Introduction to Deep Learning

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MIT 6.S191

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Training Neural Networks

Loss Optimization

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

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

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

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

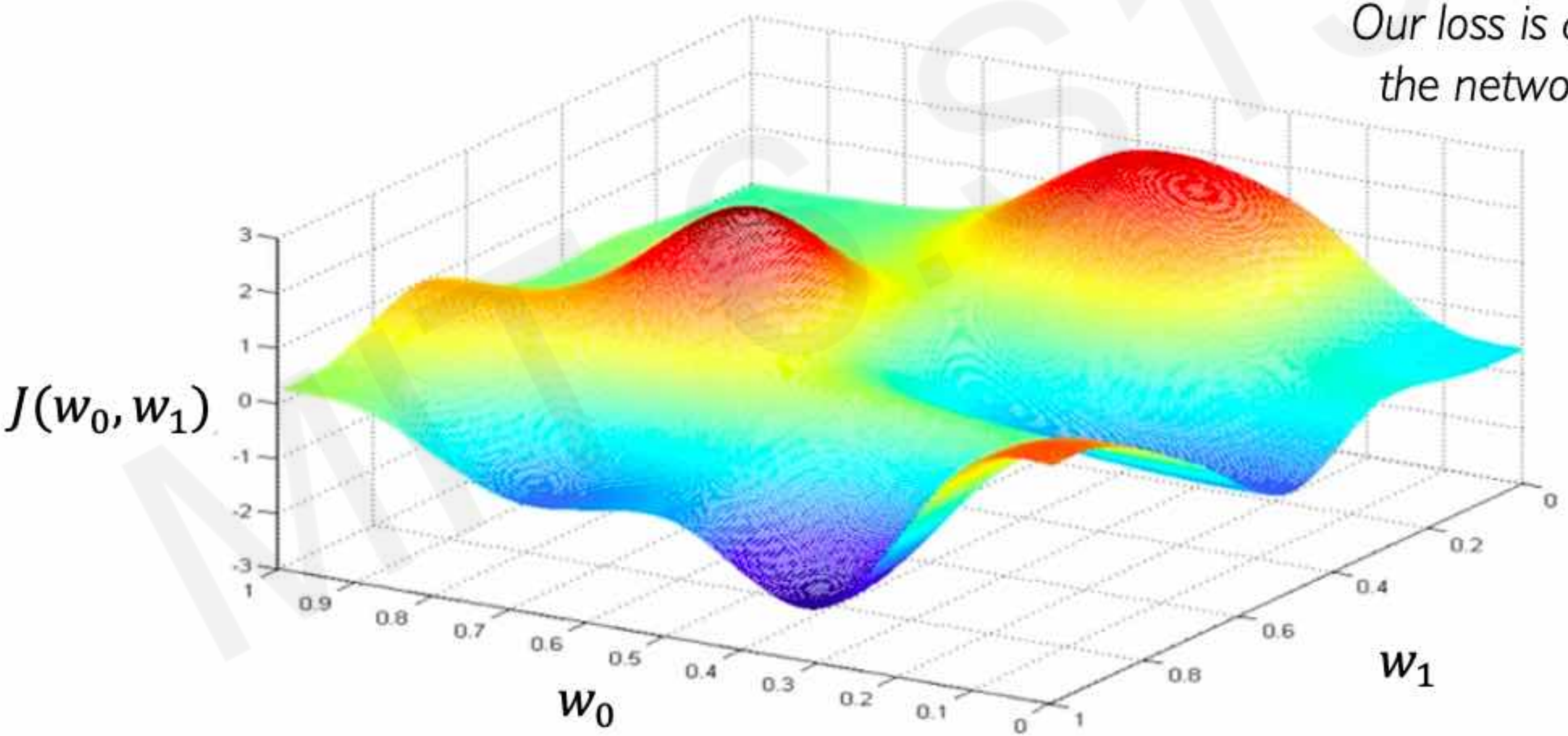
Remember:

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

Loss Optimization

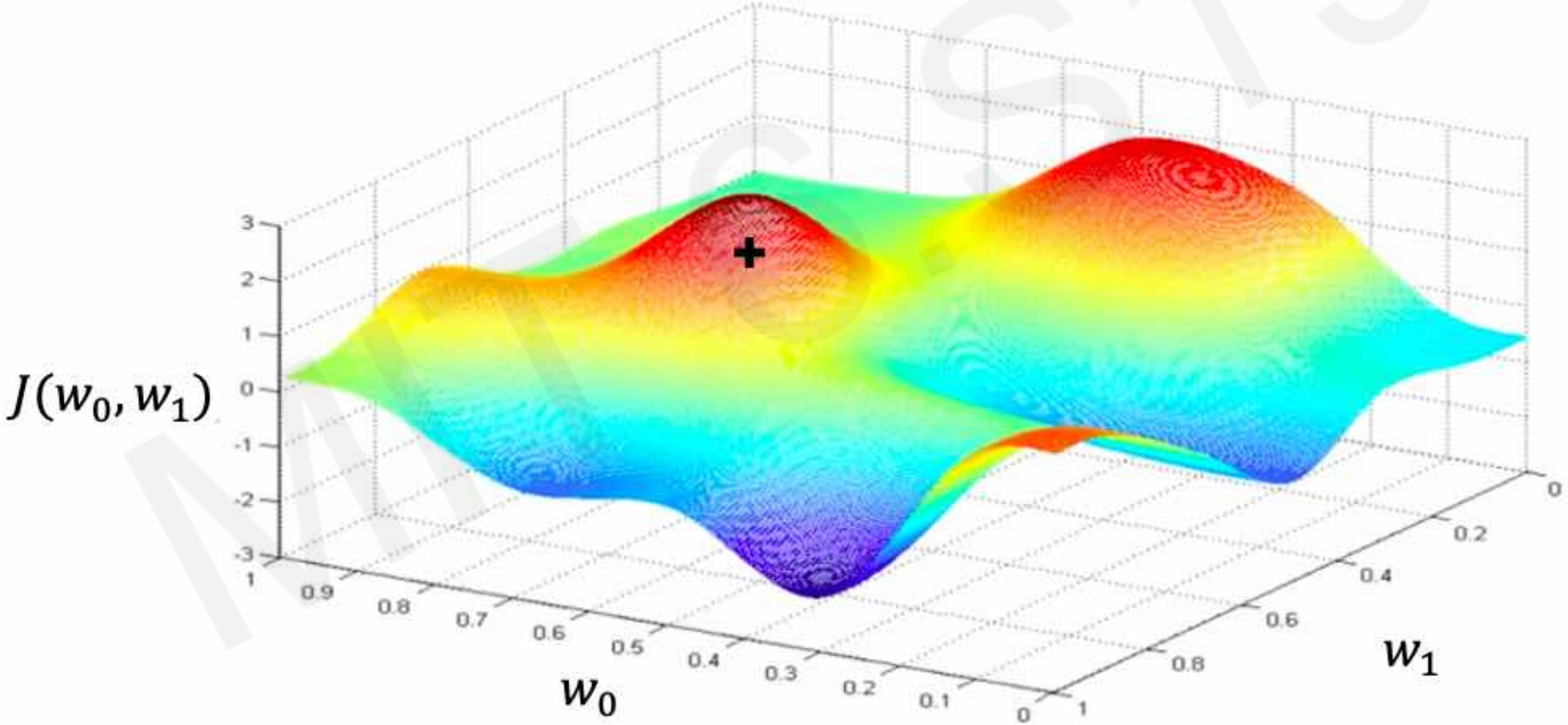
$$W^* = \underset{W}{\operatorname{argmin}}\, J(W)$$

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



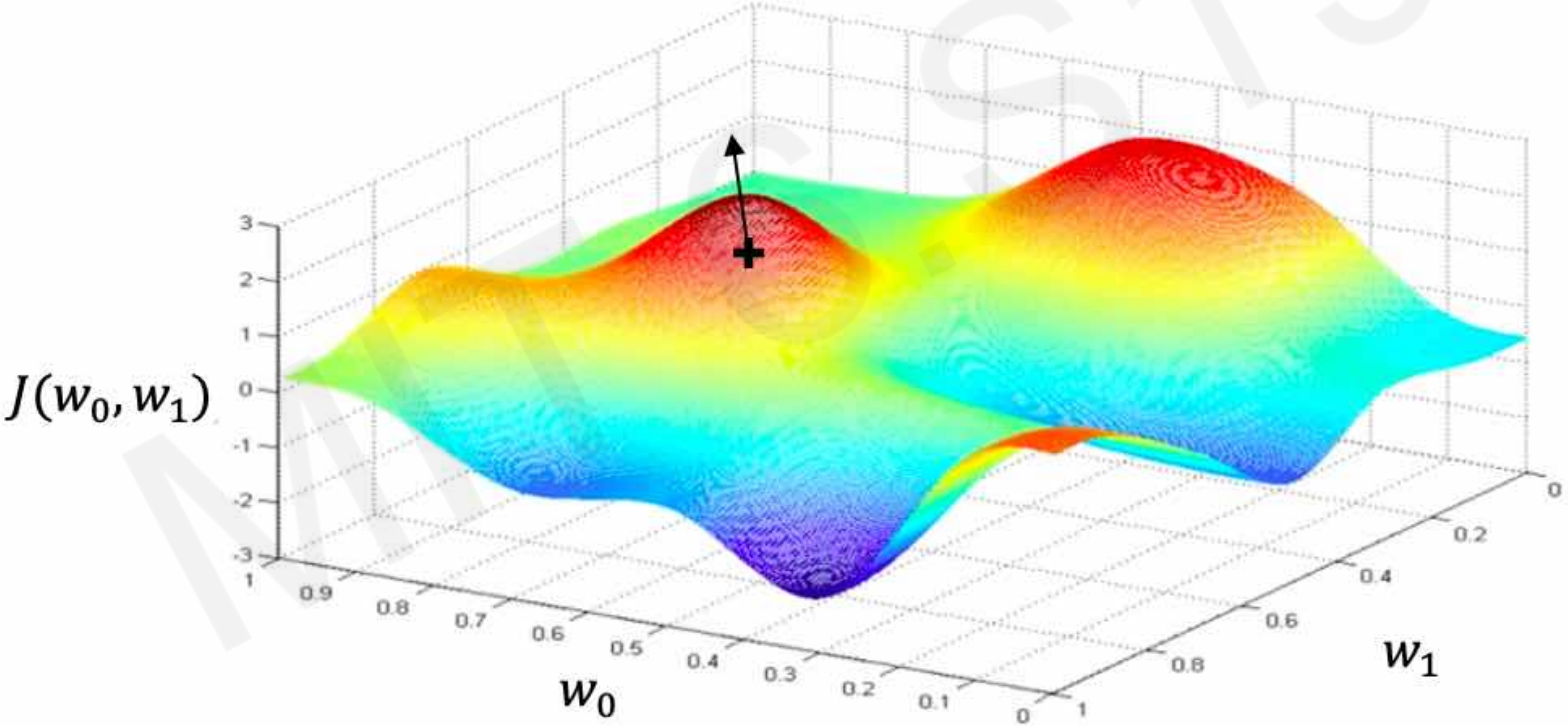
Loss Optimization

Randomly pick an initial (w_0, w_1)



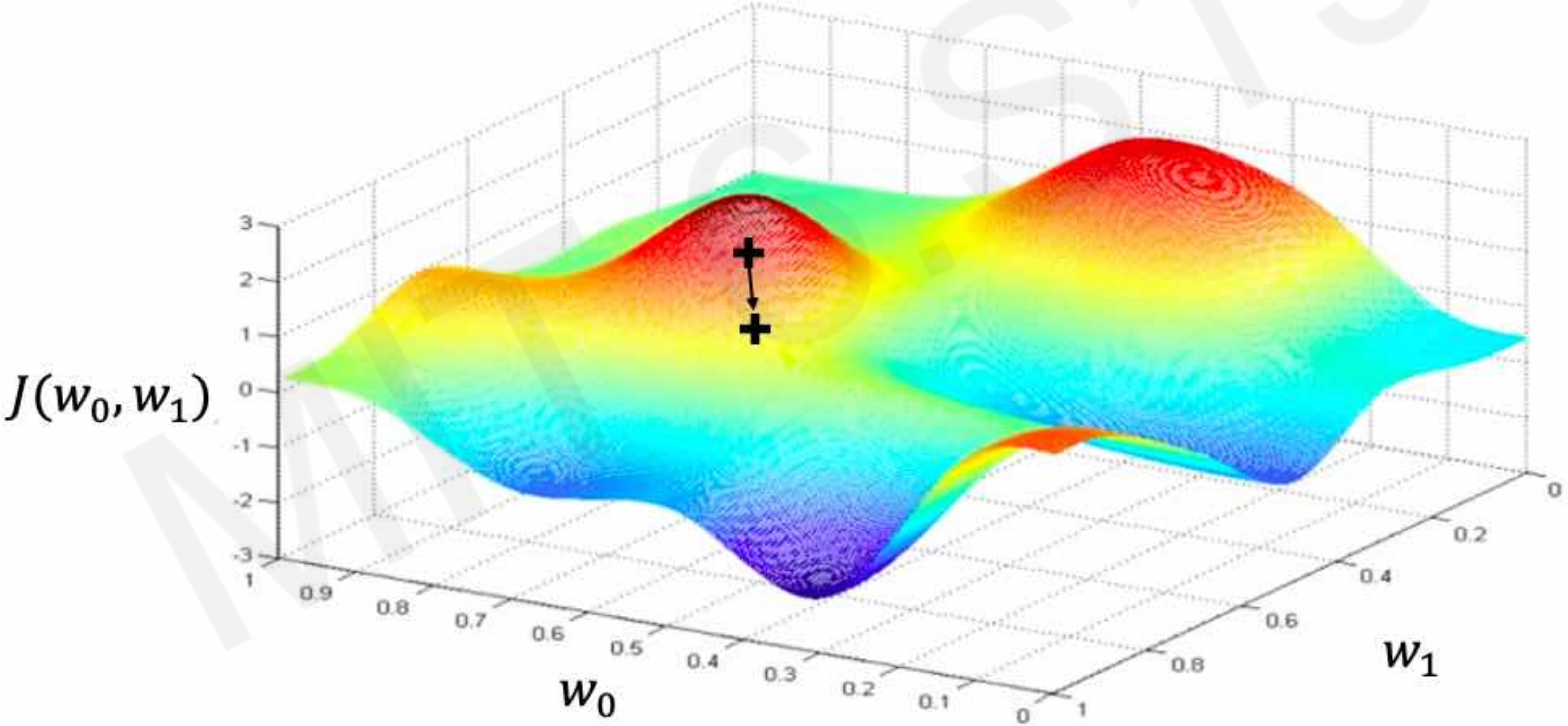
Loss Optimization

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



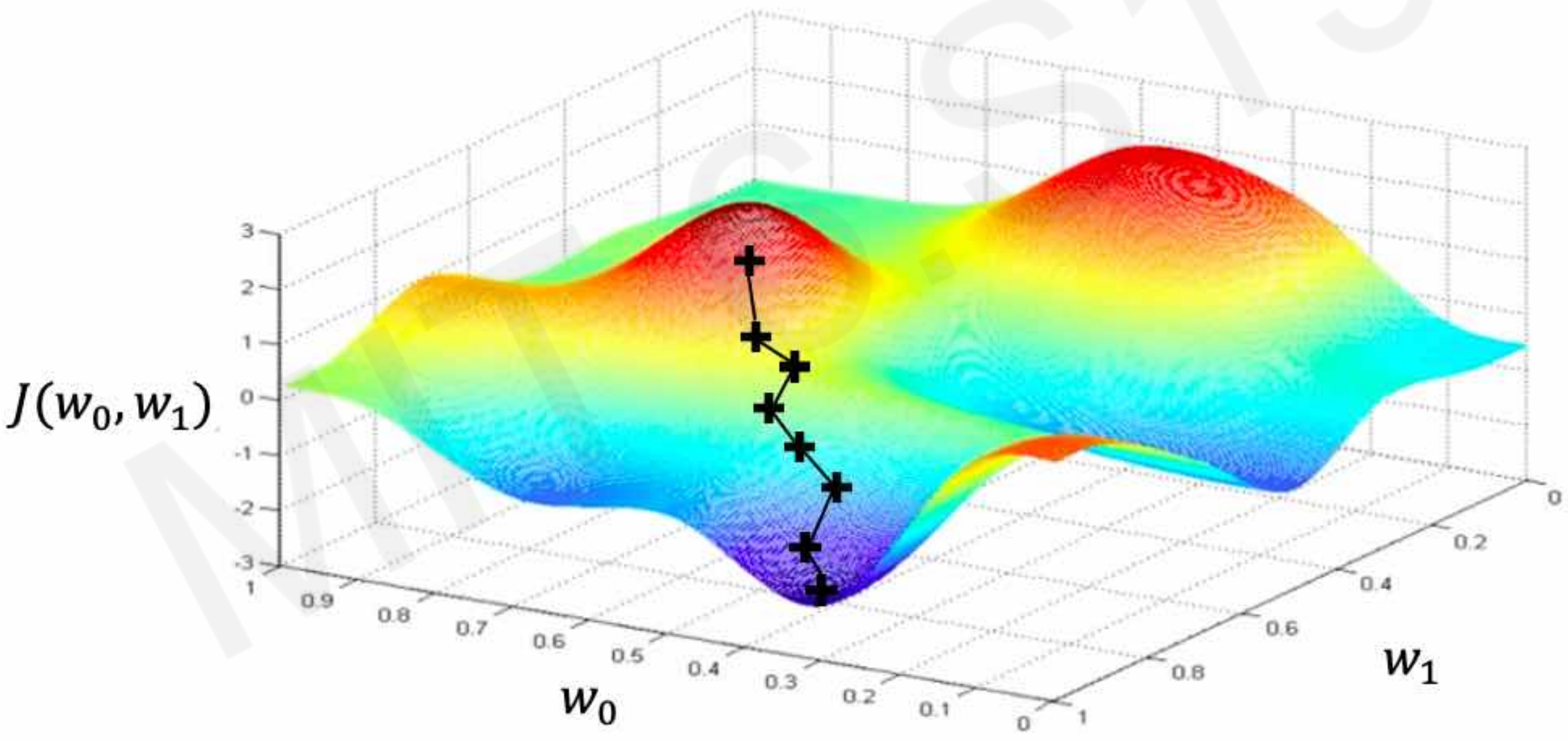
Loss Optimization

Take small step in opposite direction of gradient



Gradient Descent

Repeat until convergence



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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```python
import tensorflow as tf

weights = tf.Variable([tf.random.normal()])

while True:    # loop forever
    with tf.GradientTape() as g:
        loss = compute_loss(weights)
        gradient = g.gradient(loss, weights)

    weights = weights - lr * gradient
```

Gradient Descent

Algorithm

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Computing Gradients: Backpropagation

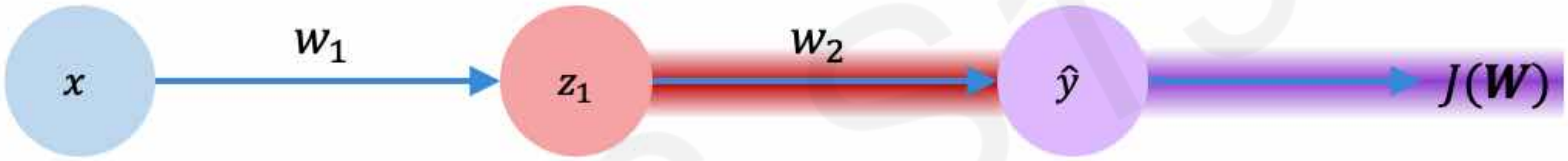
How does a small change in one weight (ex. $\boldsymbol{w_2}$) affect the final loss $\boldsymbol{J(W)}$?

Computing Gradients: Backpropagation

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

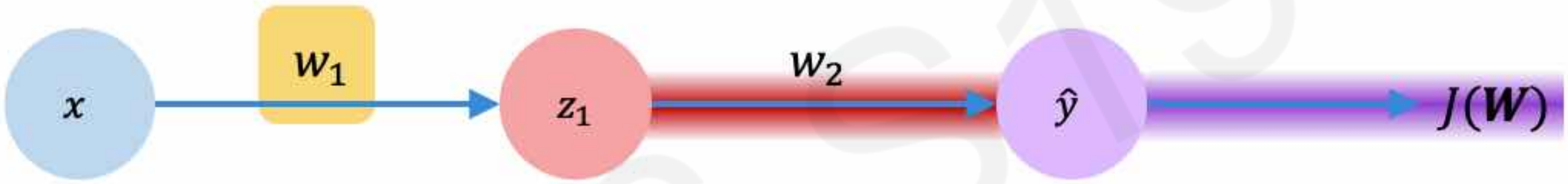
Let's use the chain rule!

Computing Gradients: Backpropagation



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

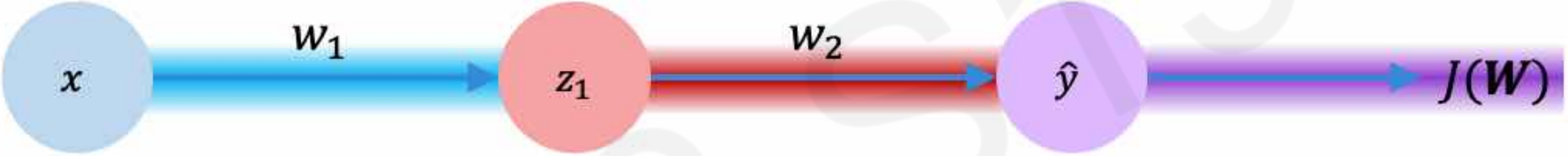
Computing Gradients: Backpropagation



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

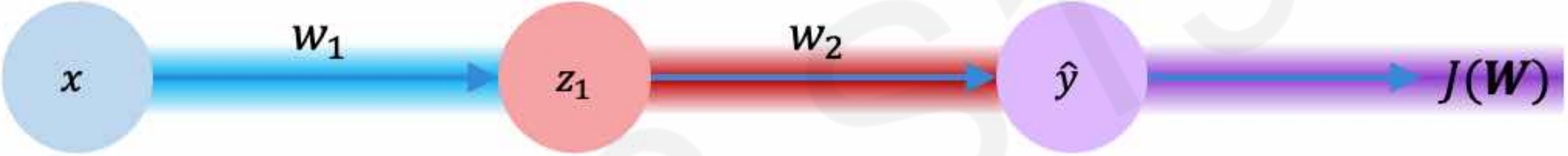
Apply chain rule! Apply chain rule!

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

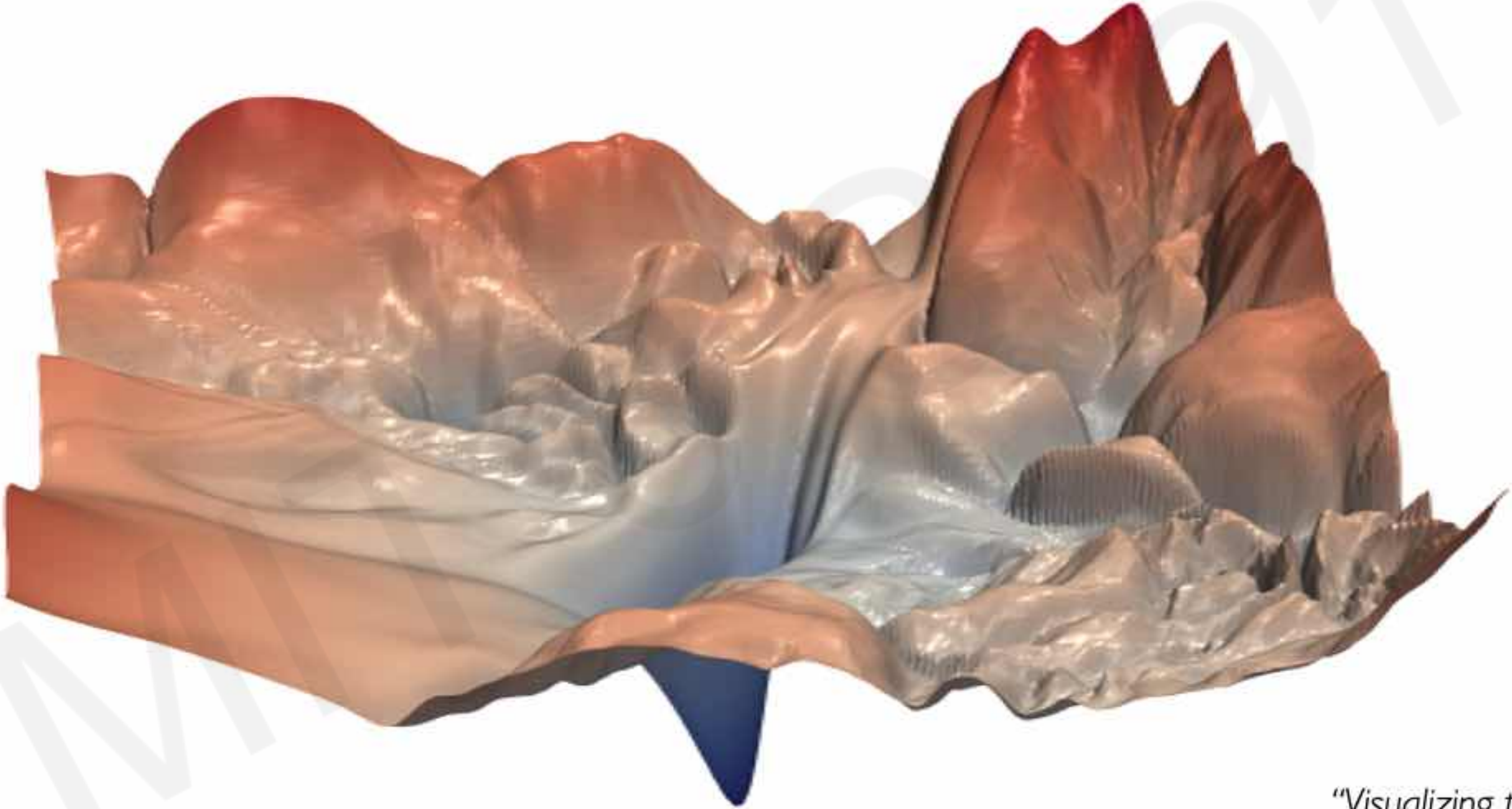


$$\frac{\partial J(\boldsymbol{W})}{\partial w_1} = \frac{\partial J(\boldsymbol{W})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

*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

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

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Optimization through gradient descent

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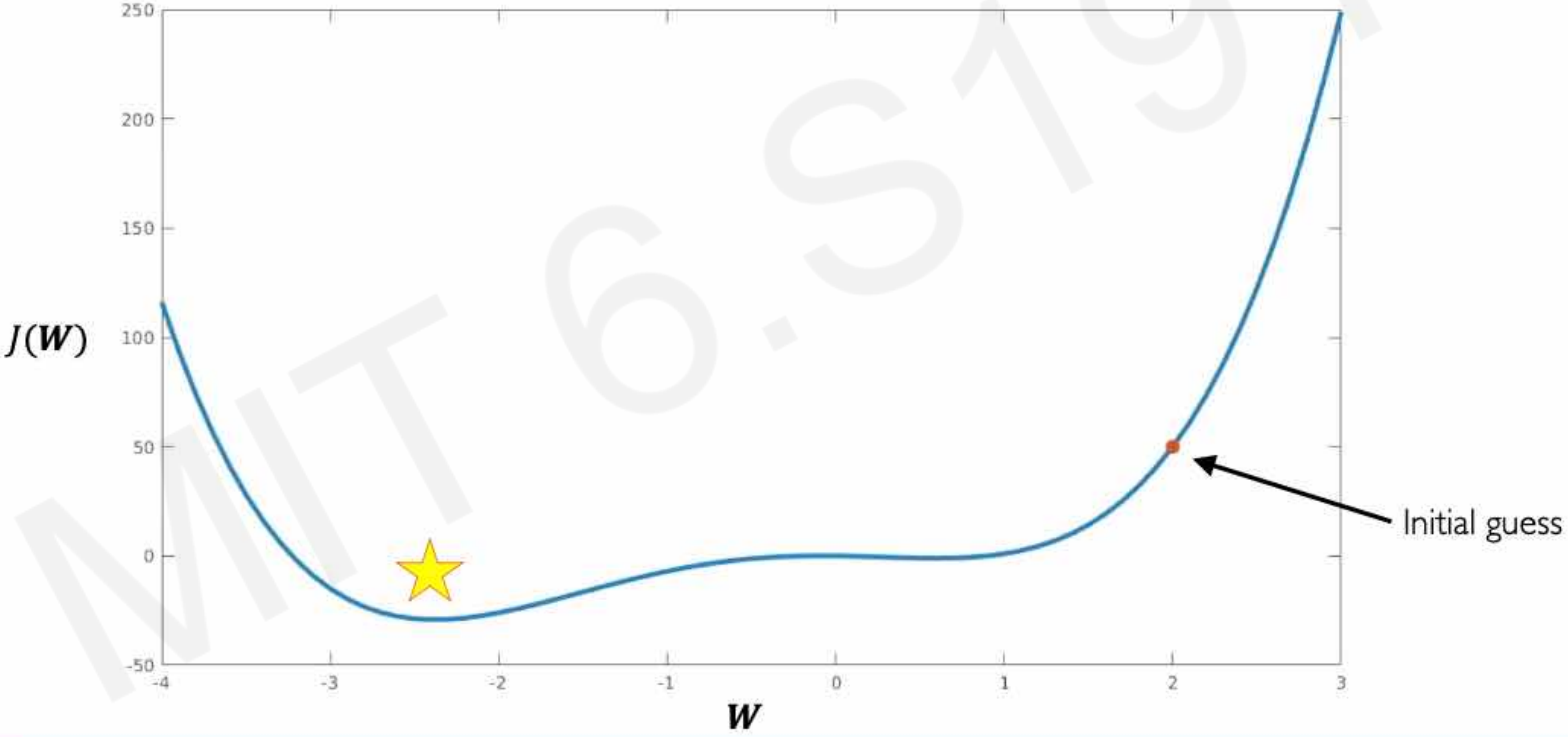
How can we set the learning rate?

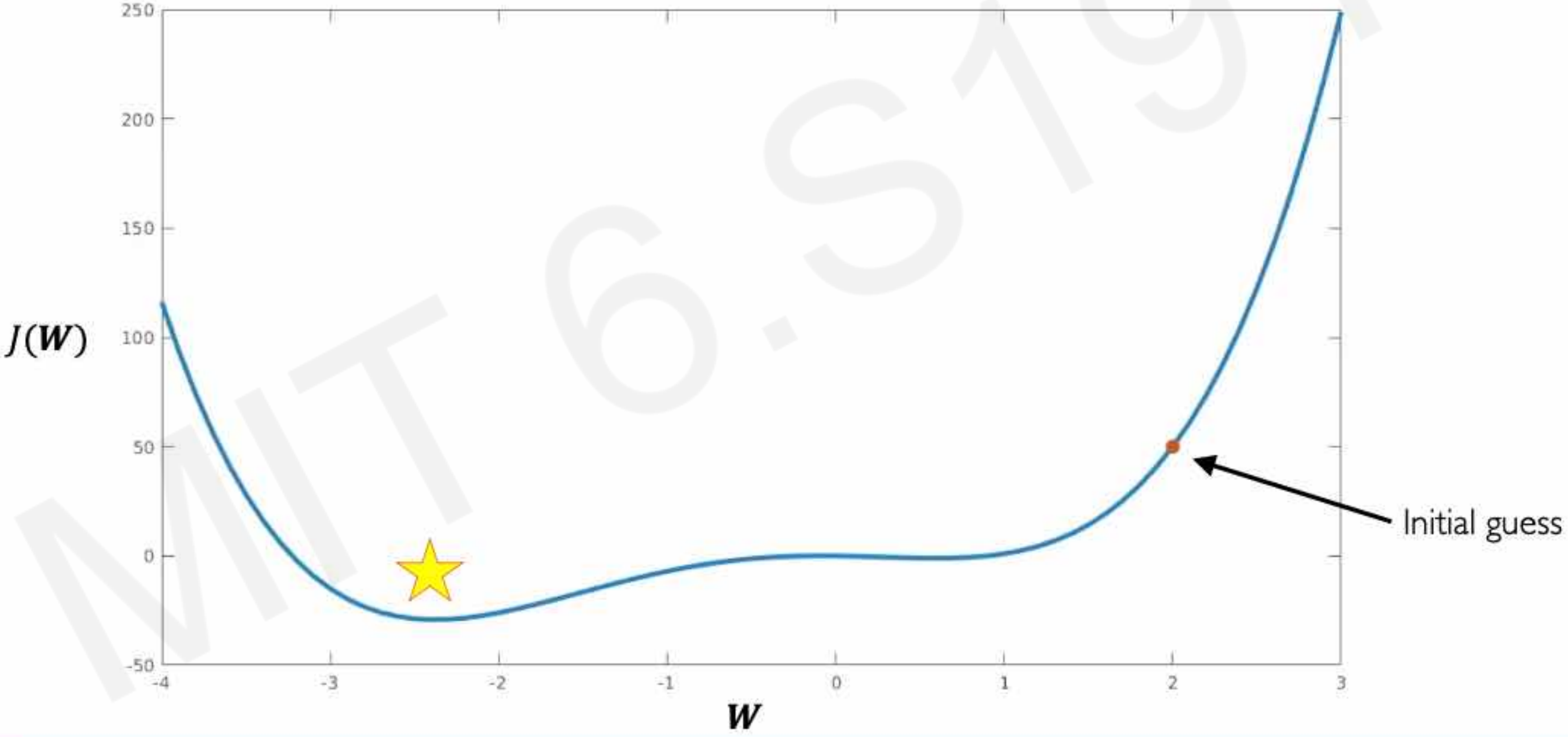
Setting the Learning Rate

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



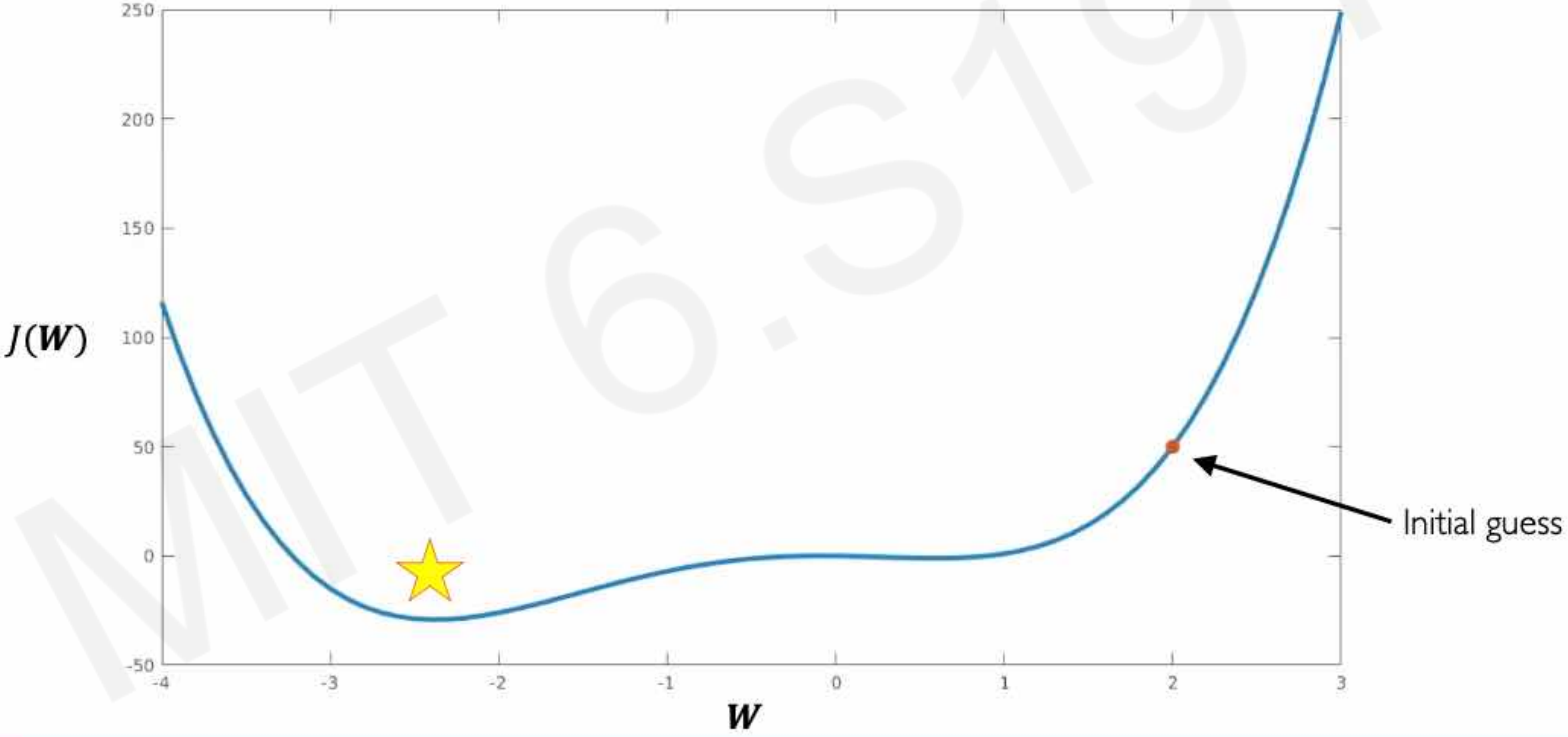
Setting the Learning Rate

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"

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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/

Putting it all together

```
import tensorflow as tf

model = tf.keras.Sequential([...])

# pick your favorite optimizer
optimizer = tf.keras.optimizer.SGD()

while True: # loop forever

    # forward pass through the network
    prediction = model(x)

    with tf.GradientTape() as tape:
        # compute the loss
        loss = compute_loss(y, prediction)

    # update the weights using the gradient
    grads = tape.gradient(loss, model.trainable_variables)
    optimizer.apply_gradients(zip(grads, model.trainable_variables)))
```

Can replace with any TensorFlow optimizer!

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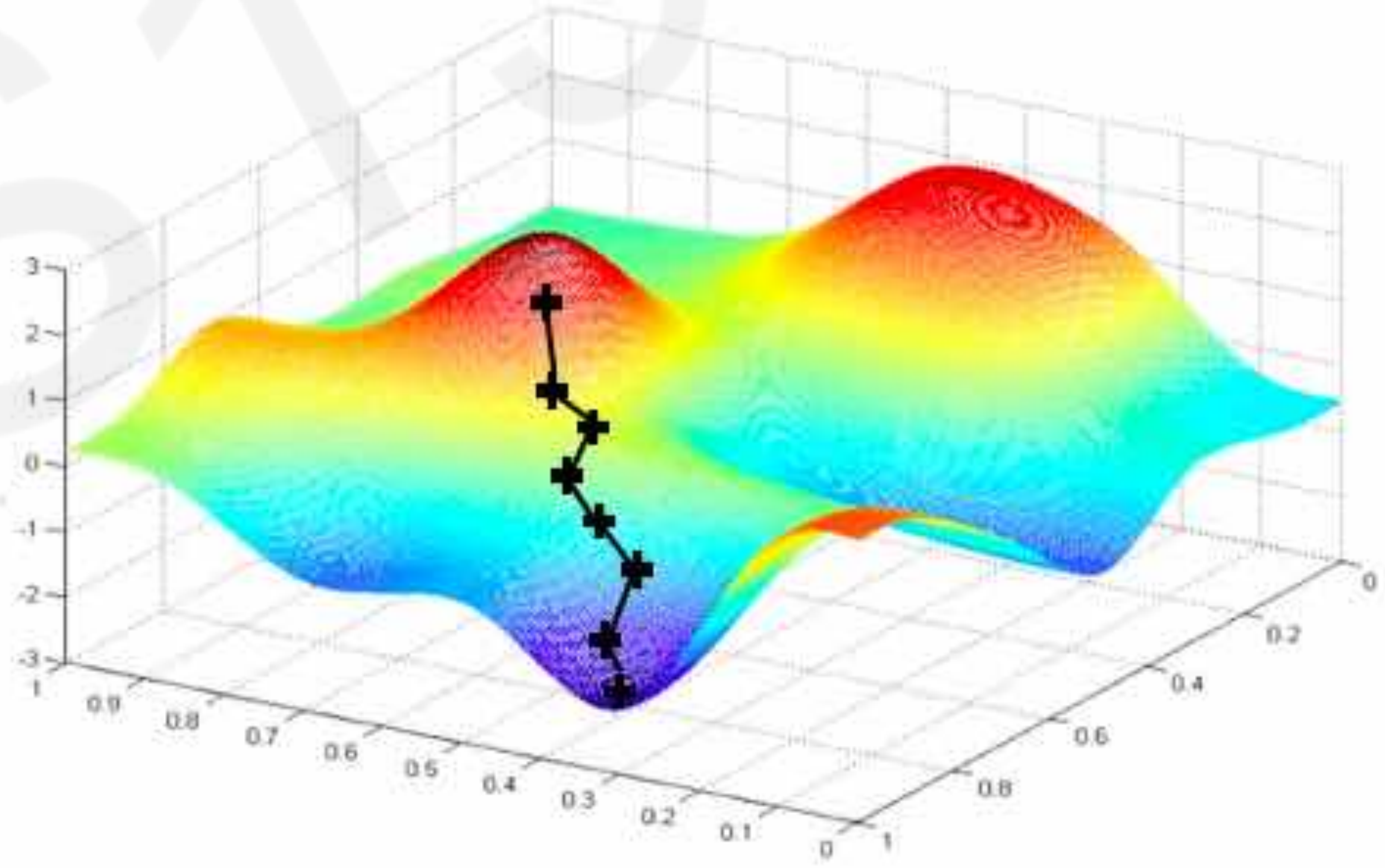

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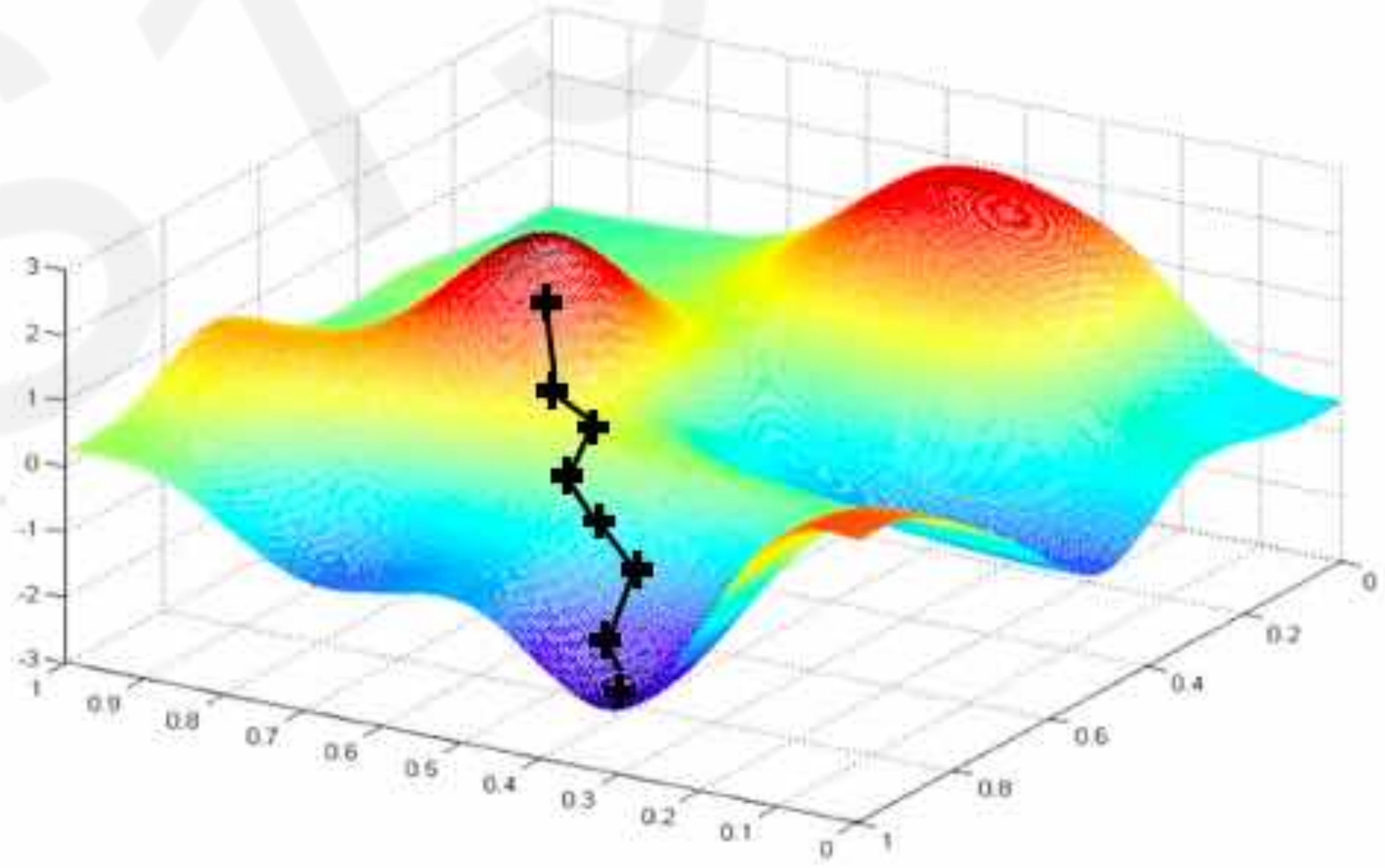
Can be very **computationally intensive** to compute!



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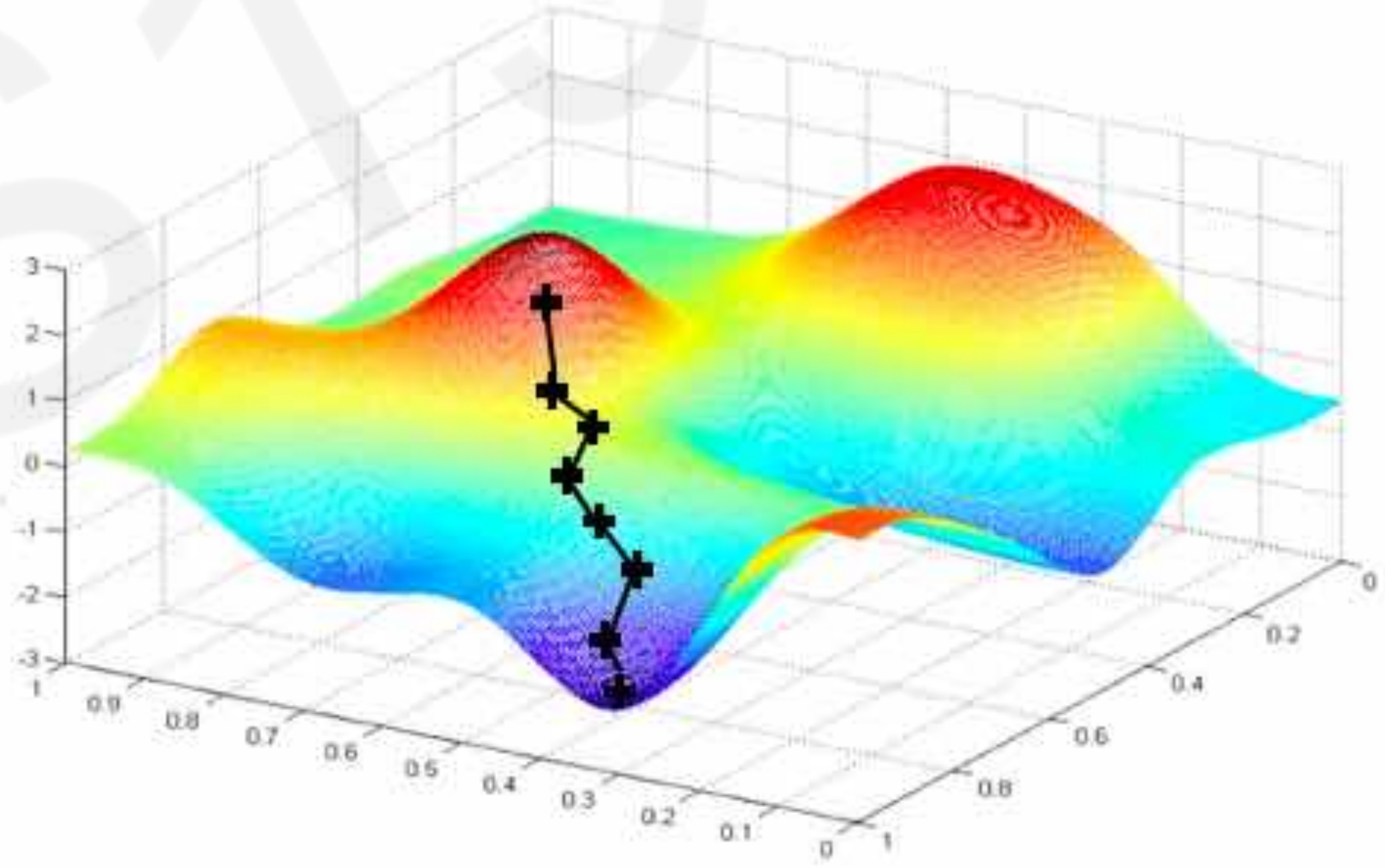

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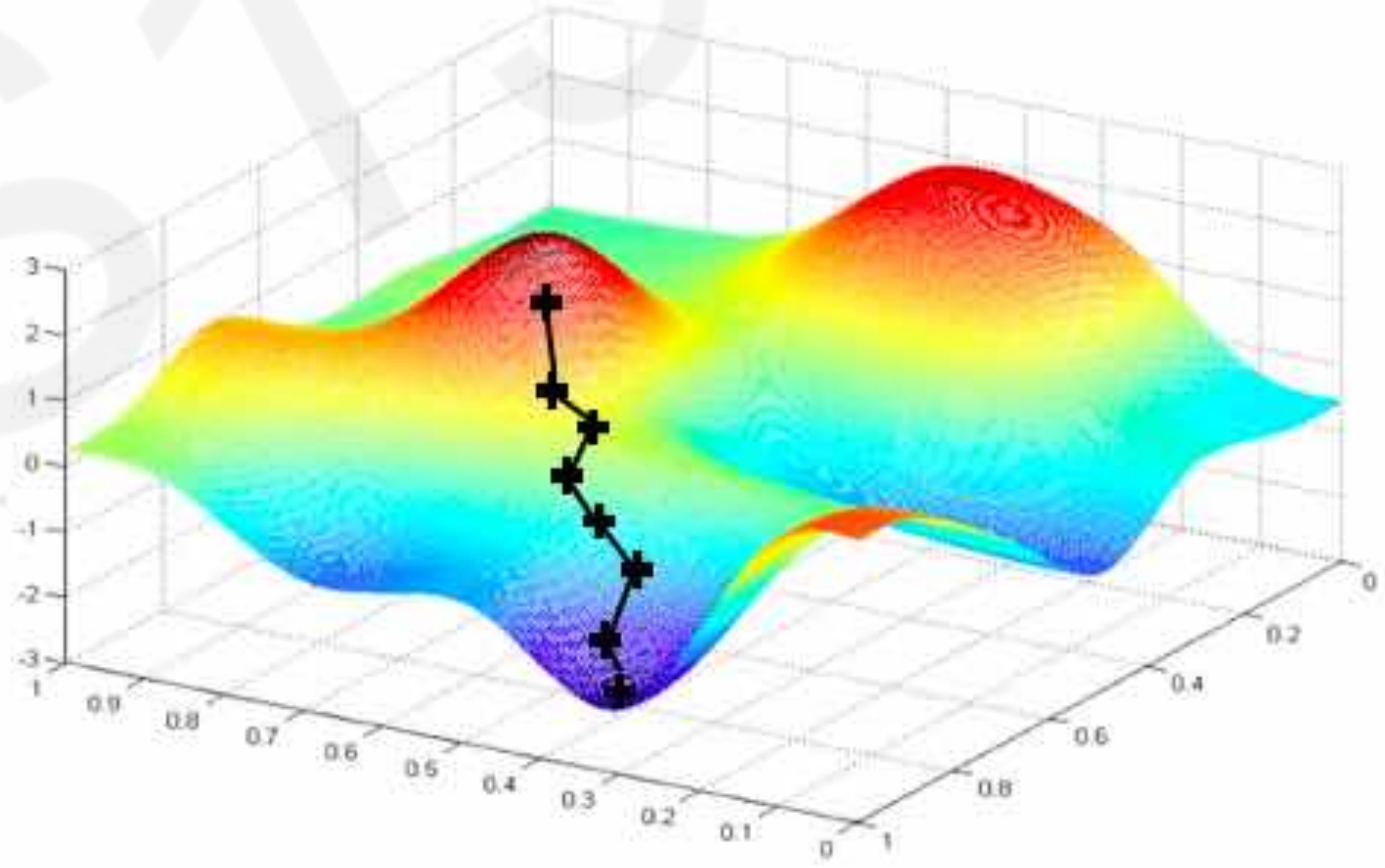
Easy to compute but **very noisy** (stochastic)!



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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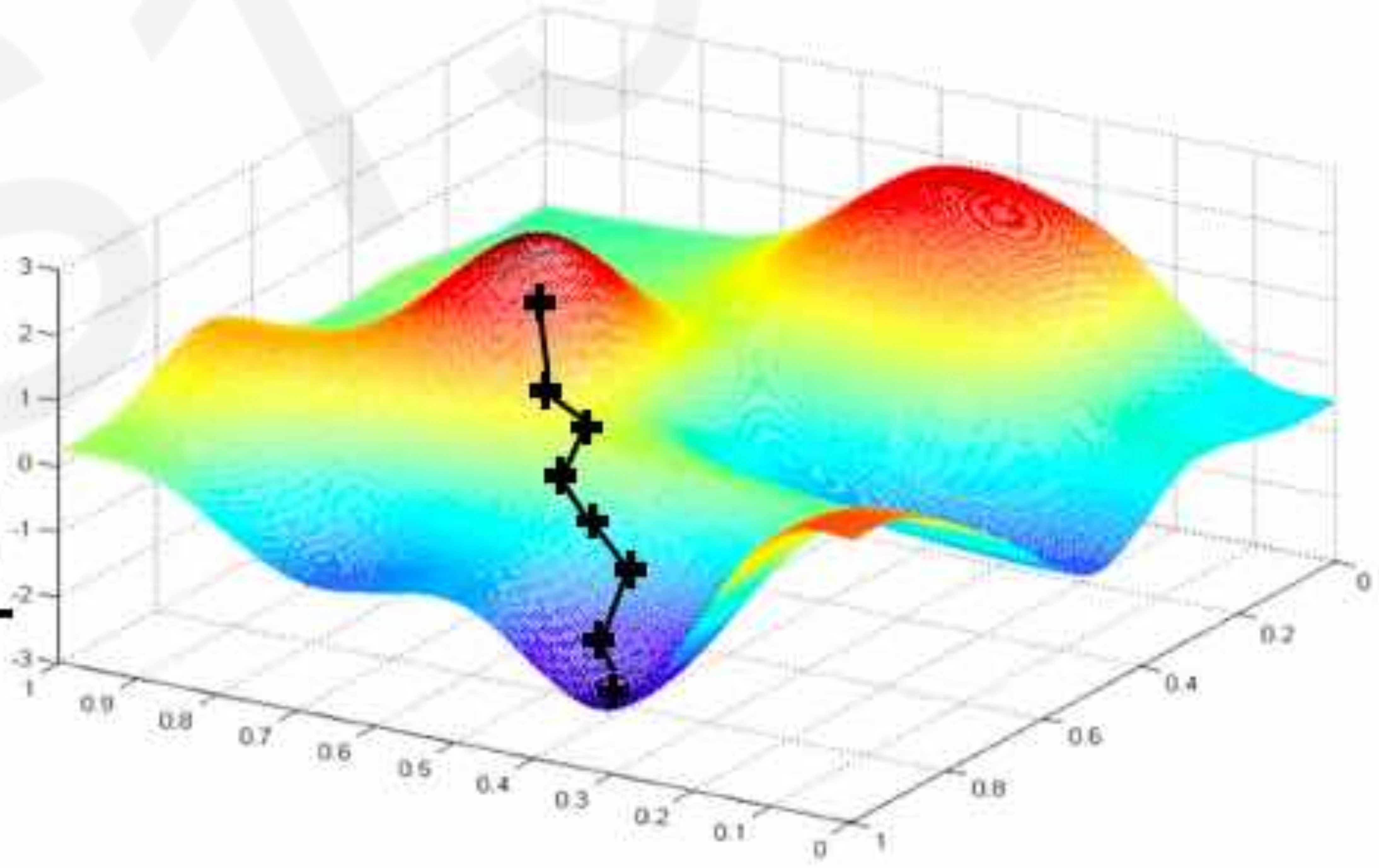

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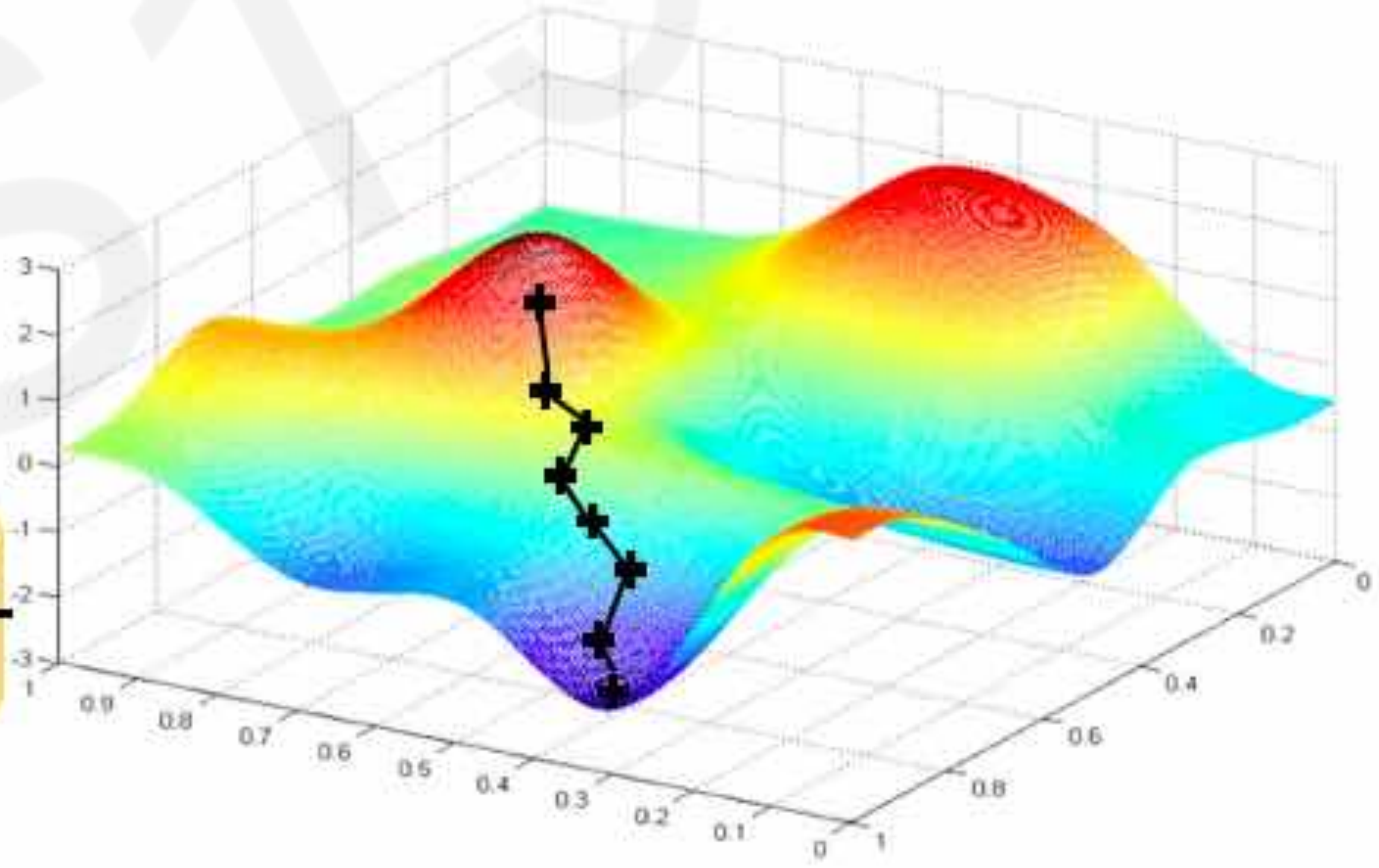

Fast to compute and a much better estimate of the true gradient!

Mini-batches while training

More accurate estimation of gradient

Smoother convergence

Allows for larger learning rates

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More accurate estimation of gradient

Smoother convergence

Allows for larger learning rates

Mini-batches lead to fast training!

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

Neural Networks in Practice: Overfitting

The Problem of Overfitting

Underfitting
Model does not have capacity to fully learn the data

Ideal fit

Overfitting
Too complex, extra parameters, does not generalize well

Regularization

What is it?

Technique that constrains our optimization problem to discourage complex models

Regularization

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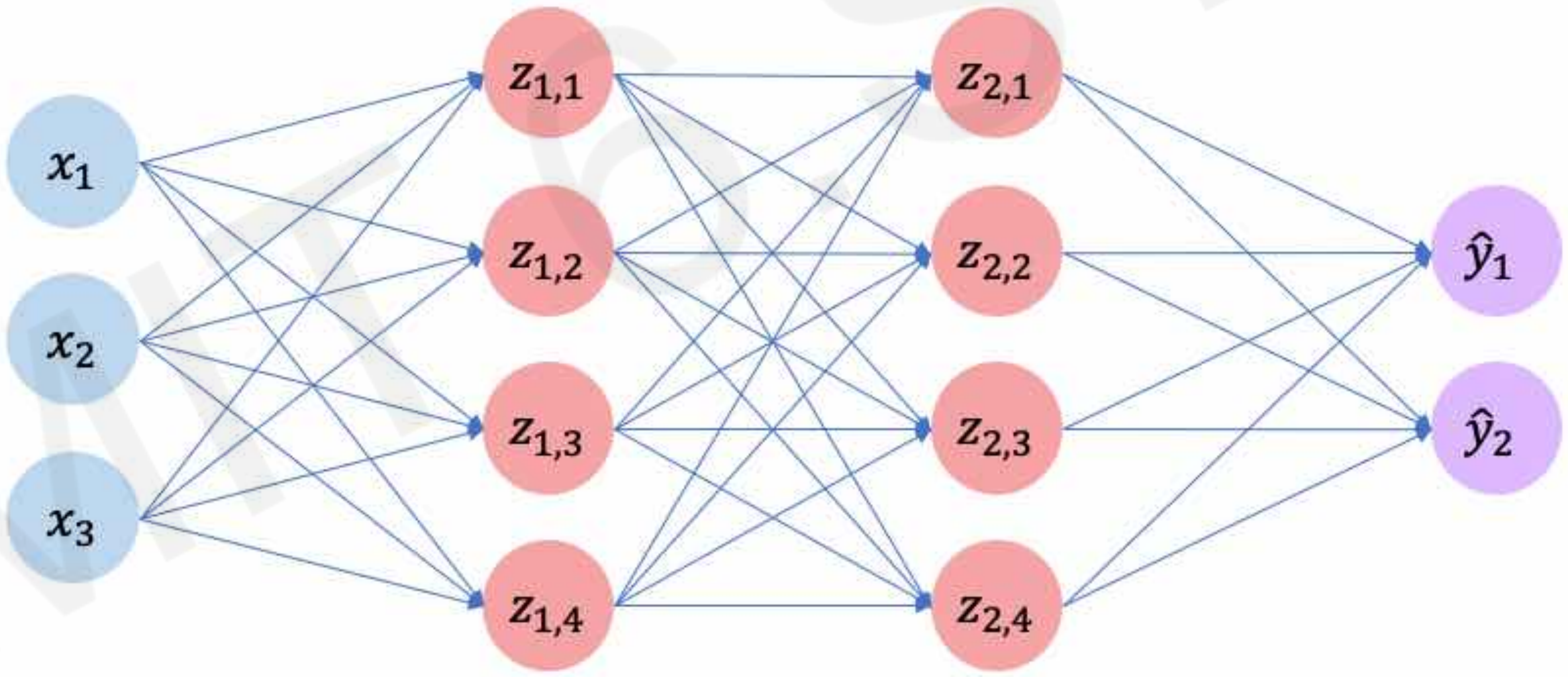
Technique that constrains our optimization problem to discourage complex models

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

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    - 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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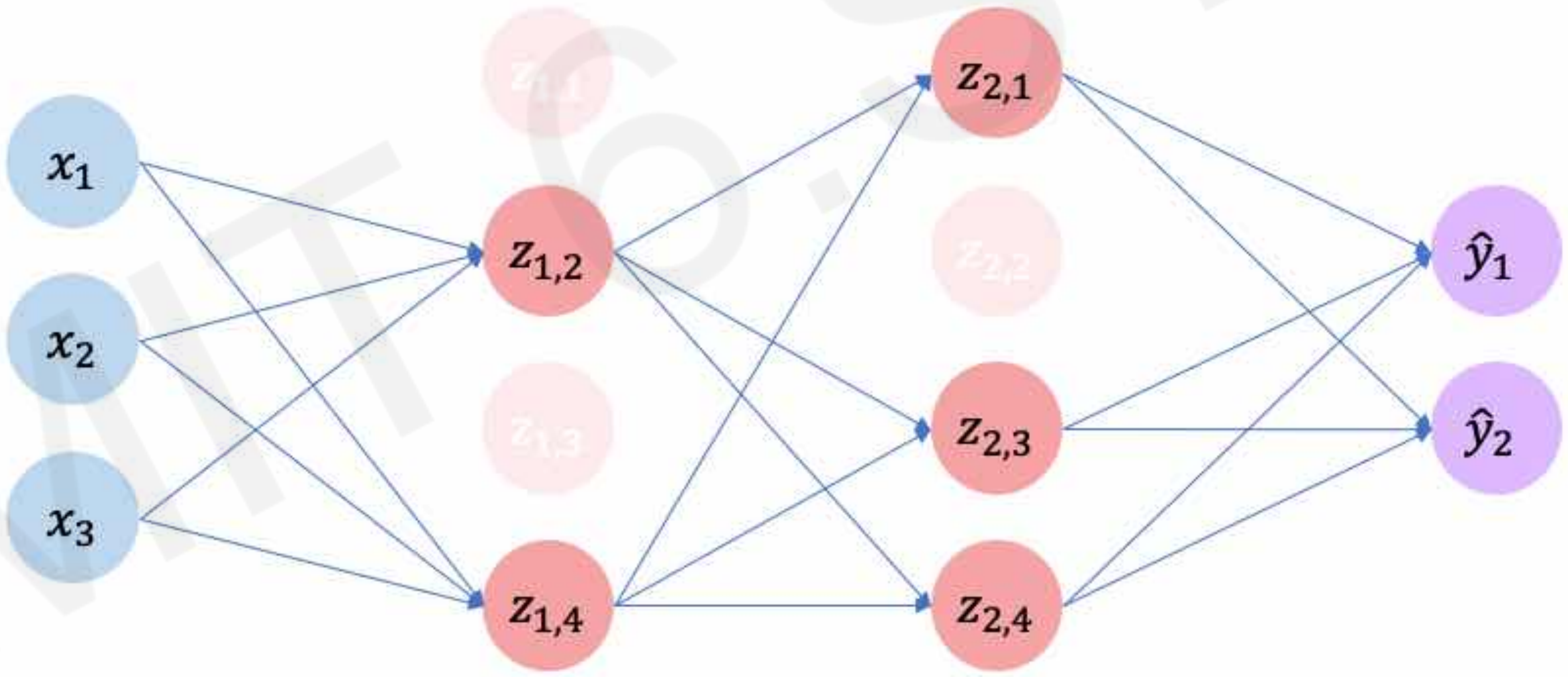

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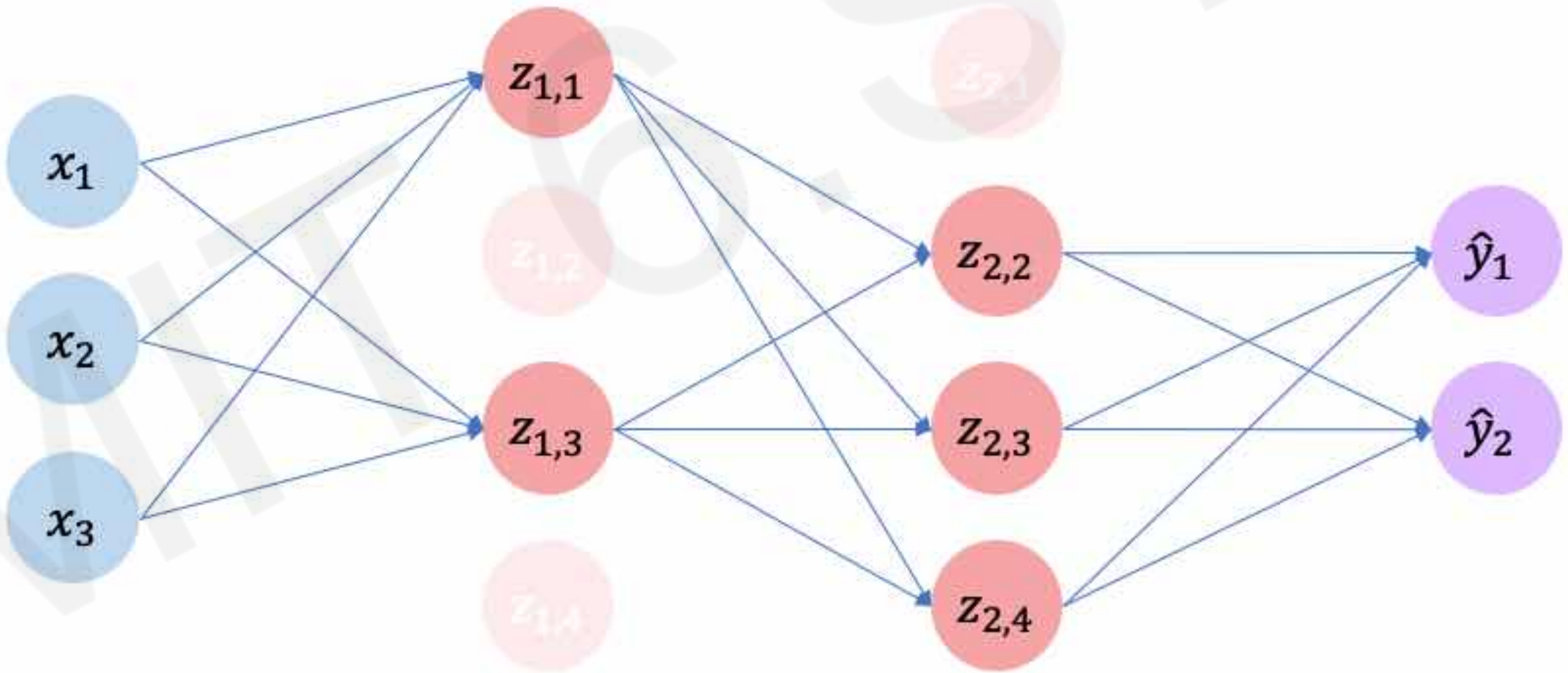

Regularization 2: Early Stopping

- Stop training before we have a chance to overfit

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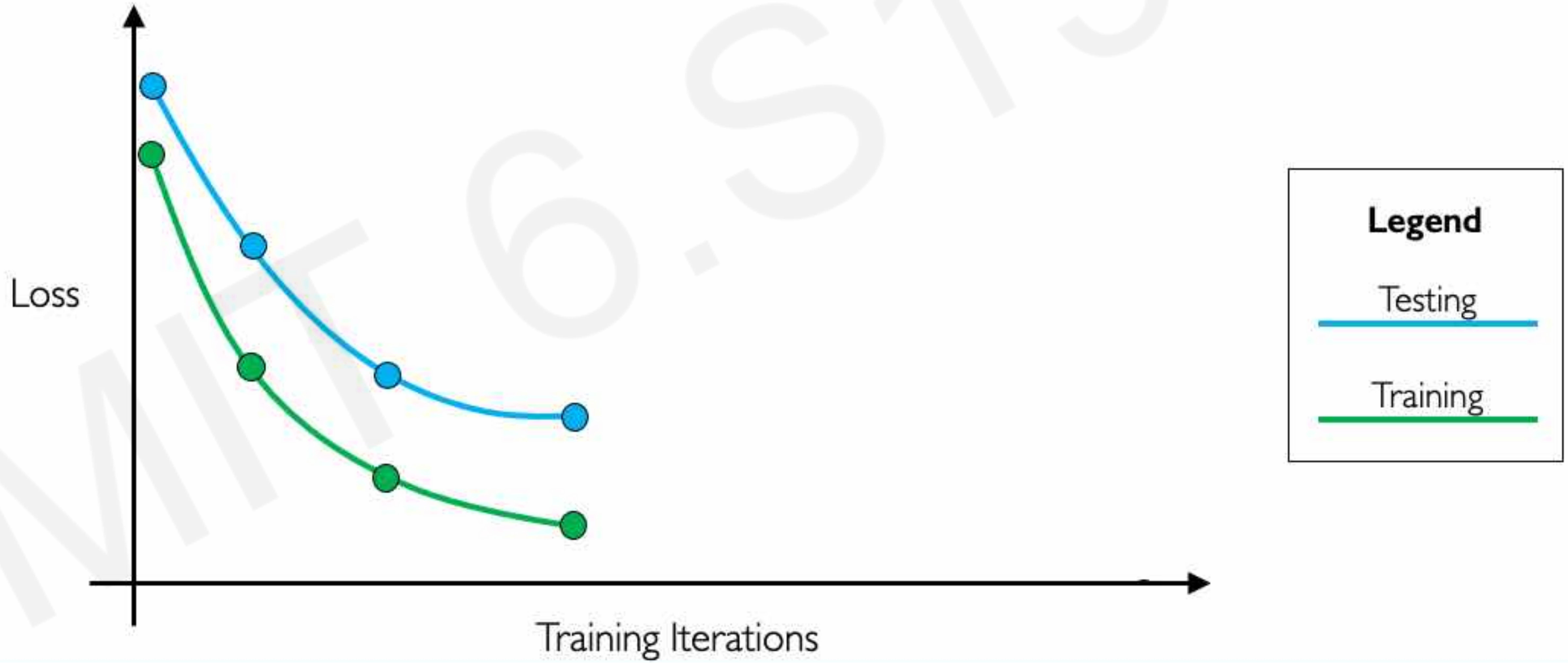

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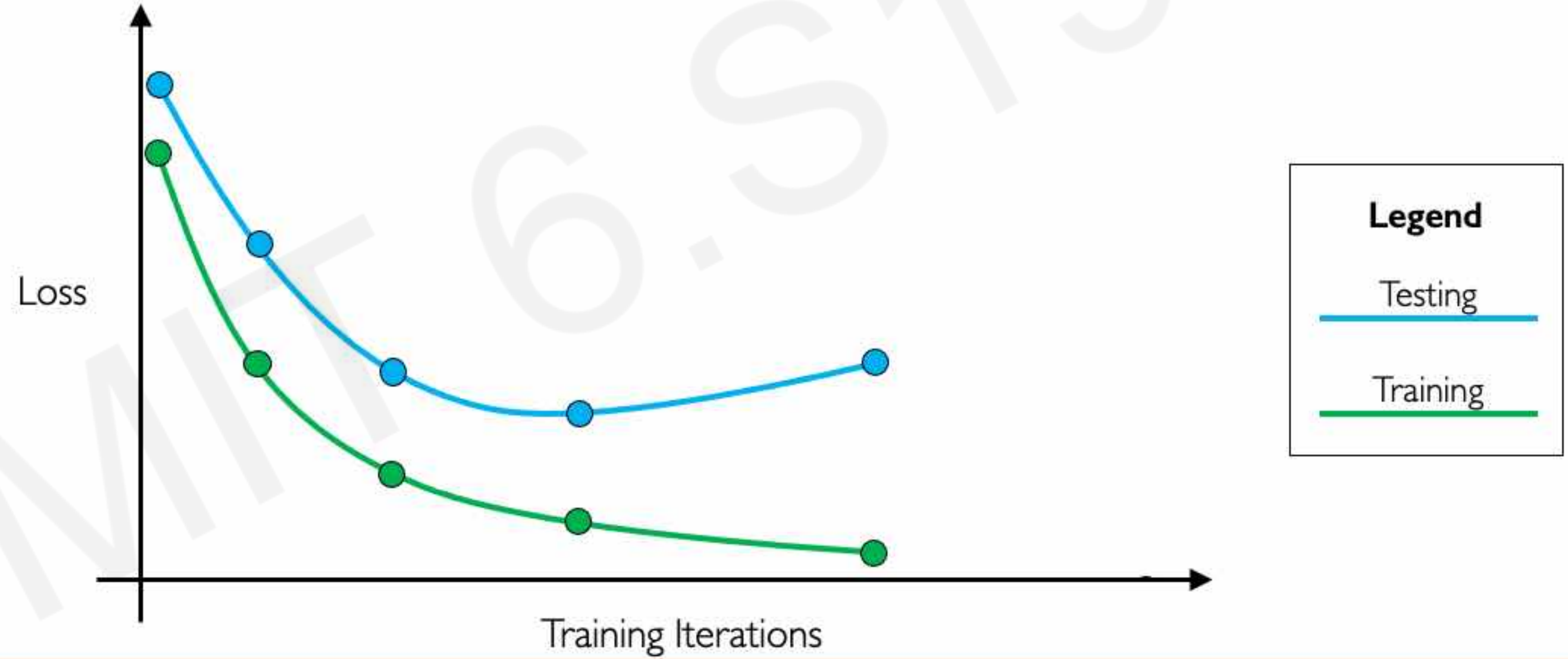

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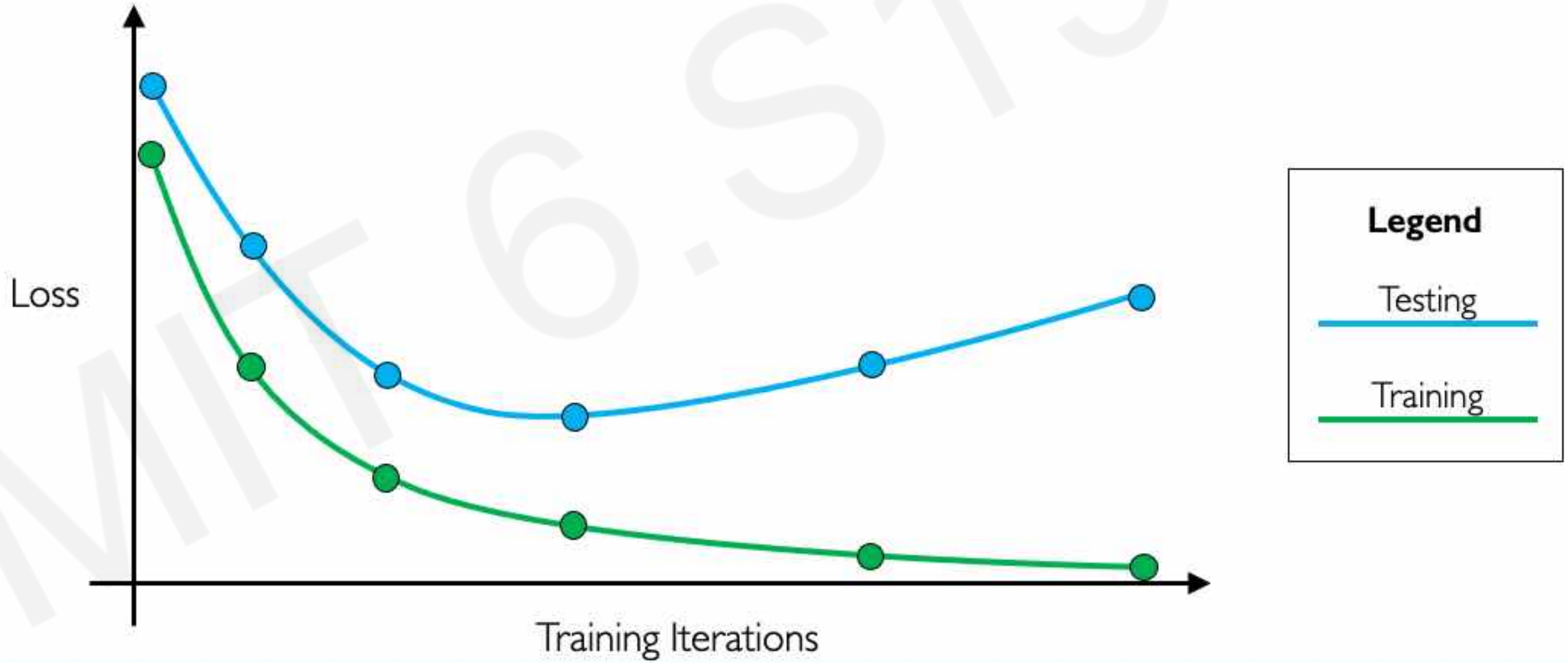

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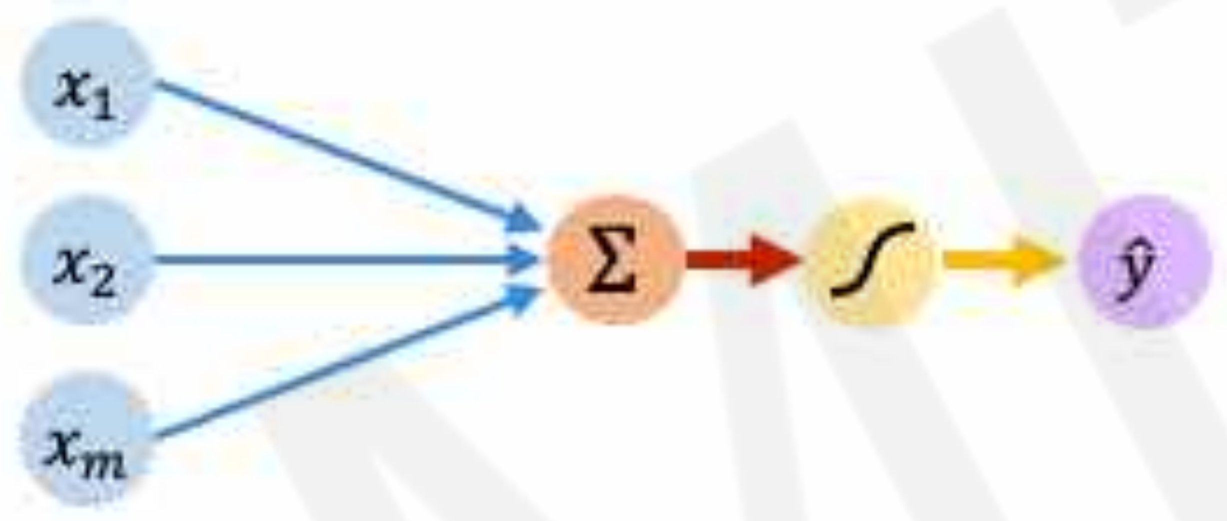
Core Foundation Review

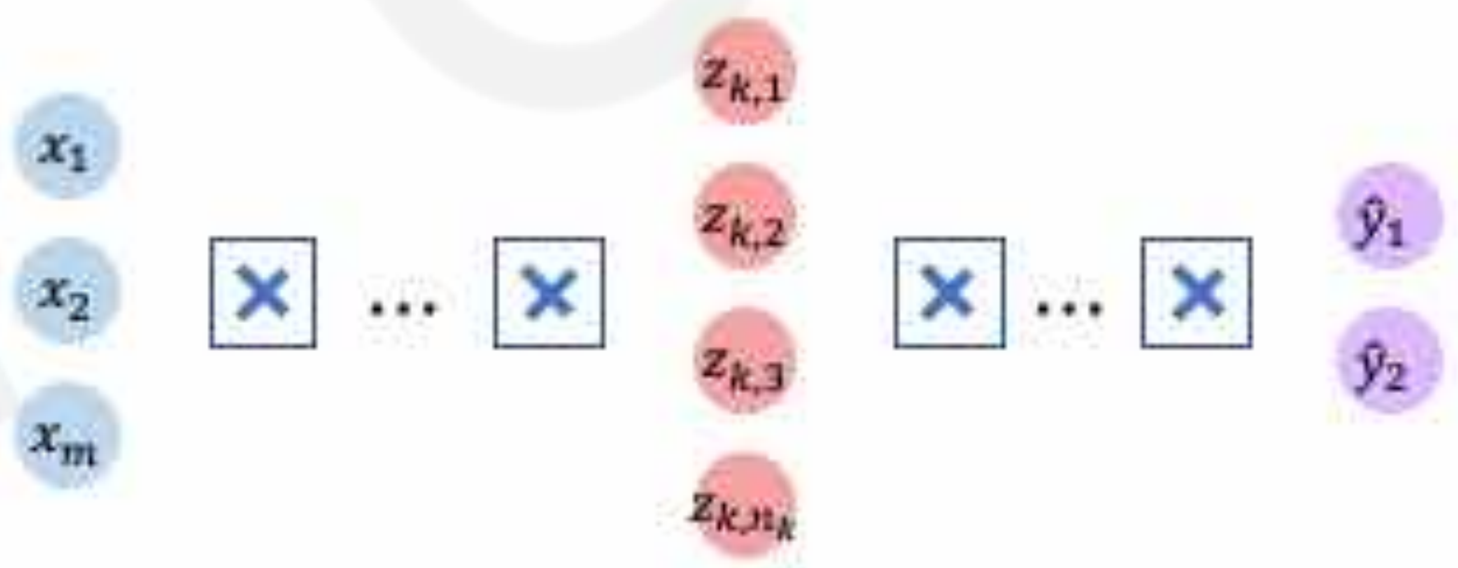
The Perceptron

- Structural building blocks
- Nonlinear activation functions



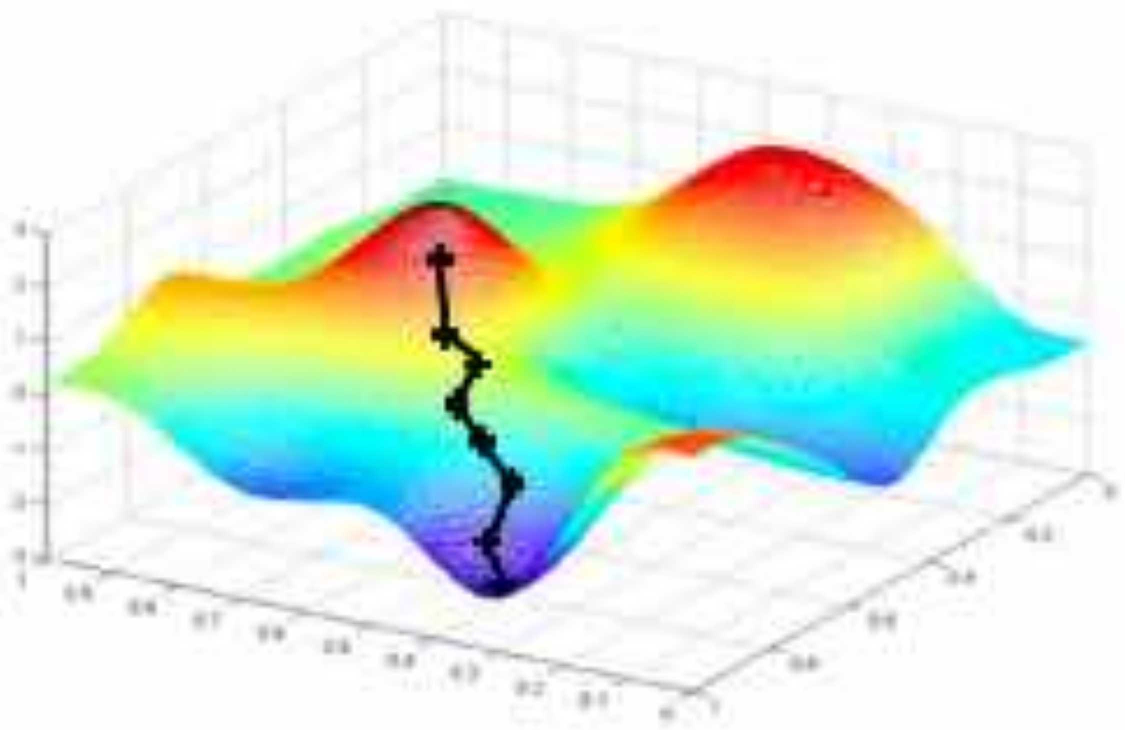
Neural Networks

- Stacking Perceptrons to form neural networks
- Optimization through backpropagation



Training in Practice

- Adaptive learning
- Batching
- Regularization



6.S191: Introduction to Deep Learning

Lab 1: Introduction to TensorFlow and Music Generation with RNNs

Link to download labs:
http://introtodeeplearning.com#schedule

1. Open the lab in Google Colab
2. Start executing code blocks and filling in the #TODOs
3. Need help? Come to the class Gather.Town or 10-250!