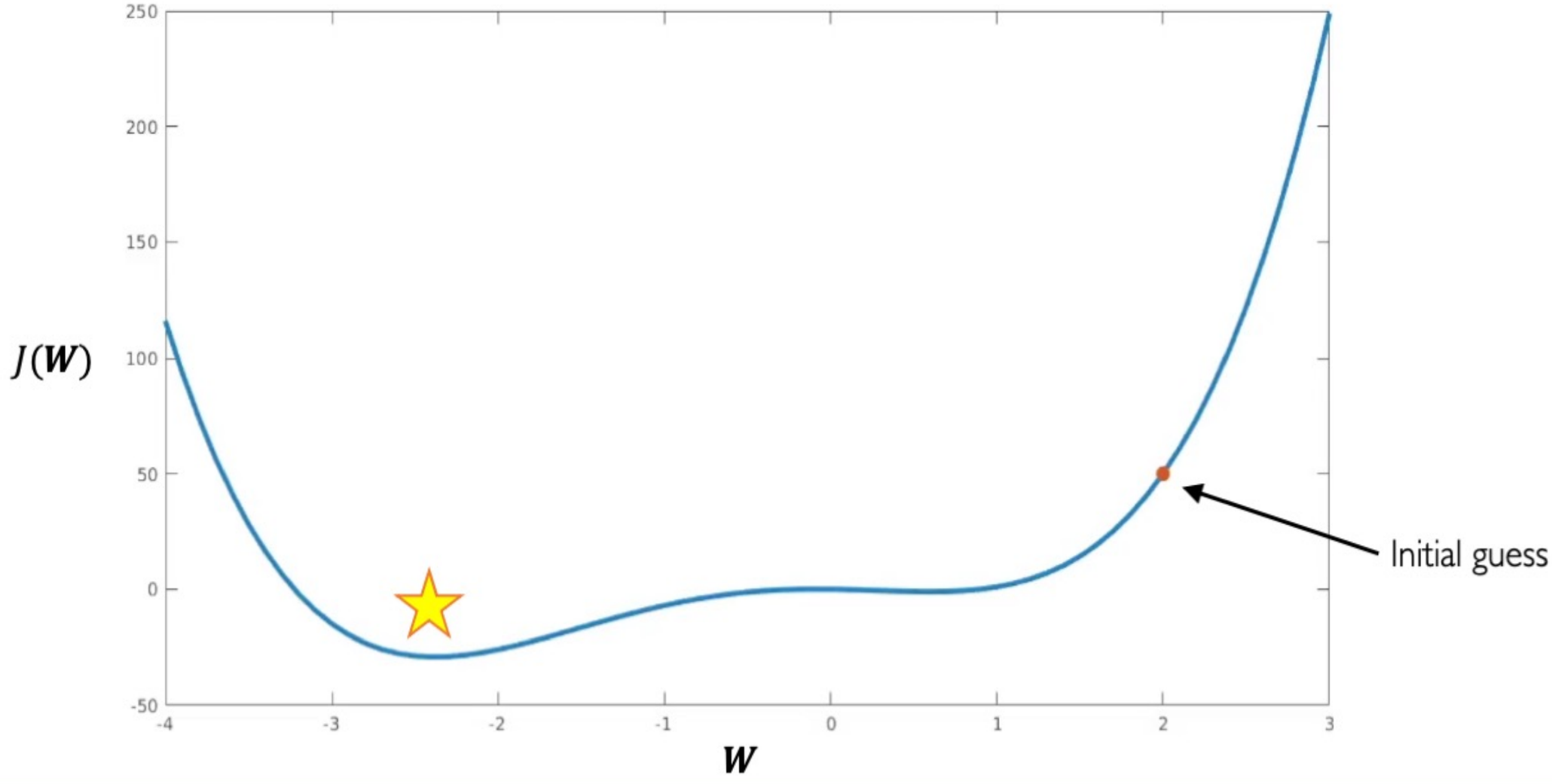
Setting the Learning Rate

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:

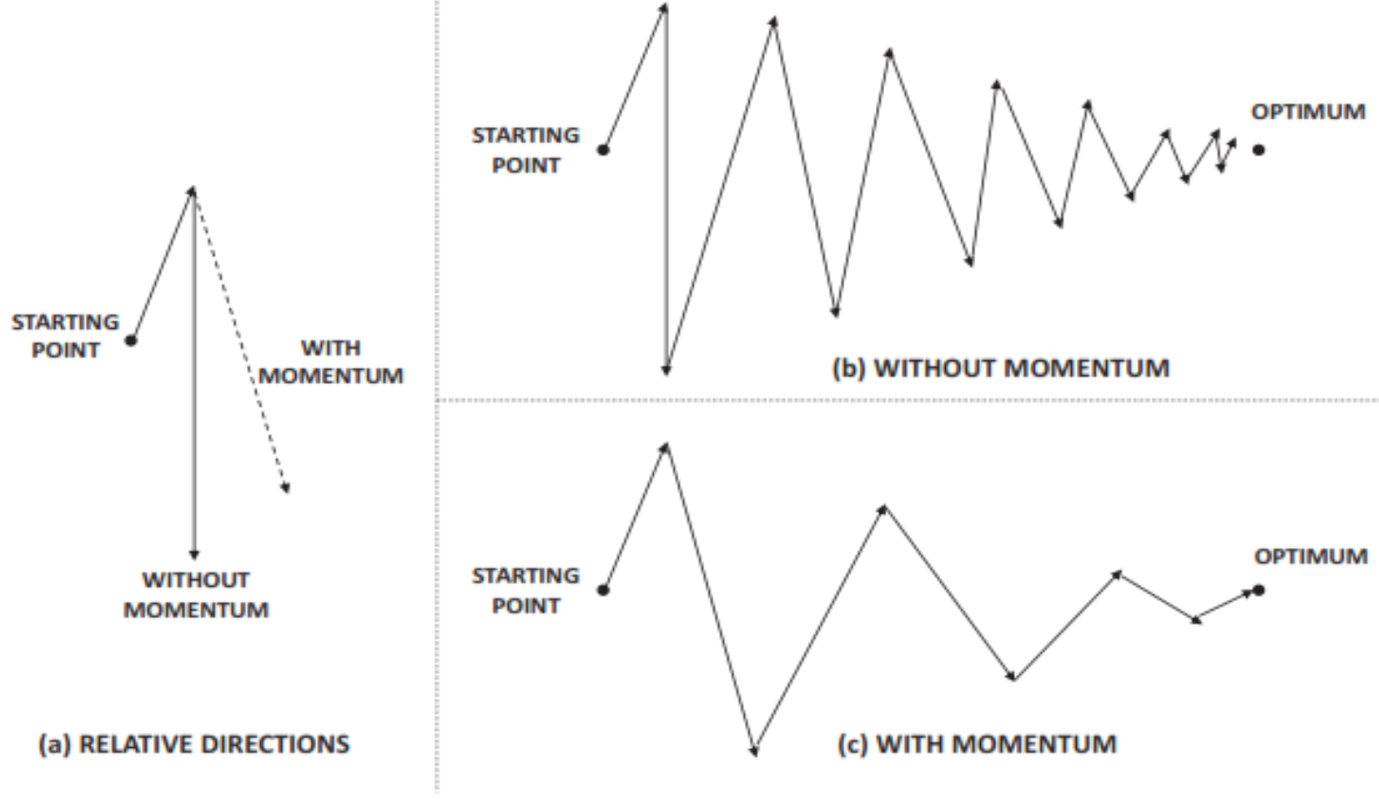
Do something smarter!
Design an adaptive learning rate that "adapts" to the landscape

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...

Momentum

- Gradient descent can be very slow if η is small, and can oscillate widely if η is too large.
- A simple way to avoid this problem is the addition of a *momentum* term
- Then the effective learning rate can be made larger without divergent oscillations occurring.



Updating Weights Using Momentum

- The idea is to give each connection w_{ji} some inertia or momentum

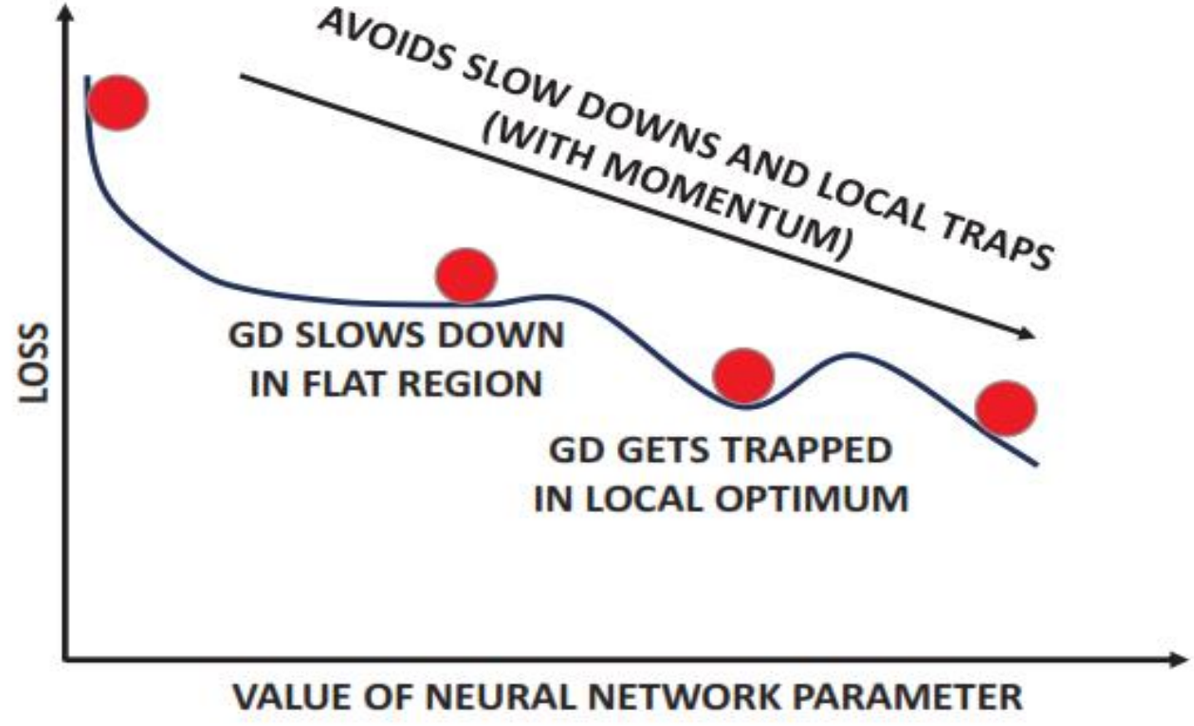
- This scheme is implemented by giving a contribution from the previous time step to each weight change: derive the weights at step $(t+1)$, using not only the weights at step t but also those at step $(t-1)$. The updating is performed by

$$\Delta w_{ji}(t+1) = -\eta \frac{\partial J(W)}{\partial w_{ji}} + \boldsymbol{\alpha \Delta w_{ji}(t)}$$

where α is called the *momentum* parameter.

- The momentum parameter α must be between 0 and 1; a value of 0.9 is often chosen

Effect of momentum in navigating complex loss surfaces



- Adding momentum can help to
  - avoid local minima
  - helps the optimization process retain speed in flat regions of the loss surface,
  - improving convergence.

Gradient Descent Algorithms

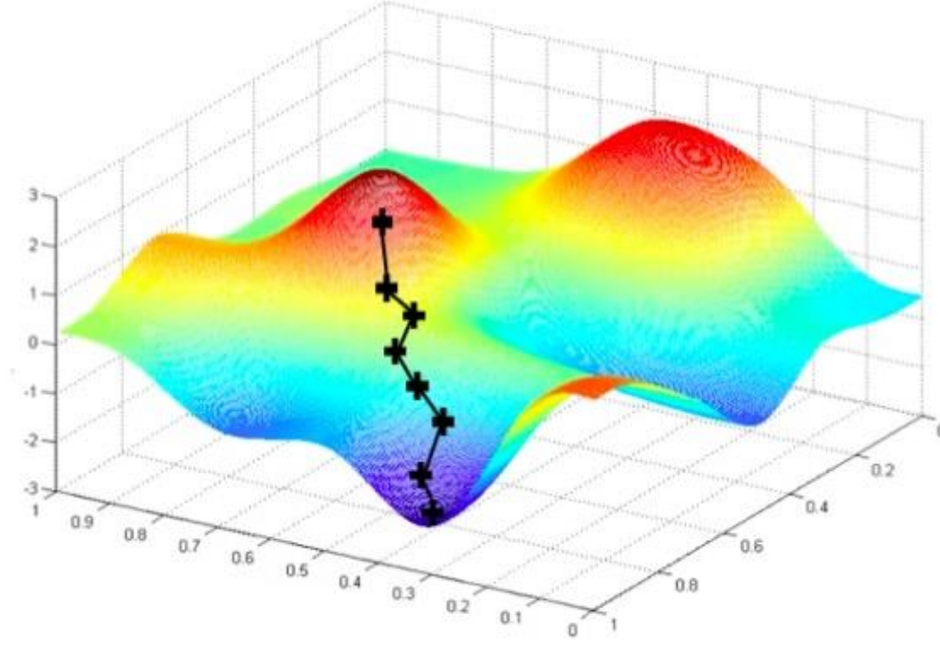
Algorithm	TF Implementation	Reference
• SGD		Kiefer & Wolfowitz. "Stochastic Estimation of the Maximum of a Regression Function." 1952.
• Adam		Kingma et al. "Adam: A Method for Stochastic Optimization." 2014.
• Adadelta		Zeiler et al. "ADADELTA: An Adaptive Learning Rate Method." 2012.
• Adagrad		Duchi et al. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." 2011.
• RMSProp		

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, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Return weights



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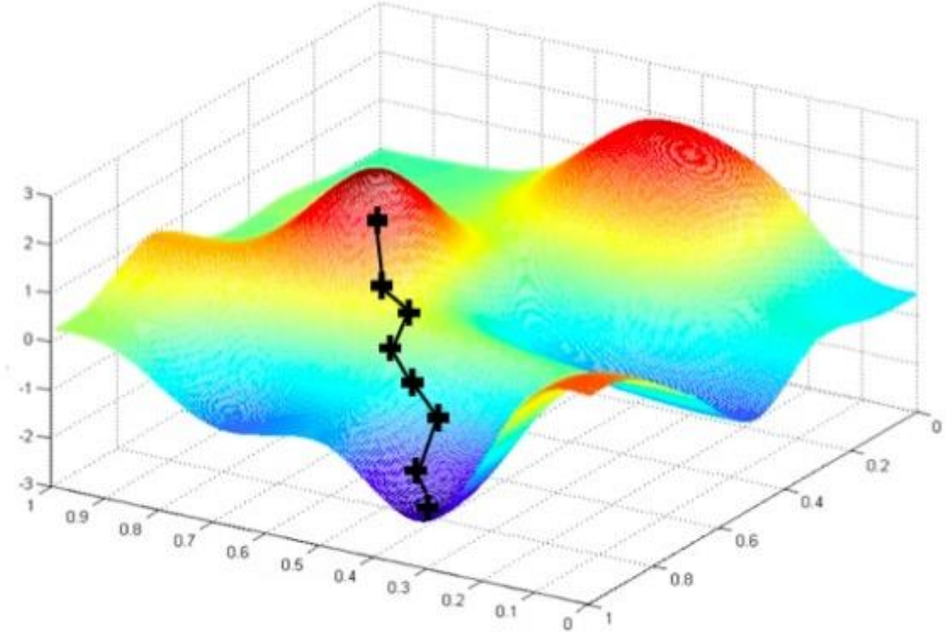

Can be very **computationally intensive** to compute!

Stochastic Gradient Descent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Pick single data point $\boldsymbol{i}$
4. Compute gradient, $\frac{\partial J_i(\boldsymbol{W})}{\partial \boldsymbol{W}}$
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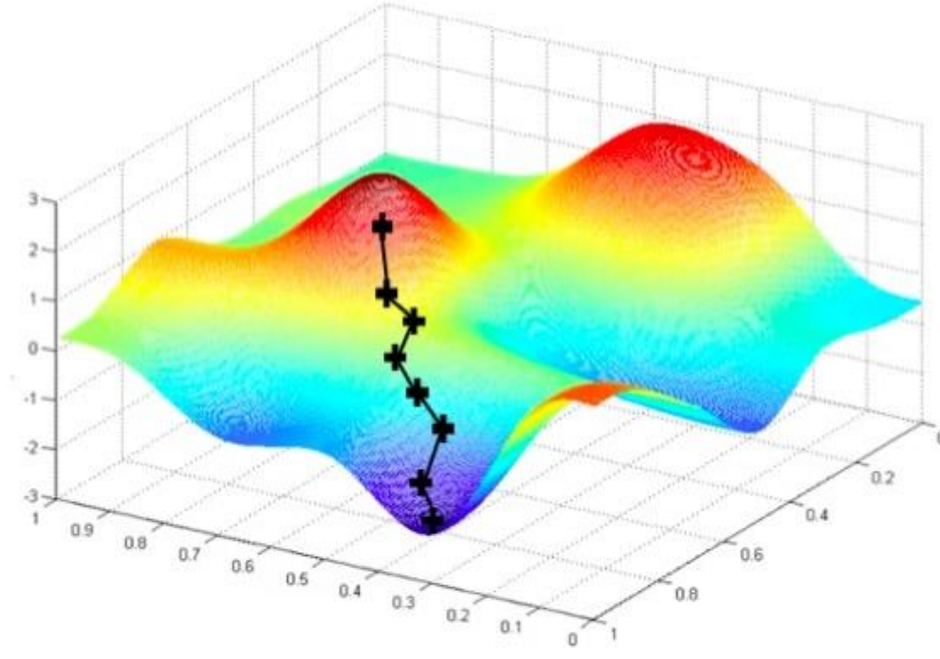

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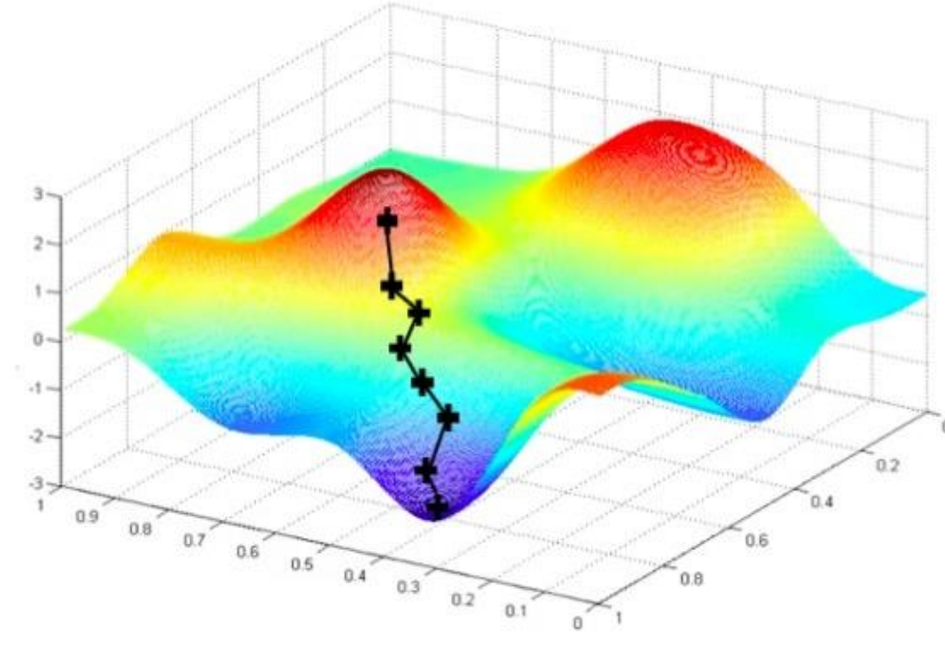
Easy to compute but
very noisy (stochastic)!



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
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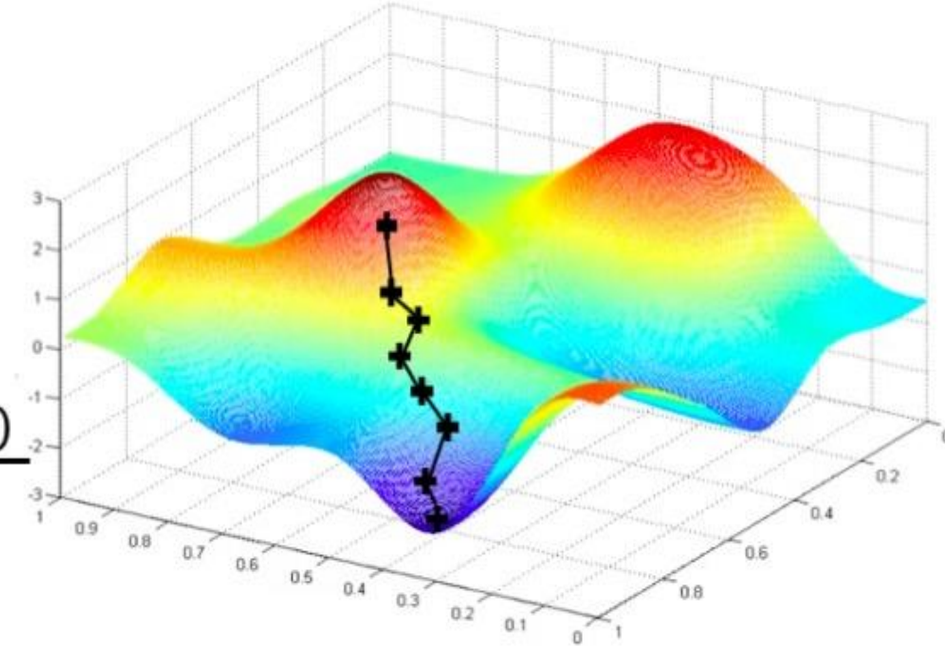

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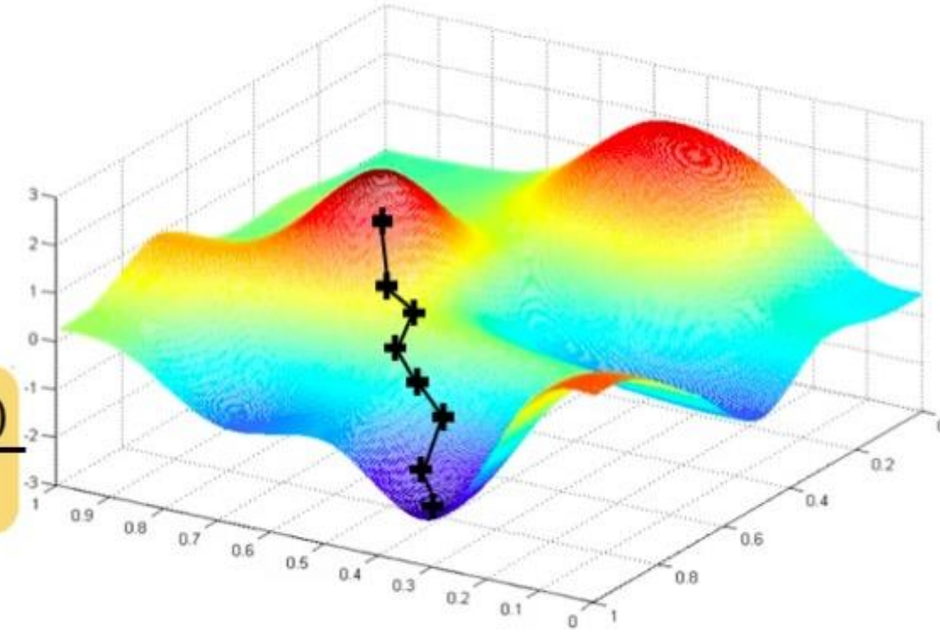

Fast to compute and a much better estimate of the true gradient!

Mini-batches while training

More accurate estimation of gradient

Smoother convergence

Allows for larger learning rates

Mini-batches while training

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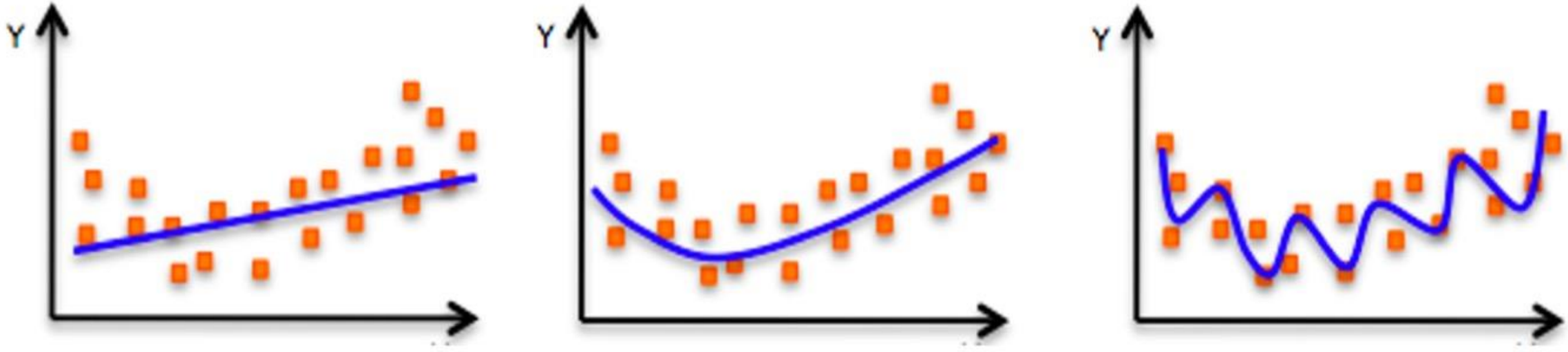
Mini-batches lead to fast training!

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

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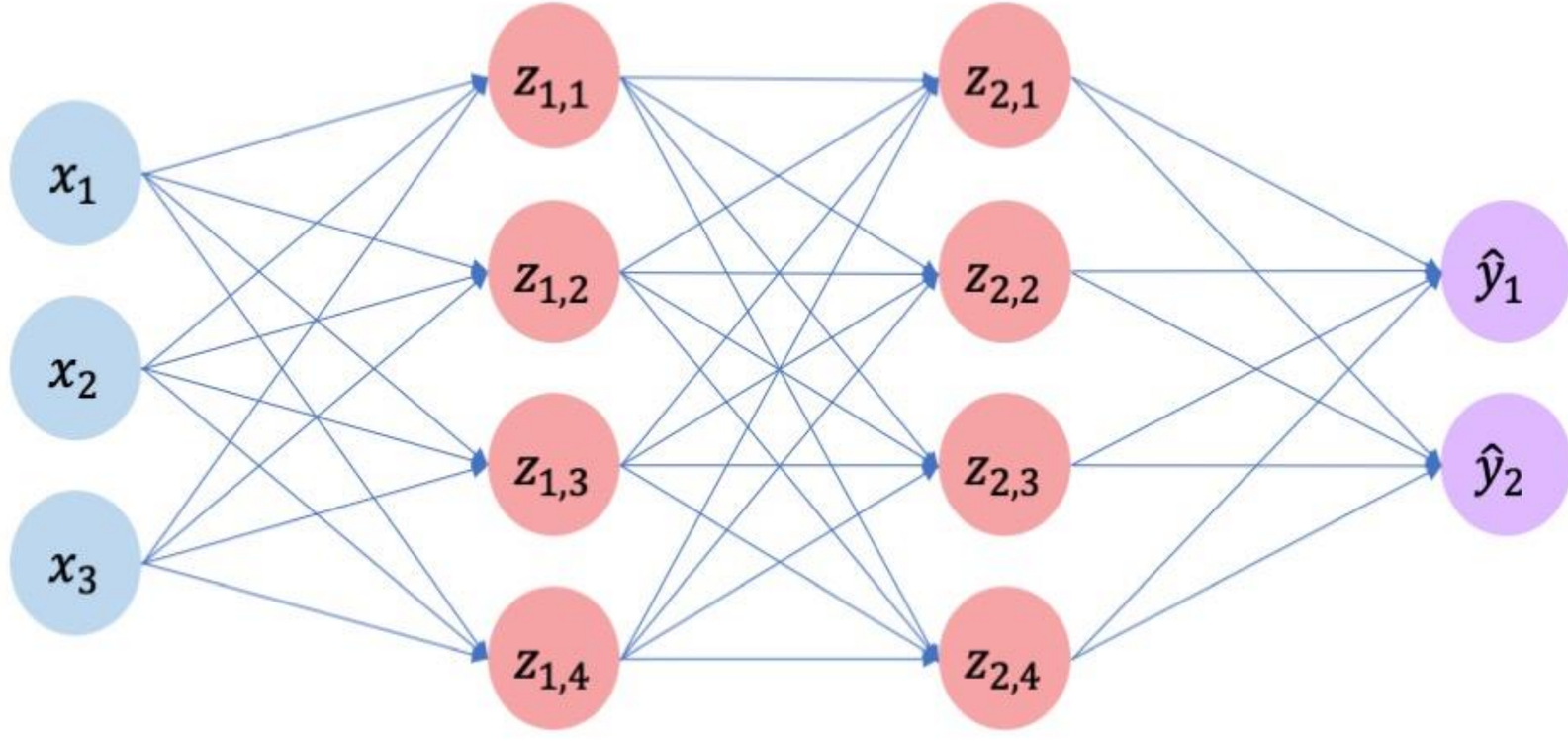
Technique that constrains our optimization problem to discourage complex models

Why do we need it?

Improve generalization of our model on unseen data

Regularization 1: Dropout

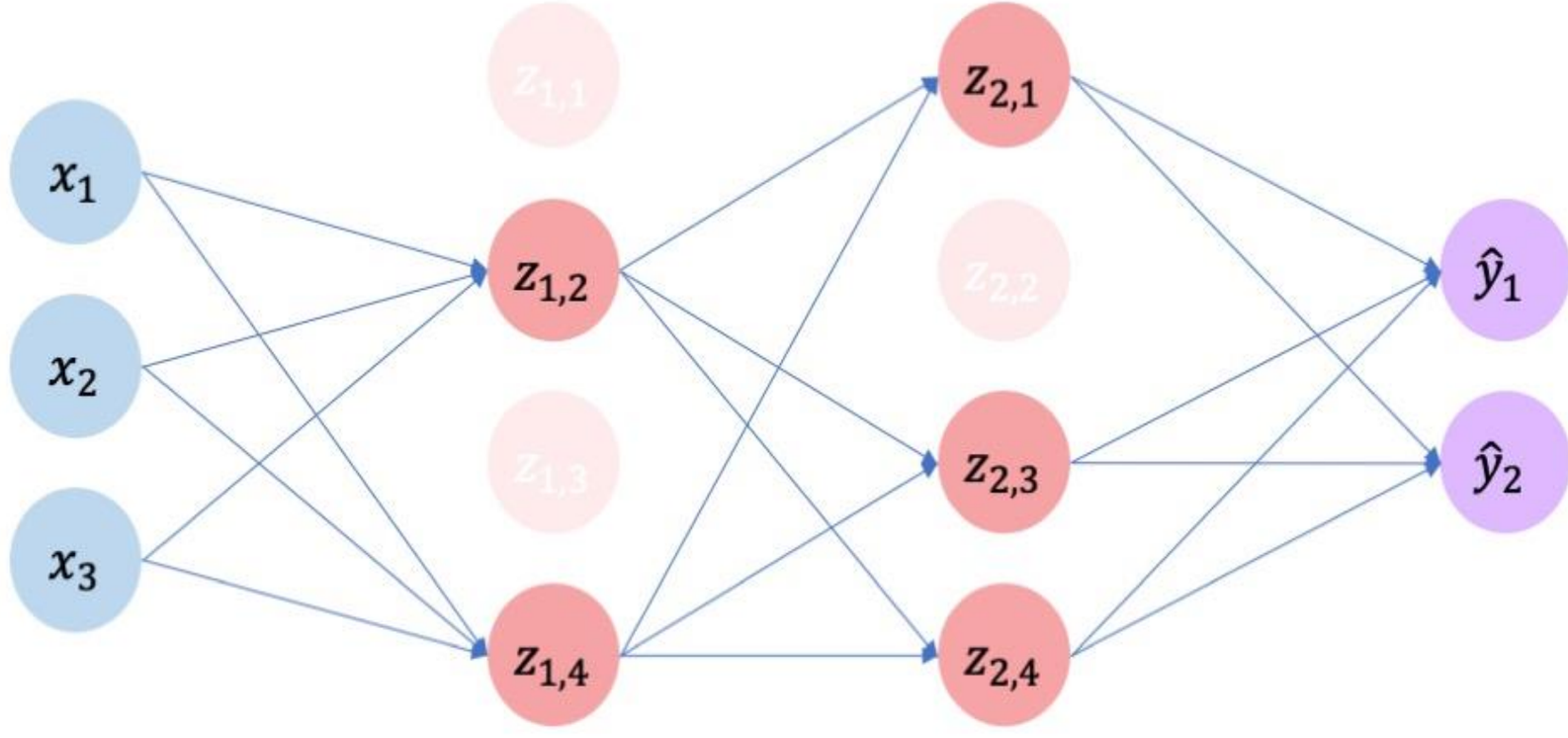
- During training, randomly set some activations to 0



Regularization 1: 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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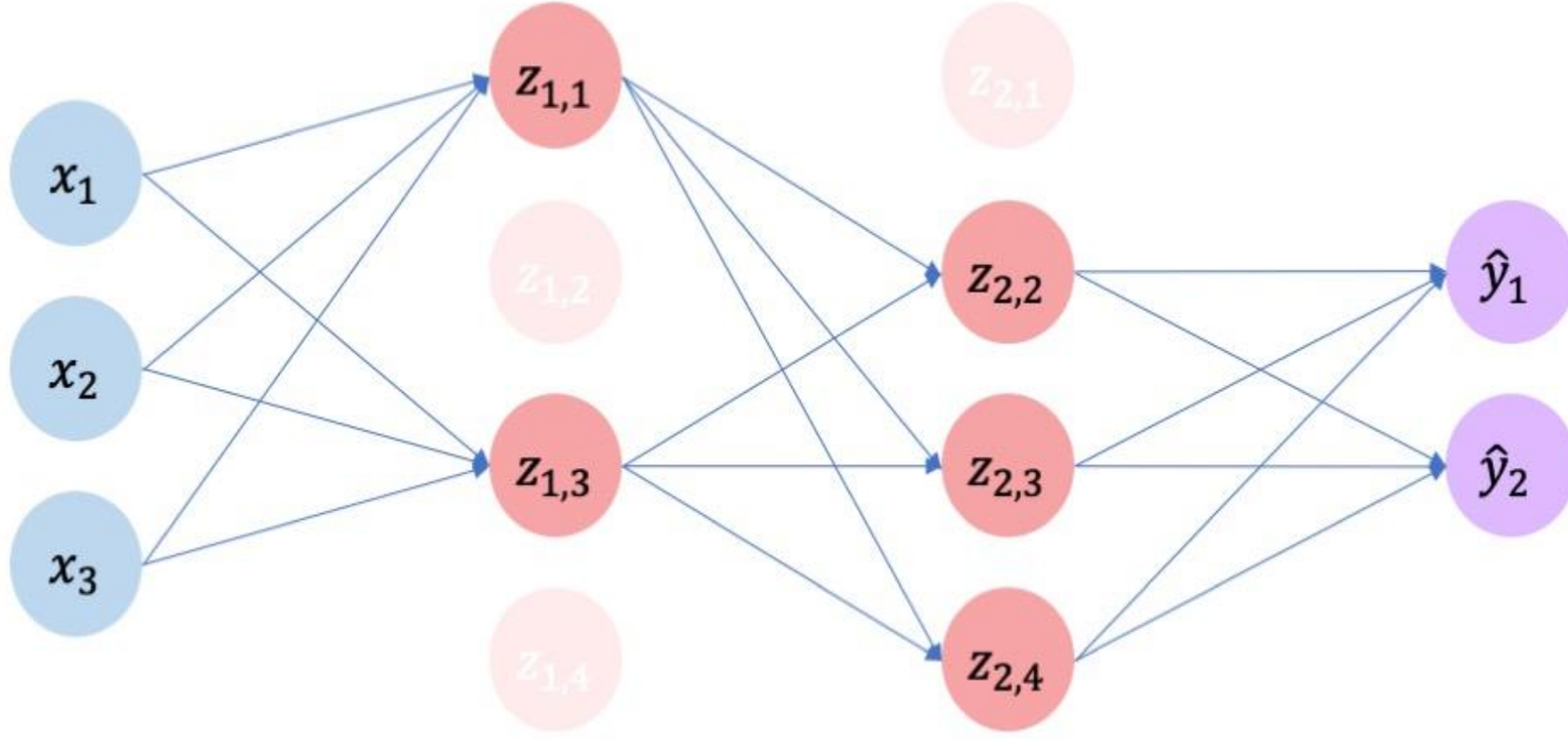
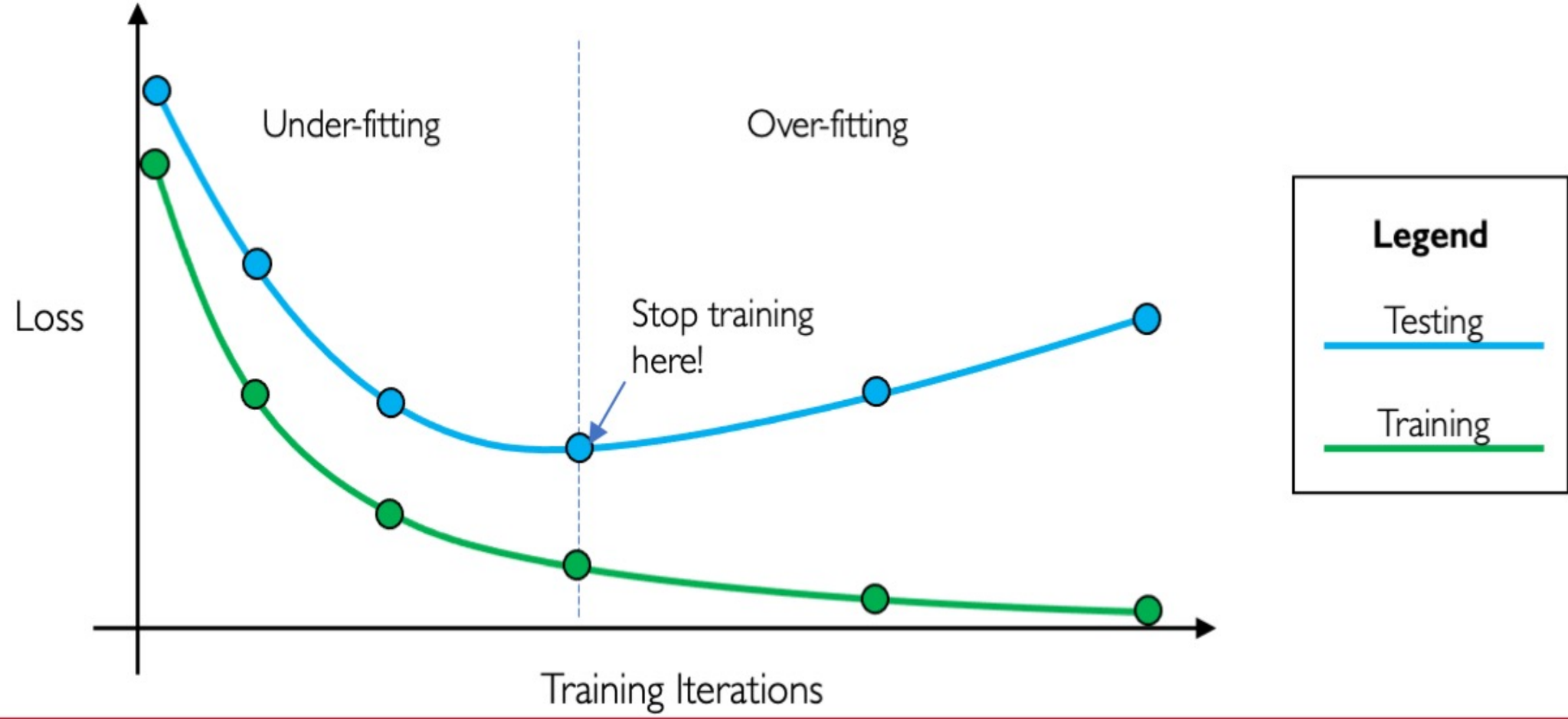


Regularization 2: Early Stopping

- Stop training before we have a chance to overfit



Regularization 3: Data augmentation

- For example in a computer vision data:
  - You can flip all your pictures horizontally this will give you more data instances.
  - You could also apply a random position and rotation to an image to get more data.

Parameters vs Hyperparameters

- Main parameters of the NN is W and b
- Hyper parameters (parameters that control the algorithm) are like:
  - Learning rate.
  - Number of iteration.
  - Number of hidden layers L.
  - Number of hidden units n.
  - Choice of activation functions.
- You have to try values yourself of hyper parameters.

Train / Dev / Test sets

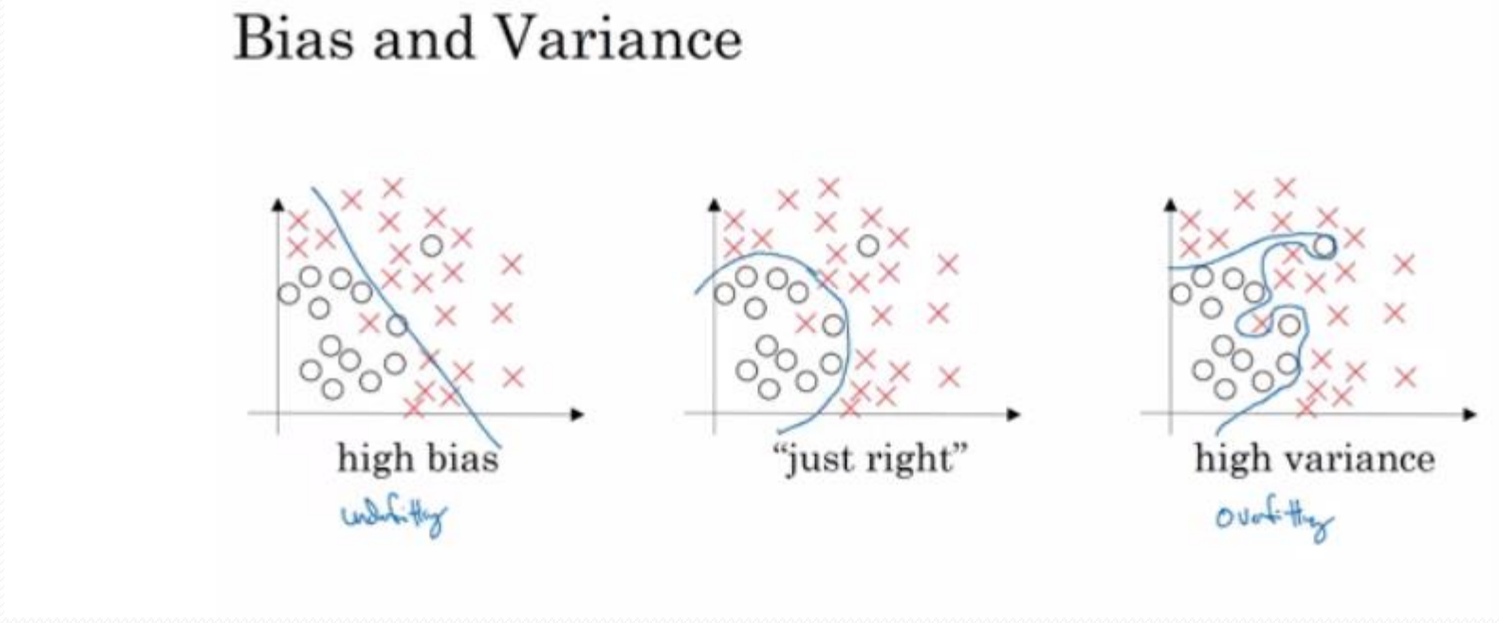
- Your data will be split into three parts:
  - Training set. (Has to be the largest set)
  - Hold-out cross validation set / Development or "dev" set.
  - Testing set.

- You will try to build a model upon training set then try to optimize hyperparameters on dev set as much as possible. Then after your model is ready you try and evaluate the testing set.

- so the trend on the ratio of splitting the models:
  - If size of the dataset is 100 to 1000000 ==> 60/20/20
  - If size of the dataset is 1000000 to INF ==> 98/1/1 or 99.5/0.25/0.25

Bias/variance tradeoff

- If your model is underfitting (logistic regression of non linear data) it has a "high bias"
- If your model is overfitting then it has a "high variance"
- Your model will be alright if you balance the Bias / Variance



Bias/variance tradeoff

- Another idea to get the bias / variance if you don't have a 2D plotting mechanism:
- High variance (overfitting) for example:
  - Training error: 1%
  - Dev error: 11%
- high Bias (underfitting) for example:
  - Training error: 15%
  - Dev error: 14%
- high Bias (underfitting) && High variance (overfitting) for example:
  - Training error: 15%
  - Test error: 30%
- Best:
  - Training error: 0.5%
  - Test error: 1%

Bias/variance tradeoff

- If your algorithm has a high bias:
  - Try to make your NN bigger (size of hidden units, number of layers)
  - Try a different model that is suitable for your data.
  - Try to run it longer.
  - Different (advanced) optimization algorithms.
- If your algorithm has a high variance:
  - More data.
  - Try regularization.
  - Try a different model that is suitable for your data.
- You should try the previous two points until you have a low bias and low variance.

Random Initialization

- In logistic regression it wasn't important to initialize the weights randomly, while in NN we have to initialize them randomly.
- If we initialize all the weights with zeros in NN it won't work (initializing bias with zero is OK):
  - all hidden units will be completely identical (symmetric) - compute exactly the same function
  - on each gradient descent iteration all the hidden units will always update the same
- To solve this we initialize the W's with a small random numbers:
- W1 = np.random.randn((2,2)) * 0.01 # 0.01 to make it small enough
- b1 = np.zeros((2,1)) # its ok to have b as zero, it won't get us to the symmetry breaking problem

Random Initialization

- We need small values because in sigmoid (or tanh), for example, if the weight is too large you are more likely to end up even at the very start of training with very large values of Z. Which causes your tanh or your sigmoid activation function to be saturated, thus slowing down learning. If you don't have any sigmoid or tanh activation functions throughout your neural network, this is less of an issue.

- Constant 0.01 is alright for ***1*** hidden layer networks, but if the NN is deep this number can be changed but it will always be a small number.

Practical Part:

Deep Neural Network for Image Classification

- Build and apply a deep neural network to supervised learning.
- Apply it to cat vs non-cat classification.

- Let’s Go

Deep L-layer neural network

- Shallow NN is a NN with one or two layers.
- Deep NN is a NN with three or more layers.
- We will use the notation `L` to denote the number of layers in a NN.
- `n[l]` is the number of neurons in a specific layer `l`.
- `n[0]` denotes the number of neurons input layer. `n[L]` denotes the number of neurons in output layer.
- `g[l]` is the activation function.
- `a[l] = g[l](z[l])`
- `w[l]` weights is used for `z[l]`
- `x = a[0]`, `a[l] = y'`
- These were the notation we will use for deep neural network.
- So we have:
  - A vector `n` of shape `(1, NoOfLayers+1)`
  - A vector `g` of shape `(1, NoOfLayers)`
  - A list of different shapes `w` based on the number of neurons on the previous and the current layer.
  - A list of different shapes `b` based on the number of neurons on the current layer.

Getting your matrix dimensions right

- The best way to debug your matrices dimensions is by a pencil and paper.
- Dimension of `W` is `(n[l],n[l-1])` . Can be thought by right to left.
- Dimension of `b` is `(n[l],1)`
- `dw` has the same shape as `W` , while `db` is the same shape as `b`
- Dimension of `Z[l]`, `A[l]` , `dZ[l]` , and `dA[l]` is `(n[l],m)`

Forward and Backward Propagation

- Pseudo code for forward propagation for layer l:

```
Input  A[l-1]
Z[l] = W[l]A[l-1] + b[l]
A[l] = g[l](Z[l])
Output A[l], cache(Z[l])
```

- Pseudo code for back propagation for layer l:

```
Input da[l], Caches
dZ[l] = dA[l] * g'[l](Z[l])
dW[l] = (dZ[l]A[l-1].T) / m
db[l] = sum(dZ[l])/m                # Dont forget axis=1, keepdims=True
dA[l-1] = w[l].T * dZ[l]            # The multiplication here are a dot product.
Output dA[l-1], dW[l], db[l]
```

- If we have used our loss function then:

```
dA[L] = (-(y/a) + ((1-y)/(1-a)))
```