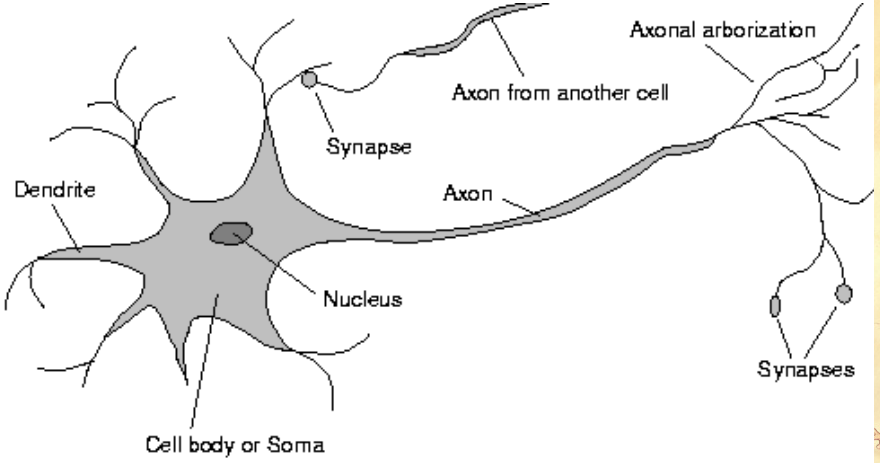
Neural networks

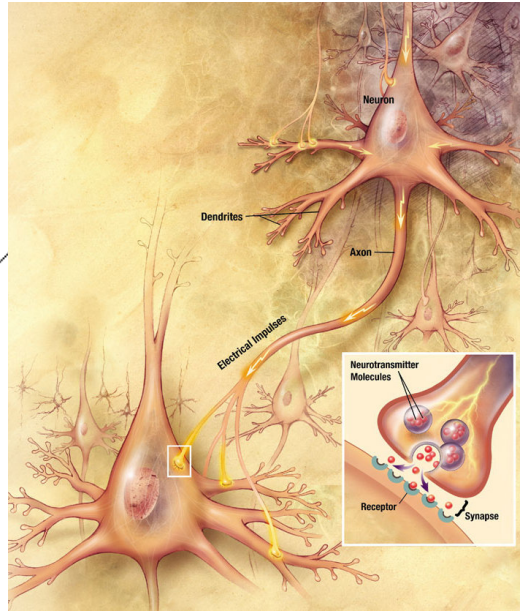
Brain function

(thought)occurs as the result of the firing of **neurons**

- Neurons connect to each other through **synapses**, which propagate **action potential** (electrical impulses) by releasing **neurotransmitters**
- Synapses can be **excitatory** (potential-increasing) or **inhibitory** (potential-decreasing), and have varying **activation thresholds**
- Learning occurs as a result of the synapses' **plasticicity**: They exhibit long-term changes in connection strength
- There are about 10^{11} neurons and about 10^{14} synapses in the human brain!

Neural networks





Neural networks

Brain structure

- Different areas of the brain have different functions
- Some areas seem to have the same function in all humans (e.g., Broca's region for motor speech); the overall layout is generally consistent
- Some areas are more plastic, and vary in their function; also, the lower-level structure and function vary greatly
- We don't know how different functions are "assigned" or acquired

Partly the result of the physical layout / connection to inputs (sensors) and outputs (effectors)

Partly the result of experience (learning)

- We *really* don't understand how this neural structure leads to what we perceive as "consciousness" or "thought"

Neural networks

Origins:

- Algorithms that try to mimic the brain.
- Very widely used in 80s and early 90s;popularity diminished in late 90s.
- Recent resurgence: State-of-the-art technique for many applications
- Artificial neural networks are not nearly as complex or intricate as the actual brain structure

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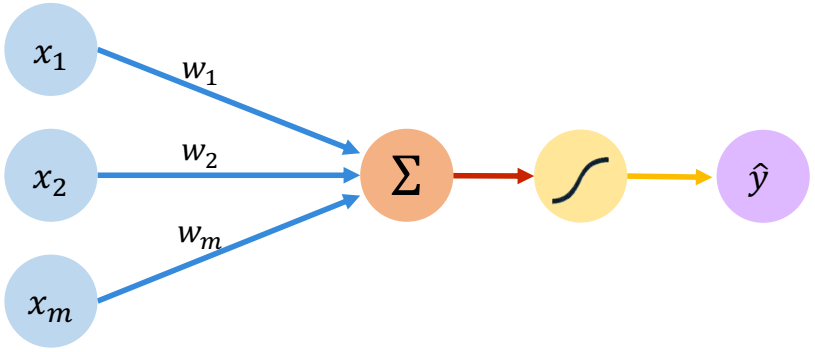
The Perceptron: Forward Propagation



Inputs Weights Sum Non-Linearity Output

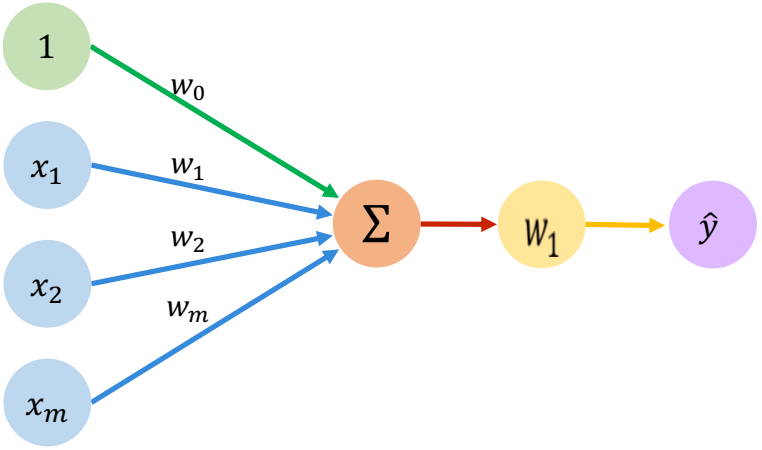
Output

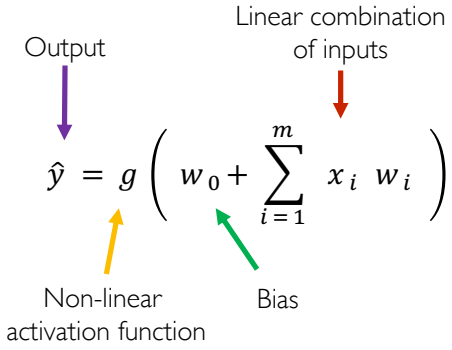
Linear combination of inputs

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

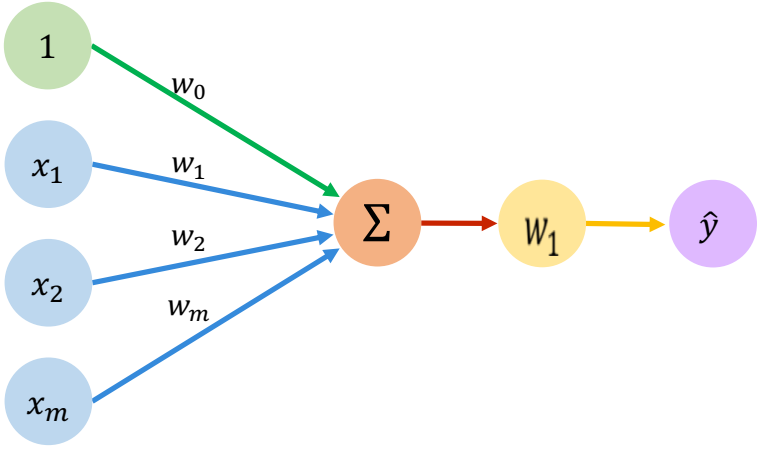
Non-linear activation function

The Perceptron: Forward Propagation





The Perceptron: Forward Propagation



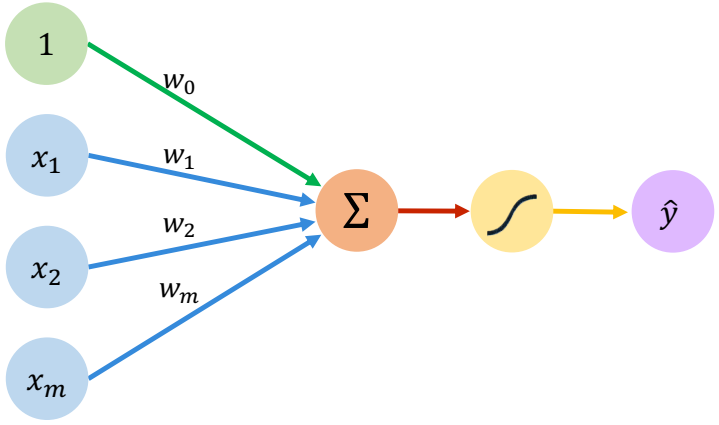
Inputs Weights Sum Non-Linearity Output

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

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

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

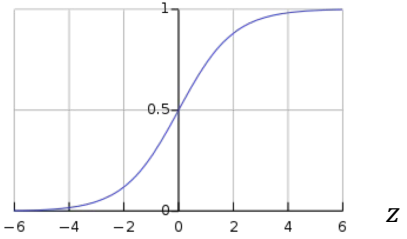


Activation Functions

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

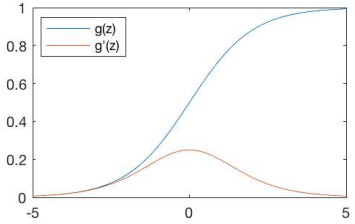
- Example: sigmoid function

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



Common Activation Functions

Sigmoid Function

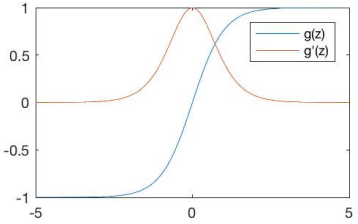


$$g(z) = \frac{1}{1 + e^{-z}}$$

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

`tf.nn.sigmoid(z)`

Hyperbolic Tangent

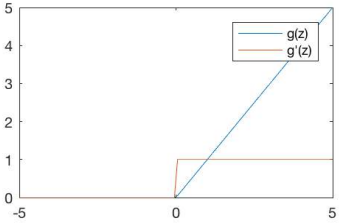


$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

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

`tf.nn.tanh(z)`

Rectified Linear Unit (ReLU)



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

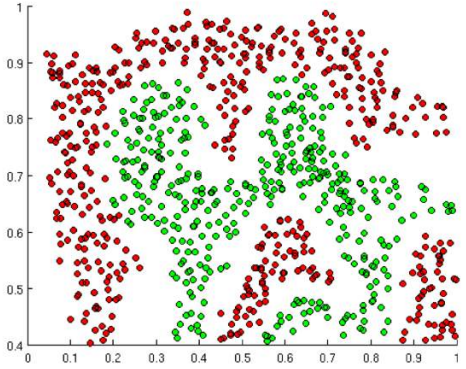
$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

`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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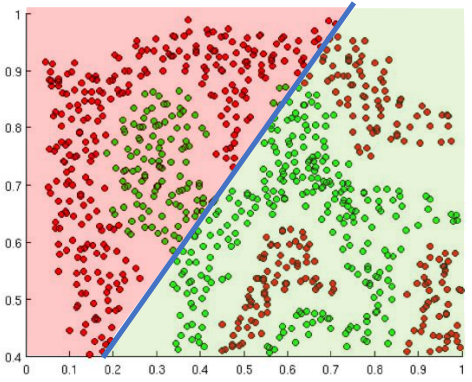
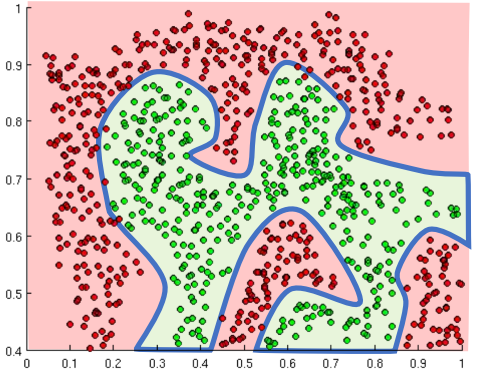
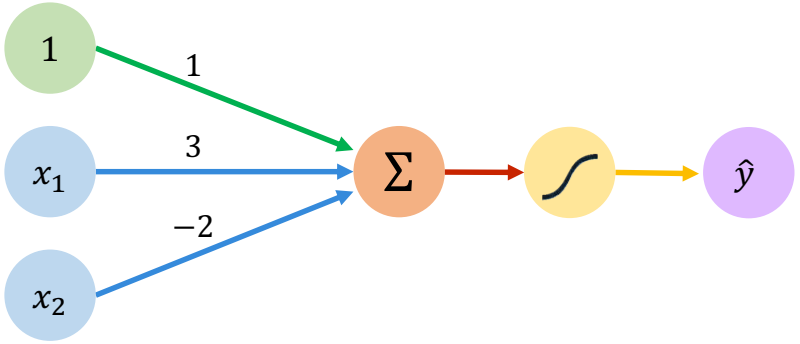


Linear Activation functions produce linear decisions no matter the network size



Non-linearities allow us to approximate arbitrarily complex functions

The Perceptron: Example



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

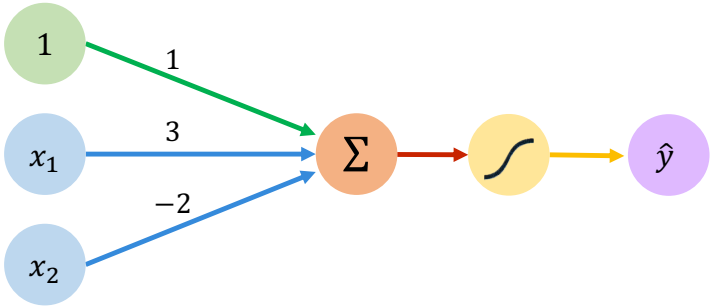
$$\hat{y} = g(w_0 + \boldsymbol{X}^T \boldsymbol{W})$$

$$= g\left(1 + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 3 \\ -2 \end{bmatrix}\right)$$

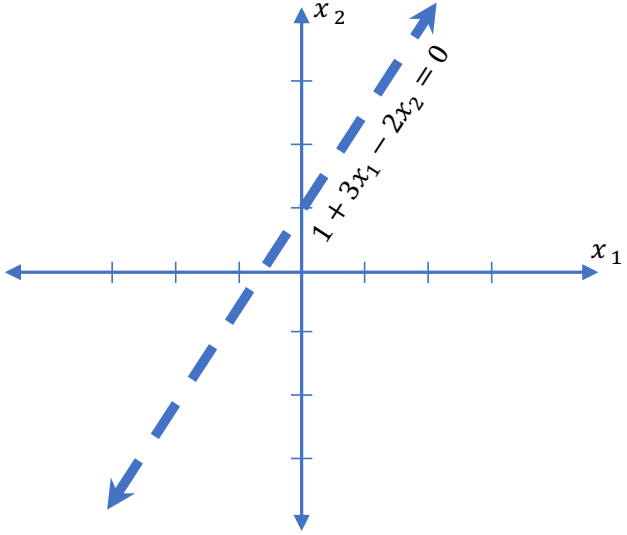
$$\hat{y} = g(1 + 3x_1 - 2x_2)$$

This is just a line in 2D!

The Perceptron: Example



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



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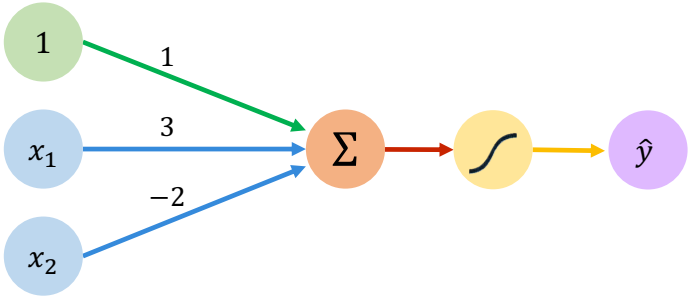
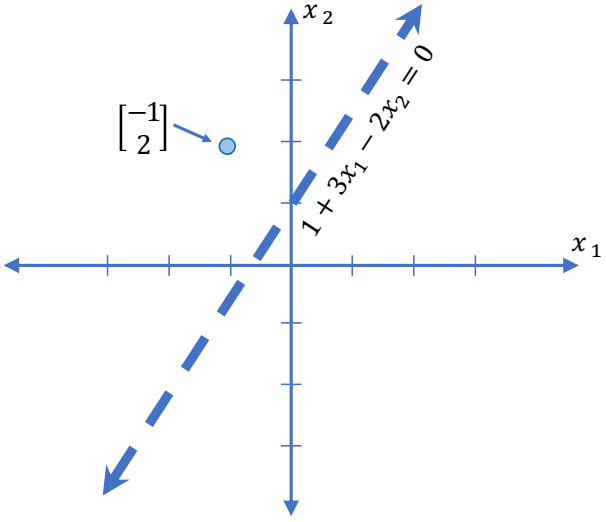


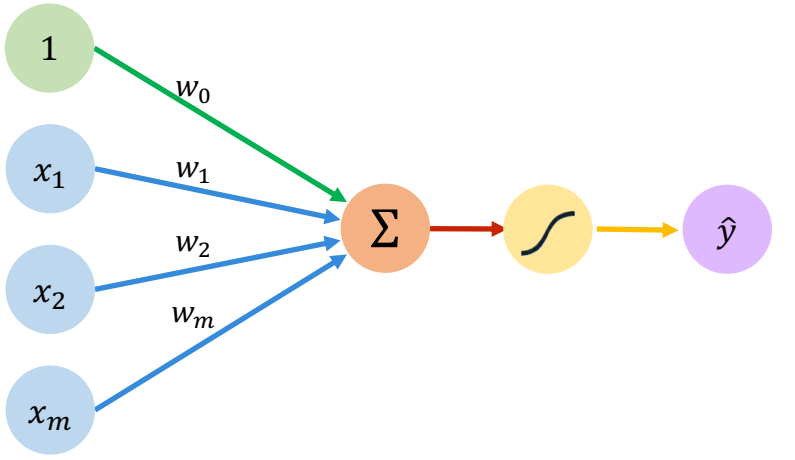
Assume we have input: $\boldsymbol{X} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$

$$\hat{y} = g\left(1 + (3 * -1) - (2 * 2)\right)$$
$$= g(-6) \approx 0.002$$

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



The Perceptron: Simplified



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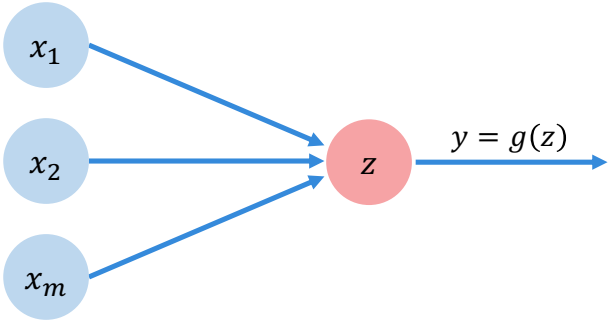
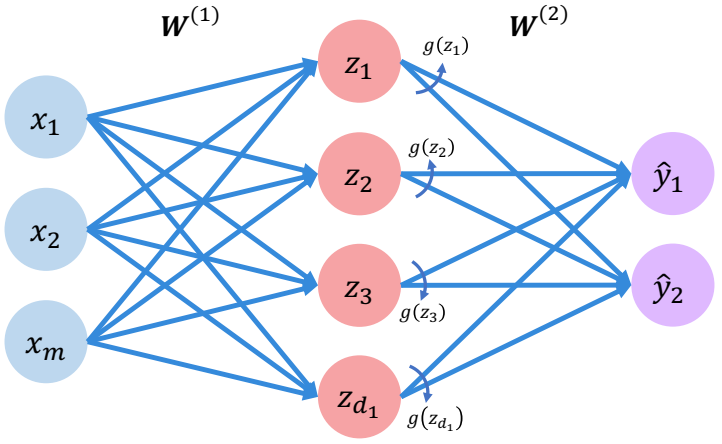


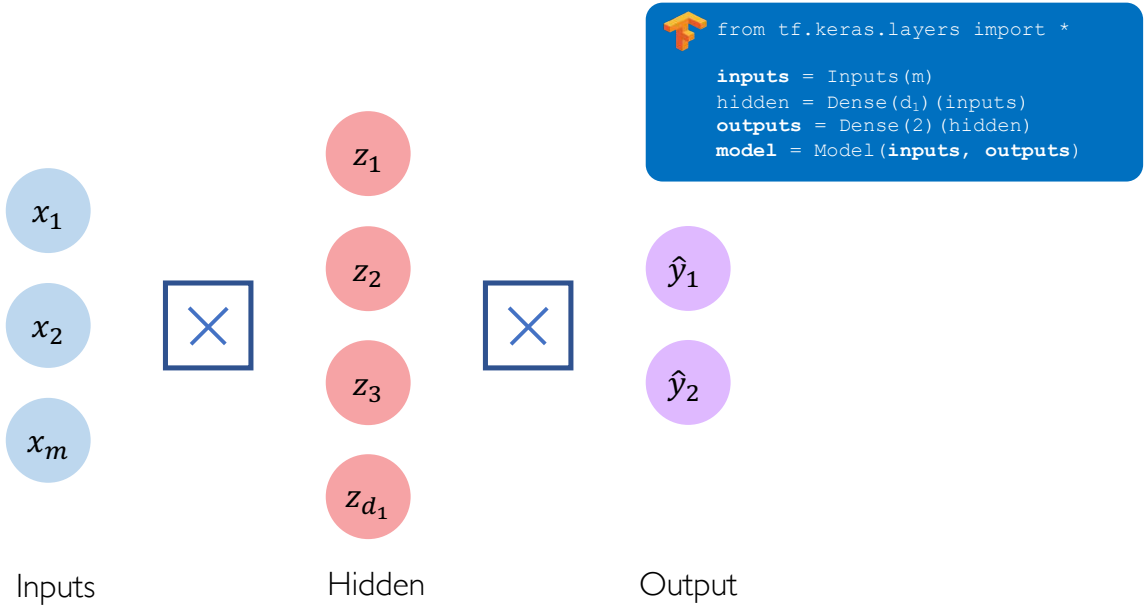
$$z = w_0 + \sum_{j=1}^{m} x_j w_j$$

Single Layer Neural Network

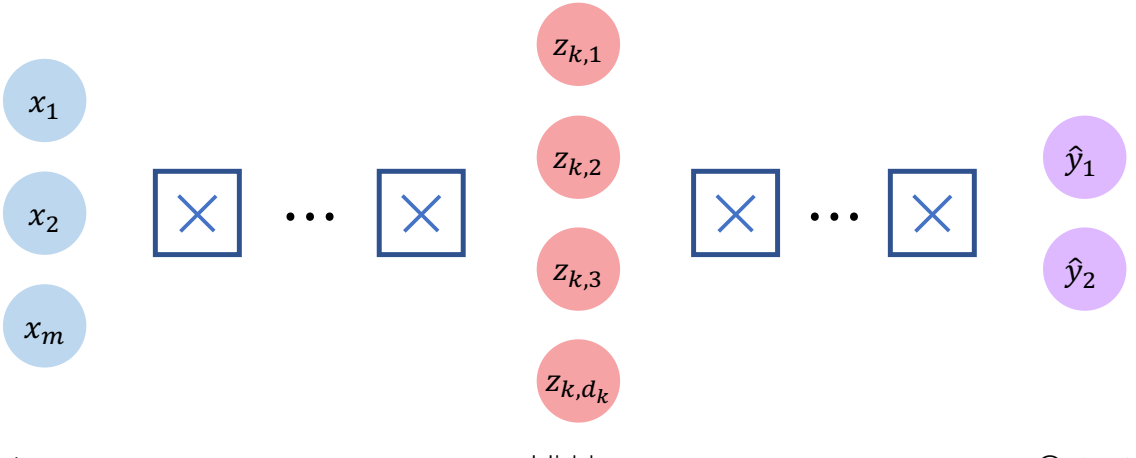


$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^{m} x_j \, w_{j,i}^{(1)} \qquad \hat{y}_i = g\left(w_{0,i}^{(2)} + \sum_{j=1}^{d_1} z_j \, w_{j,i}^{(2)}\right)$$

Multi Output Perceptron

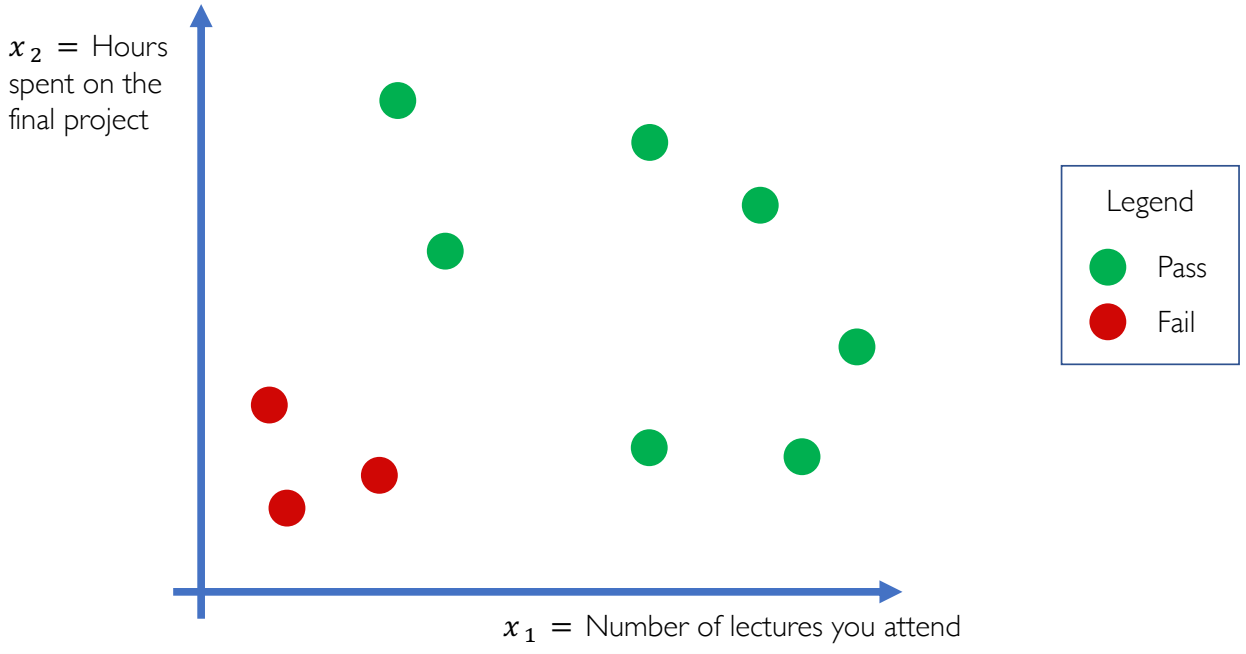


Deep Neural Network



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

Example Problem: Will I pass this class?



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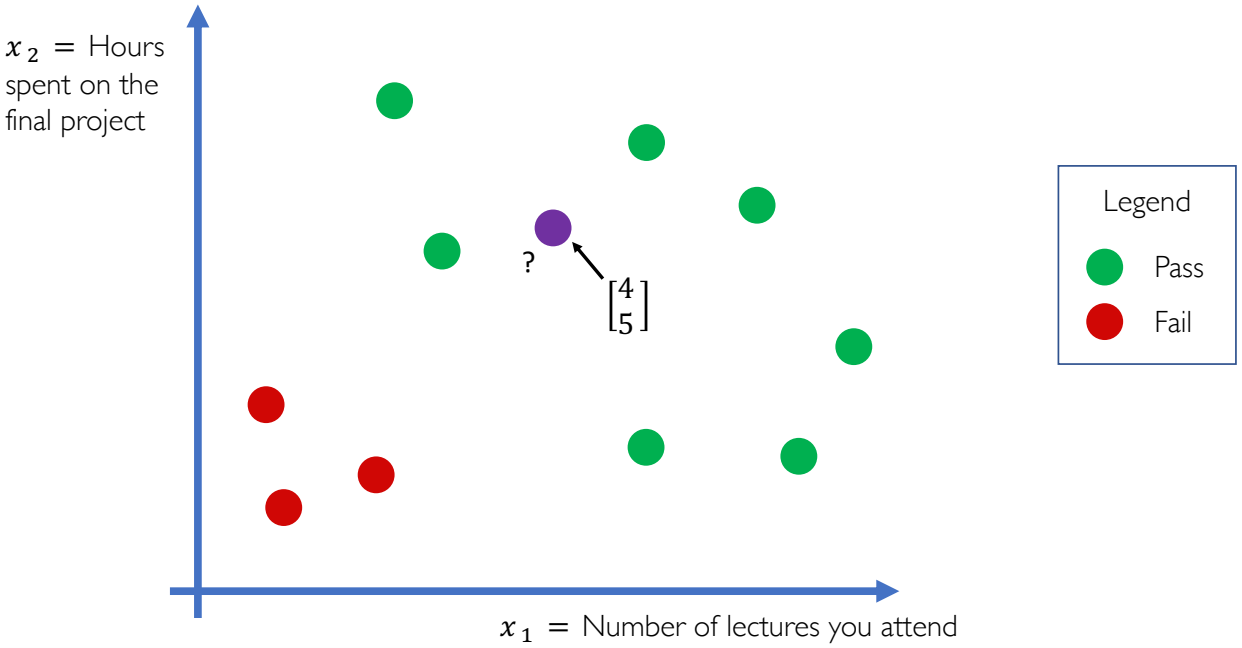

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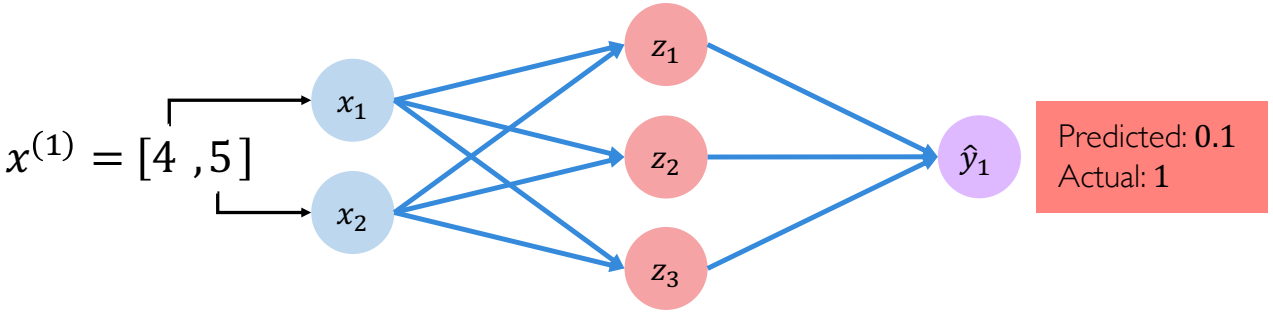
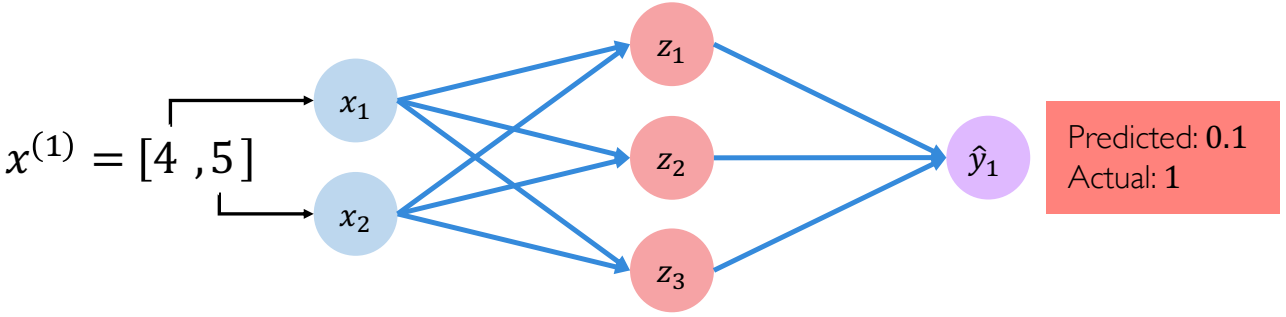


Quantifying Loss

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

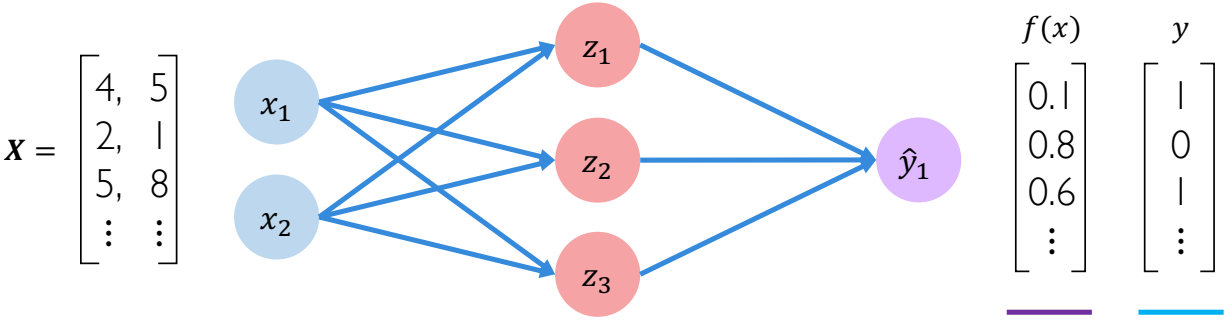


$$\mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

Predicted Actual

Empirical Loss

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



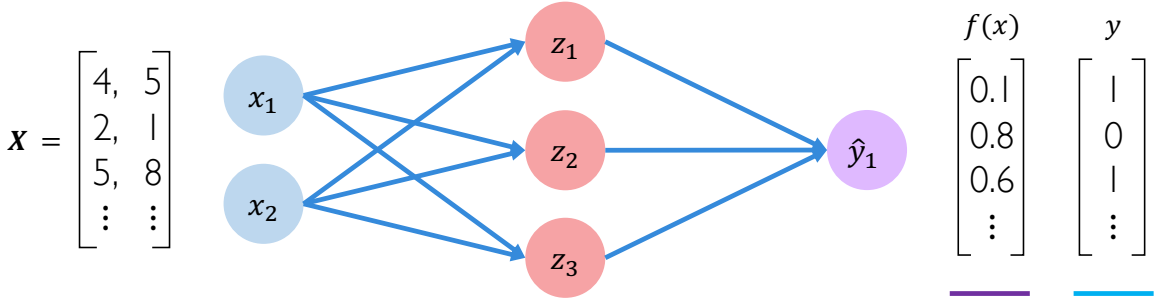
$$J(\boldsymbol{W}) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

Predicted Actual

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

Binary Cross Entropy Loss

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

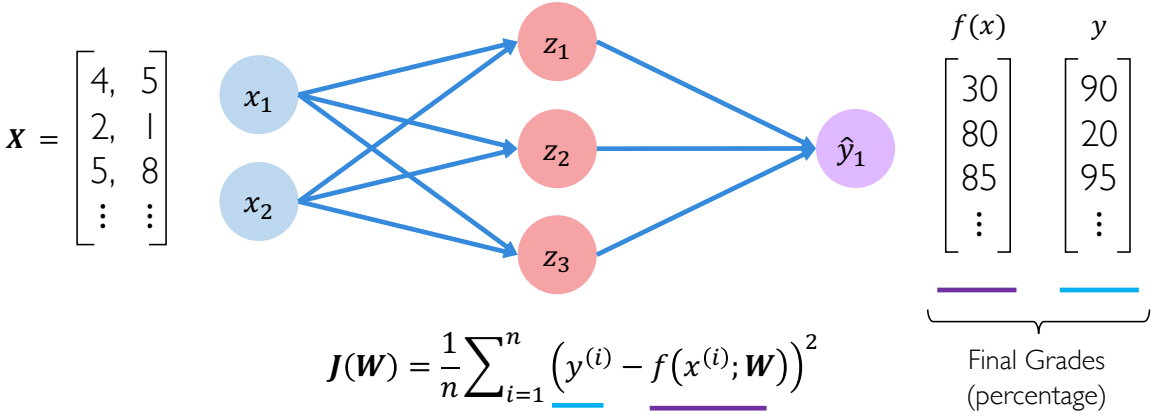


$$J(W) = \frac{1}{n}\sum_{i=1}^{n} \underbrace{y^{(i)}}_{\text{Actual}} \log\Big(\underbrace{f\big(x^{(i)}; W\big)}_{\text{Predicted}}\Big) + (1 - \underbrace{y^{(i)}}_{\text{Actual}}) \log\Big(1 - \underbrace{f\big(x^{(i)}; W\big)}_{\text{Predicted}}\Big)$$

```
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) )
```

Neural networks: training

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

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

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

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Remember:

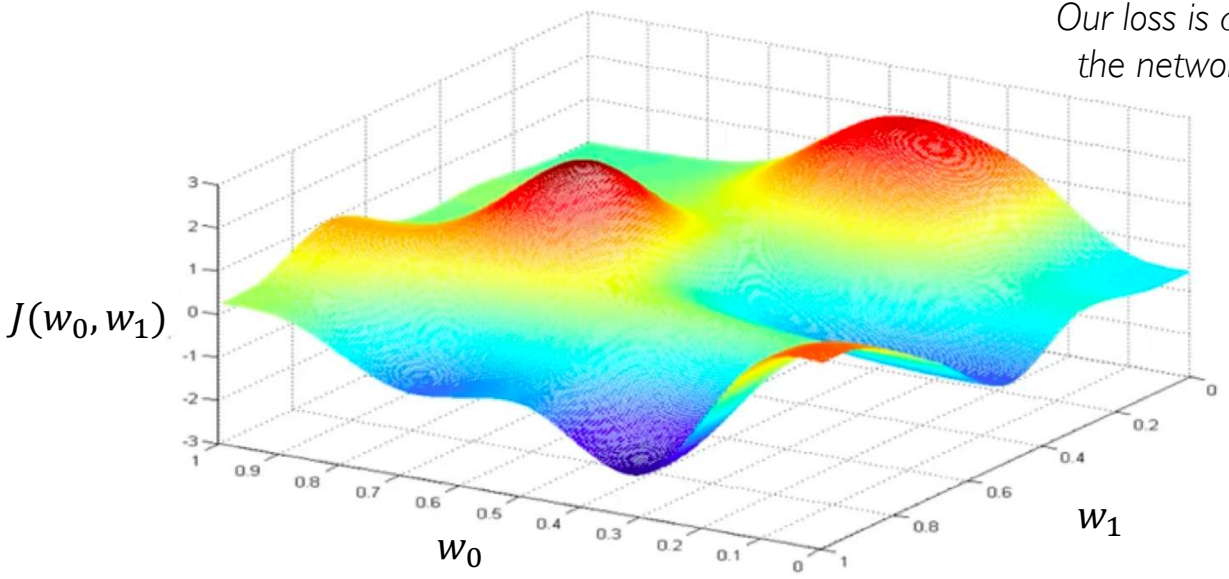
$$\boldsymbol{W} = \left\{\boldsymbol{W}^{(0)}, \boldsymbol{W}^{(1)}, \dots\right\}$$

Neural networks: training

Many local minima – want to achieve a global minimum

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

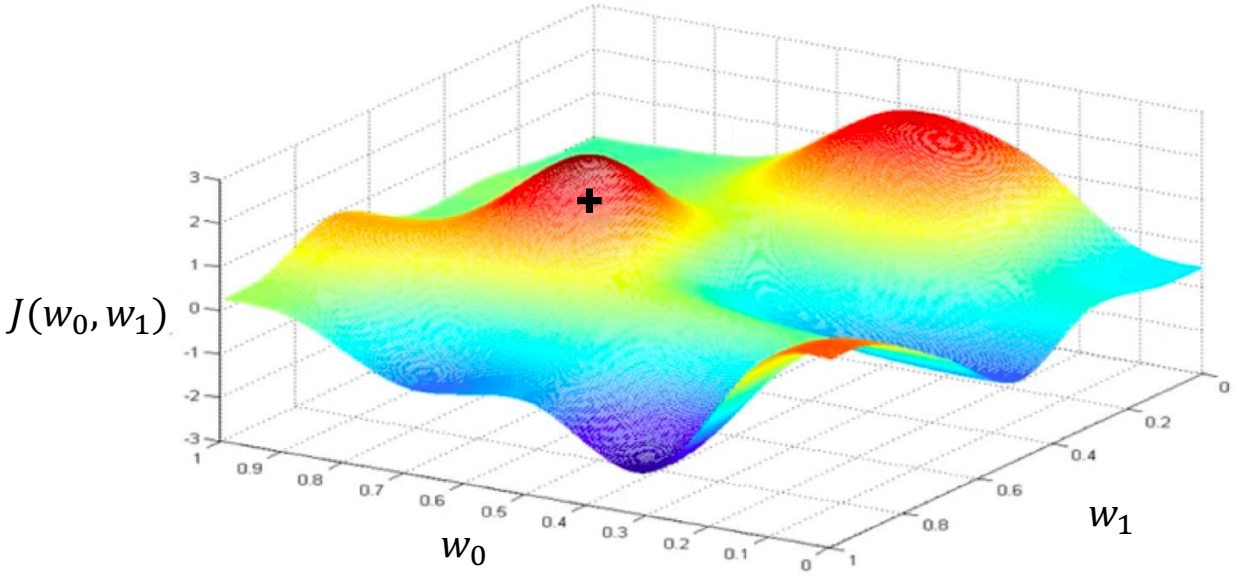
Remember:
Our loss is a function of the network weights!



Neural networks: training

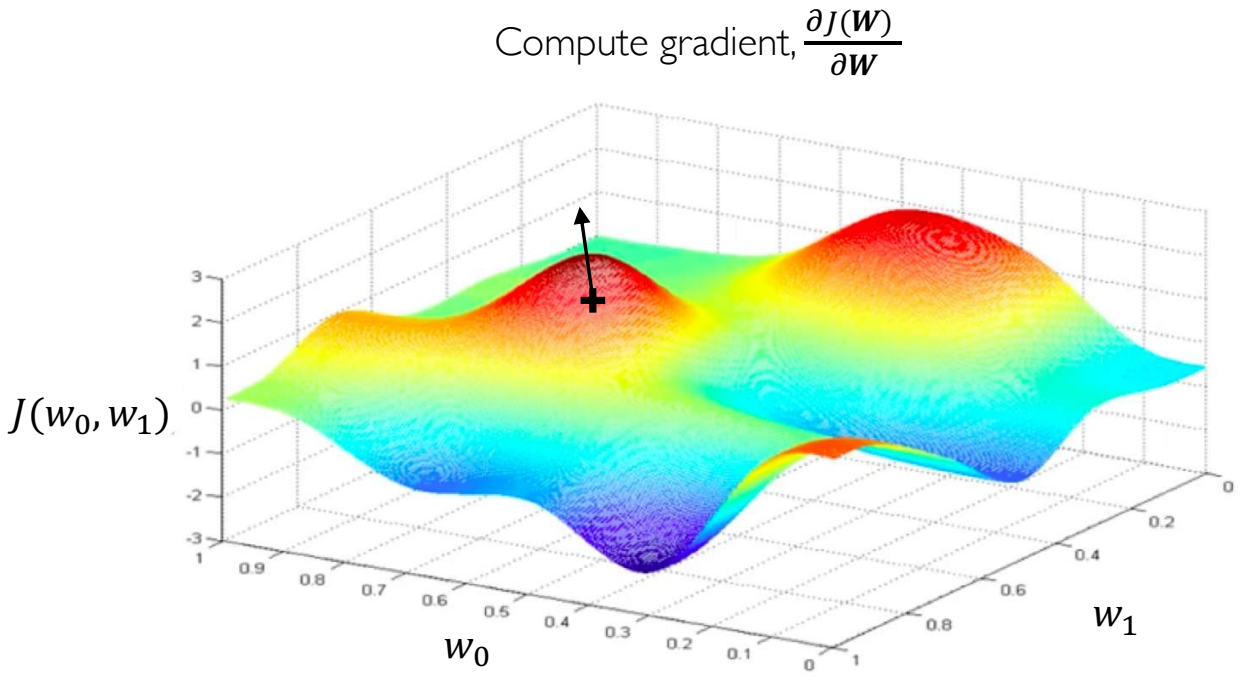
Initial weights and biases – typically from normal unit distribution

Randomly pick an initial (w_0, w_1)



Neural networks: training

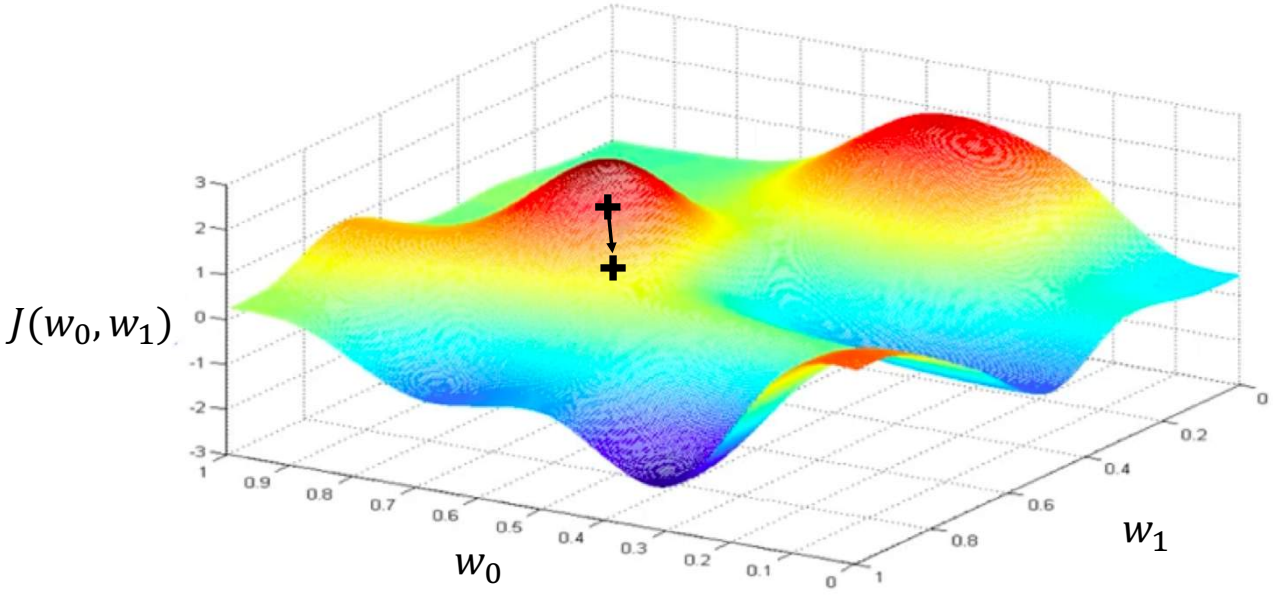
"Local" gradients – nonlinear need to compute it on sample/minibatch



Neural networks: training

Gradient descent

Take small step in opposite direction of gradient



Neural networks: training

Gradient descent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$

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

2. Loop until convergence:
3. Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$

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

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

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

5. Return weights

Neural networks: training

Gradient descent

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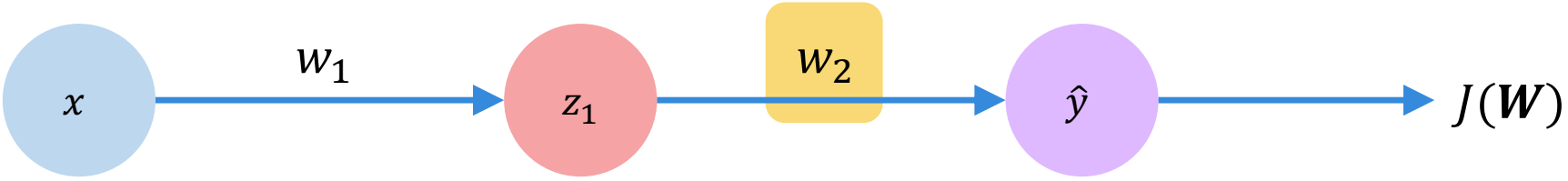
Neural networks: gradients

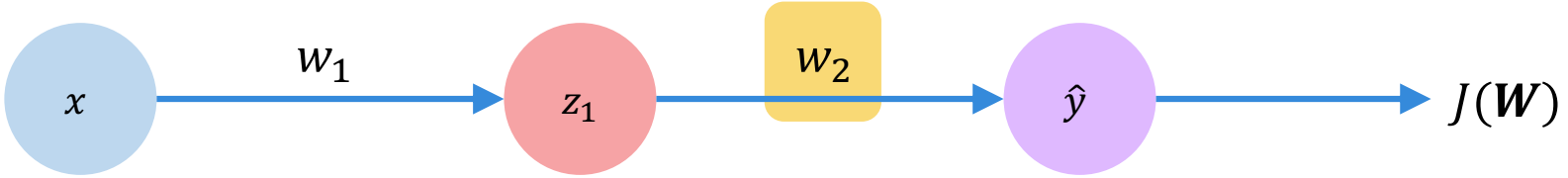
How do we compute gradients?



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

Neural networks: gradients

How do we compute gradients?
Backpropagation

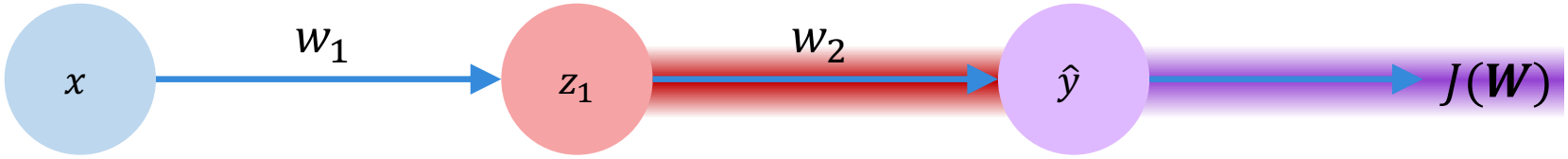


$$\frac{\partial J(\boldsymbol{W})}{\partial w_2} =$$

Let's use the chain rule!

Neural networks: gradients

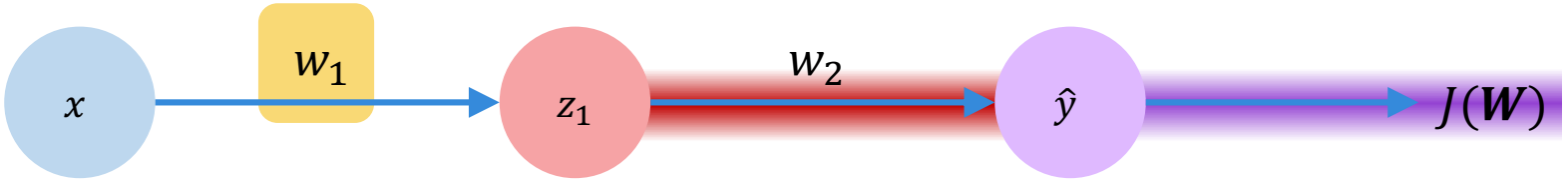
How do we compute gradients?
Backpropagation



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

Neural networks: gradients

How do we compute gradients?
Backpropagation



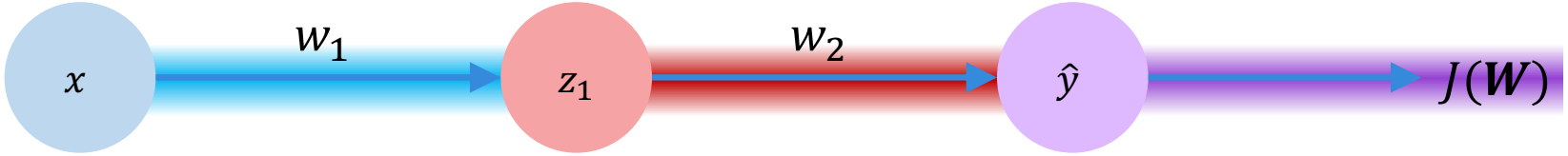
$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_1}$$

Apply chain rule!

Apply chain rule!

Neural networks: gradients

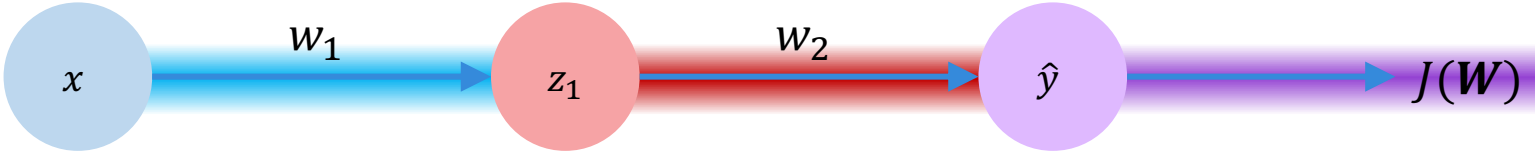
How do we compute gradients?
Backpropagation



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

Neural networks: gradients

How do we compute gradients?
Backpropagation

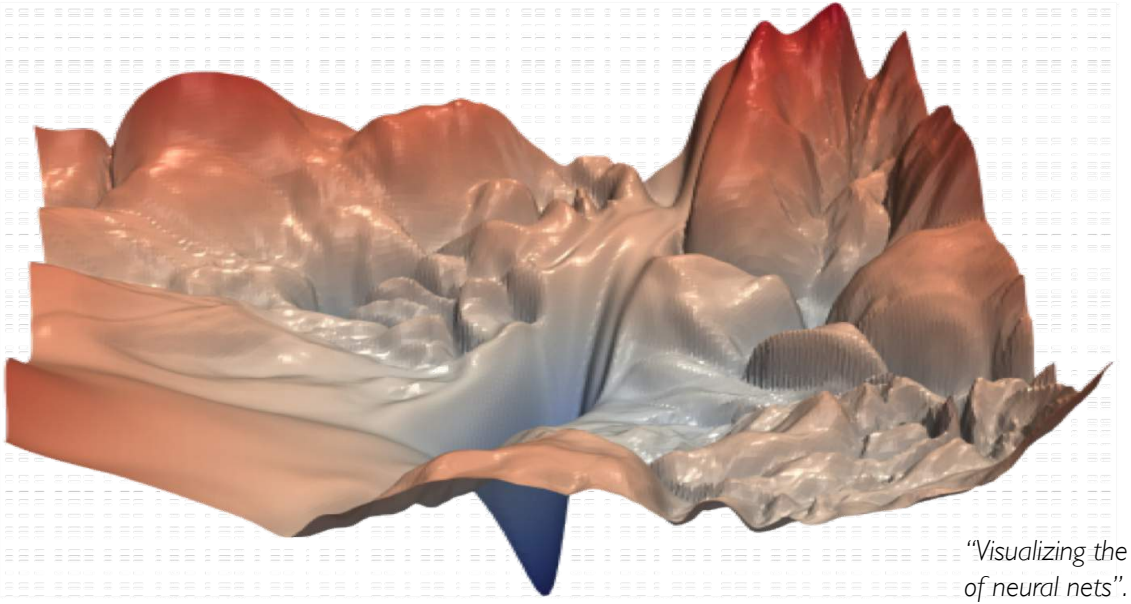


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

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

Neural networks: training

Loss function is complex



"Visualizing the loss landscape of neural nets". Dec 2017.

Neural networks: training

Loss function is complex
Learning rate?

Remember:

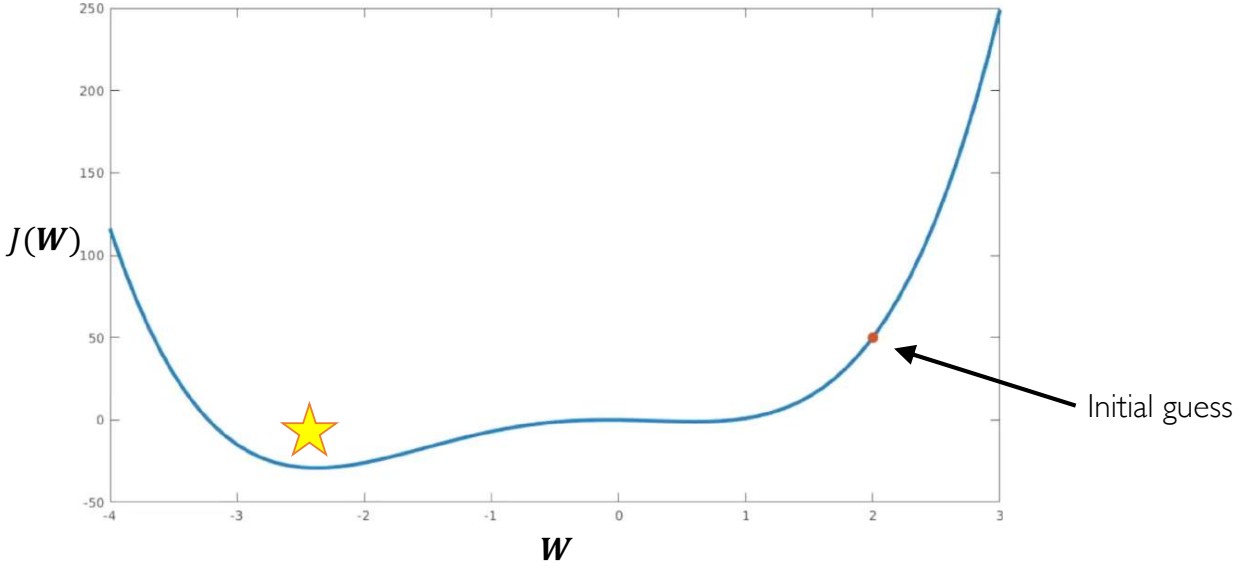
Optimization through gradient descent

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

Neural networks: training

Loss function is complex
Learning rate?

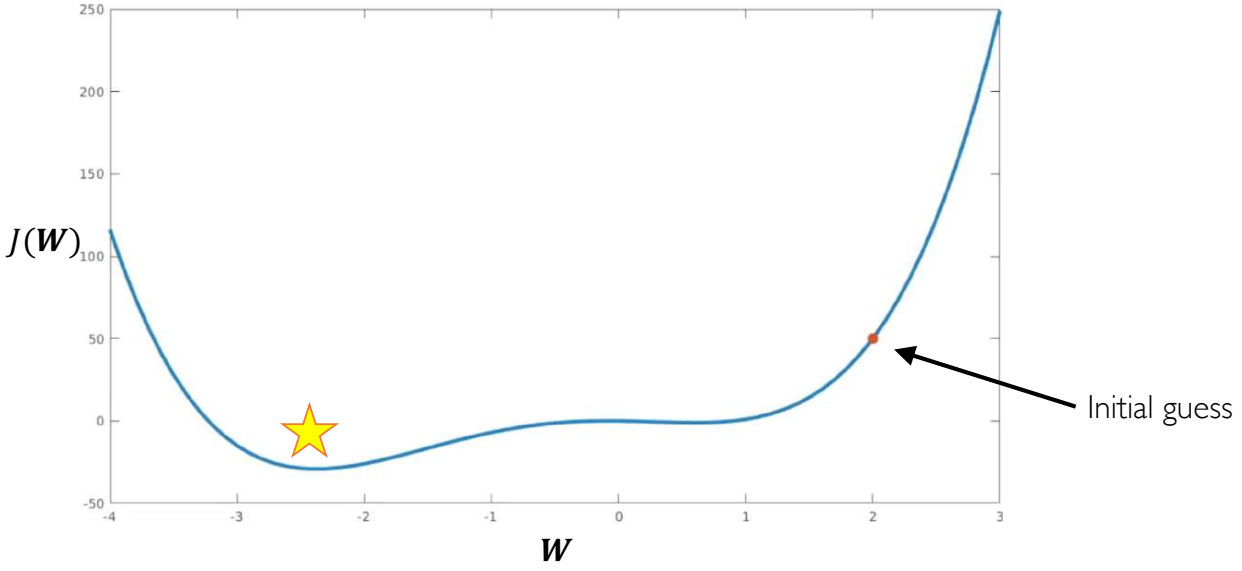
Small learning rate *converges slowly and gets stuck in false local minima*



Neural networks: training

Loss function is complex
Learning rate?

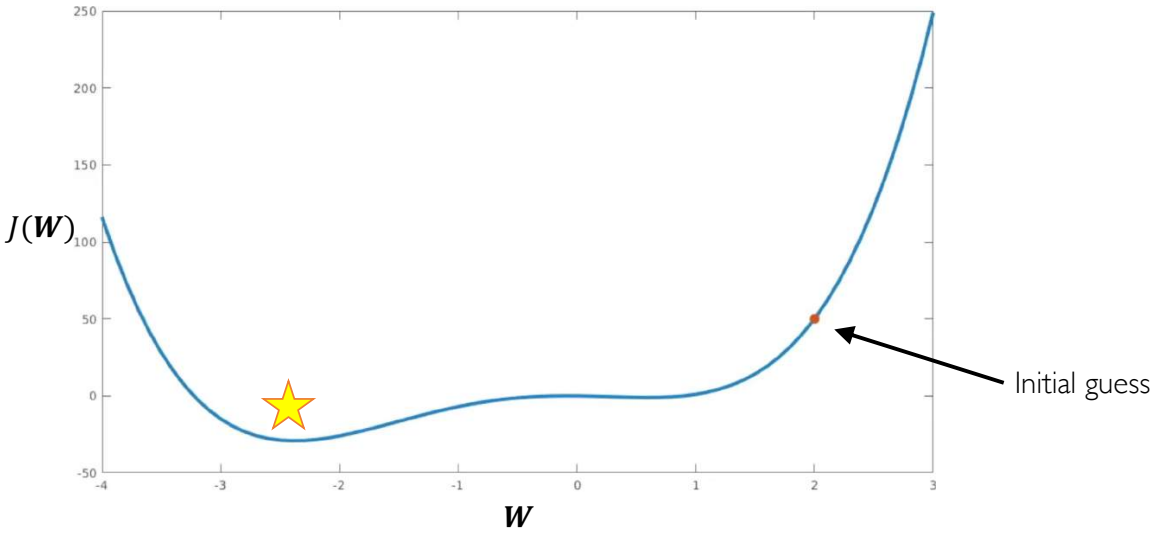
Small learning rate *converges slowly and gets stuck in false local minima*



Neural networks: training

Loss function is complex
Learning rate?

Large learning rates *overshoot, become unstable and diverge*



Neural networks: training

How can we handle 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

Neural networks: training

How can we handle this?

- 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...

Neural networks: training

Learning rates

- Momentum
- Adagrad
- Adadelta
- Adam
- RMSProp

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

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

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

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

Neural networks: training

Learning rates

Momentum – large rate but dampens oscillations

Image 2: SGD without momentum

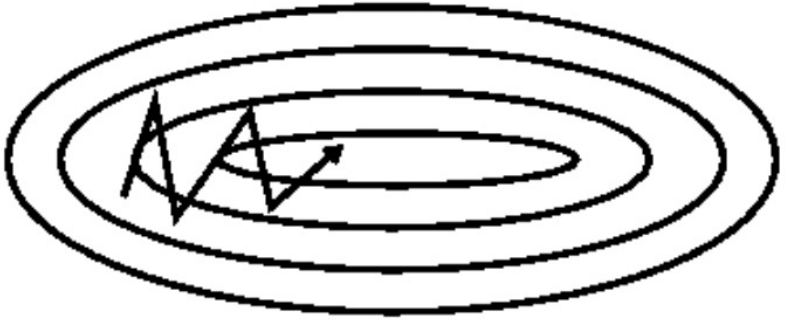


Image 3: SGD with momentum

Neural networks: training

Learning rates

Adagrad - adapts the learning rate to the parameters, performing smaller updates (i.e. low learning rates) for parameters associated with frequently occurring features, and larger updates (i.e. high learning rates) for parameters associated with infrequent features. Accumulates past gradients. Well-suited for dealing with sparse data

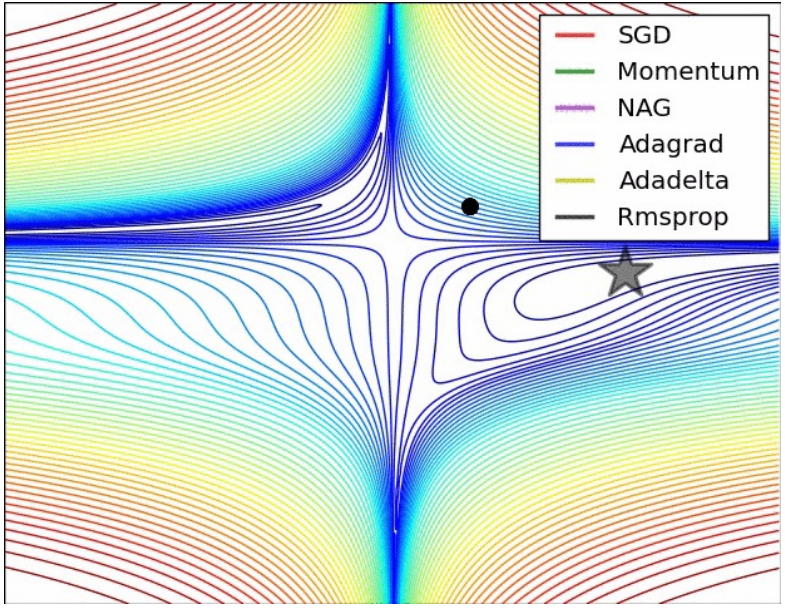
Adadelta - is an extension of Adagrad that seeks to reduce its aggressive, monotonically decreasing learning rate. Instead of accumulating all past squared gradients, Adadelta restricts the window of accumulated past gradients to some fixed size w.

Neural networks: training

Learning rates

Adam - Adaptive Moment Estimation (Adam) is another method that computes adaptive learning rates. In addition to storing an exponentially decaying average of past squared gradients like Adadelta, Adam also keeps an exponentially decaying average of past gradients mt, similar to momentum. Whereas momentum can be seen as a ball running down a slope, Adam behaves like a heavy ball with friction, which thus prefers flat minima in the error surface.

Neural networks: training

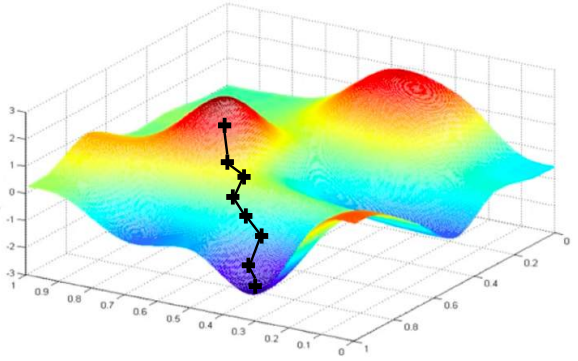


Gradient Descent

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

Can be very computational to compute!

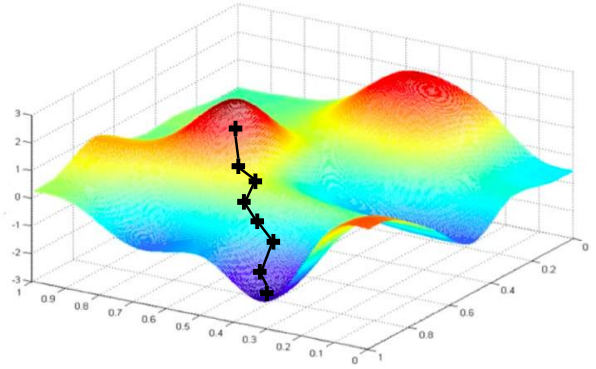


Stochastic Gradient Descent

Algorithm

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

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



Neural networks in practices: mini batches

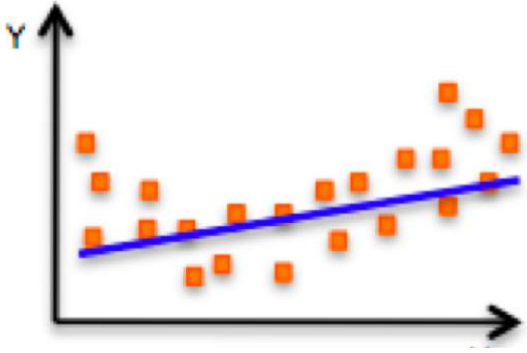
More accurate estimation of gradient

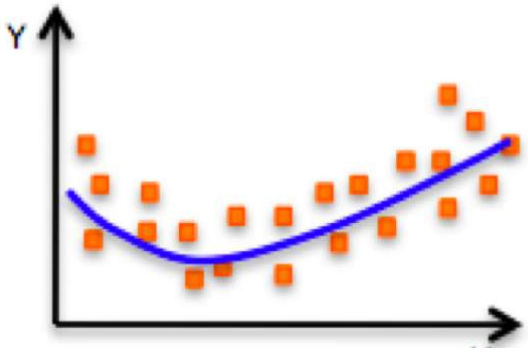
- Smoother convergence
- Allows for larger learning rates

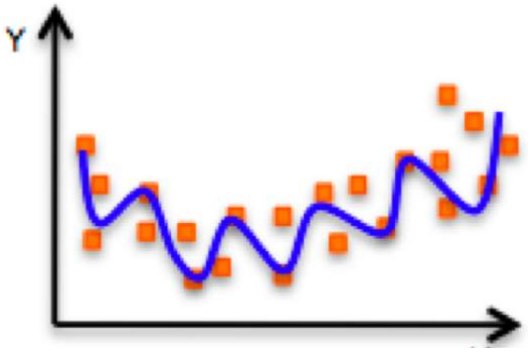
Mini-batches lead to fast training!

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

Neural networks in practices: overfitting







Underfitting
Model does not have capacity to fully learn the data

Ideal fit

Overfitting
Too complex, extra parameters, does not generalize well

Neural networks in practices: overfitting

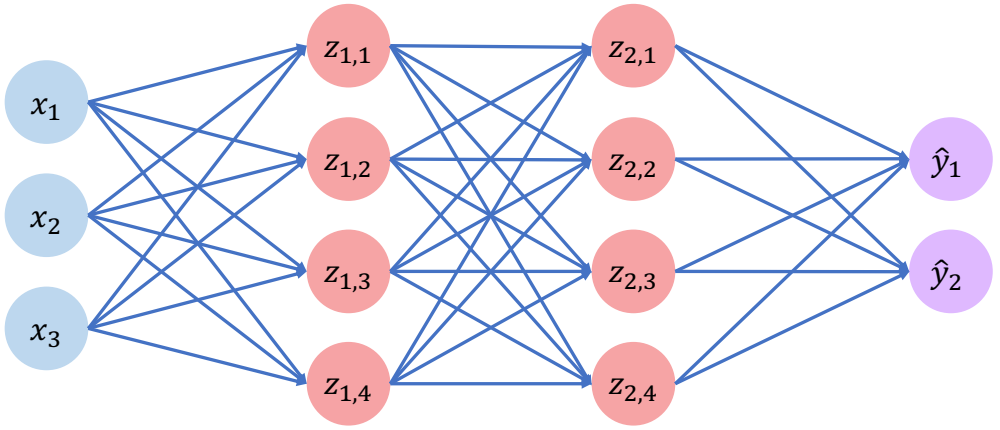
Regularization

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 1: Dropout

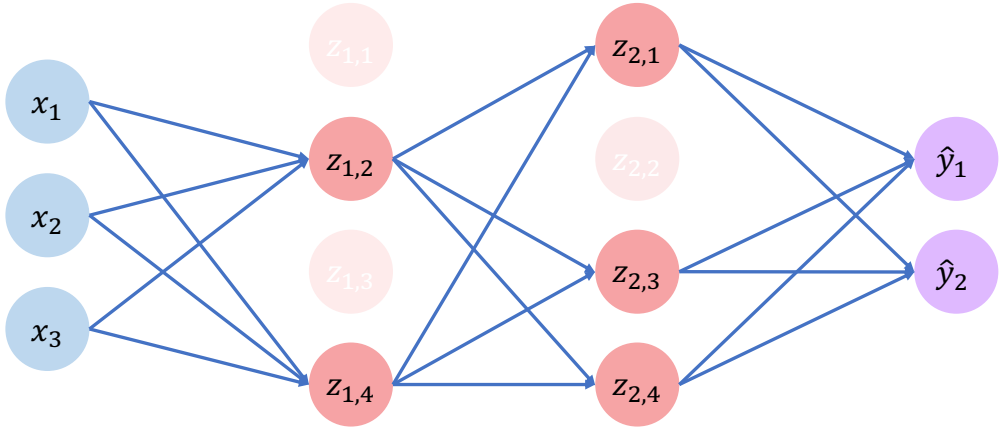
- During training, randomly set some activations to 0



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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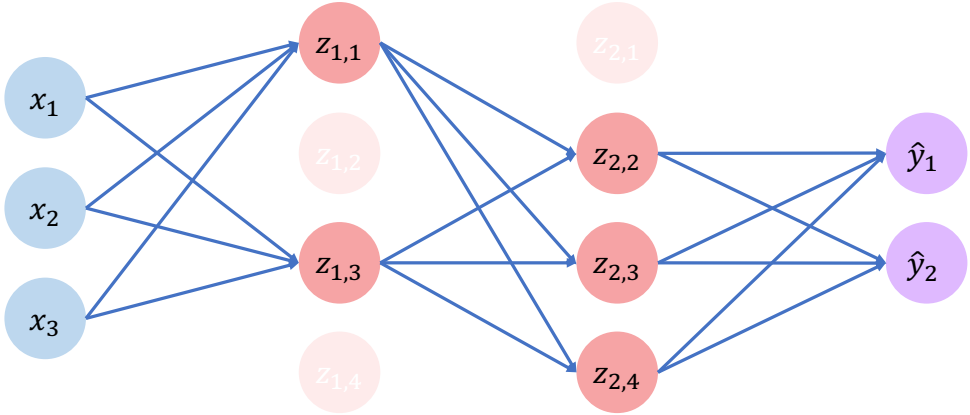

Regularization 2: Early Stopping

- Stop training before we have a chance to overfit

Regularization 2: Early Stopping

- Stop training before we have a chance to overfit

Regularization 3: equal weight variance across layers

Minimize difference in total weights of each layers – avoid vanishing gradients