PennState College of the Liberal Arts

C-SoDA Center for Social Data Analytics

Day 4/5 - Introduction to Neural Nets / Deep Learning for NLP

Advanced Text as Data: Natural Language Processing
Essex Summer School in Social Science Data Analysis

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Pennsylvania State University

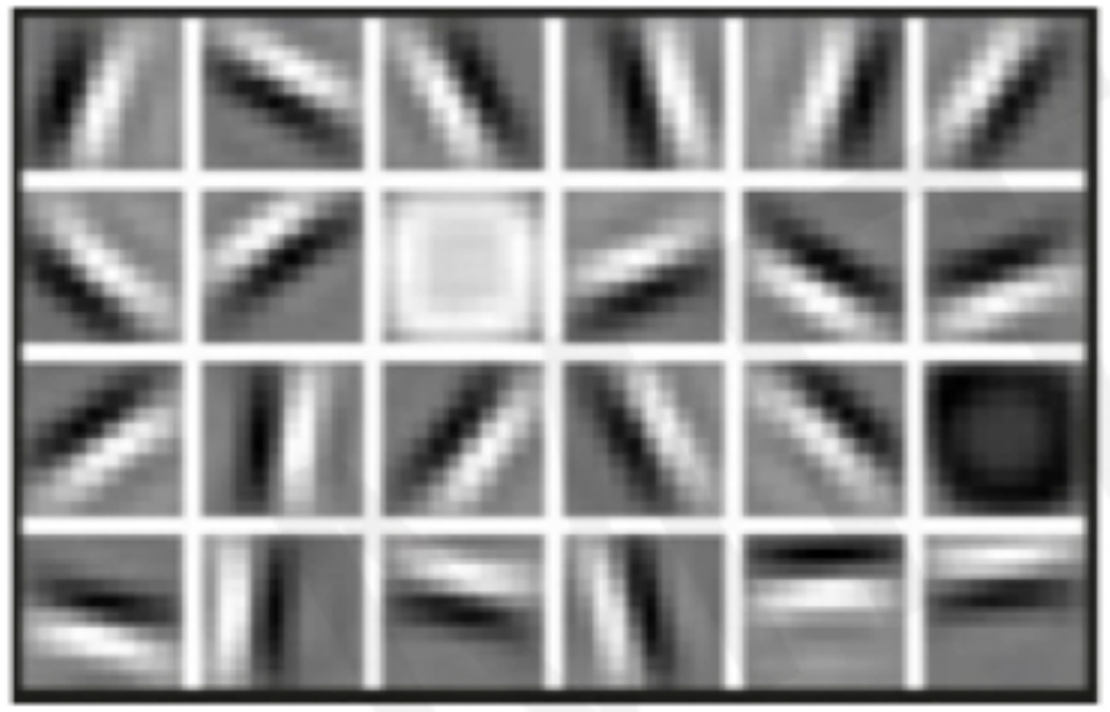
July 29-30, 2021

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

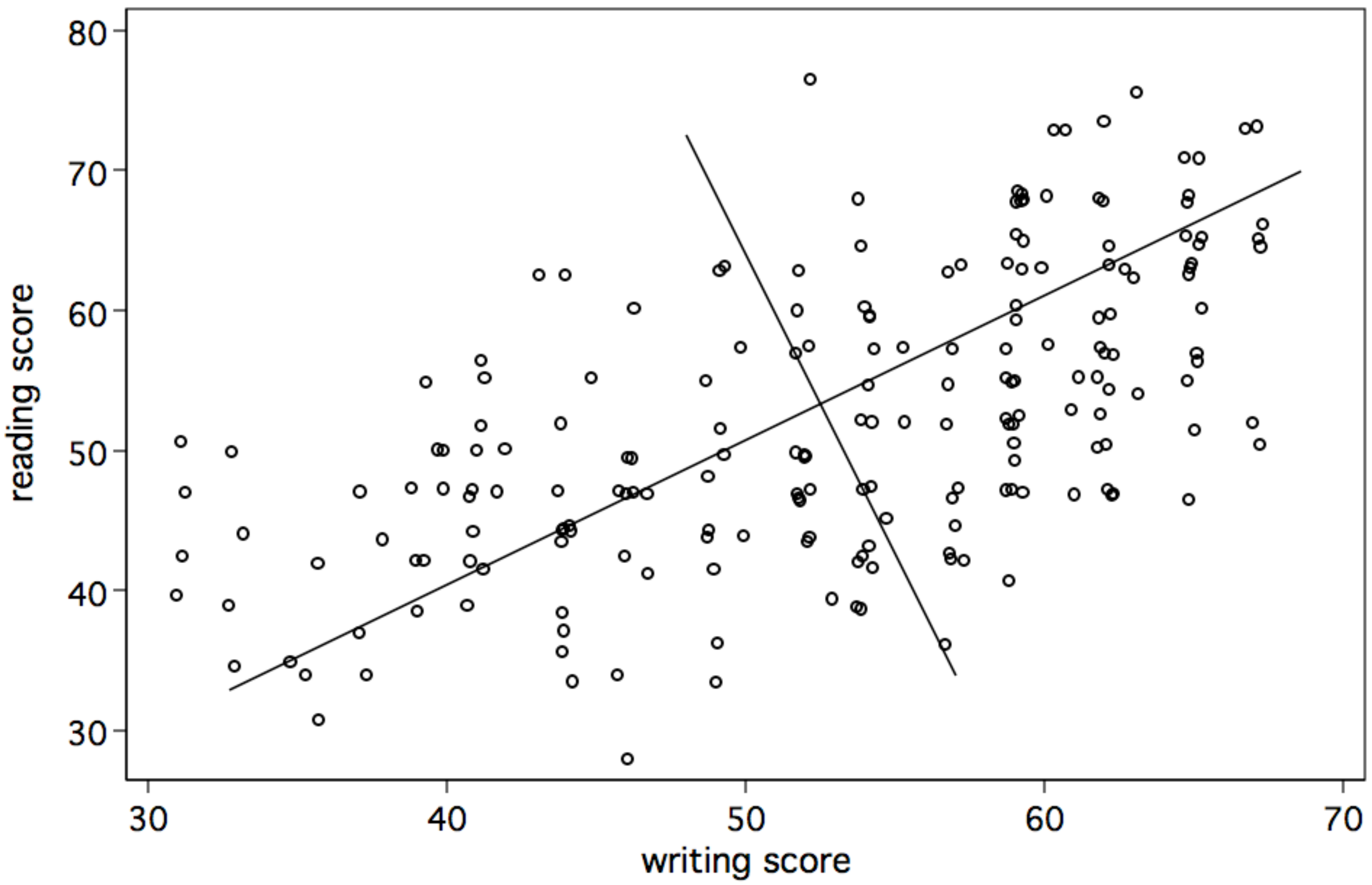
Mid Level Features

Eyes & Nose & Ears

High Level Features

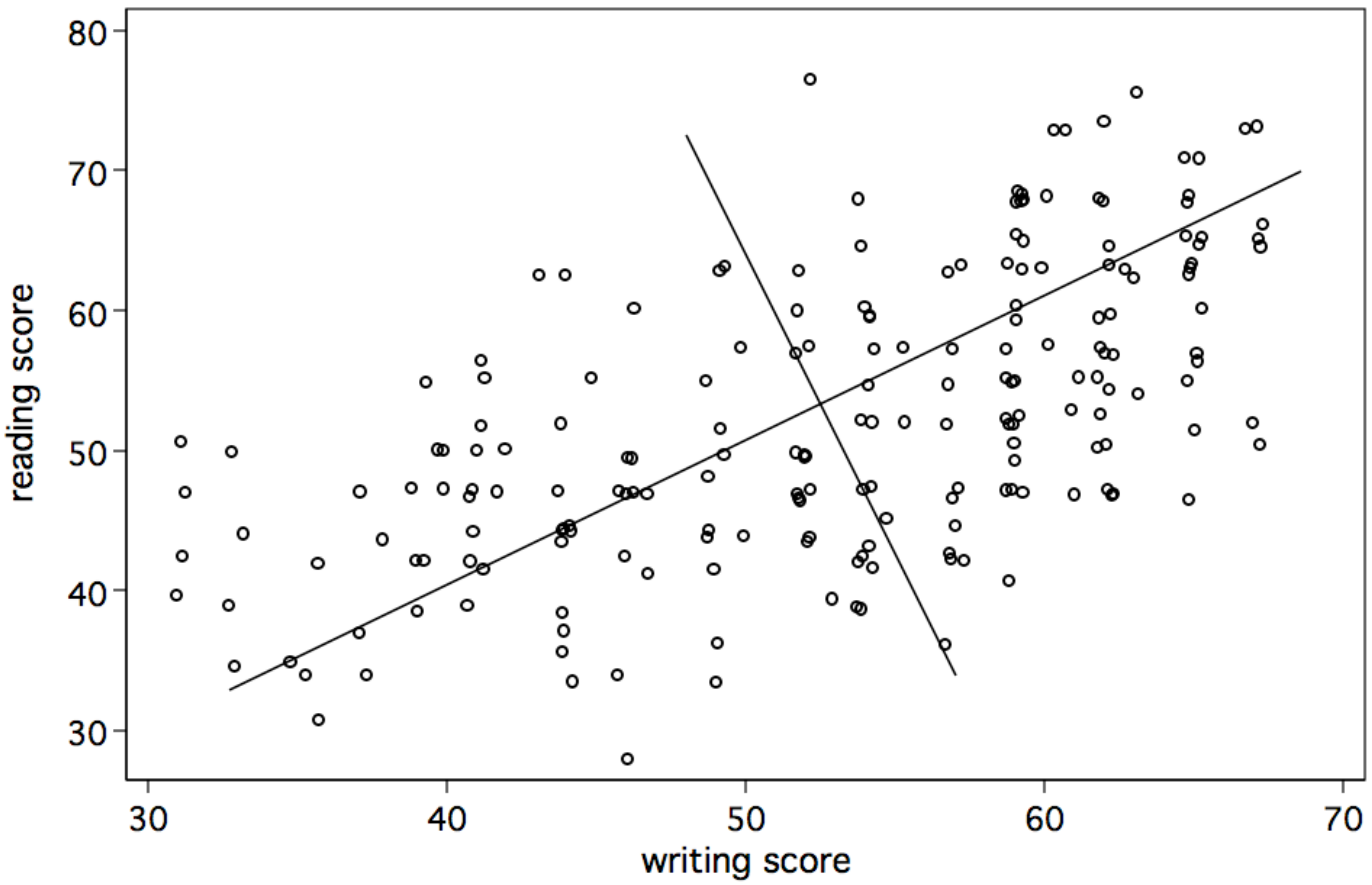
Facial Structure

You've probably seen a lot of linear approaches to finding new feature representations:



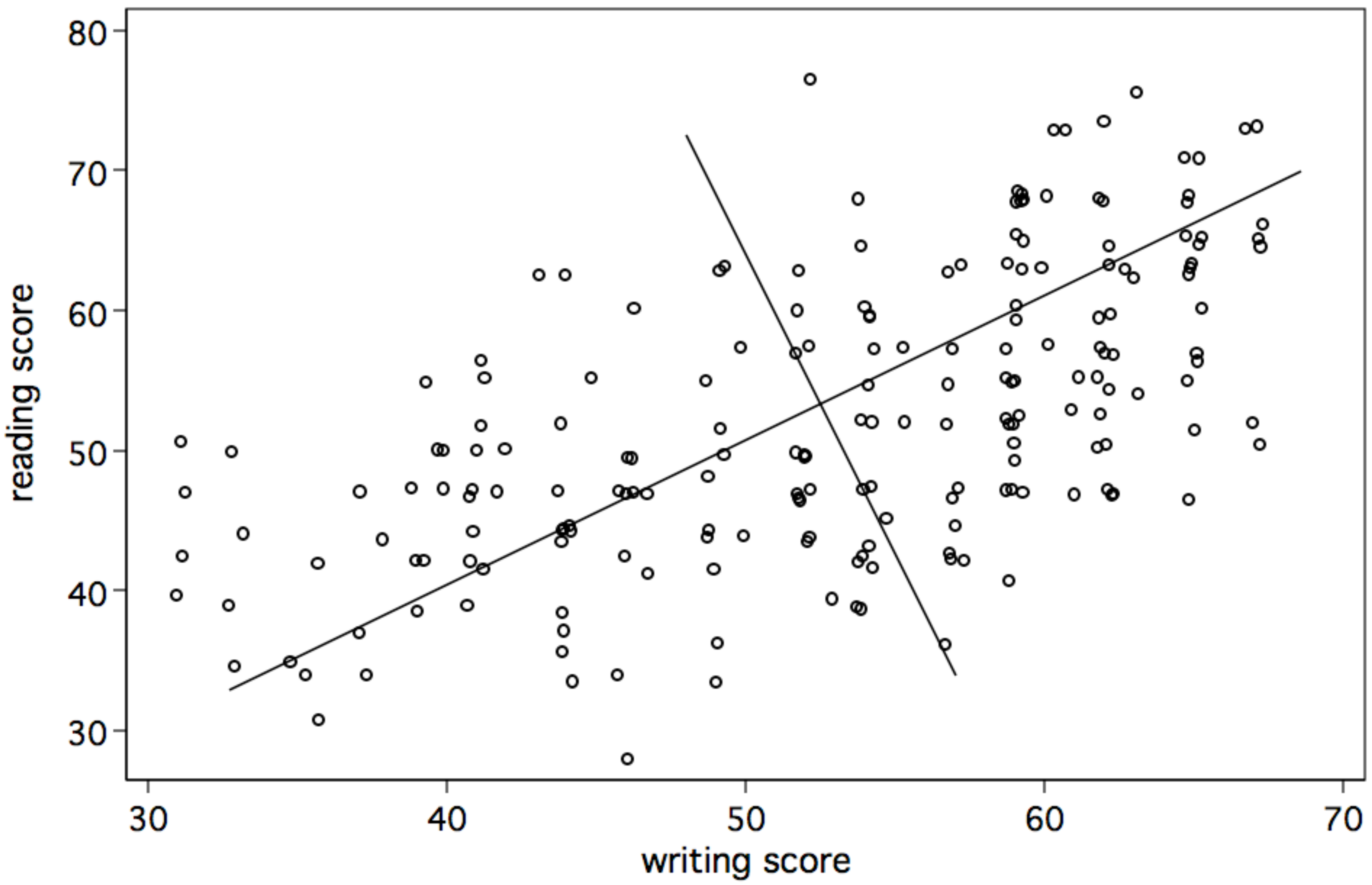
You've probably seen a lot of linear approaches to finding new feature representations:

We might do this to find interpretable or intuitive latent concepts.



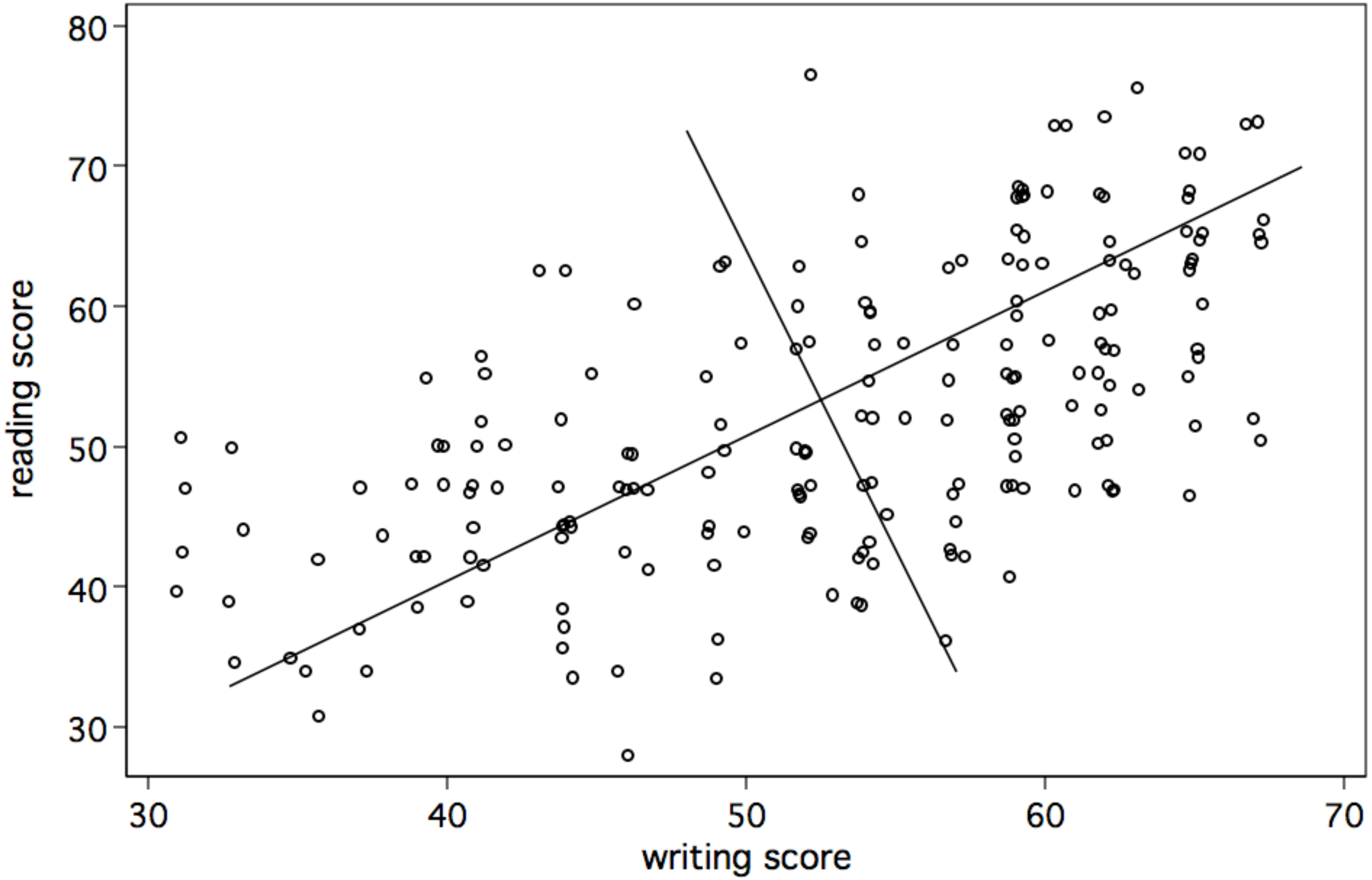
You've probably seen a lot of linear approaches to finding new feature representations:

We might do this to make computing more efficient (e.g., orthogonalization).



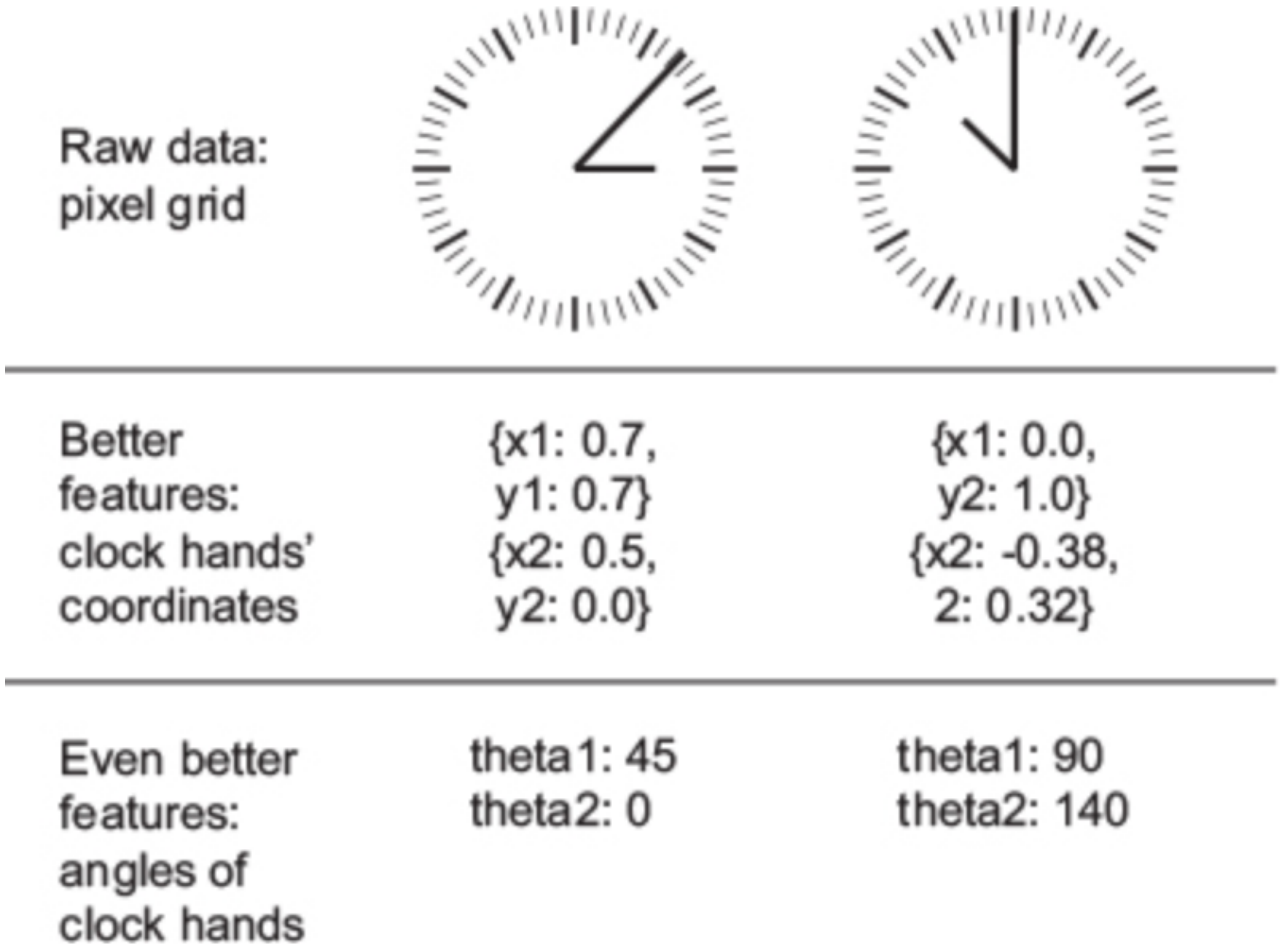
You've probably seen a lot of linear approaches to finding new feature representations:

We might do this to reduce dimensionality for generalizability or compression

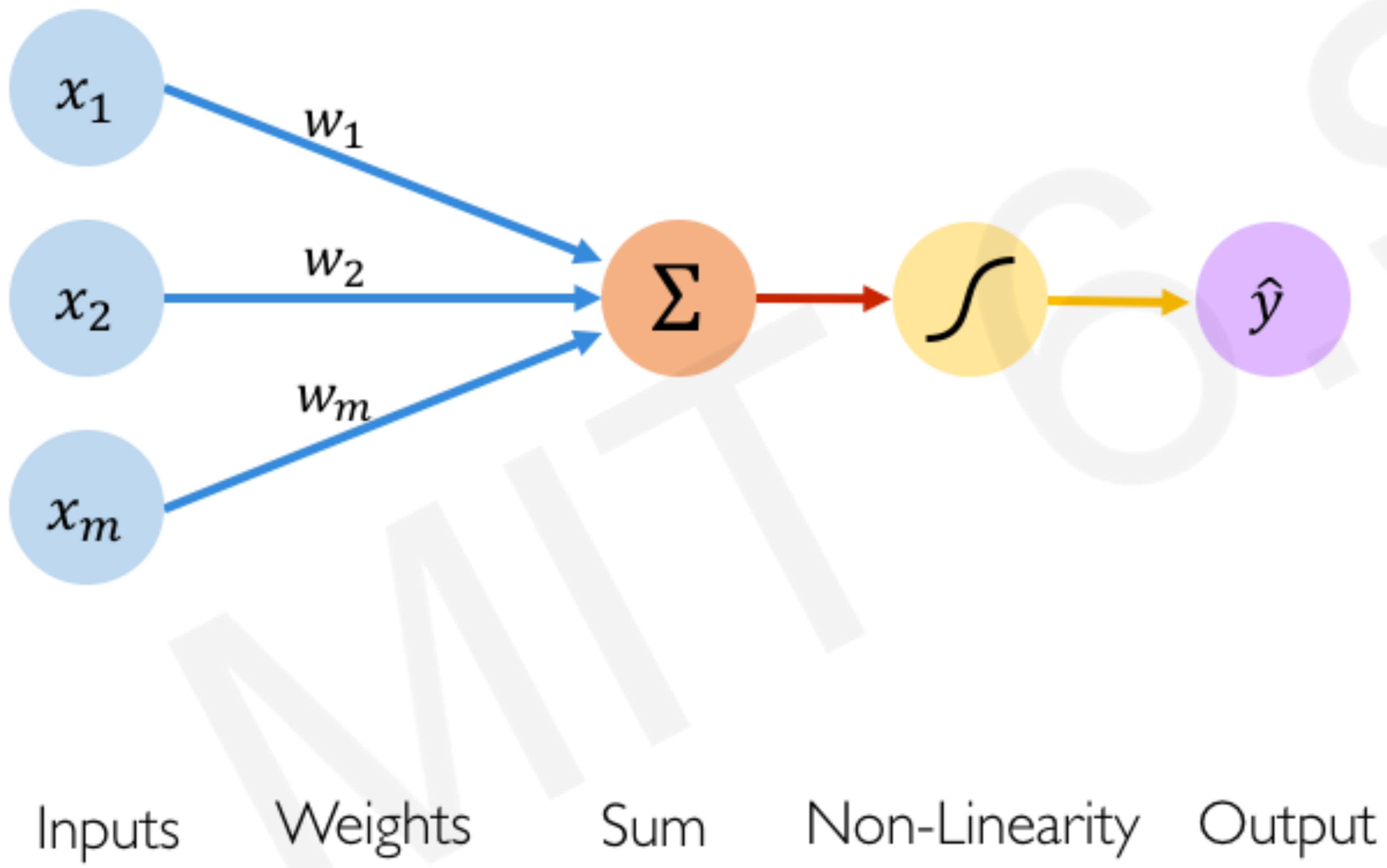


Domain knowledge may allow us to do successful *feature engineering.*

Figure 4.3. Feature engineering for reading the time on a clock



The Perceptron: Forward Propagation



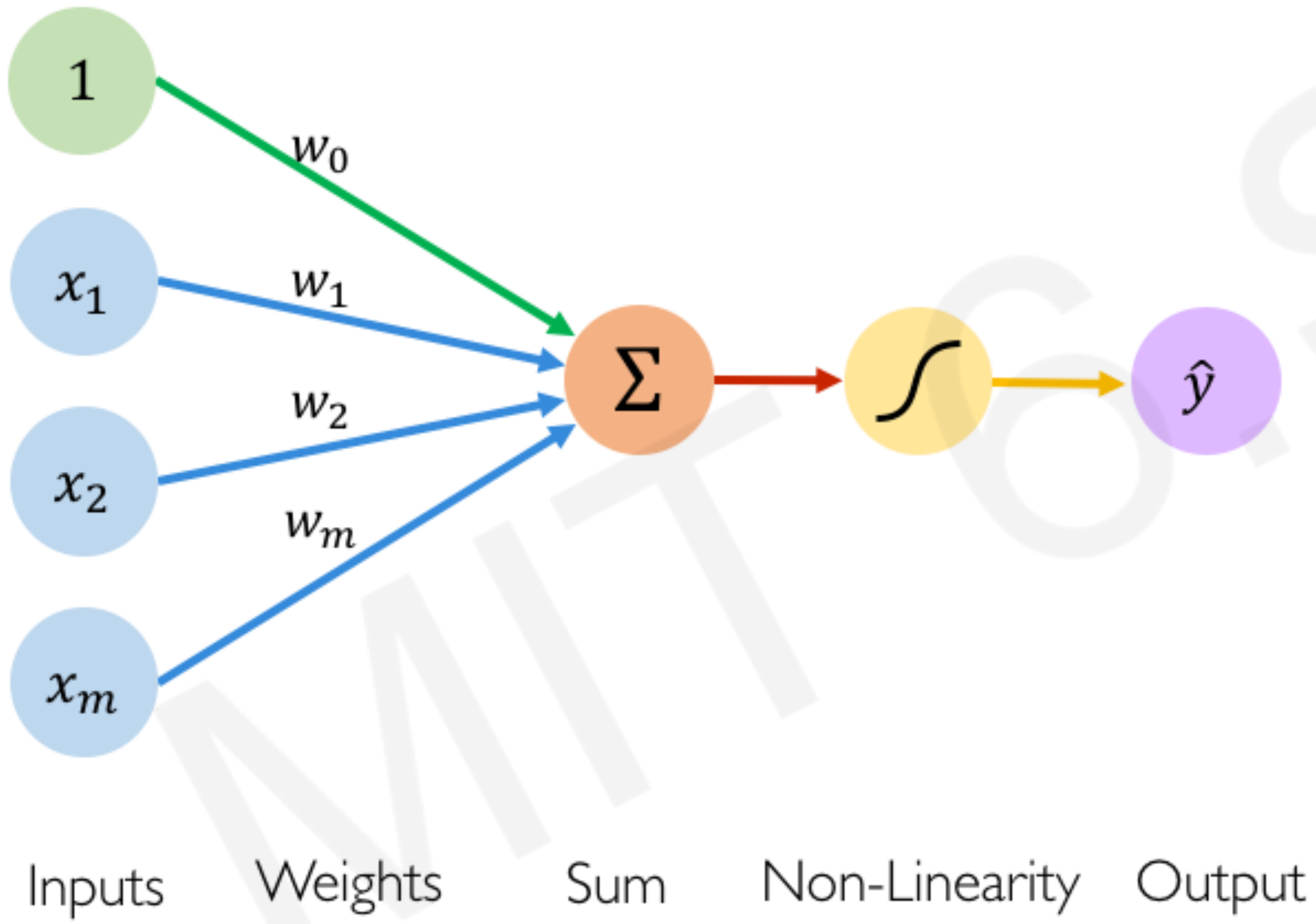
Output

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



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

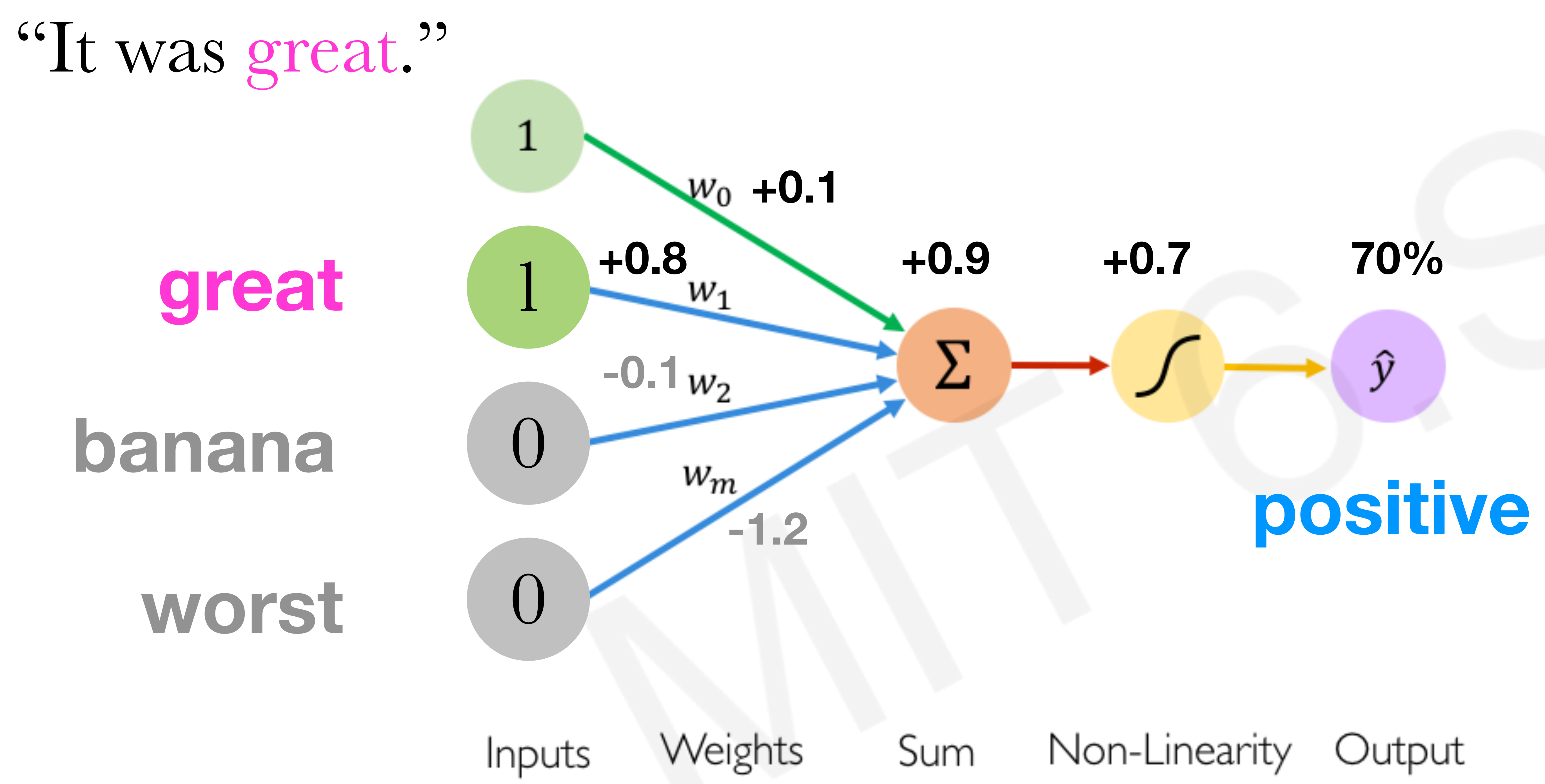
Output

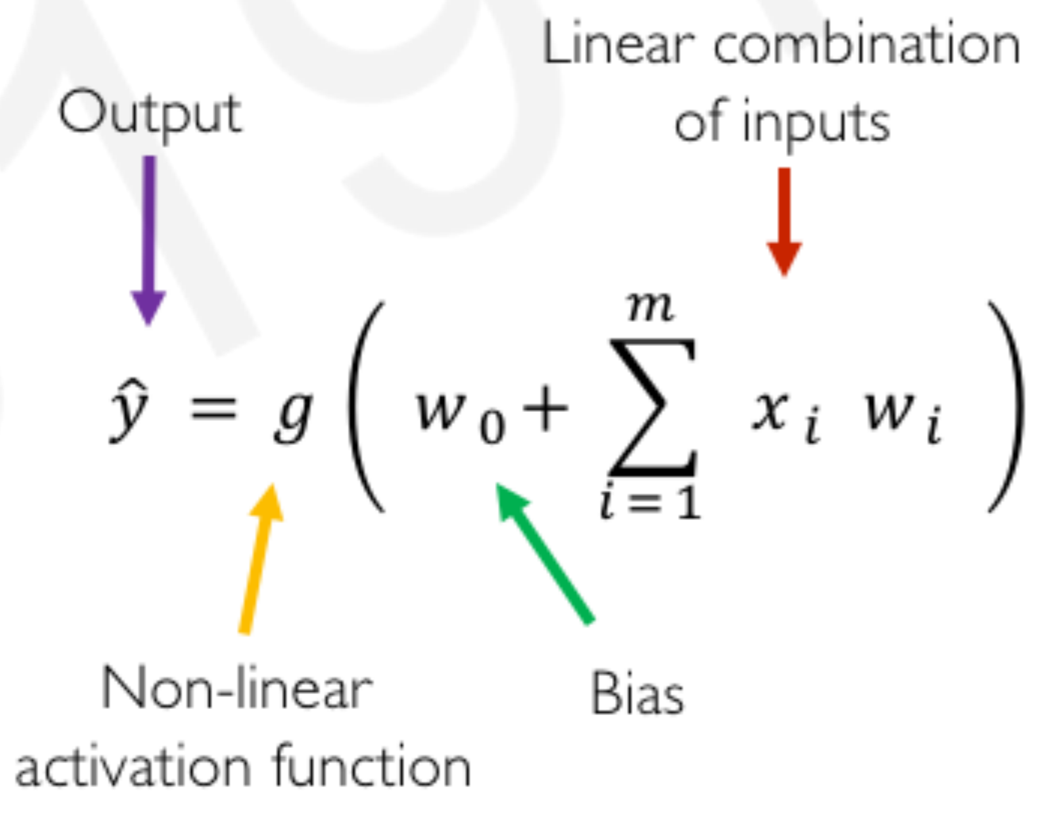
Linear combination of inputs

Non-linear activation function

Bias

The Perceptron: Forward Propagation





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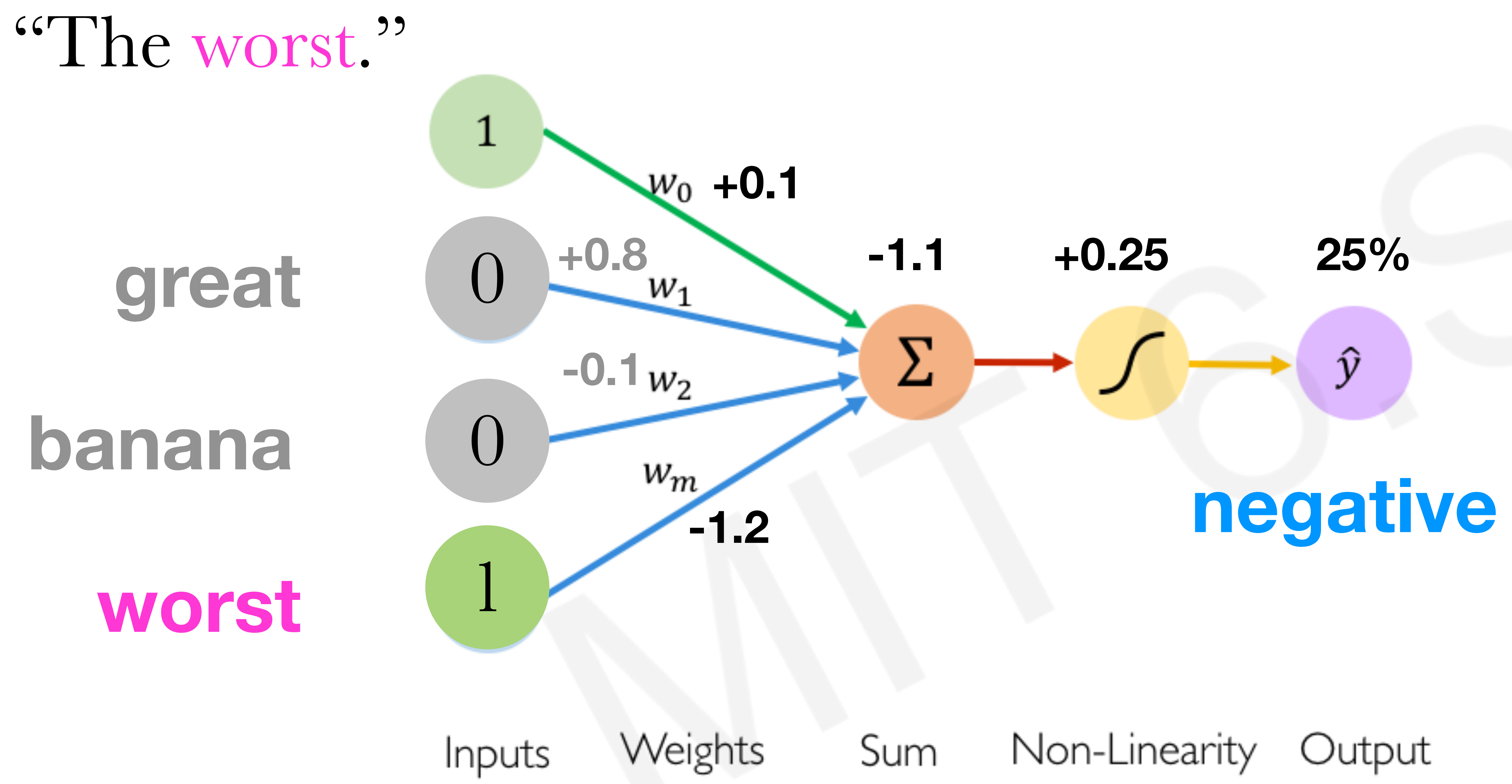

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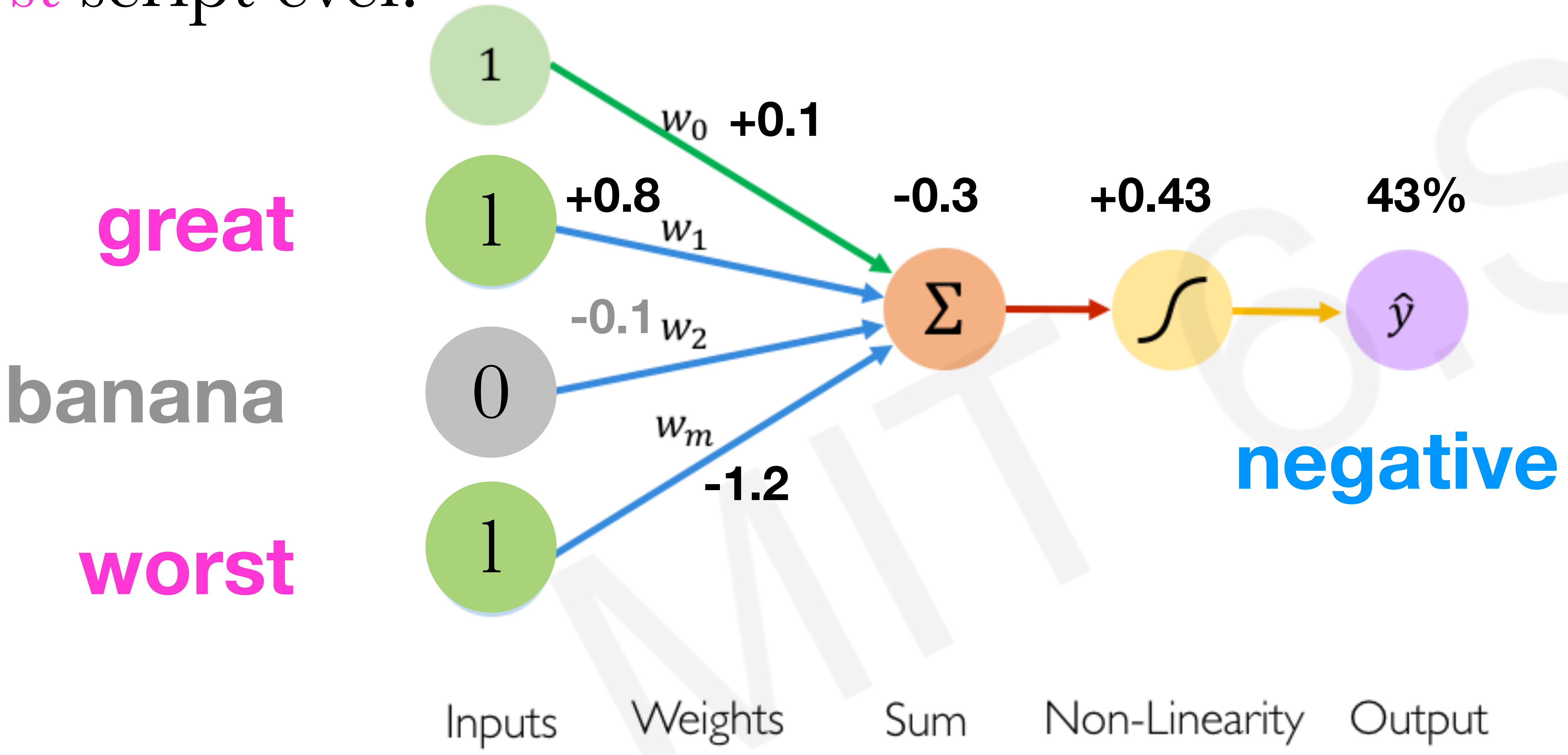
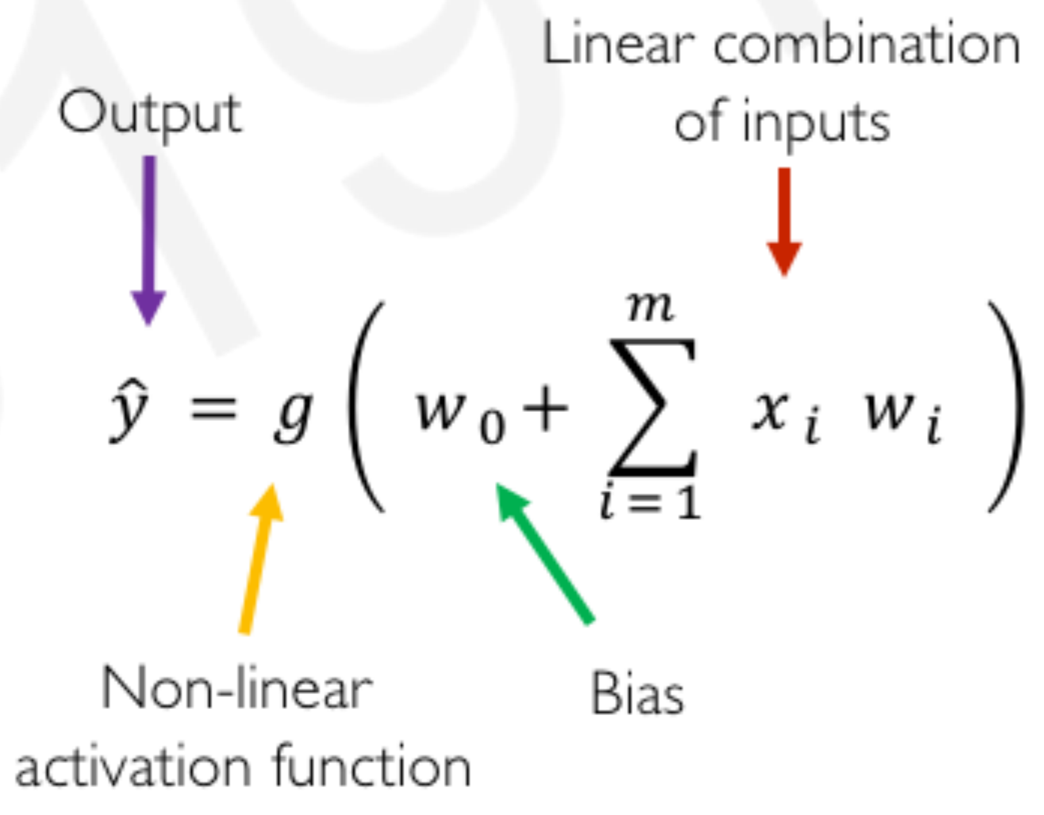
Bias

The Perceptron: Forward Propagation

"Acting was great.
Worst script ever."

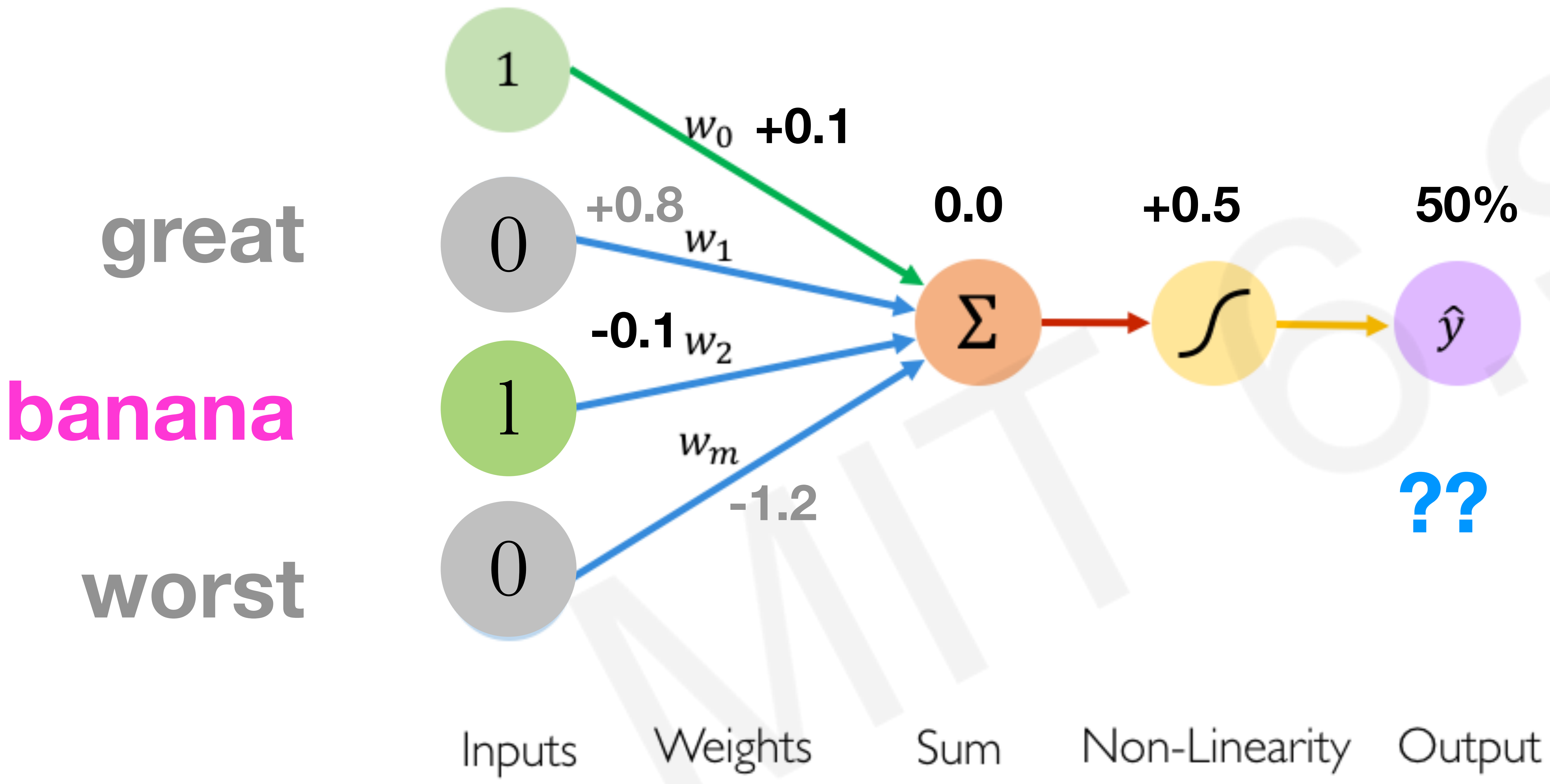


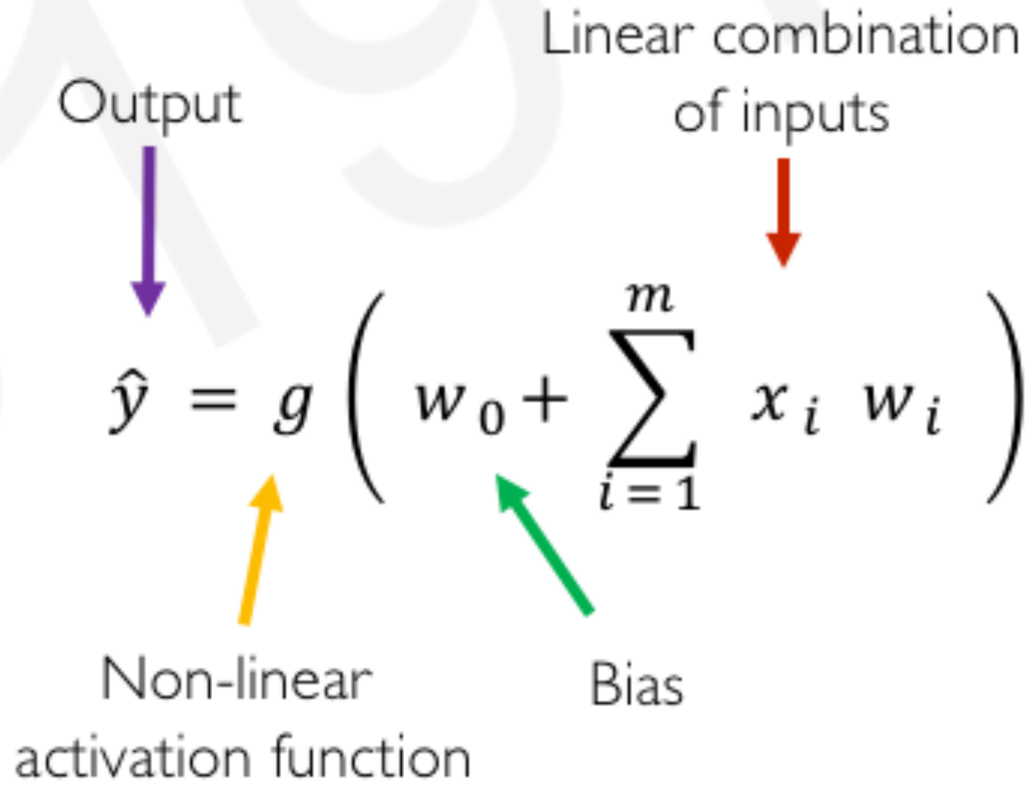


$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i \, w_i \right)$$

The Perceptron: Forward Propagation

"I want a banana."





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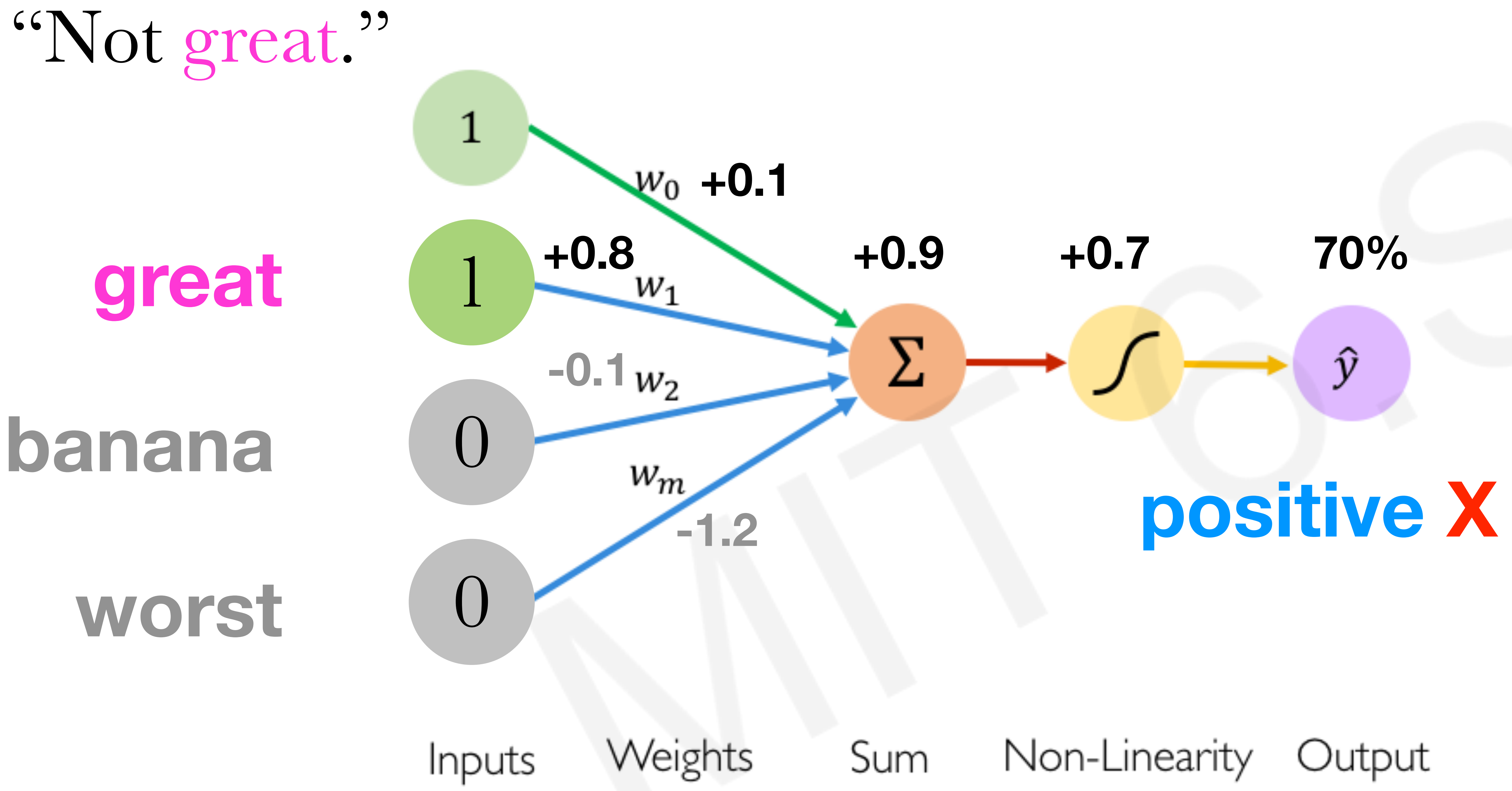

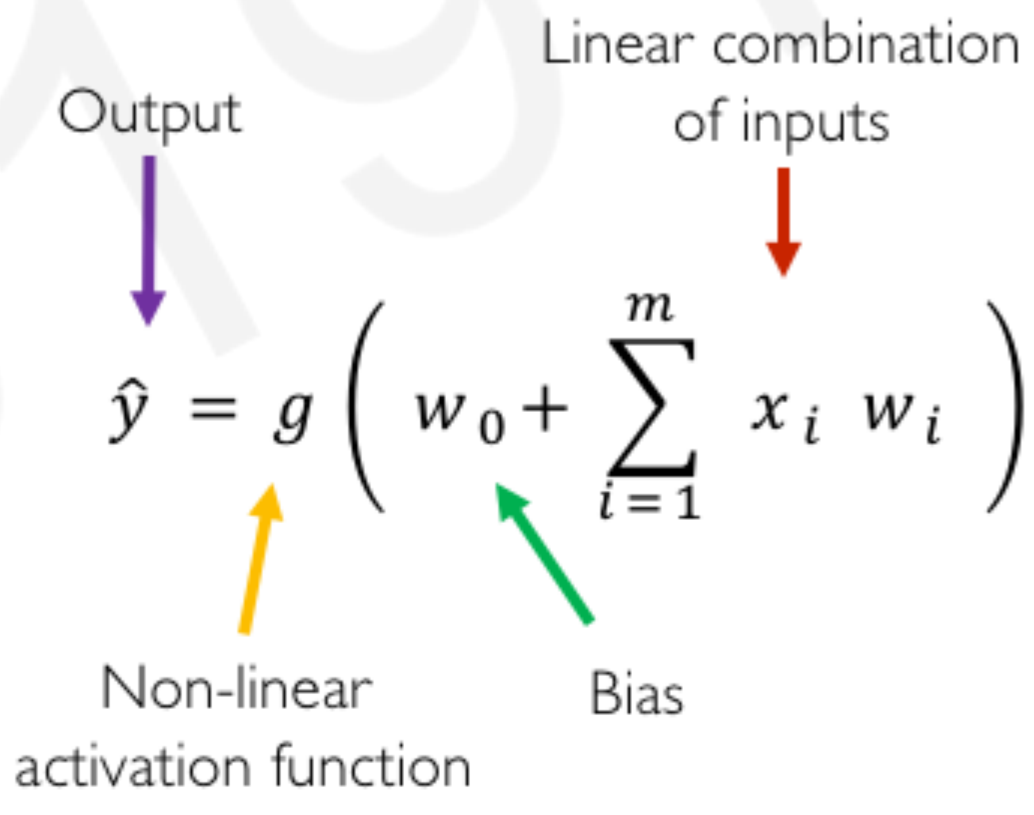

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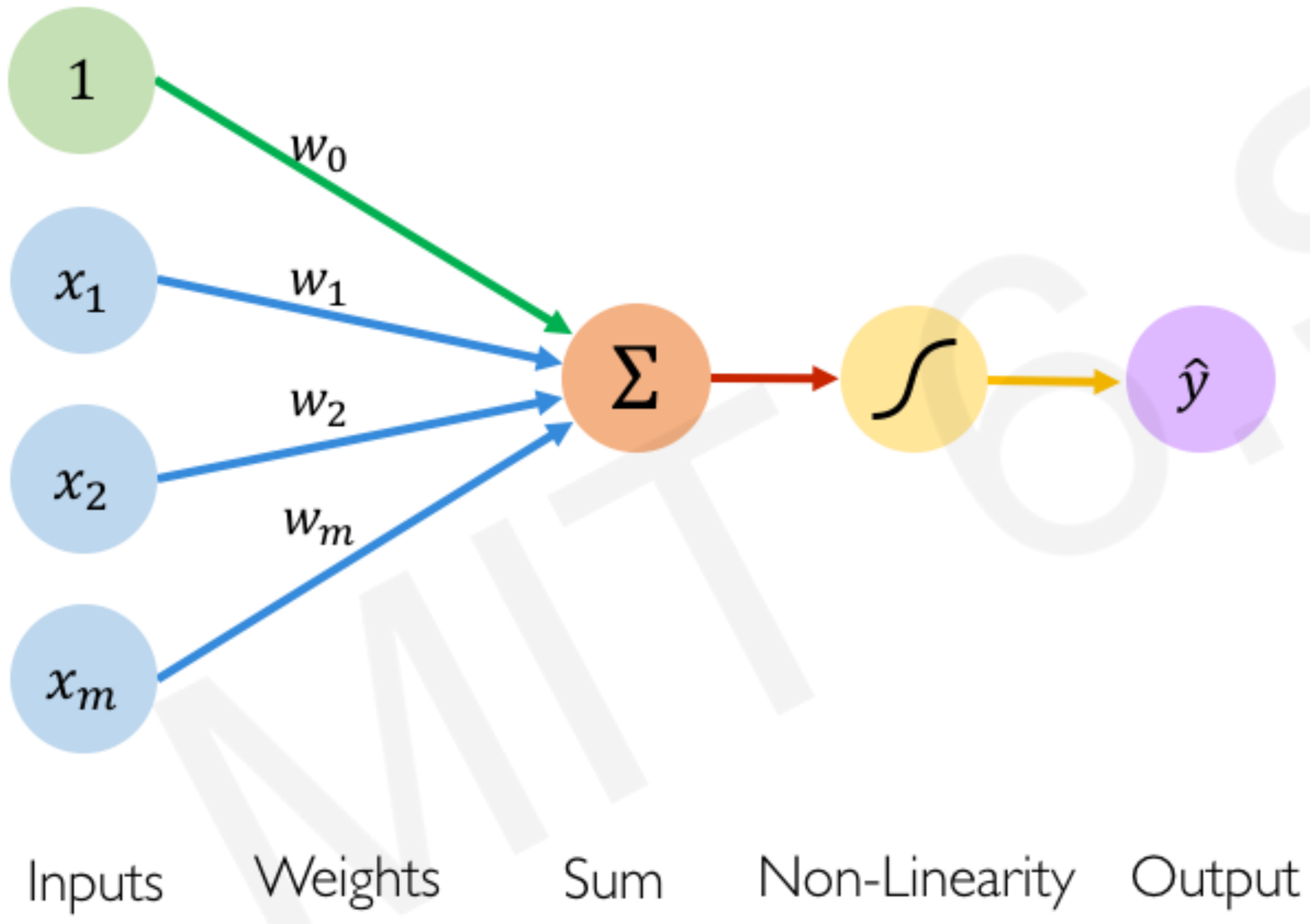
The Perceptron: Forward Propagation

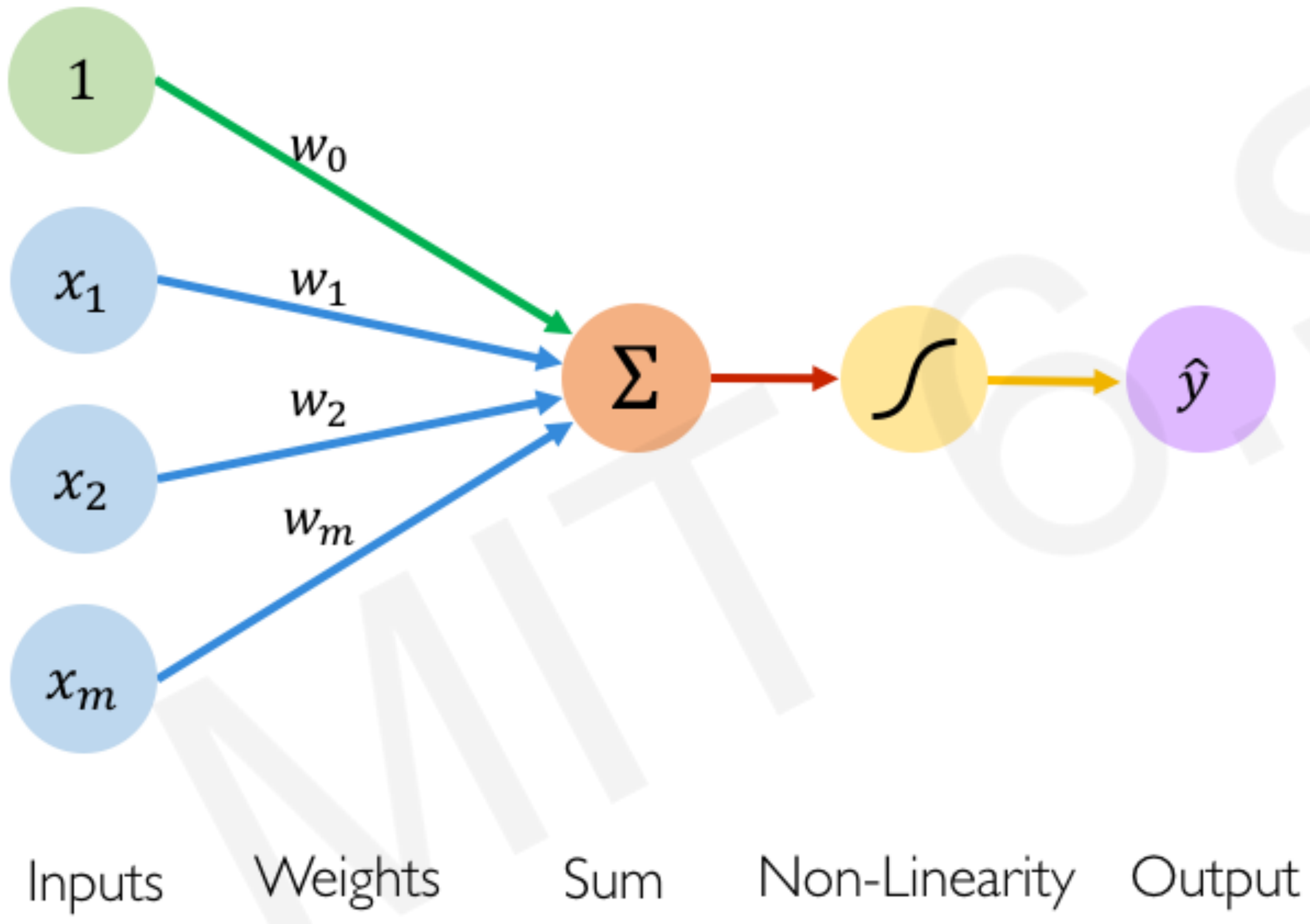


$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i \, w_i \right)$$

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

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

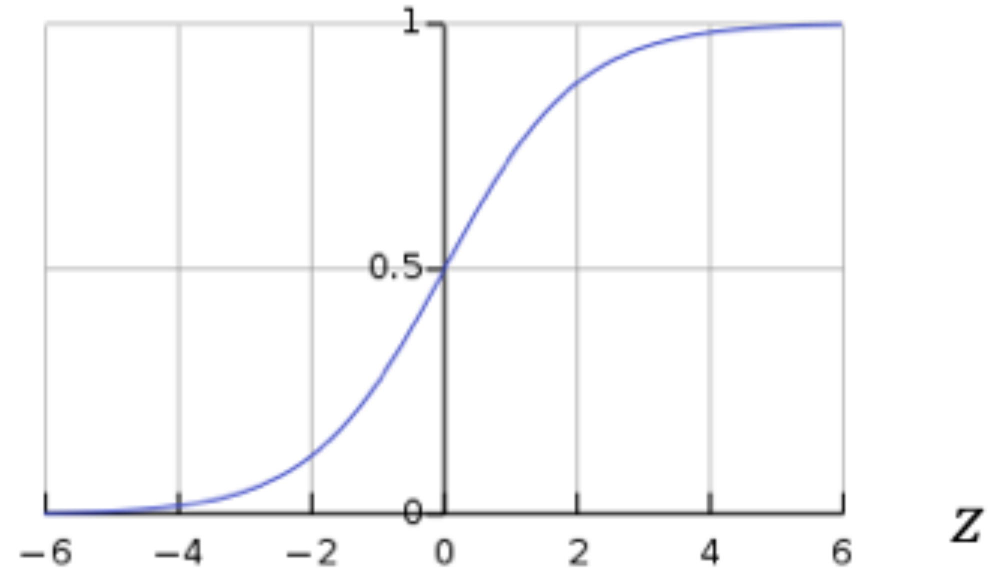


Activation Functions

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

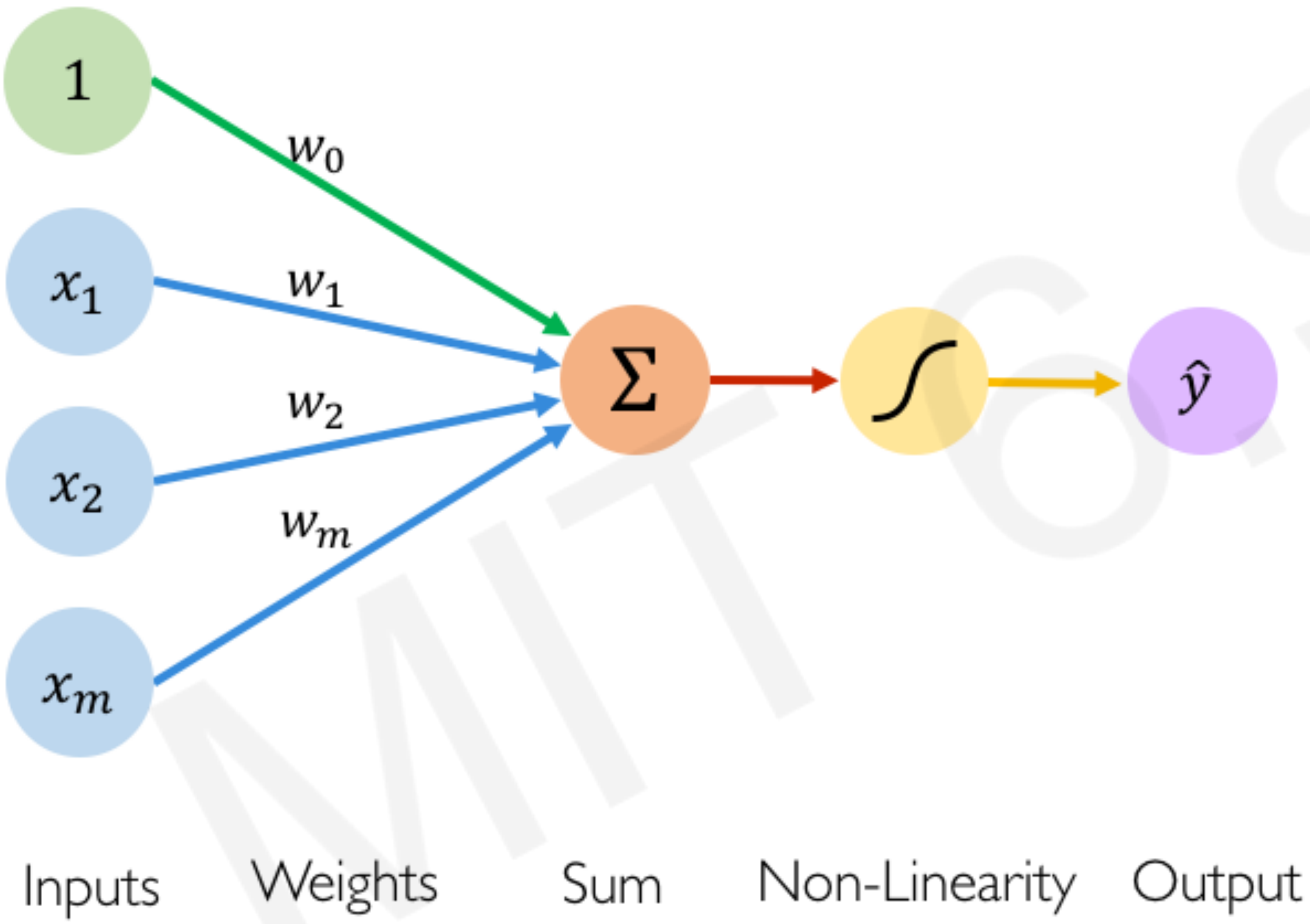
- Example: sigmoid function

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



This is *exactly the same* as the logit / logistic regression “inverse link function.”

The Perceptron: Forward Propagation



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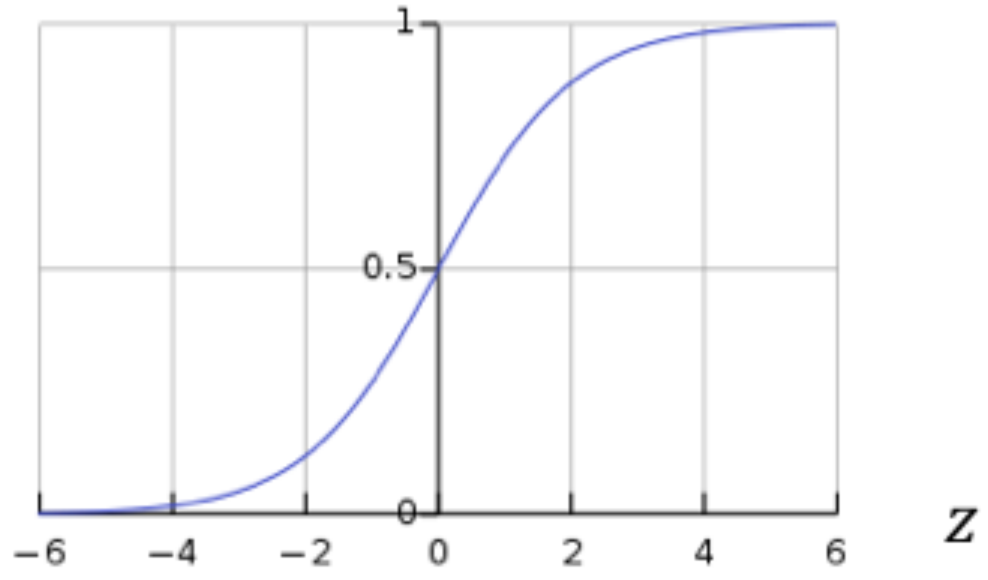
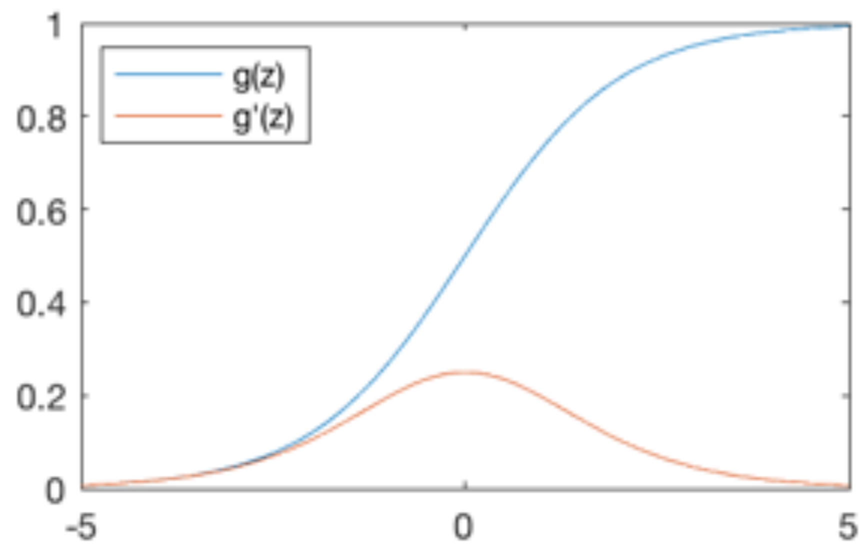


Machine learning in one slide

Social science (inference)	**Machine learning (prediction)**
GLM inverse link function $\mathbb{E}(y) = f(\mathbf{x}'\boldsymbol{\beta})$	Activation function $\mathbb{E}(y) = f(\mathbf{x}'\boldsymbol{\beta})$
Preferred objective function	
Log-likelihood $\log \mathcal{L} = \sum_{i=1}^{n} \log P(y_i \mid \mathbf{x}_i, \boldsymbol{\beta})$	Cross-entropy $-\log \mathcal{L} = -\sum_{i=1}^{n} \log P(y_i \mid \mathbf{x}_i, \boldsymbol{\beta})$
Solving algorithm	
Newton-Raphson $\boldsymbol{\beta}_t := \boldsymbol{\beta}_{t-1} - [\boldsymbol{H} \log \mathcal{L}]^{-1} \nabla \log \mathcal{L}$	Gradient descent $\boldsymbol{\beta}_t := \boldsymbol{\beta}_{t-1} - \eta \nabla(-\log \mathcal{L})$
Quantities of interest	
$\widehat{\boldsymbol{\beta}}; Var(\widehat{\boldsymbol{\beta}})$	$\widehat{\mathbf{y}}; \sum \mathbf{1}(\widehat{y} = y)/n$

Common Activation Functions

Sigmoid Function

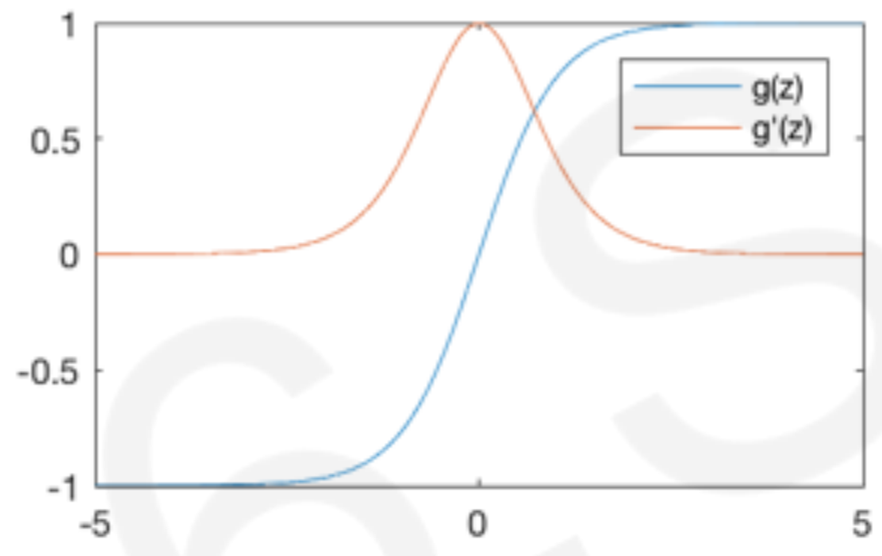


$$g(z) = \frac{1}{1 + e^{-z}}$$

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

```
tf.math.sigmoid(z)
```

Hyperbolic Tangent

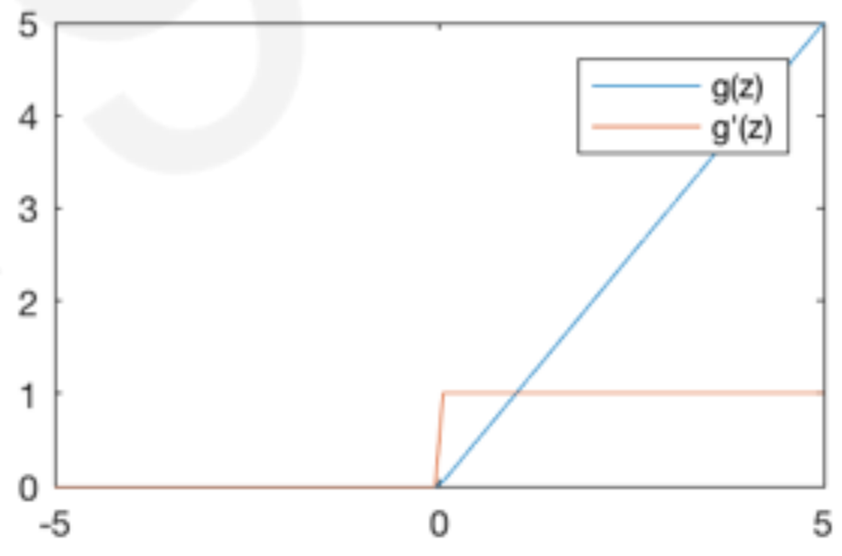


$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

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

```
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

Common Activation Functions

```
model = models.Sequential()
model.add(layers.Dense(16, activation = 'relu', input_shape=(5000,)))
model.add(layers.Dense(16, activation = 'relu'))
model.add(layers.Dense(1, activation= 'sigmoid'))

model.compile(optimizer='adam',
             loss='binary_crossentropy',
             metrics=['accuracy'])

history = model.fit(partial_x_train,
                    partial_y_train,
                    epochs=4,
                    batch_size=512,
                    validation_data=(x_val,y_val))
```

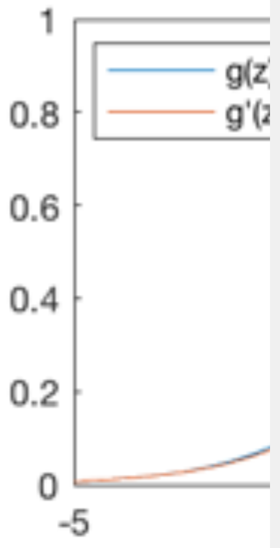
TensorFlow code blocks

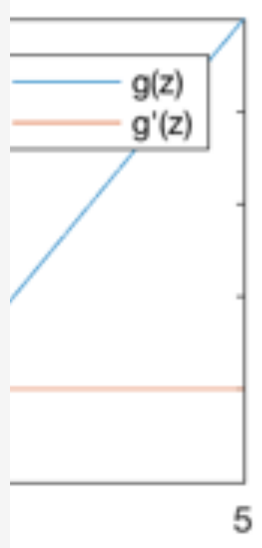
NOTE: All activation functions are non-linear

```{r}
model <- keras_model_sequential() %>%
  layer_dense(units = 16, activation = "relu", input_shape = c(5000)) %>%
  layer_dense(units = 16, activation = "relu") %>%
  layer_dense(units = 1, activation = "sigmoid")

model %>% compile(
  optimizer = "adam",
  loss = "binary_crossentropy",
  metrics = c("accuracy")
)

model %>% fit(x_train, y_train, epochs = 4, batch_size = 512)
results <- model %>% evaluate(x_test, y_test)
```

Sig

(ReLU)





g (z

z)

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

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

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

`tf.math.sigmoid(z)`

`tf.math.tanh(z)`

`tf.nn.relu(z)`

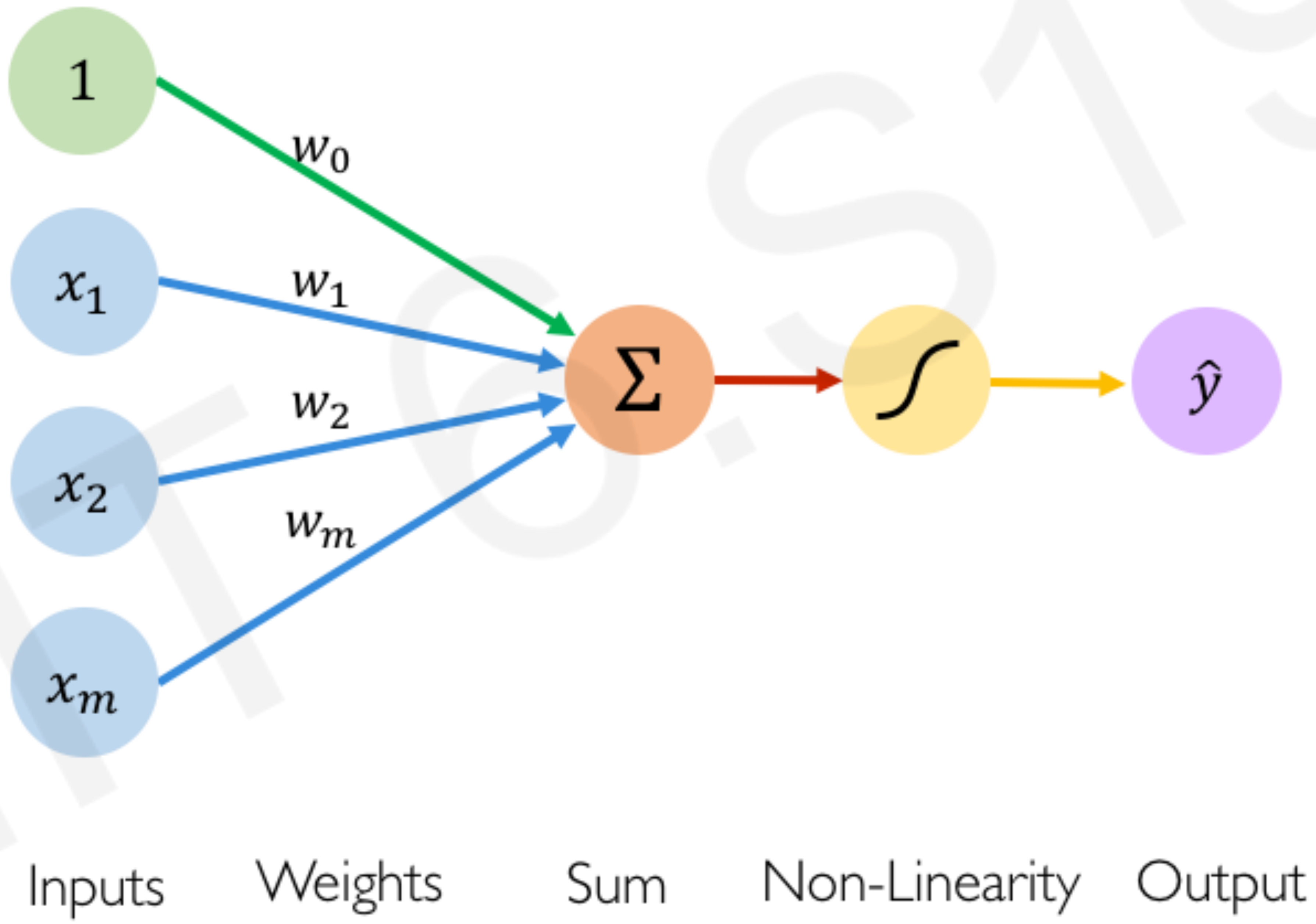
TensorFlow code blocks

NOTE: All activation functions are non-linear

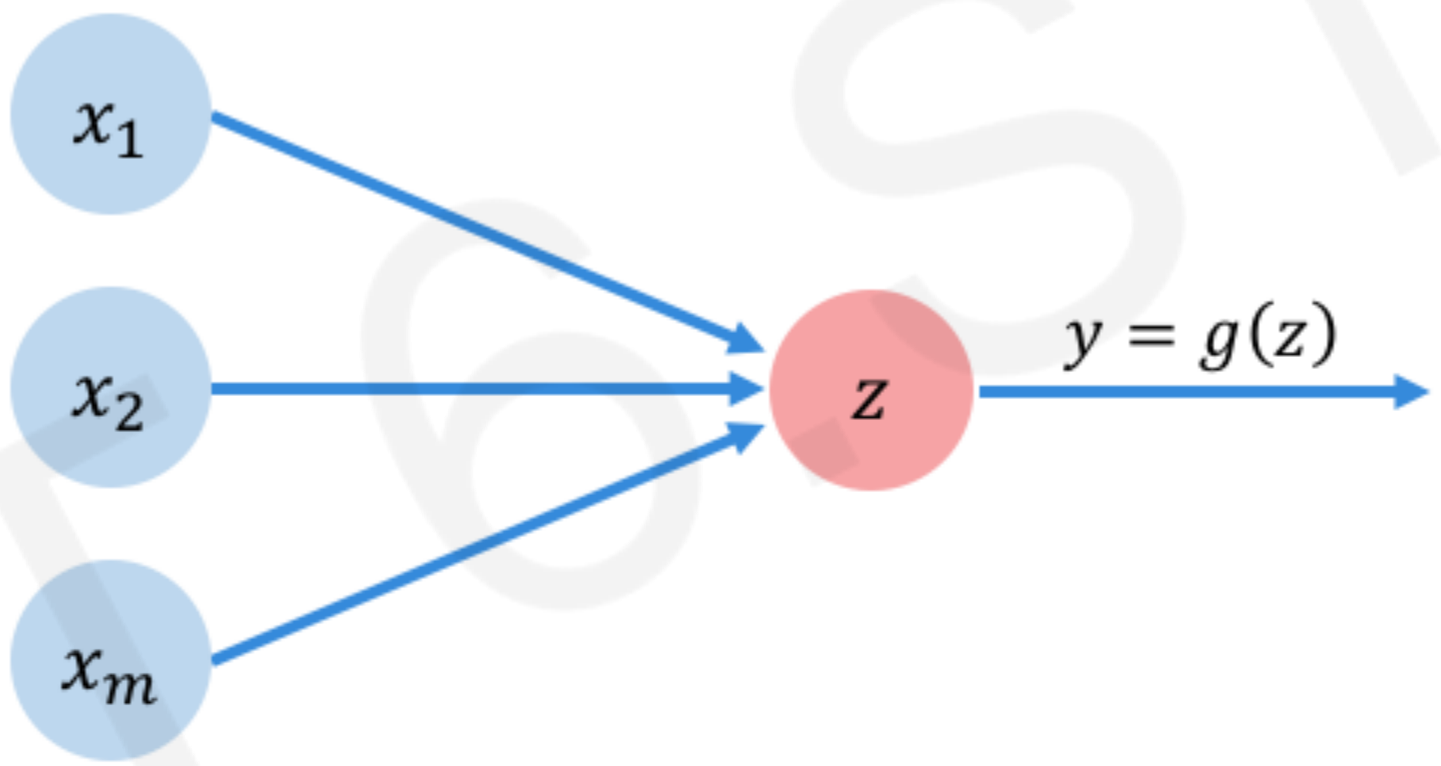
Building Neural Networks with Perceptrons

The Perceptron: Simplified

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



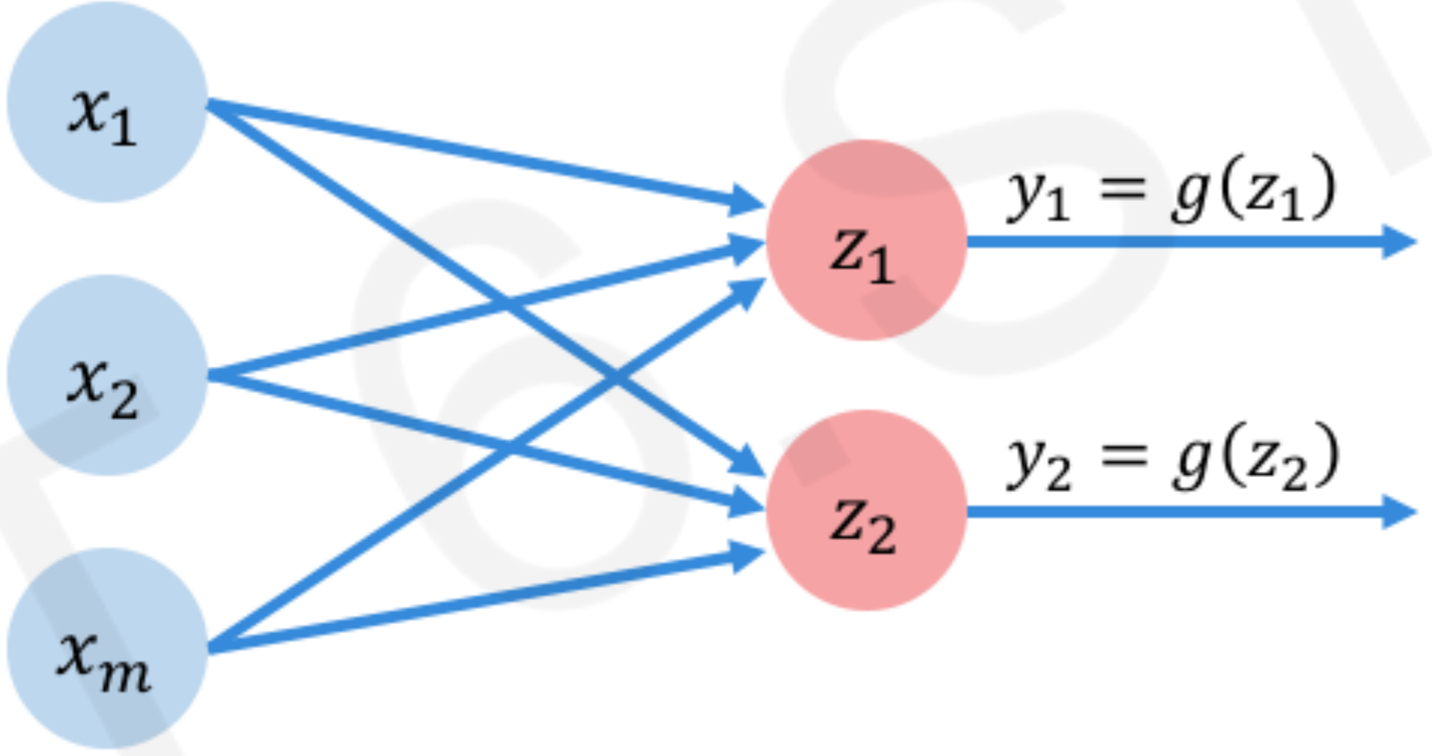
The Perceptron: Simplified



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

Multi Output Perceptron

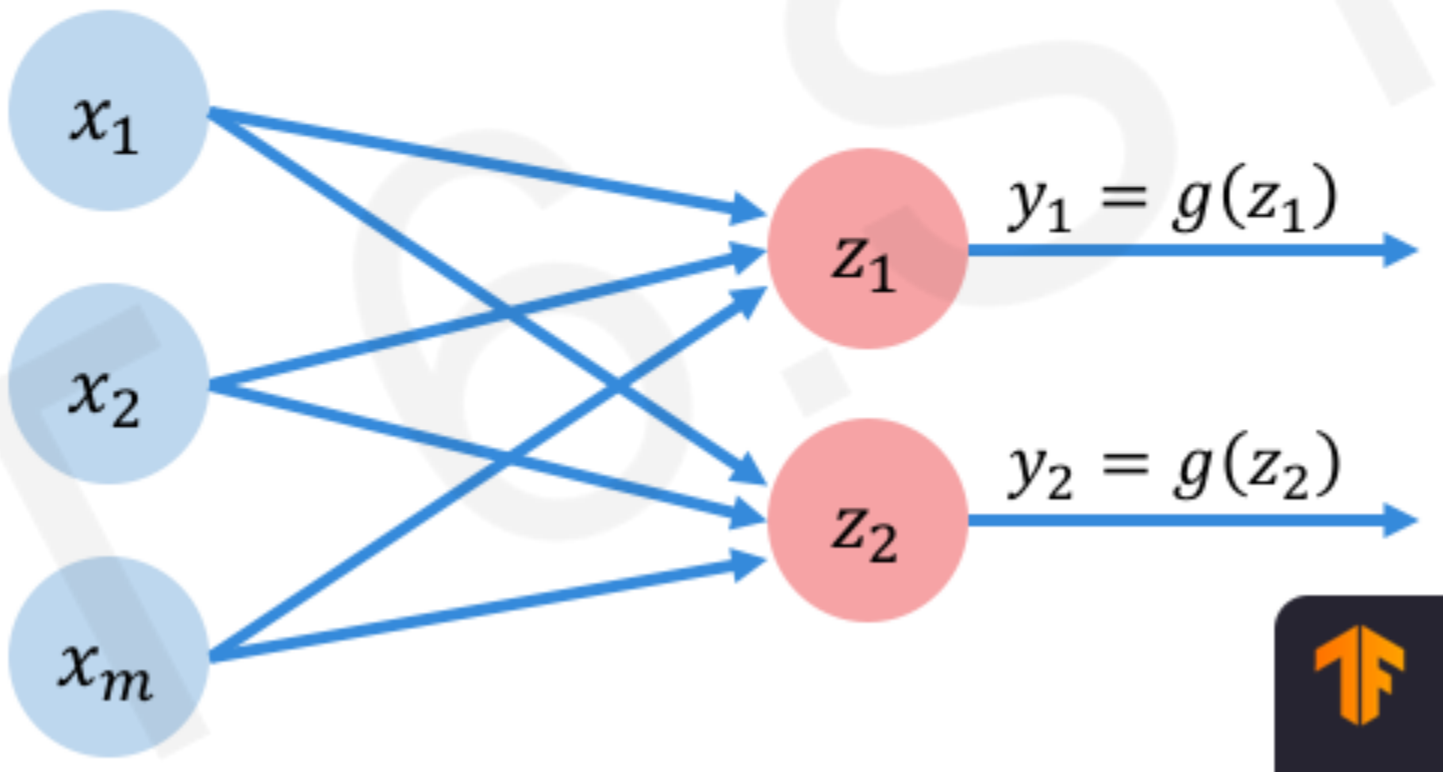
Because all inputs are densely connected to all outputs, these layers are called **Dense** layers



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

Multi Output Perceptron

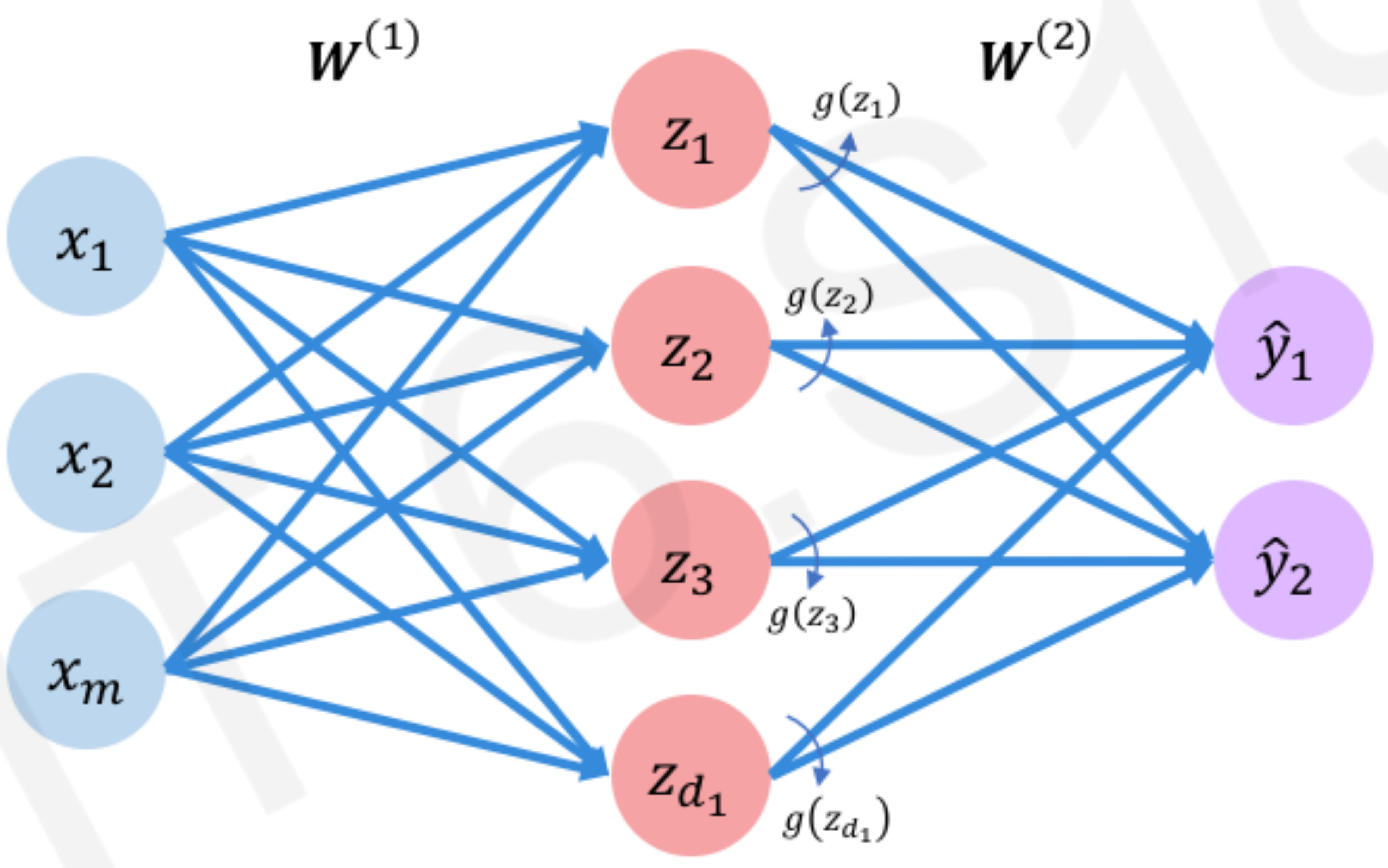
Because all inputs are densely connected to all outputs, these layers are called **Dense** layers




```python
import tensorflow as tf

layer = tf.keras.layers.Dense(
    units=2)
```

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

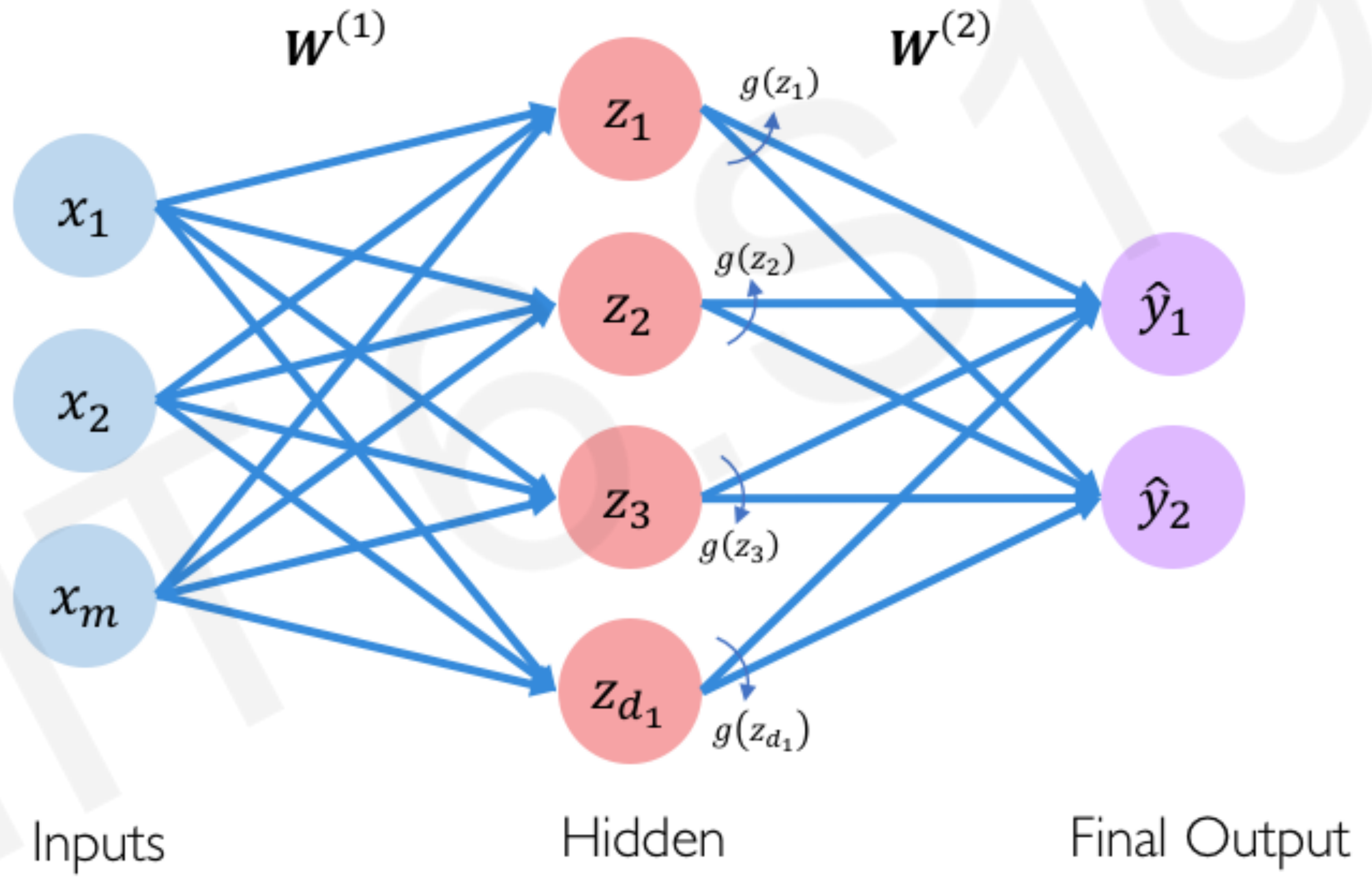
Single Layer Neural Network



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

There are important contexts — like modeling with Keras — where we would refer to this as a "two-layer" neural network

Single Layer Neural Network



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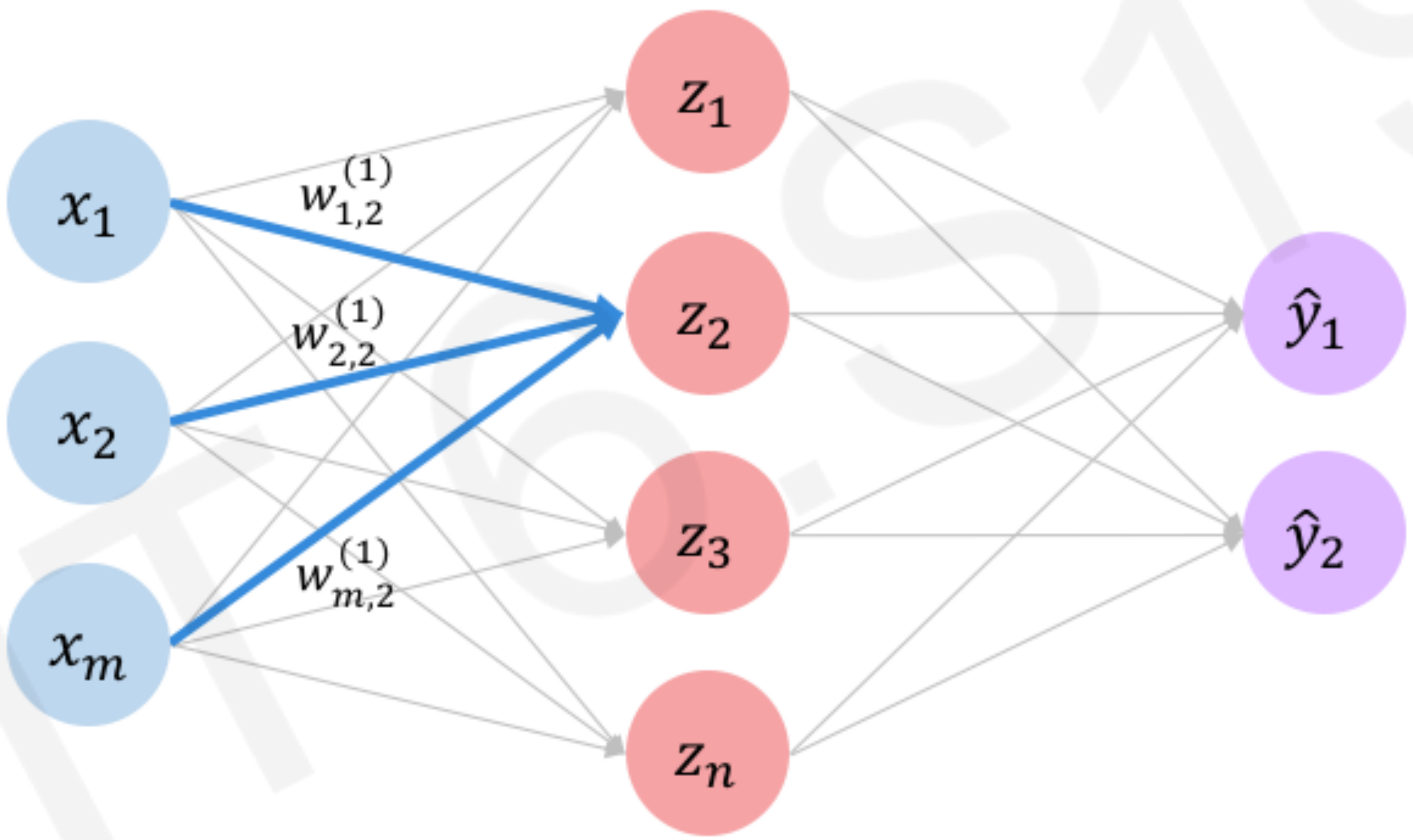
Single Layer Neural Network

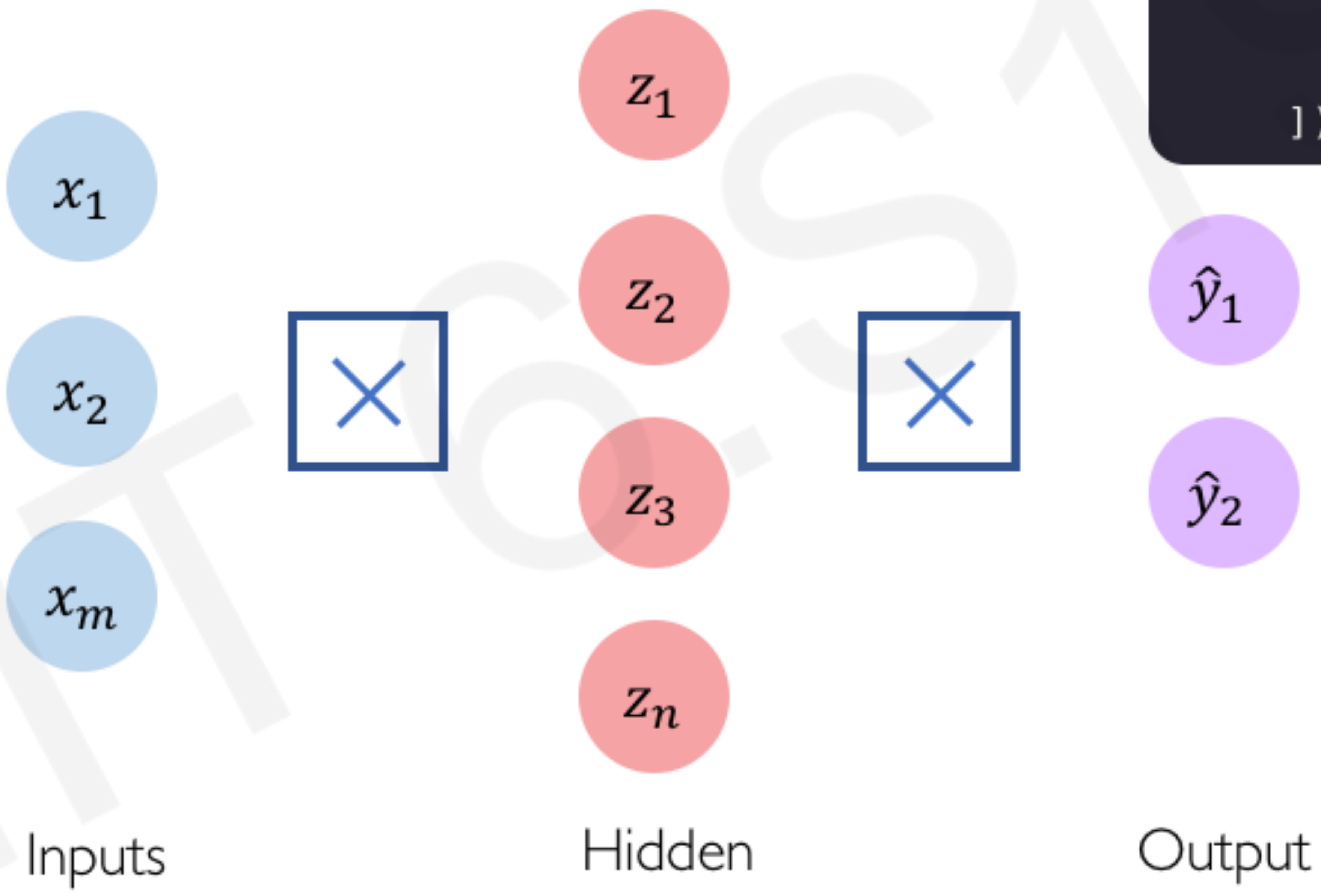


$$z_2 = w_{0,2}^{(1)} + \sum_{j=1}^{m} x_j \, w_{j,2}^{(1)}$$
$$= w_{0,2}^{(1)} + x_1 \, w_{1,2}^{(1)} + x_2 \, w_{2,2}^{(1)} + x_m \, w_{m,2}^{(1)}$$

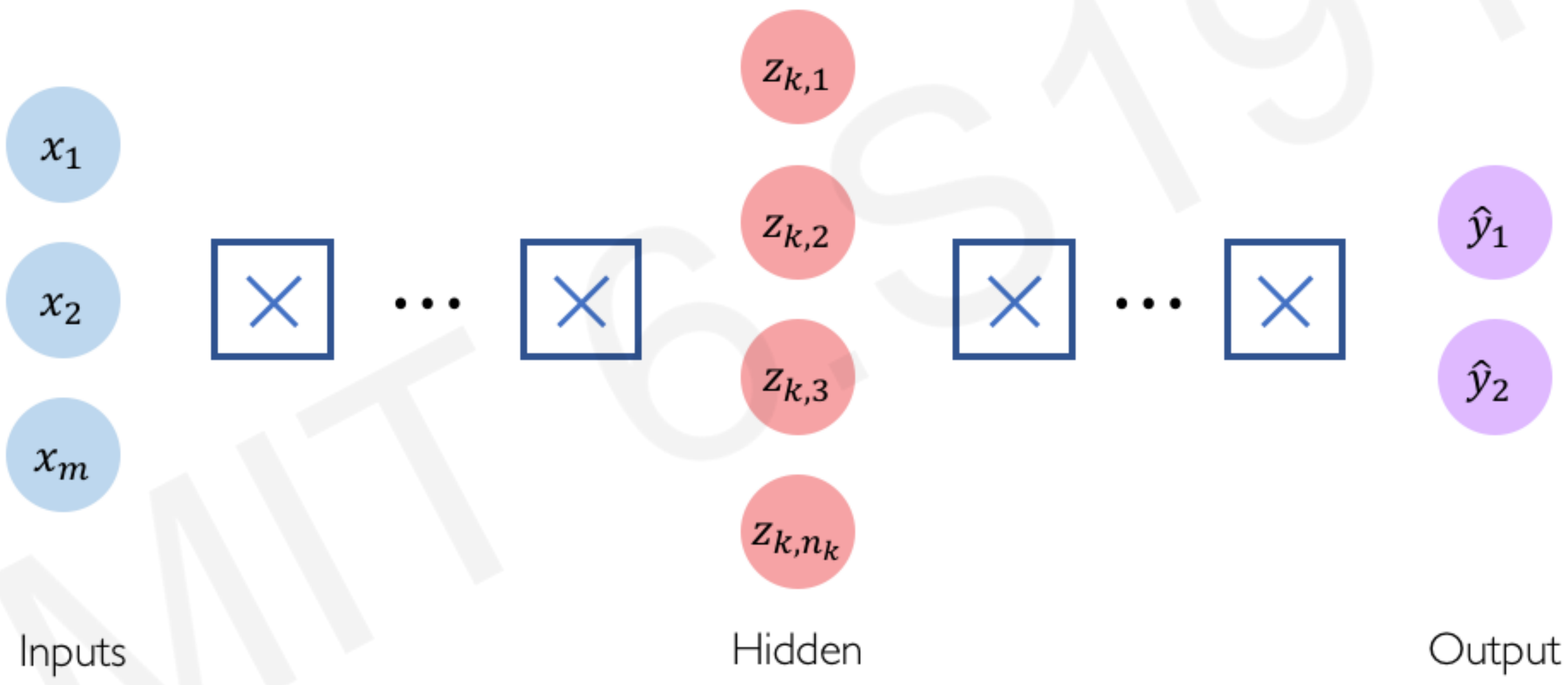
Multi Output Perceptron

```python
import tensorflow as tf

model = tf.keras.Sequential([
    tf.keras.layers.Dense(n),
    tf.keras.layers.Dense(2)
])
```

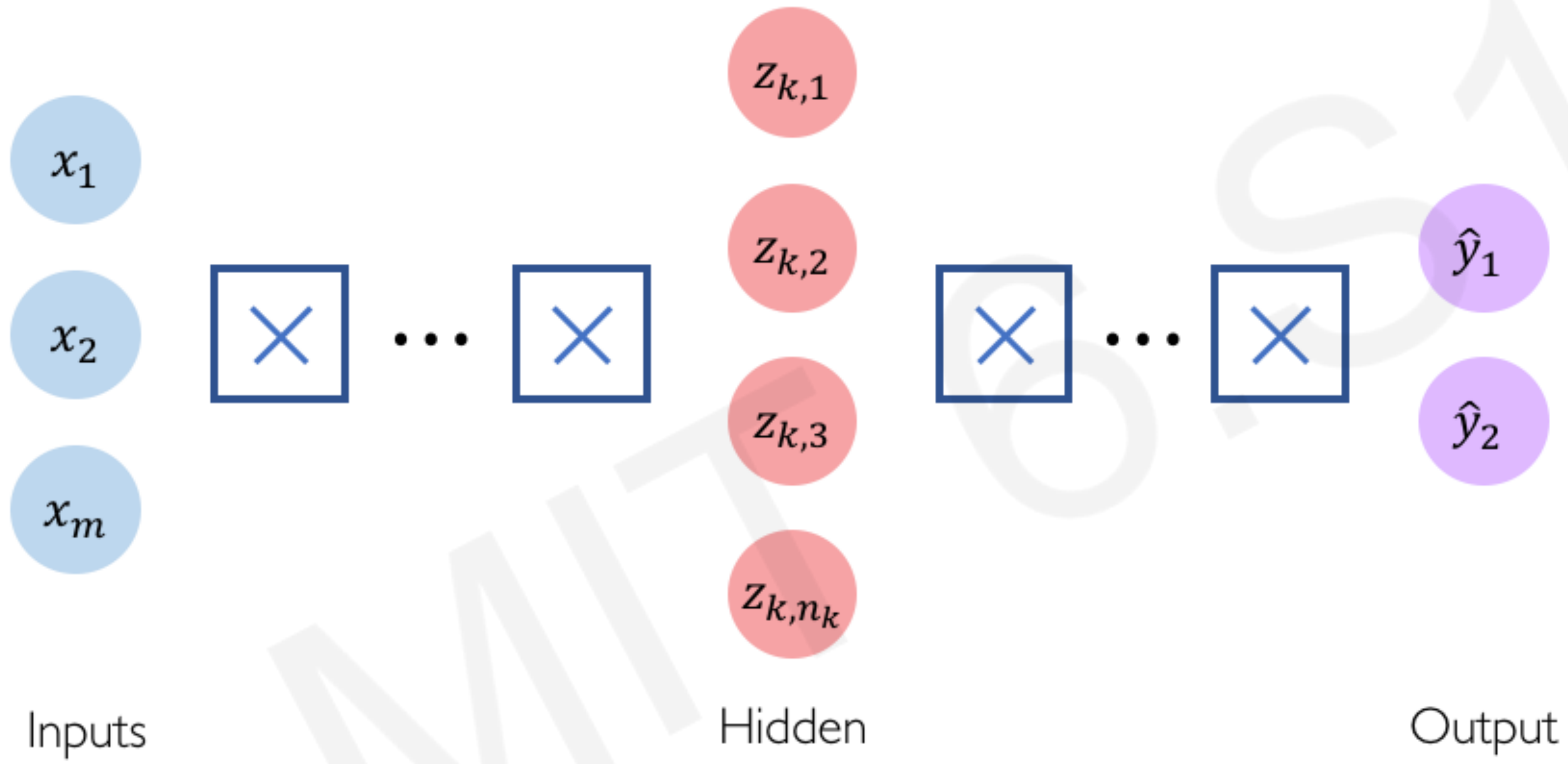


Deep Neural Network



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

Deep Neural Network



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model = tf.keras.Sequential([
  tf.keras.layers.Dense(n₁),
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  ⋮
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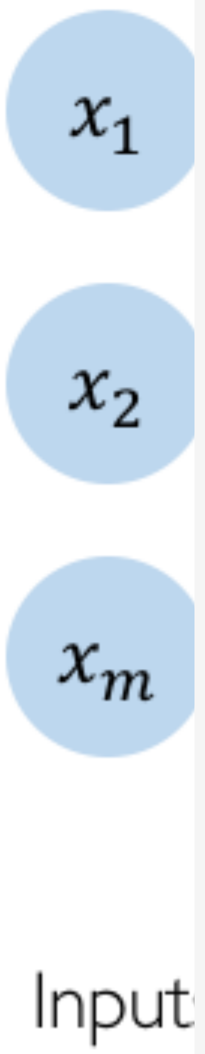
```

Deep Neural Network

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Deep Neural Network

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  ⋮
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])
```

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

Applying Neural Networks

Example Problem

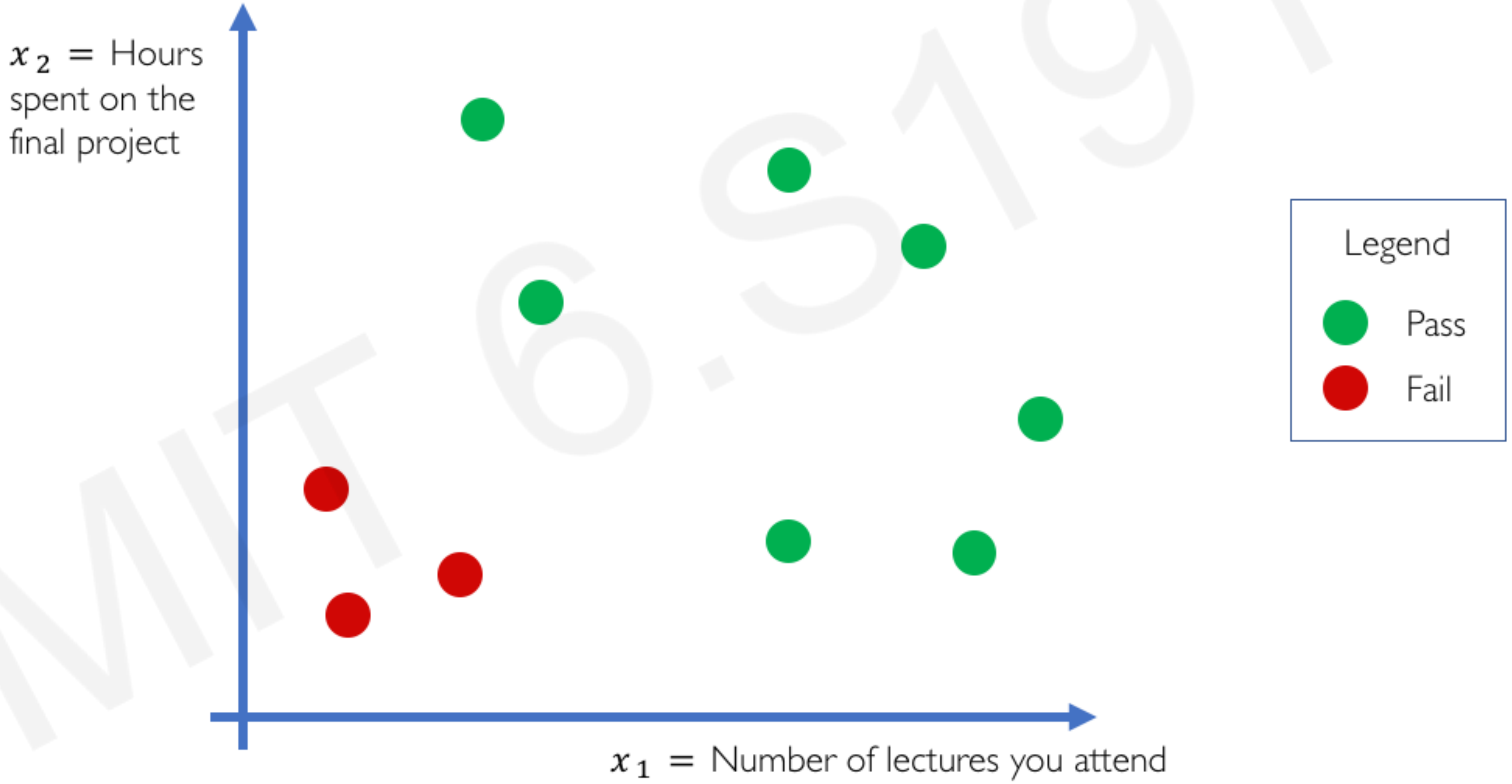
Will I pass this class?

Let's start with a simple two feature model

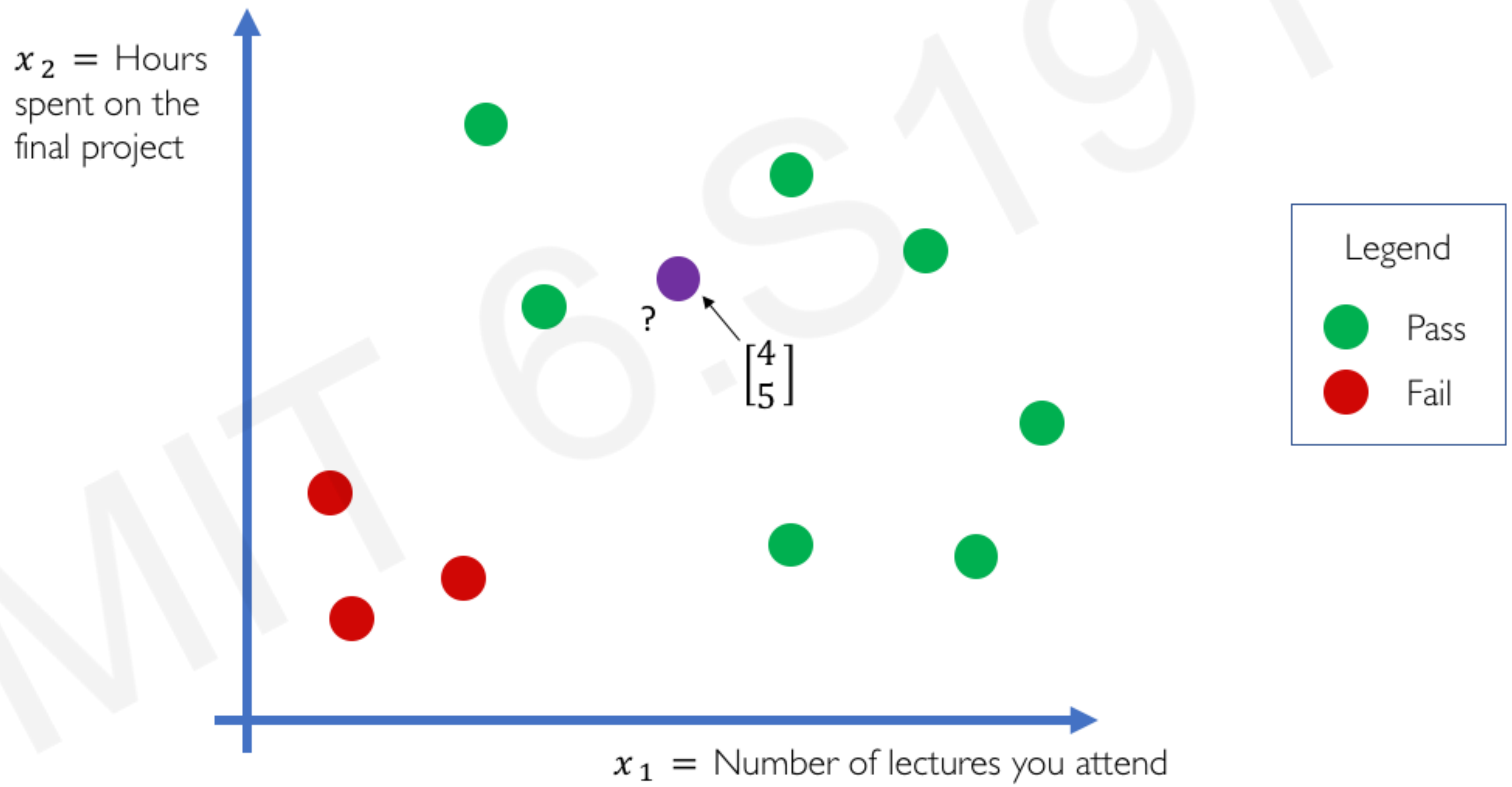
x_1 = Number of lectures you attend

x_2 = Hours spent on the final project

Example Problem: Will I pass this class?



Example Problem: Will I pass this class?



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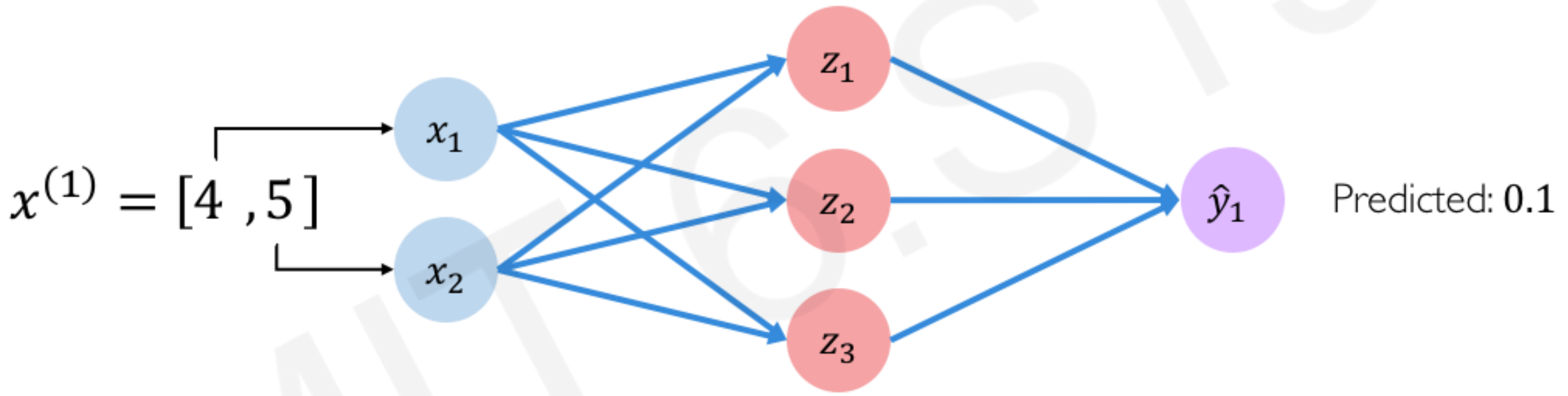

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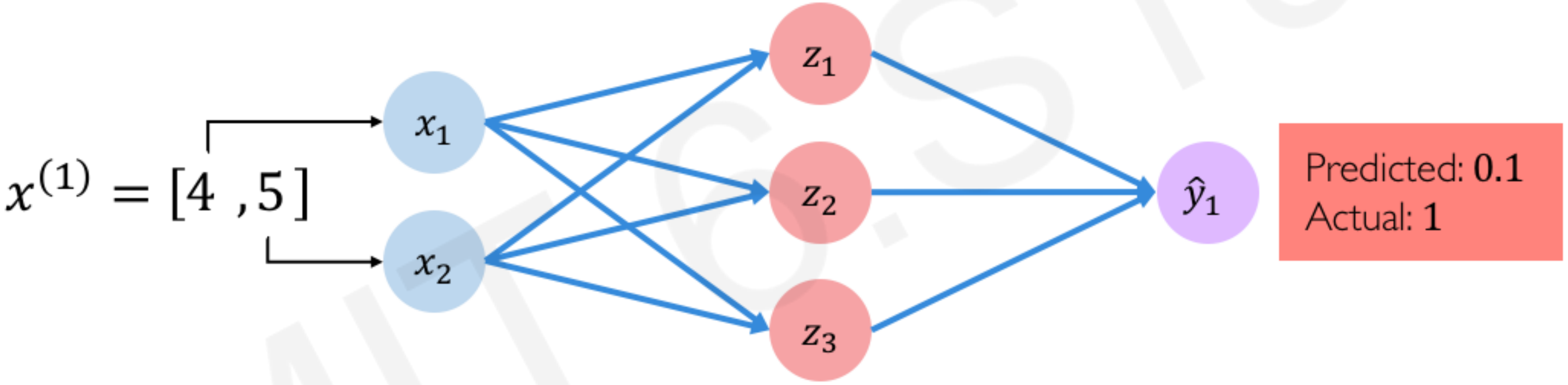
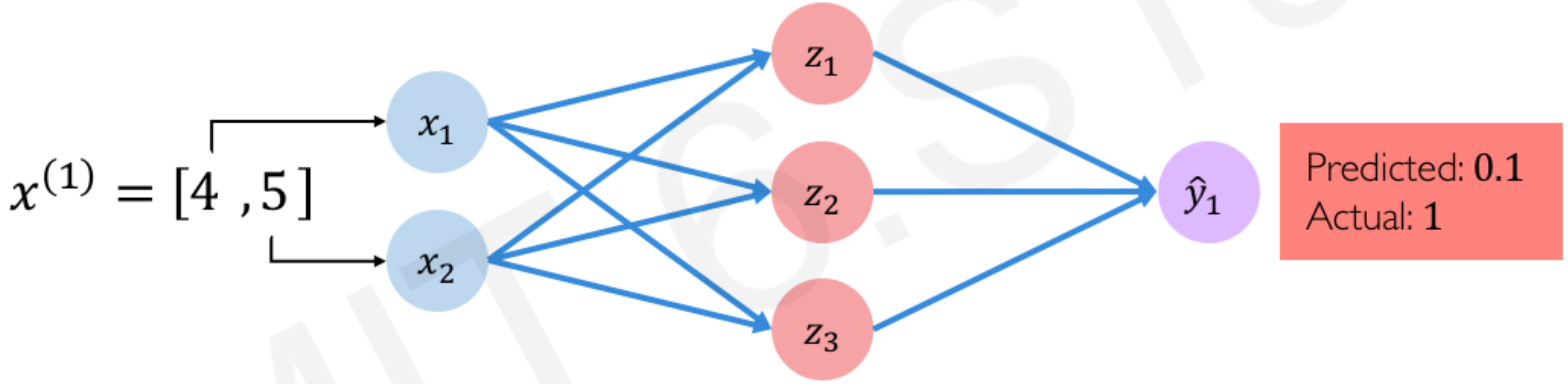


Quantifying Loss

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

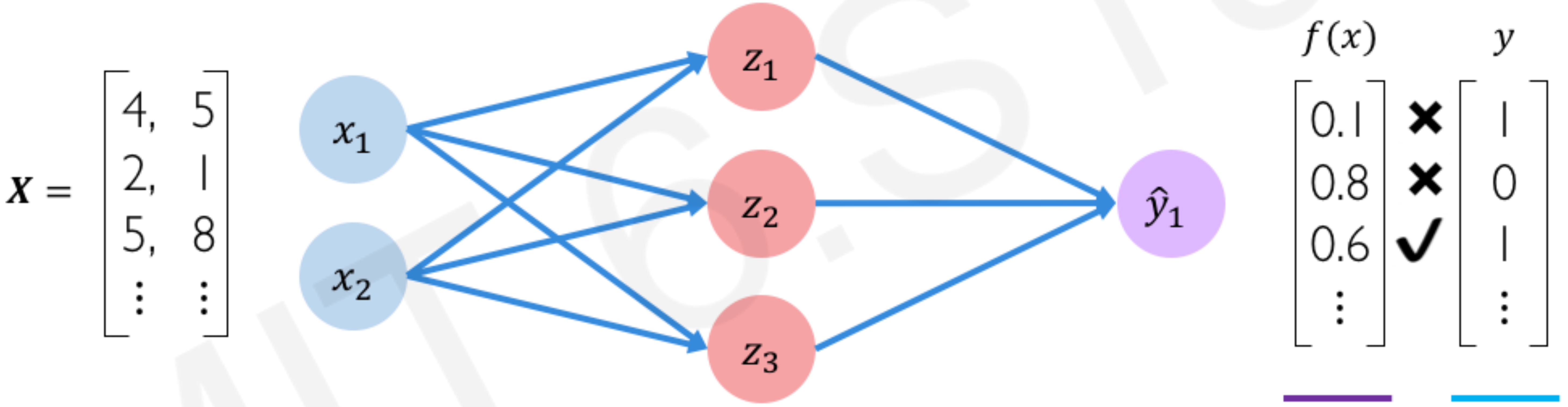


$$\mathcal{L}\left(f\left(x^{(i)}; \boldsymbol{W}\right), y^{(i)}\right)$$

Predicted Actual

Empirical Loss

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



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

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

Binary Cross Entropy Loss

```
model = models.Sequential()
model.add(layers.Dense(16, activation = 'relu', input_shape=(5000,)))
model.add(layers.Dense(16, activation = 'relu'))
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model.compile(optimizer='adam',
             loss='binary_crossentropy',
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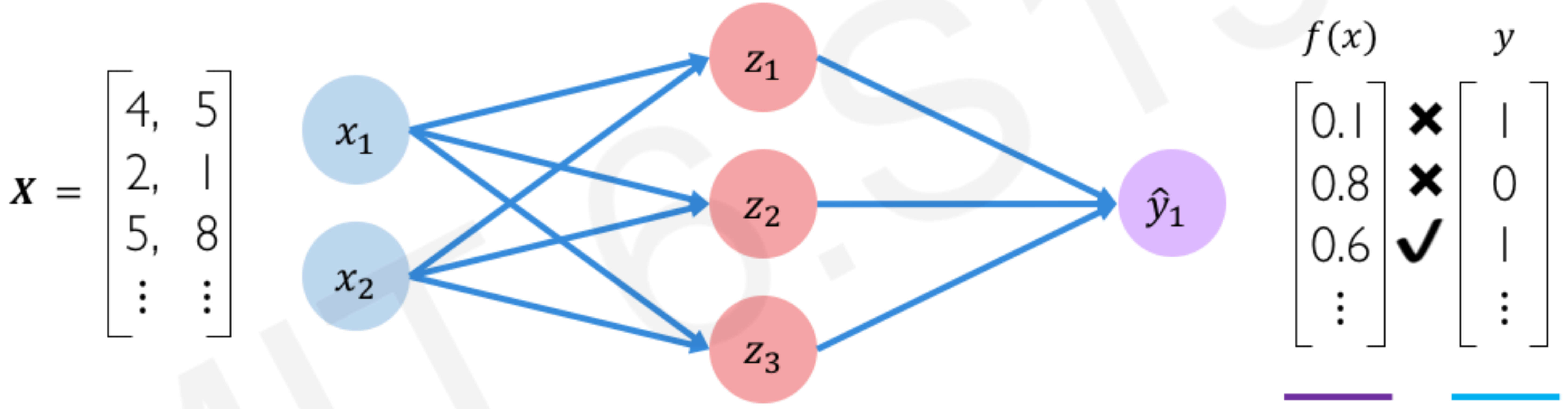
history = model.fit(partial_x_train,
                   partial_y_train,
                   epochs=4,
                   batch_size=512,
                   validation_data=(x_val,y_val))
```

Actual Predicted Actual Predicted

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

Binary Cross Entropy Loss

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



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

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loss = tf.reduce_mean( tf.nn.softmax_cross_entropy_with_logits(y, predicted) )
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Binary Cross Entropy Loss

Cro

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```

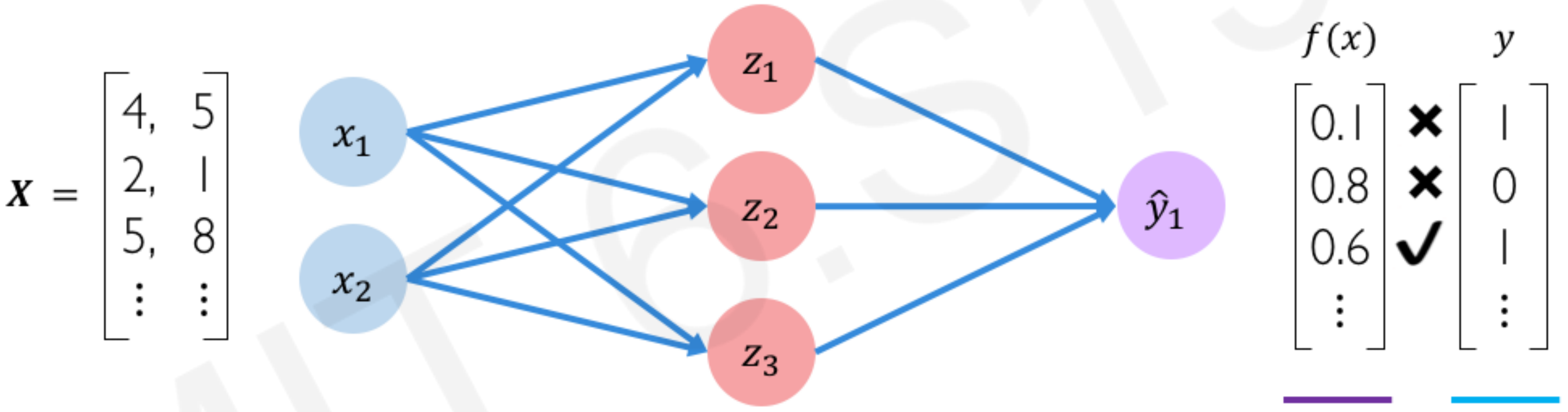
Actual Predicted Actual Predicted

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

This is exactly equivalent to the negative log-likelihood.
So this is so far identical to logit/logistic regression.

Binary Cross Entropy Loss

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



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loss = tf.reduce_mean( tf.nn.softmax_cross_entropy_with_logits(y, predicted) )
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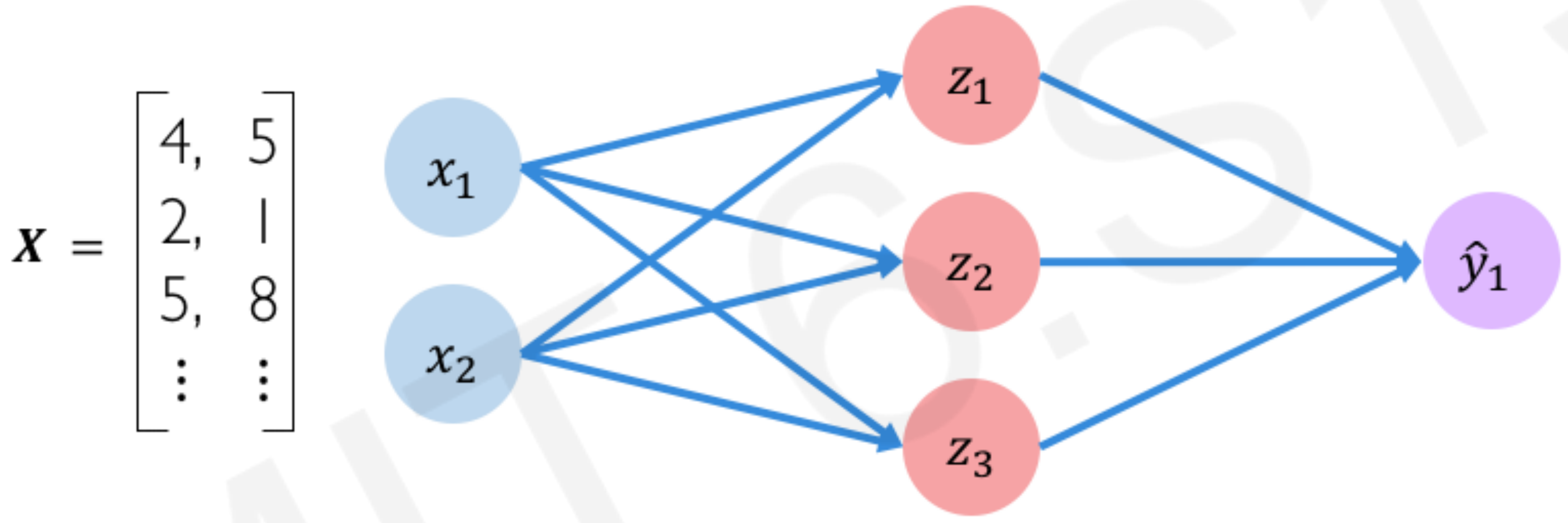
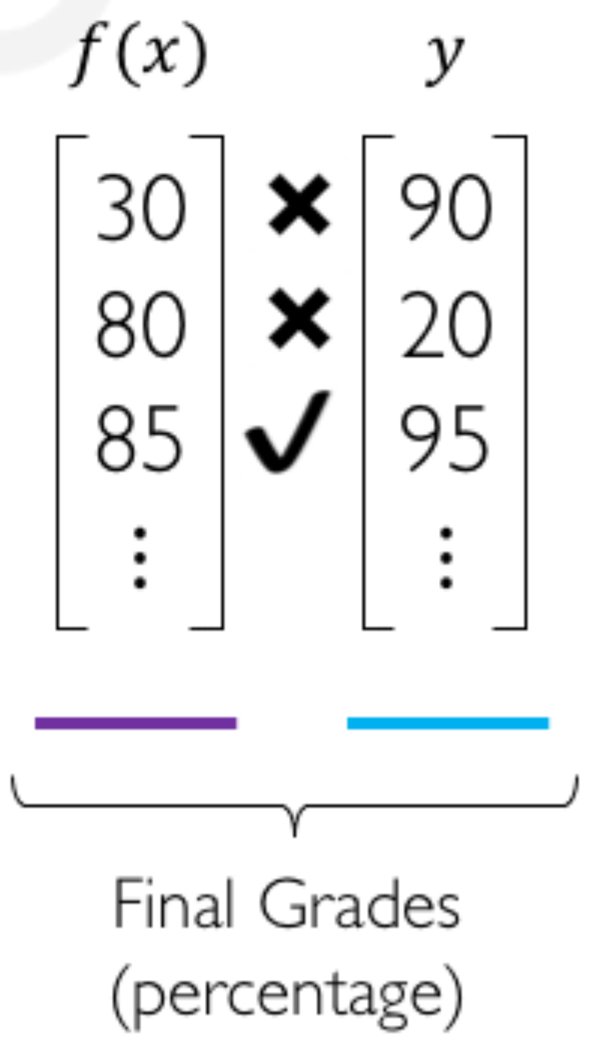
Machine learning in one slide

Social science (inference)	**Machine learning (prediction)**
GLM inverse link function $\mathbb{E}(y) = f(\mathbf{x}'\boldsymbol{\beta})$	Activation function $\mathbb{E}(y) = f(\mathbf{x}'\boldsymbol{\beta})$
Preferred objective function	
Log-likelihood $\log \mathcal{L} = \sum_{i=1}^{n} \log P(y_i \mid \mathbf{x}_i, \boldsymbol{\beta})$	Cross-entropy $-\log \mathcal{L} = -\sum_{i=1}^{n} \log P(y_i \mid \mathbf{x}_i, \boldsymbol{\beta})$
Solving algorithm	
Newton-Raphson $\boldsymbol{\beta}_t := \boldsymbol{\beta}_{t-1} - [\boldsymbol{H} \log \mathcal{L}]^{-1} \nabla \log \mathcal{L}$	Gradient descent $\boldsymbol{\beta}_t := \boldsymbol{\beta}_{t-1} - \eta \nabla(-\log \mathcal{L})$
Quantities of interest	
$\widehat{\boldsymbol{\beta}}; Var(\widehat{\boldsymbol{\beta}})$	$\widehat{\mathbf{y}}; \sum \mathbf{1}(\widehat{y} = y)/n$

Mean Squared Error Loss

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





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

Actual Predicted

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

Training Neural Networks

Loss Optimization

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

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

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

Loss Optimization

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

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

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

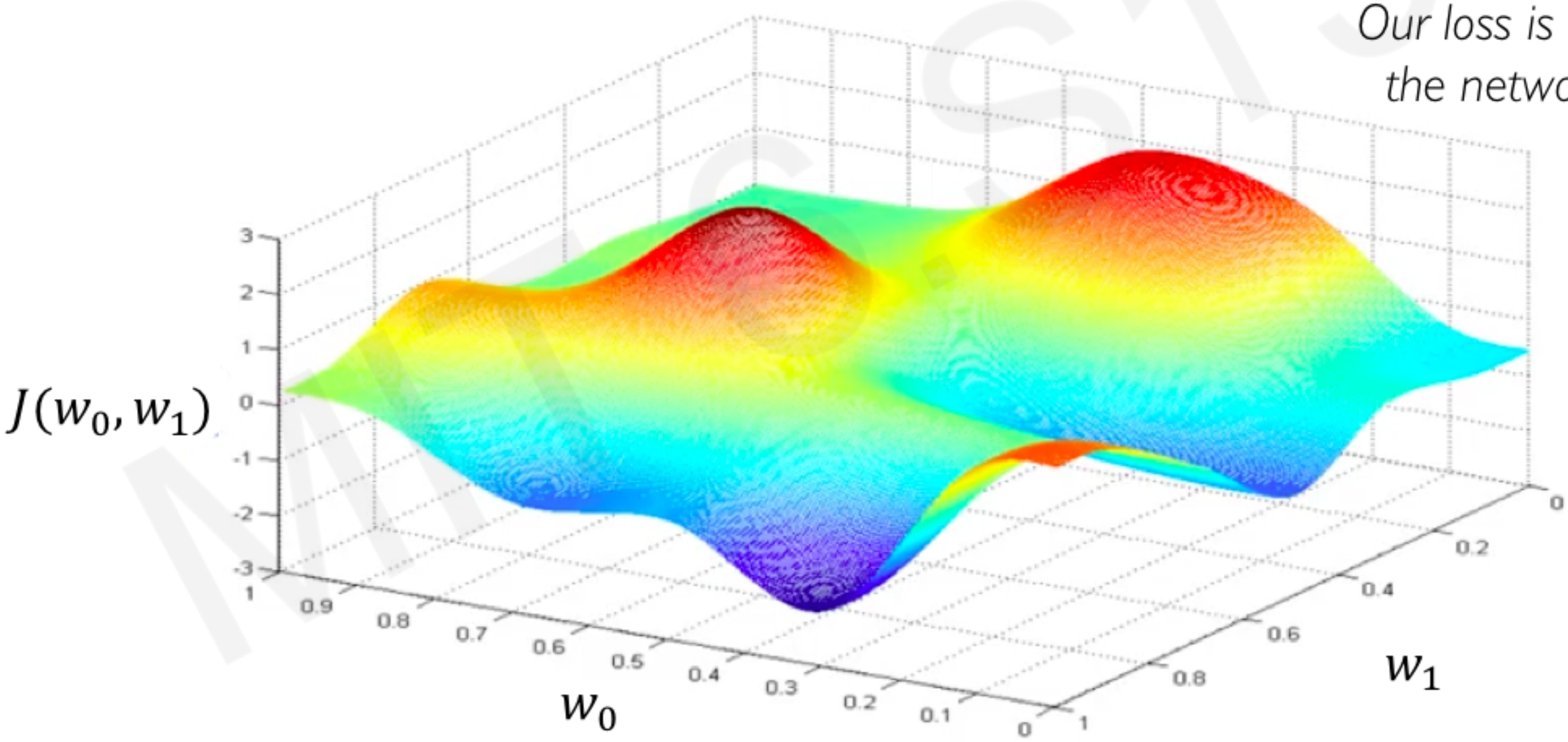
Remember:

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

Loss Optimization

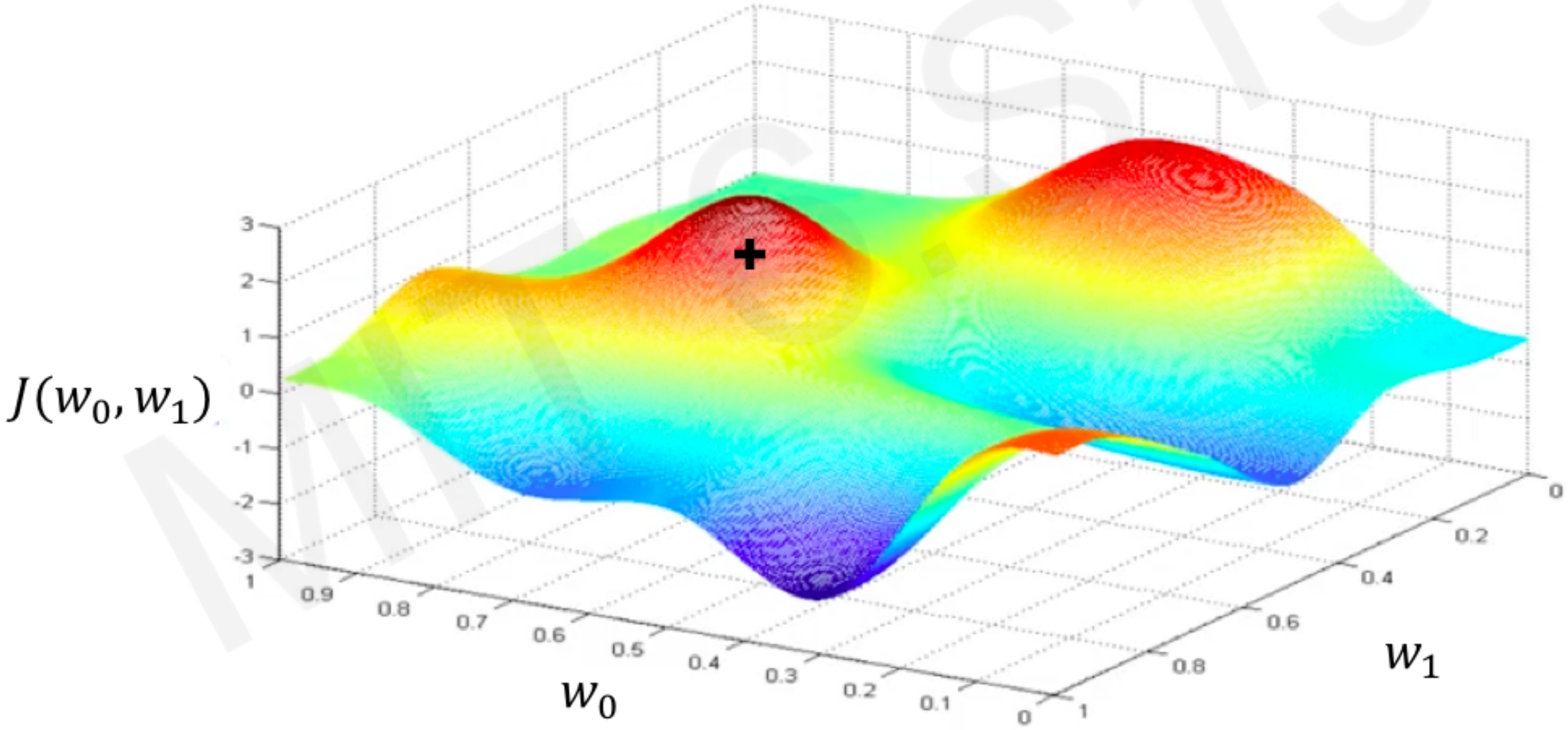
$$W^* = \underset{W}{\operatorname{argmin}}\, J(W)$$

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



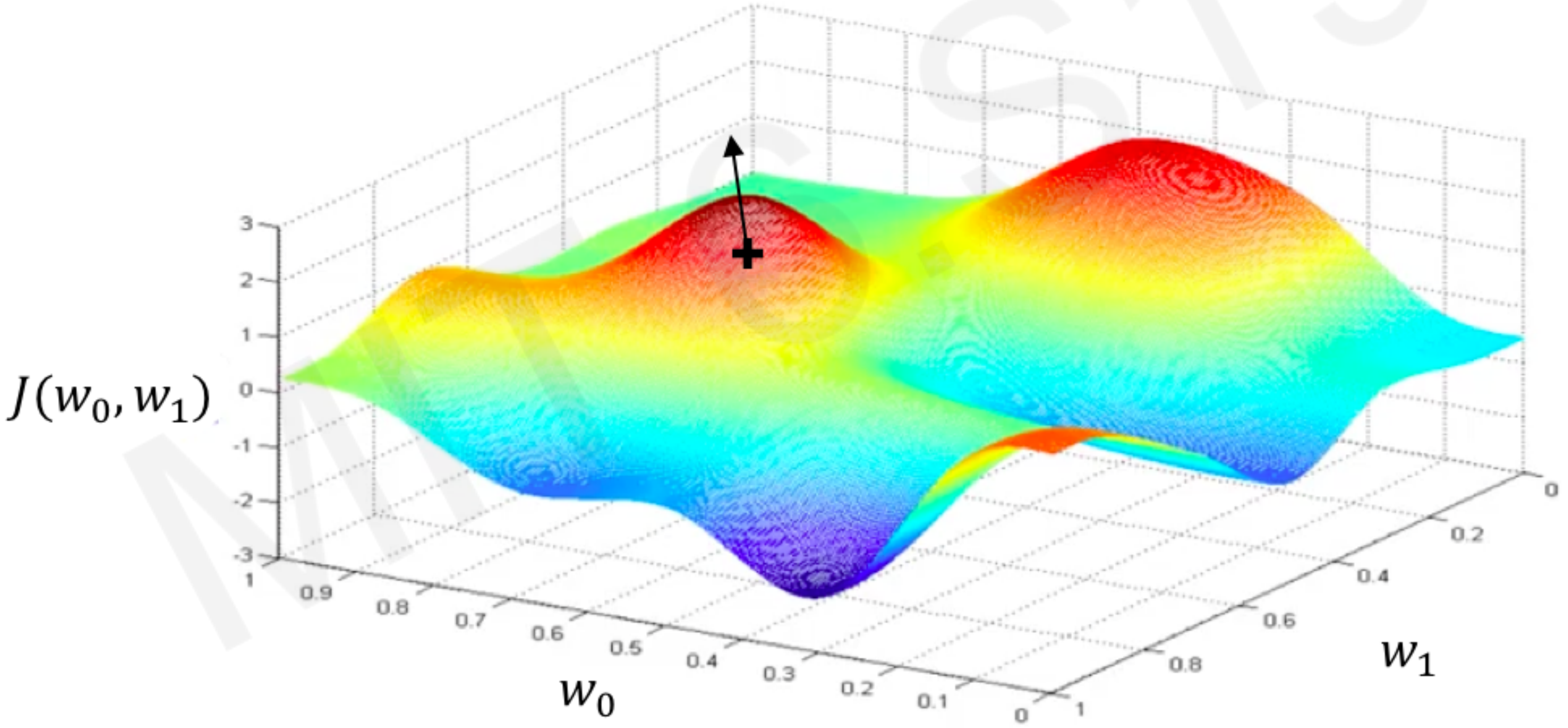
Loss Optimization

Randomly pick an initial (w_0, w_1)



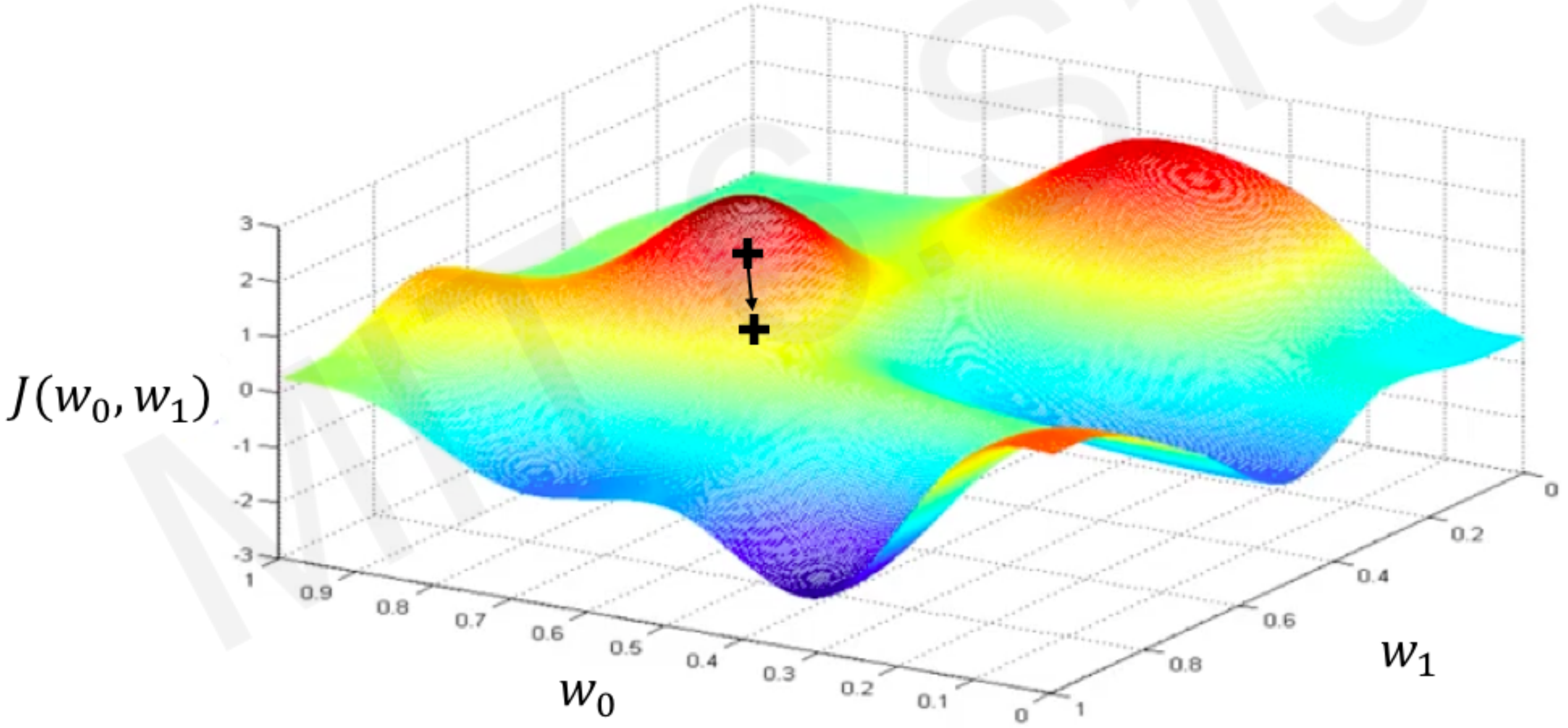
Loss Optimization

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



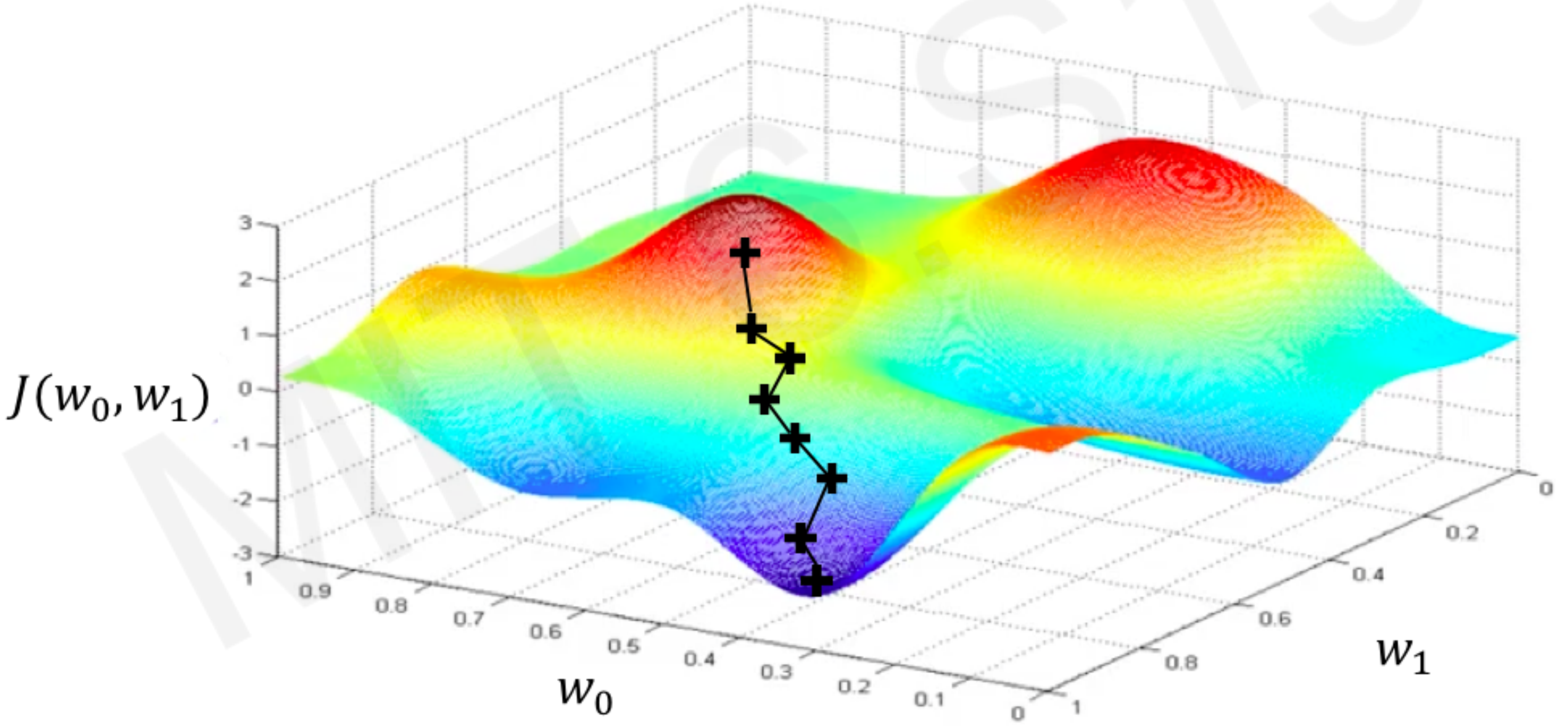
Loss Optimization

Take small step in opposite direction of gradient



Gradient Descent

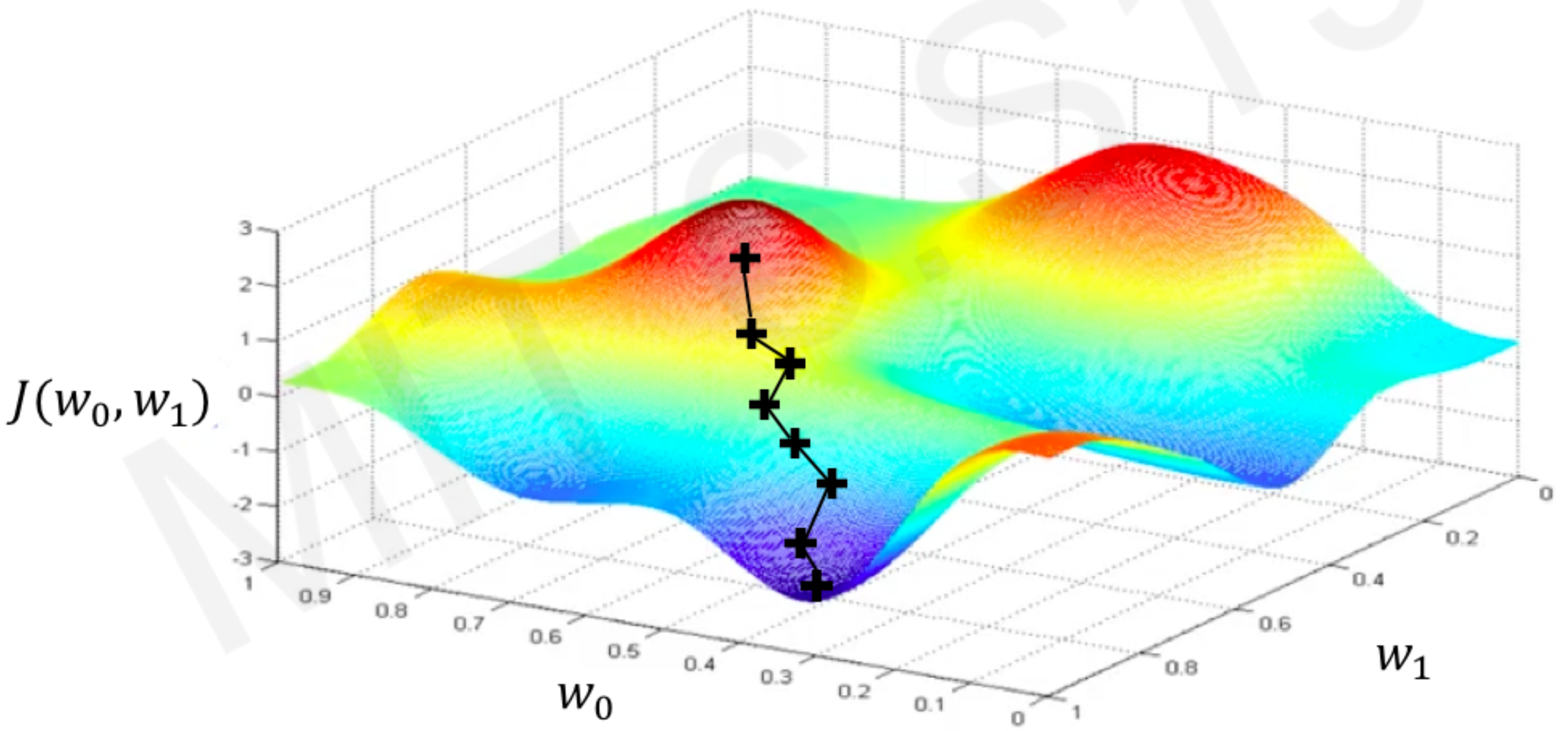
Repeat until convergence



Contrast with Newton-Raphson, which also uses *second derivative* (Hessian)

Gradient Descent

Repeat until convergence



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Gradient Descent

Algorithm

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

Computing Gradients: Backpropagation

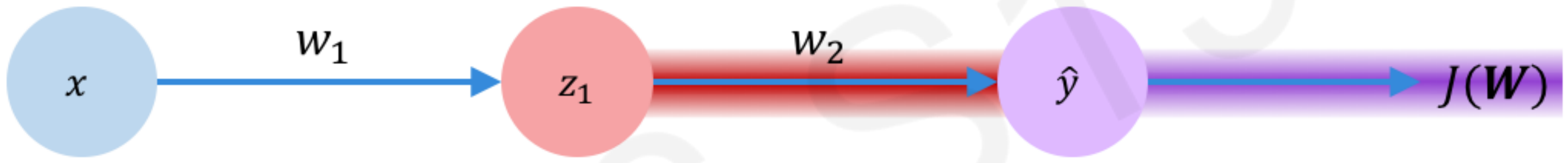
How does a small change in one weight (ex. $\boldsymbol{w_2}$) affect the final loss $\boldsymbol{J(W)}$?

Computing Gradients: Backpropagation

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

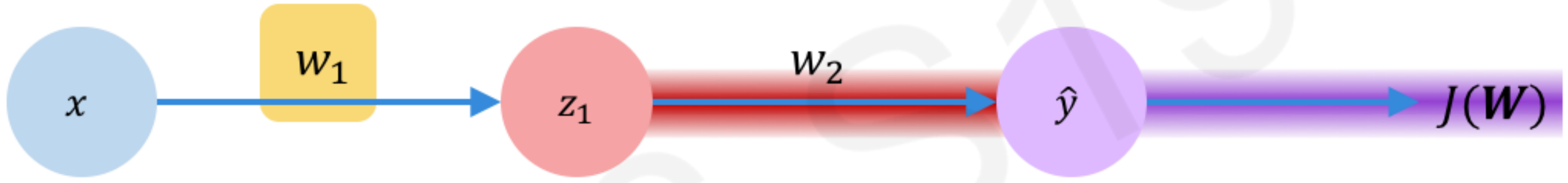
Let's use the chain rule!

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

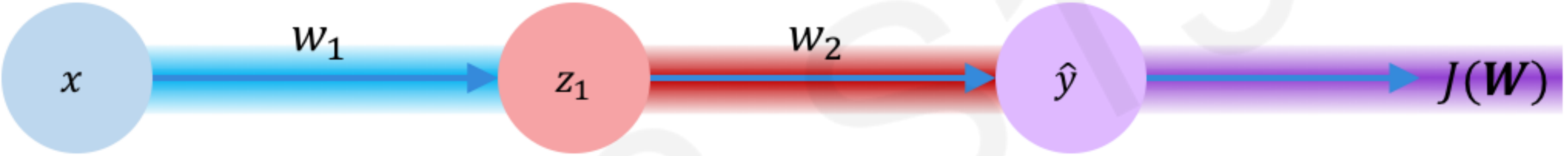


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial w_1}$$

Apply chain rule!

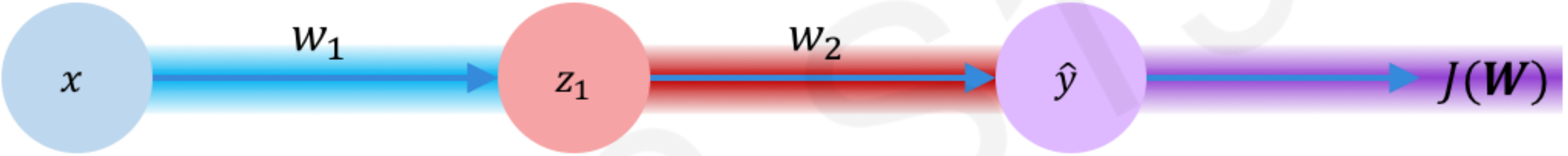
Apply chain rule!

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

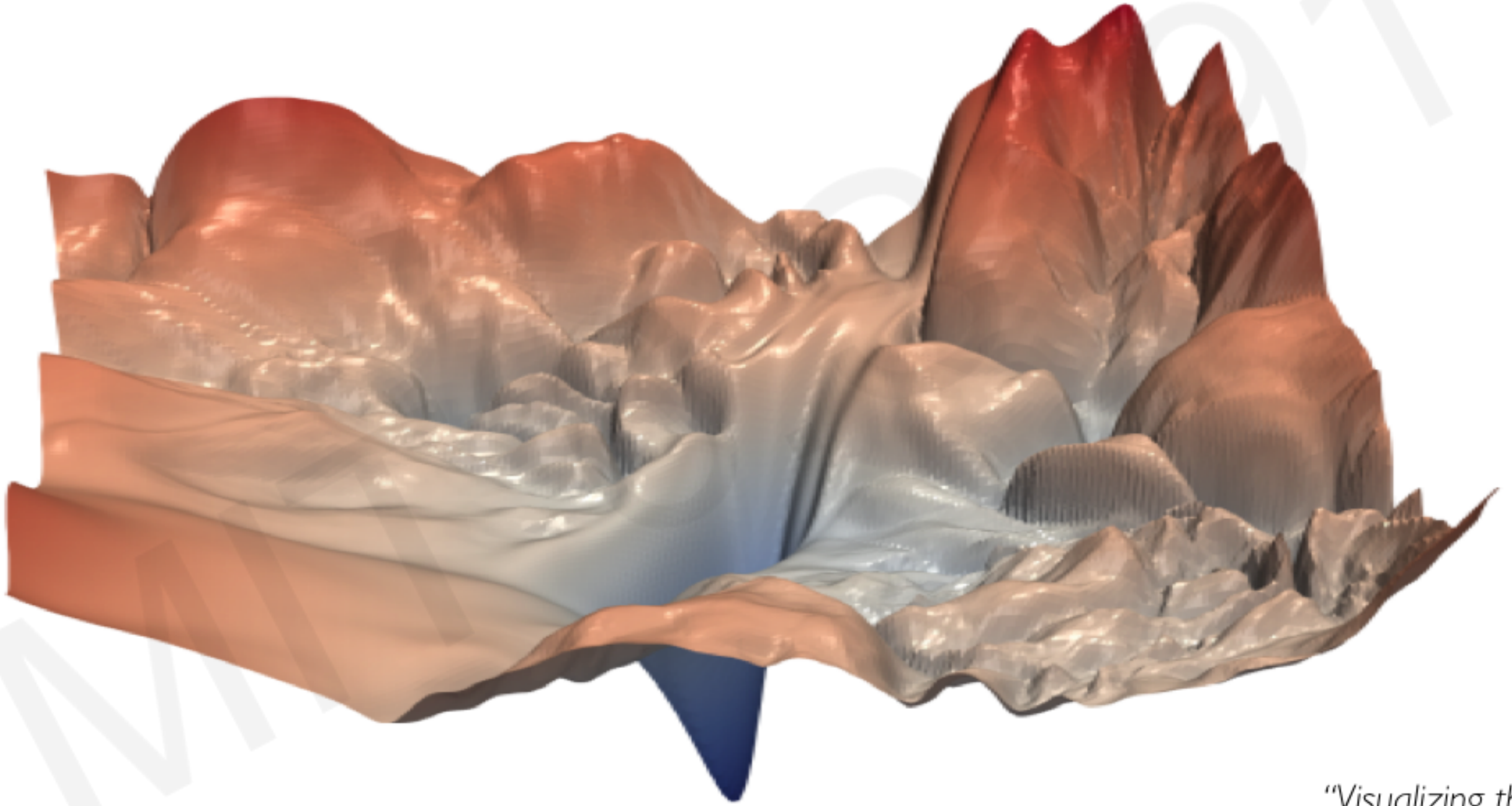


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

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:

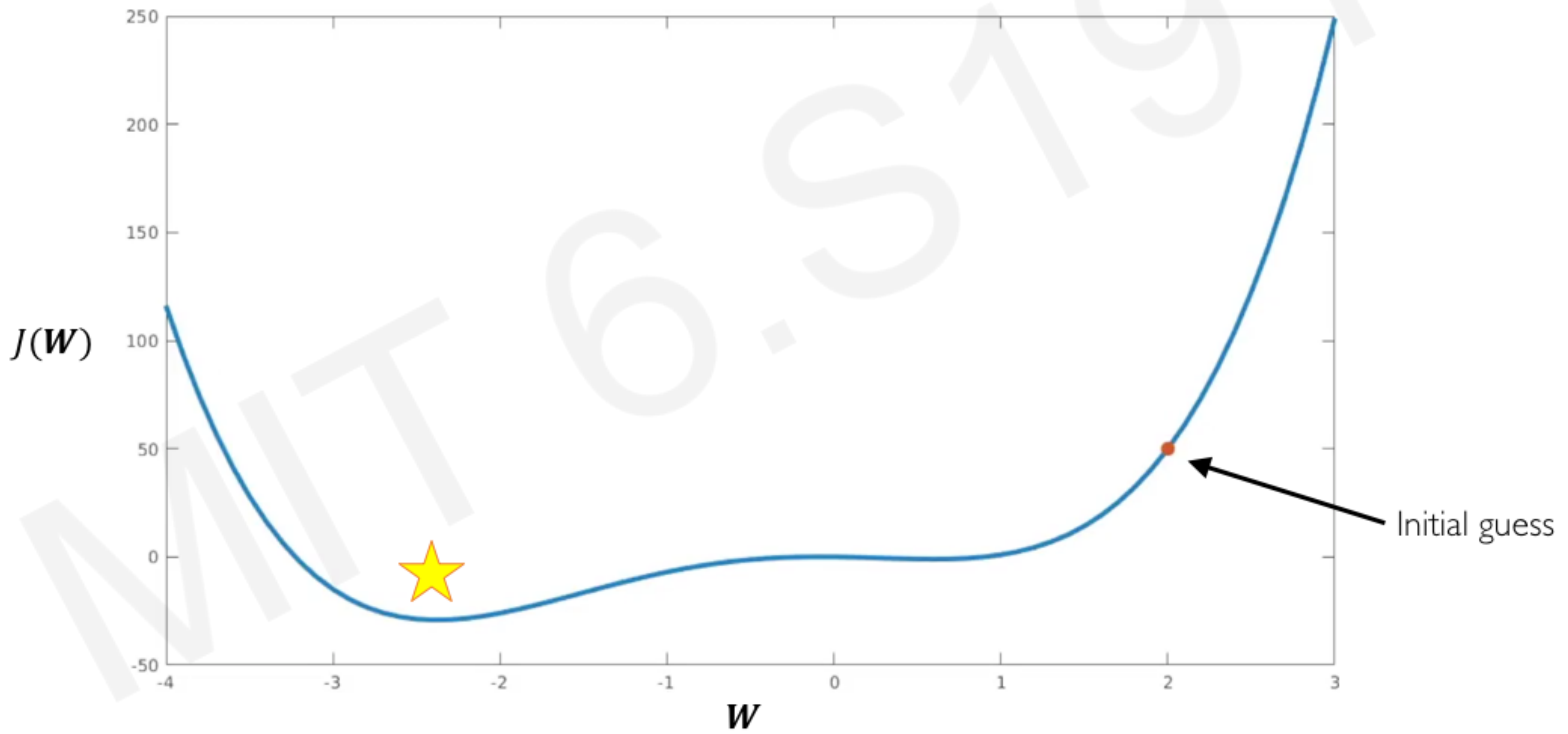
Optimization through gradient descent

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

How can we set the learning rate?

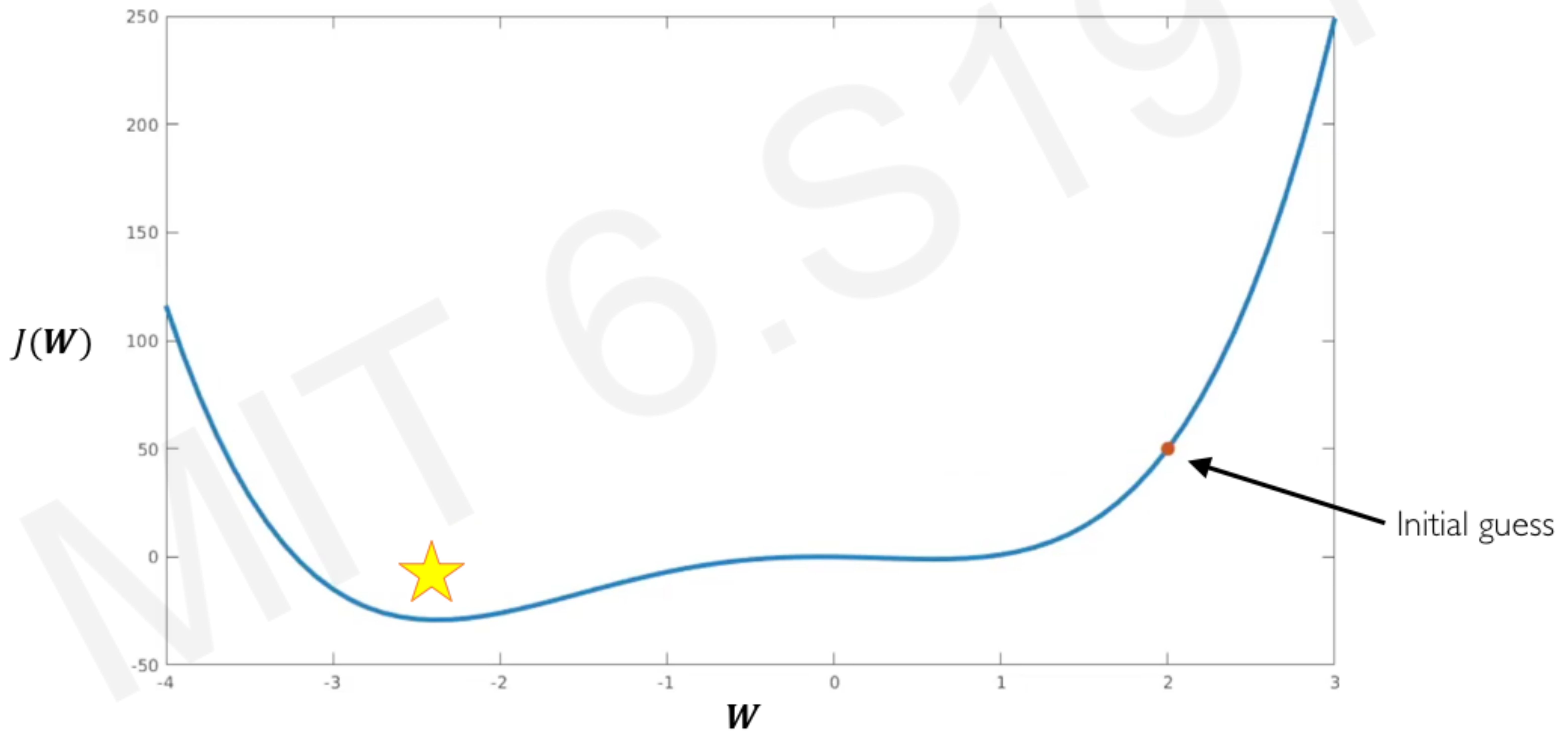
Setting the Learning Rate

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



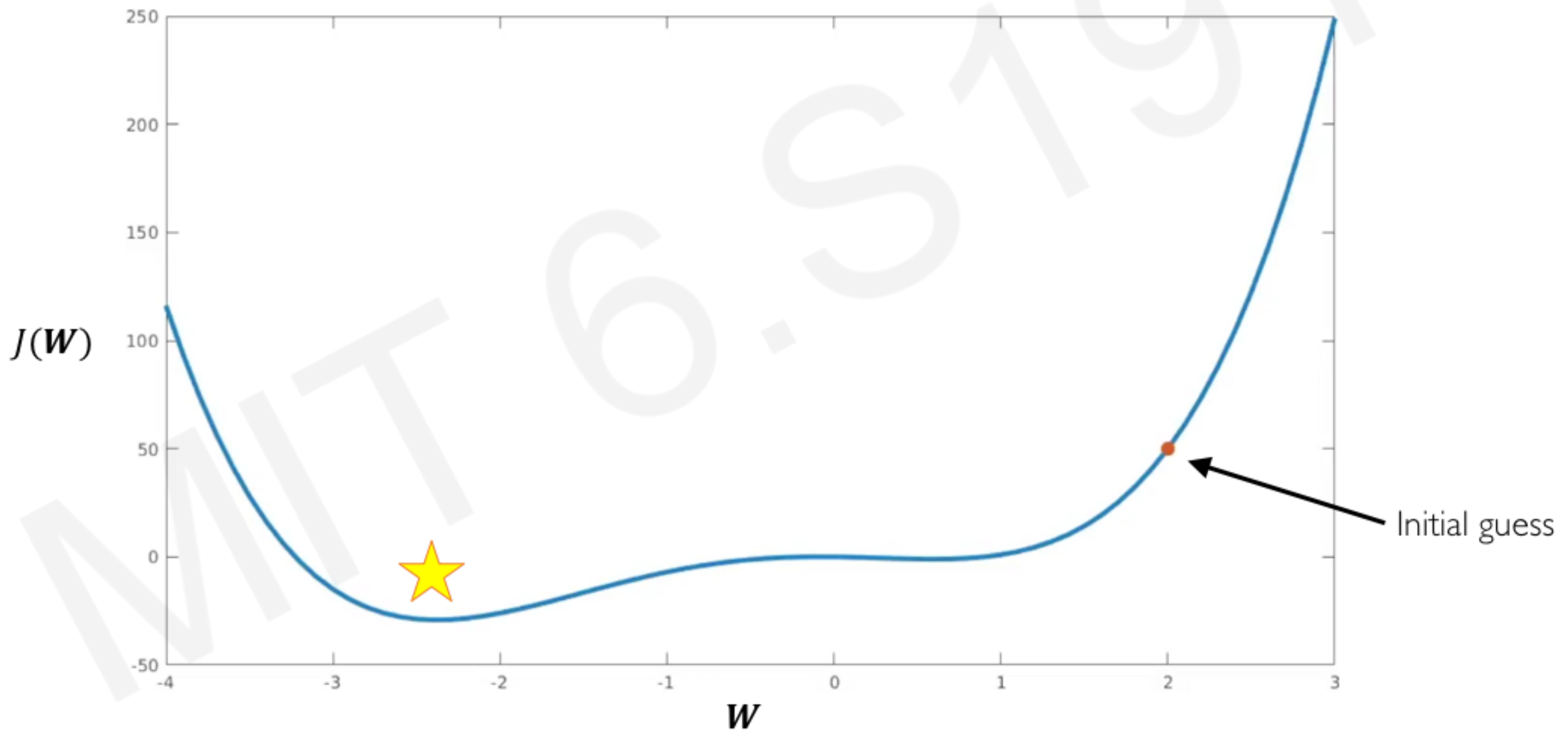
Setting the Learning Rate

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...

Gradient Descent Algorithms

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

Additional details: http://ruder.io/optimizing-gradient-descent/

Gradient Descent Algorithms

```
model = models.Sequential()
model.add(layers.Dense(16, activation = 'relu', input_shape=(5000,)))
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model.compile(optimizer='adam',
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history = model.fit(partial_x_train,
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                    epochs=4,
                    batch_size=512,
                    validation_data=(x_val,y_val))
```

Rate

Online

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Gradient Descent Algorithms

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- A
- R

```r
```{r}
model <- keras_model_sequential() %>%
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```

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Neural Networks in Practice: Mini-batches

Gradient Descent

Algorithm

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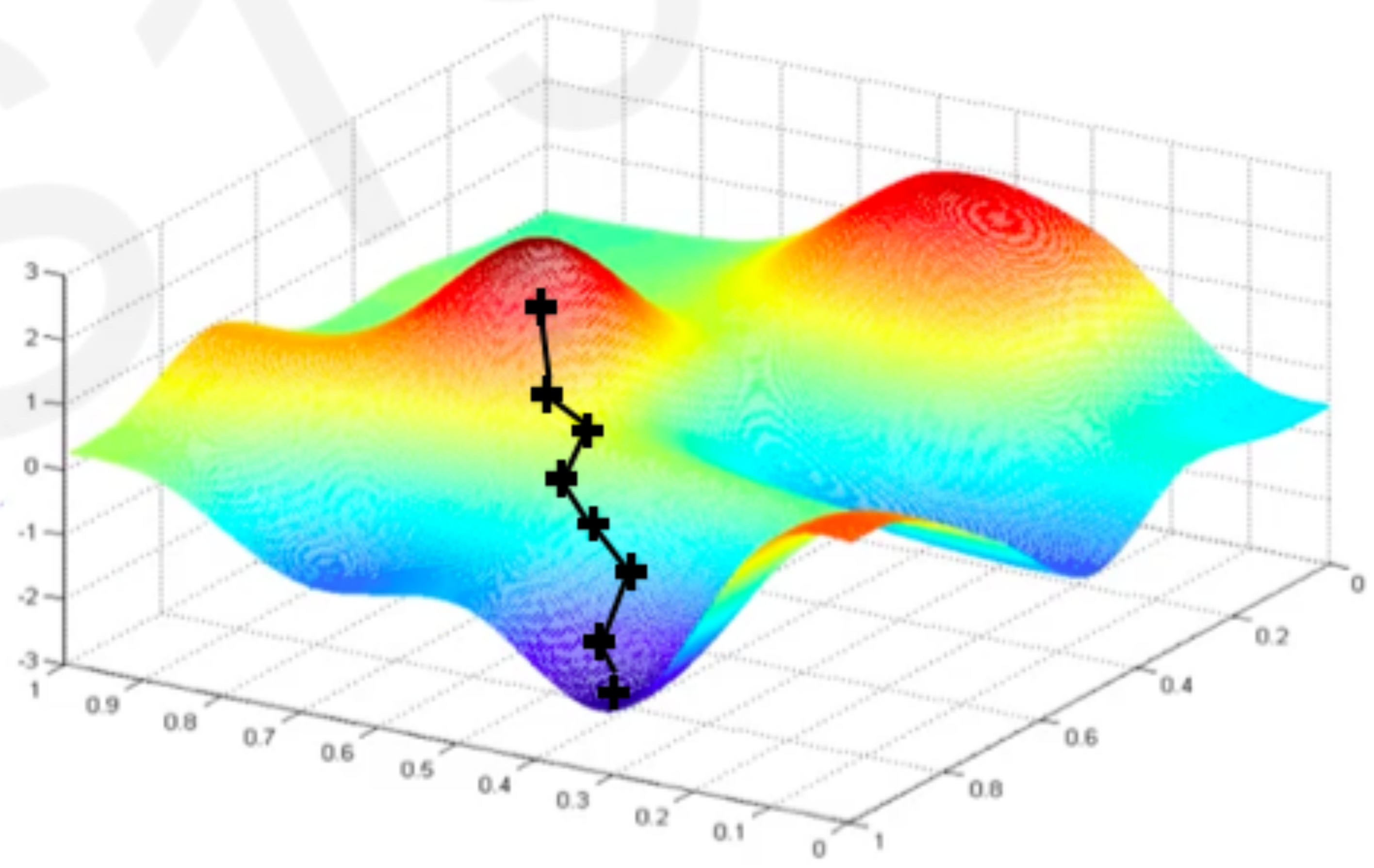

Gradient Descent

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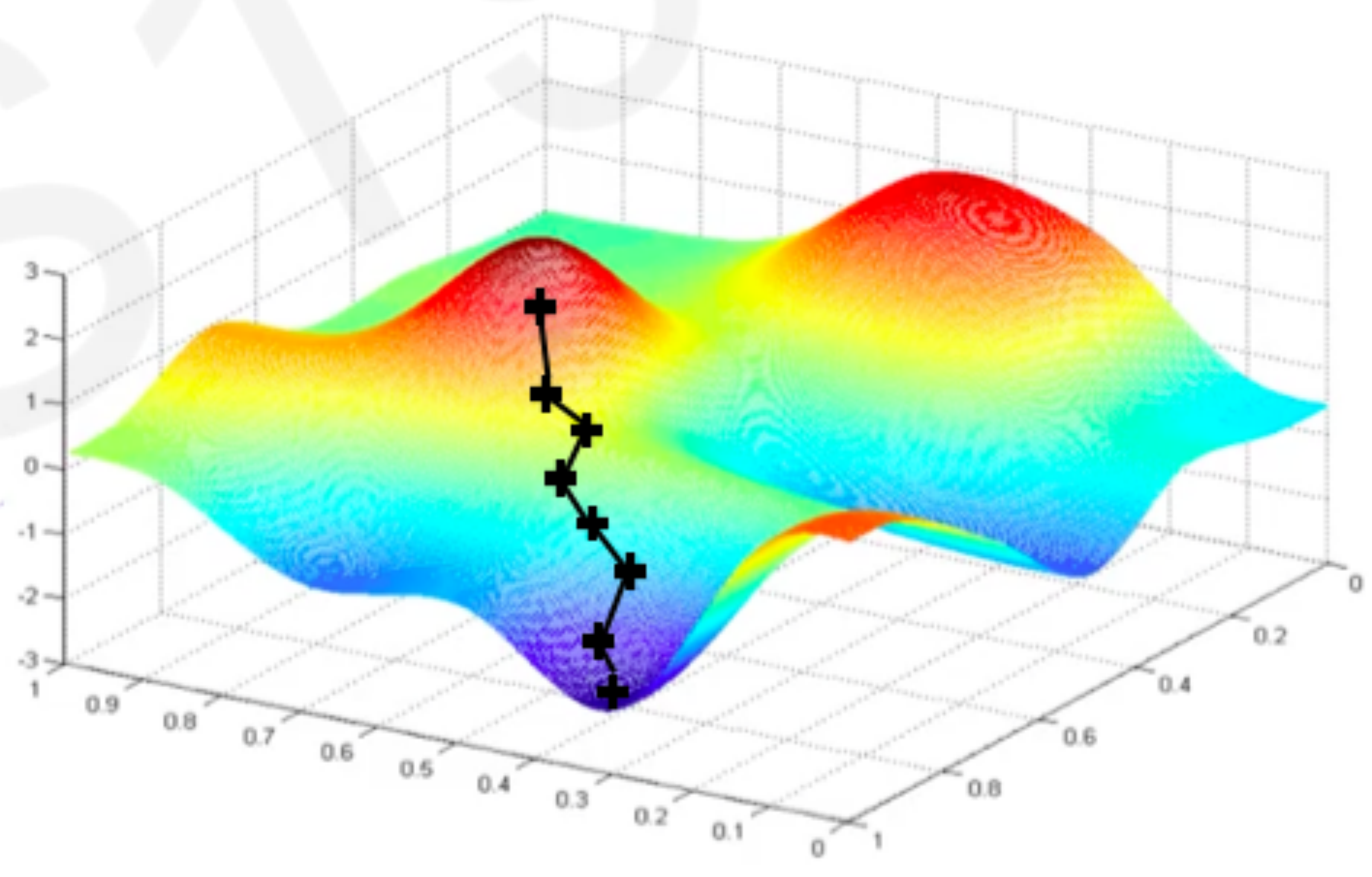

Can be very **computationally intensive** to compute!

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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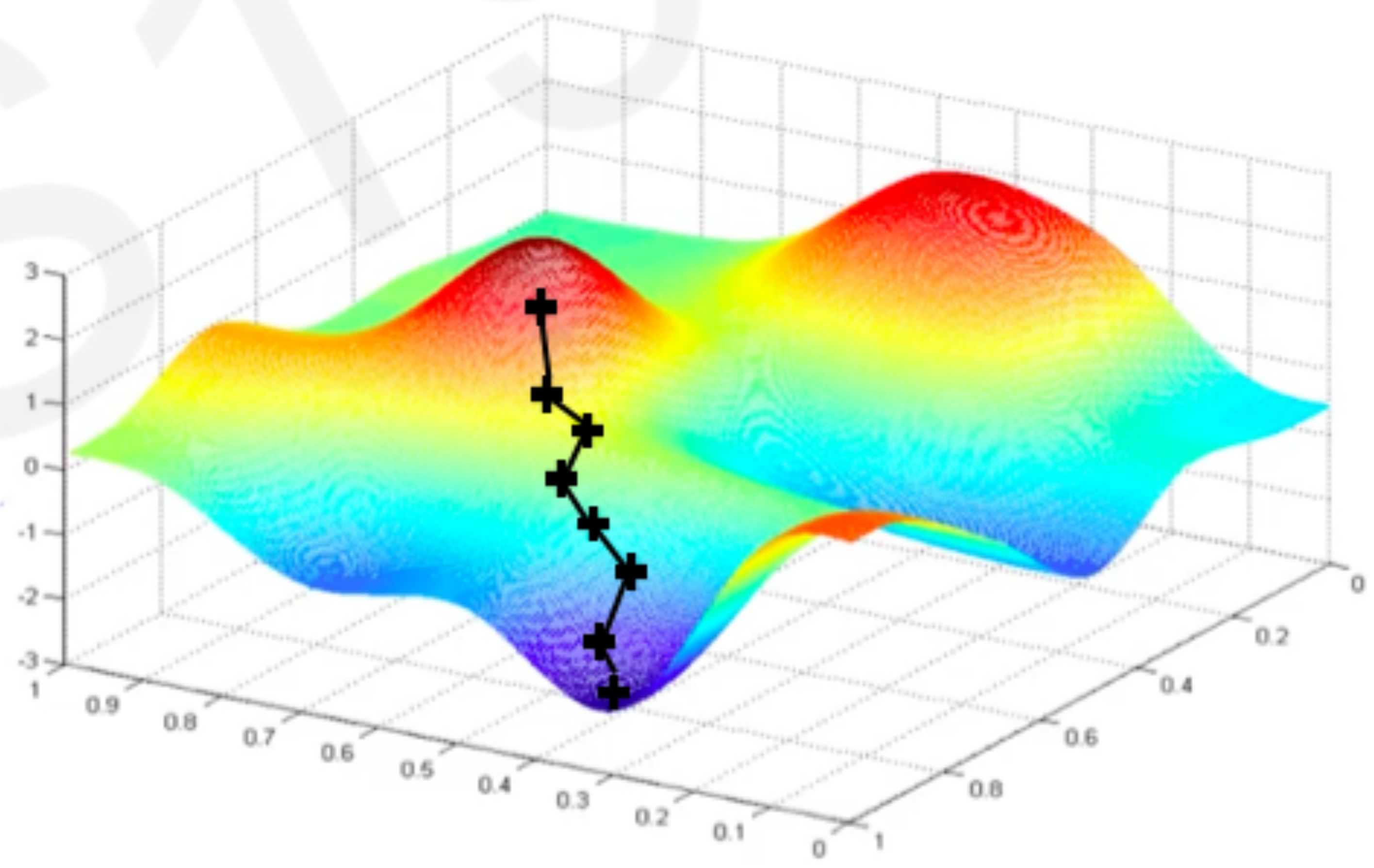
6. Return weights



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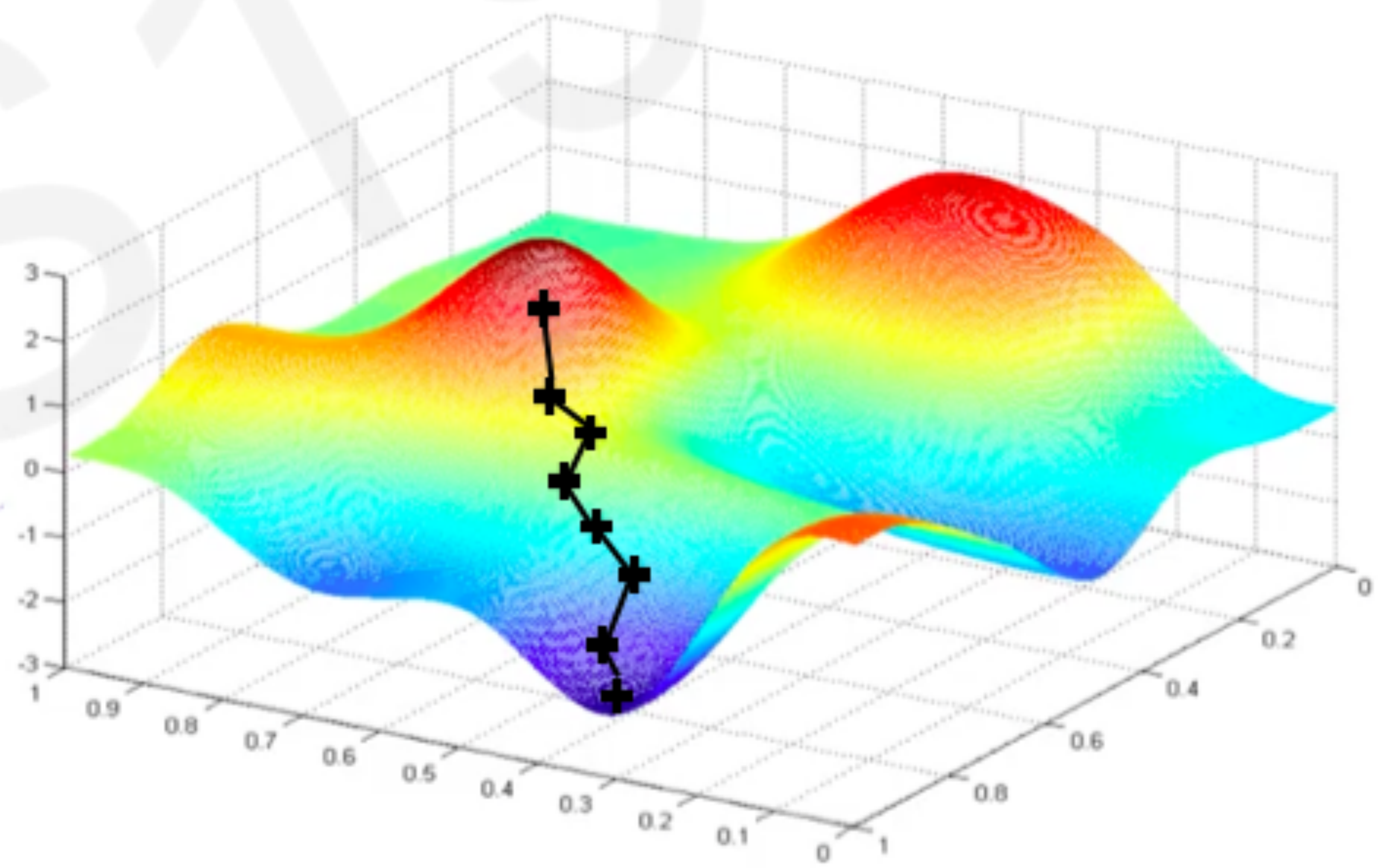

Easy to compute but **very noisy** (stochastic)!

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, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}} = \frac{1}{B}\sum_{k=1}^{B} \frac{\partial J_k(\boldsymbol{W})}{\partial \boldsymbol{W}}$
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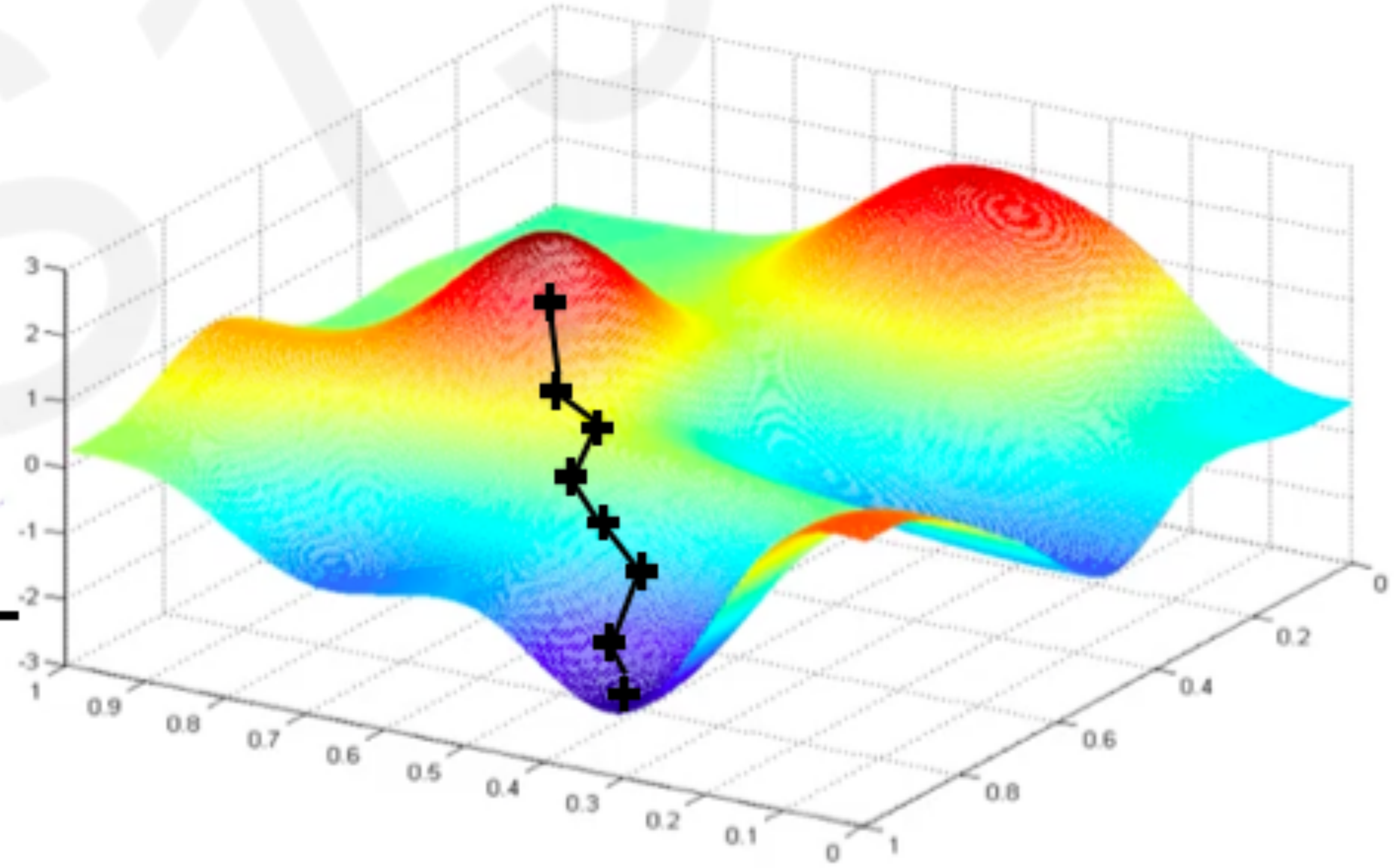

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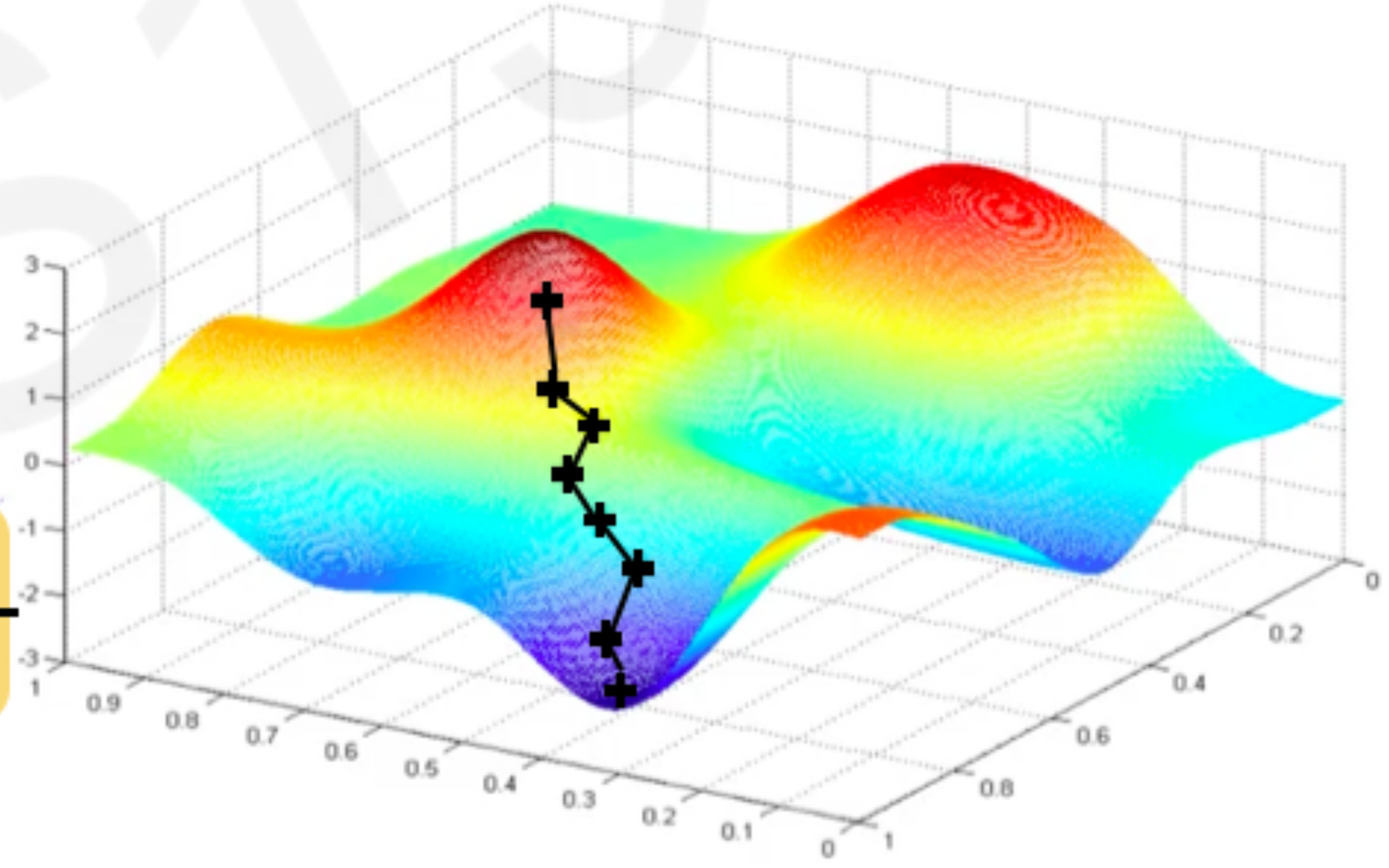

Fast to compute and a much better estimate of the true gradient!

Stochastic Gradient Descent

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Stochastic Gradient Descent

Algo

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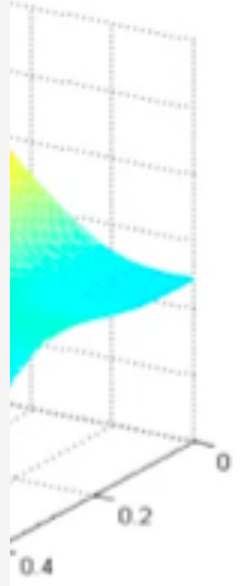


Fast to compute and a much better estimate of the true gradient!

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

So, SGD is different from Newton-Raphson in derivative information used, *and* in its optimization over small subsets of the data at a time and in parallel.

Mini-batches while training

More accurate estimation of gradient

Smoother convergence

Allows for larger learning rates

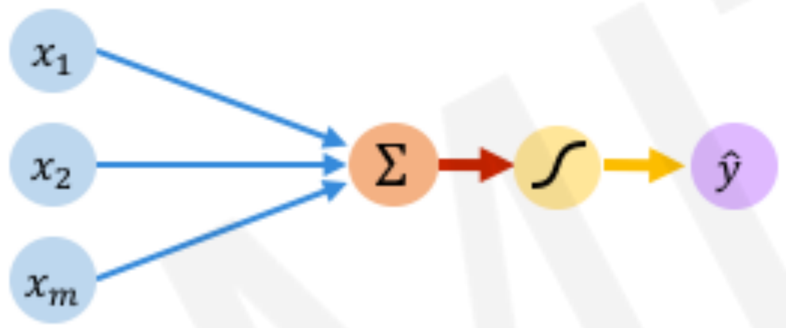
Mini-batches lead to fast training!

Can parallelize computation + achieve significant speed increases on GPU's https://playground.tensorflow.org

Core Foundation Review

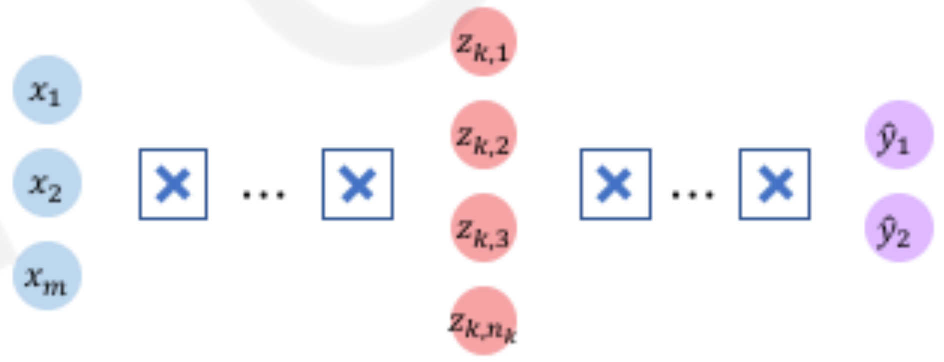
The Perceptron

- Structural building blocks
- Nonlinear activation functions



Neural Networks

- Stacking Perceptrons to form neural networks
- Optimization through backpropagation



Training in Practice

- Adaptive learning
- Batching
- Regularization