Intro to Neural Nets

Sessions 2-3: Mathematical Building Blocks
& Working with Keras API

Session Agenda

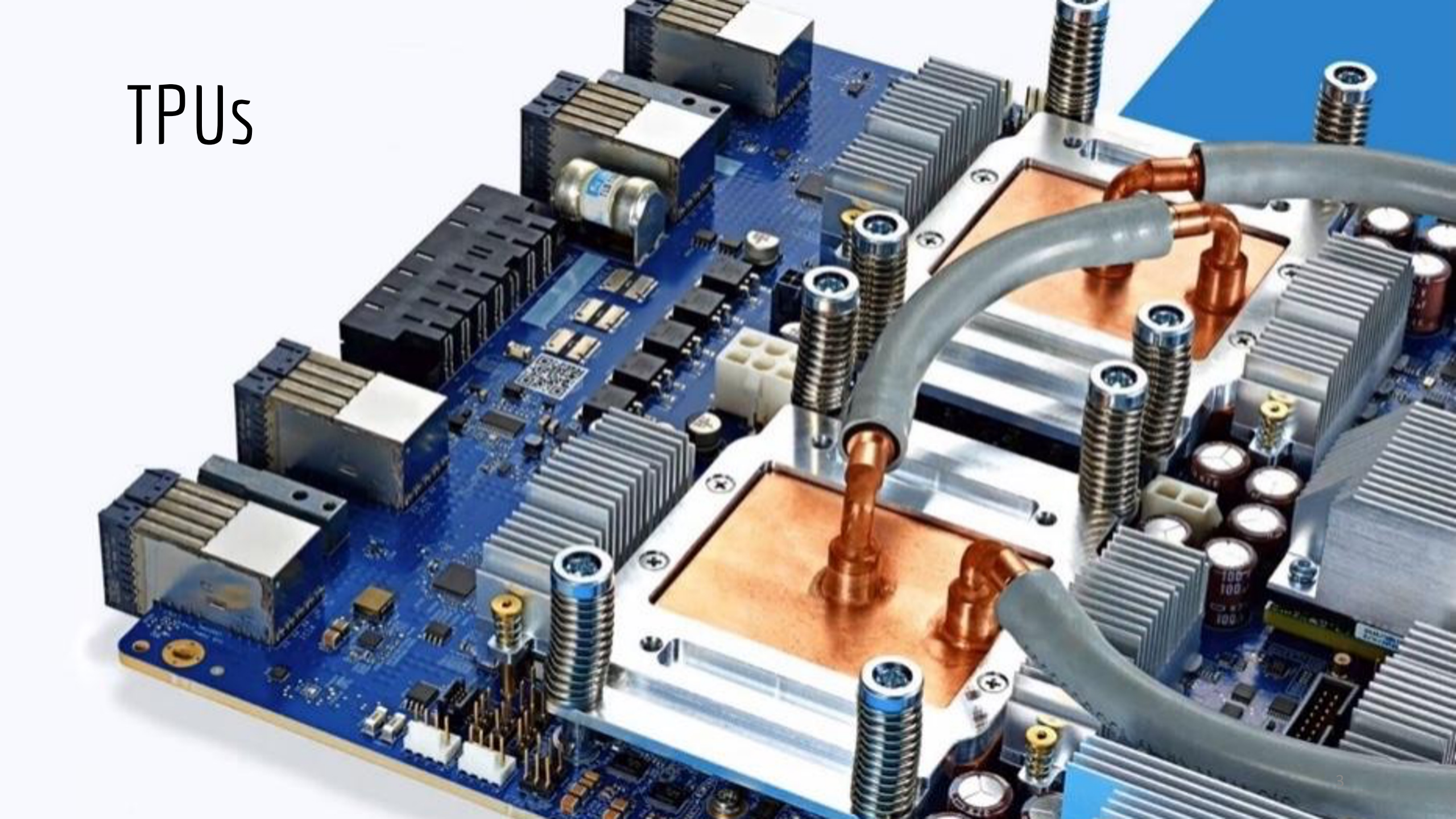
1. Building Blocks of NNs

- Tensors (and relevant mathematical operations)
- Loss Functions
- Backpropagation: Derivatives, Gradients & the Chain Rule (quick examples)
- Optimizers

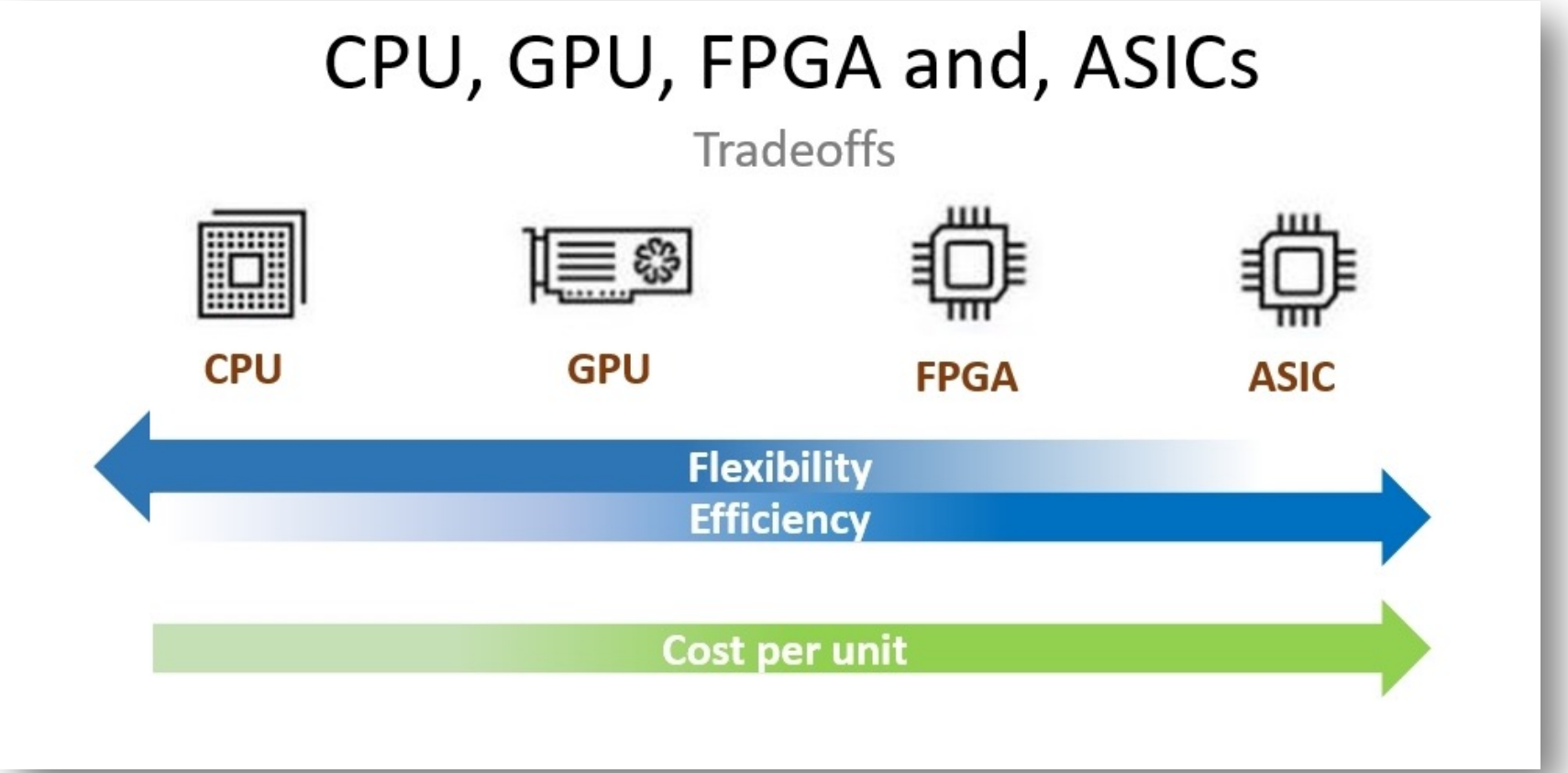
2. Building a Linear Classifier

- Overview of Keras and Tensorflow.
- Implementing a linear classifier in Keras (now that we know the components).

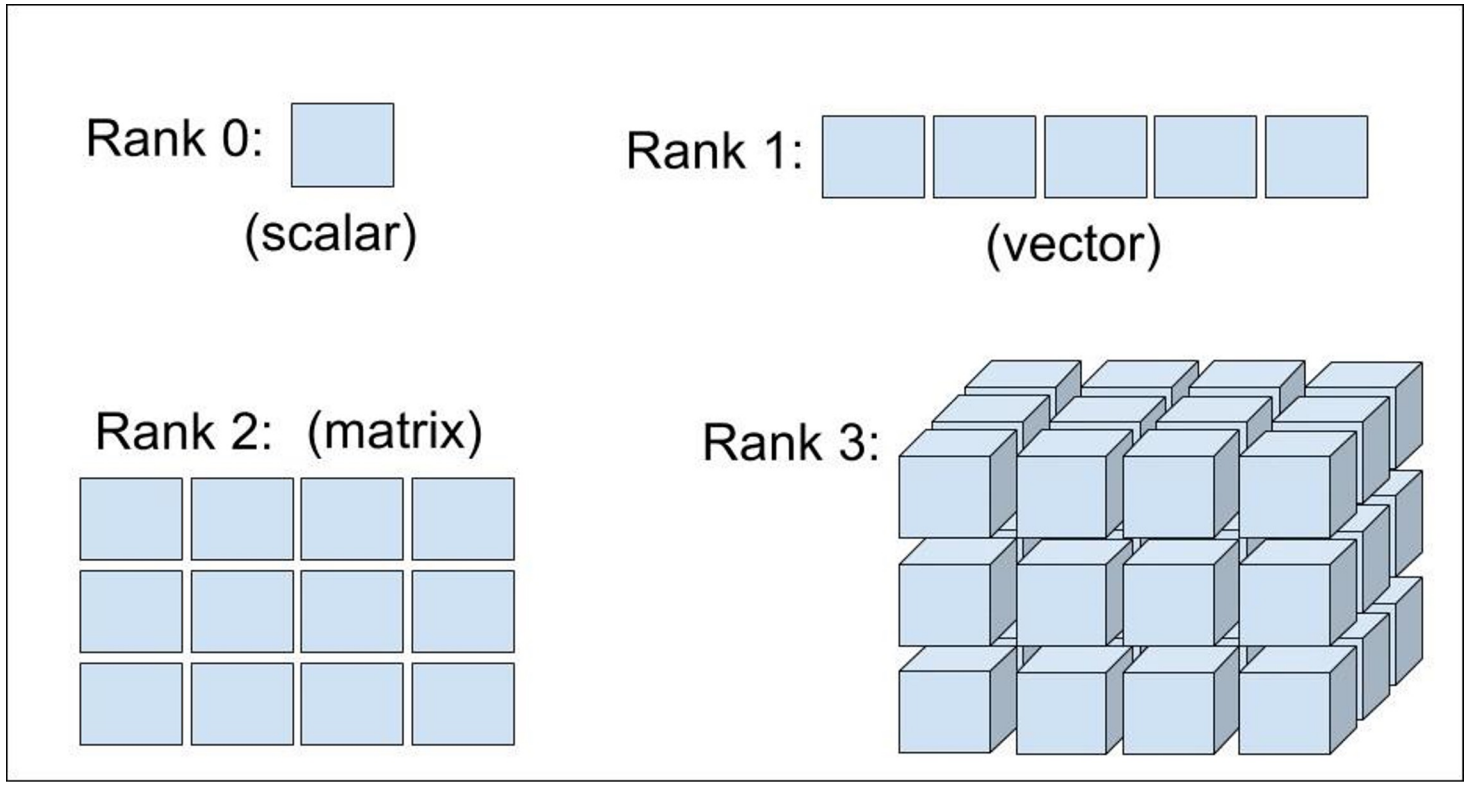
TPUs



An Aside: GPU vs. ASIC

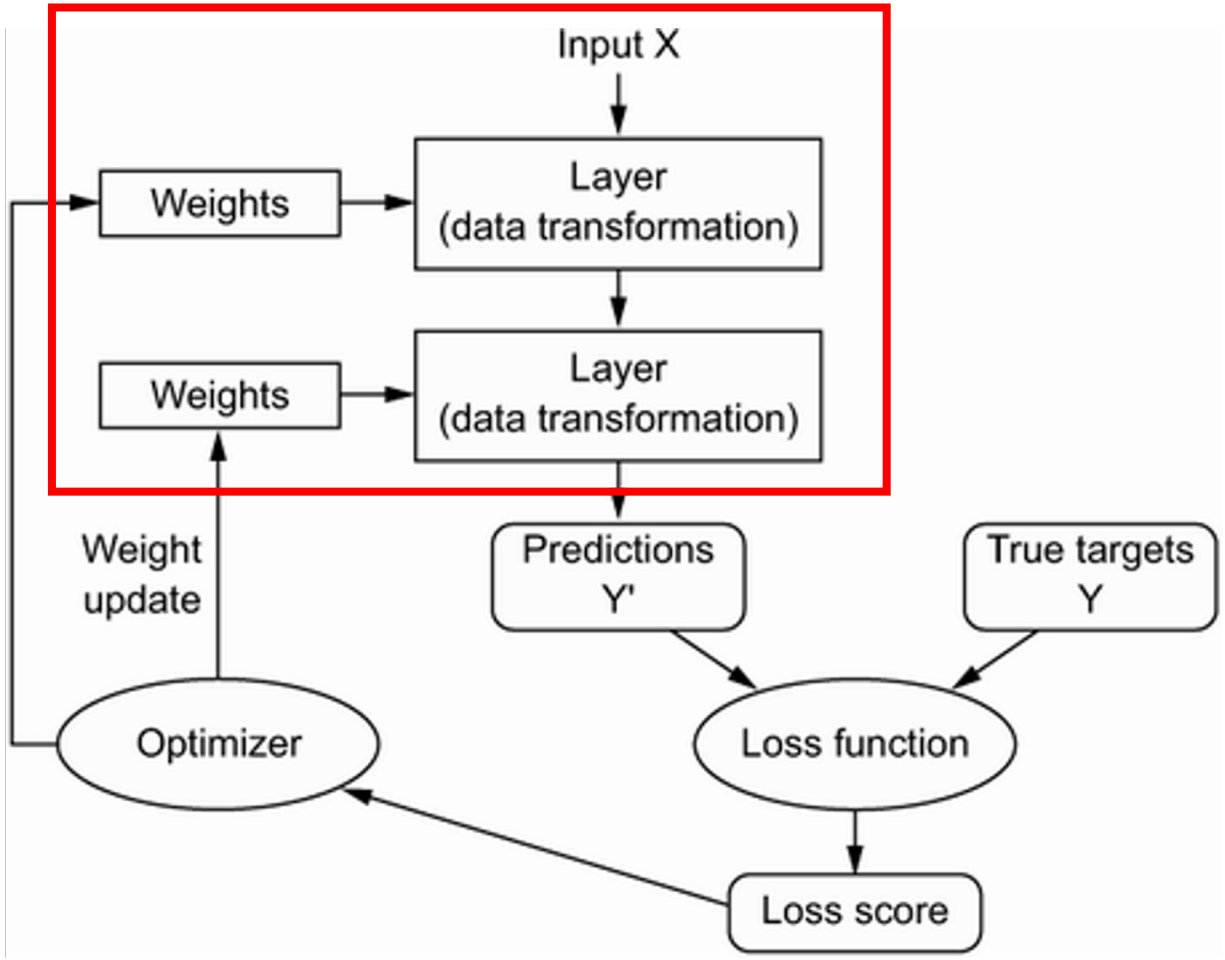


Tensors

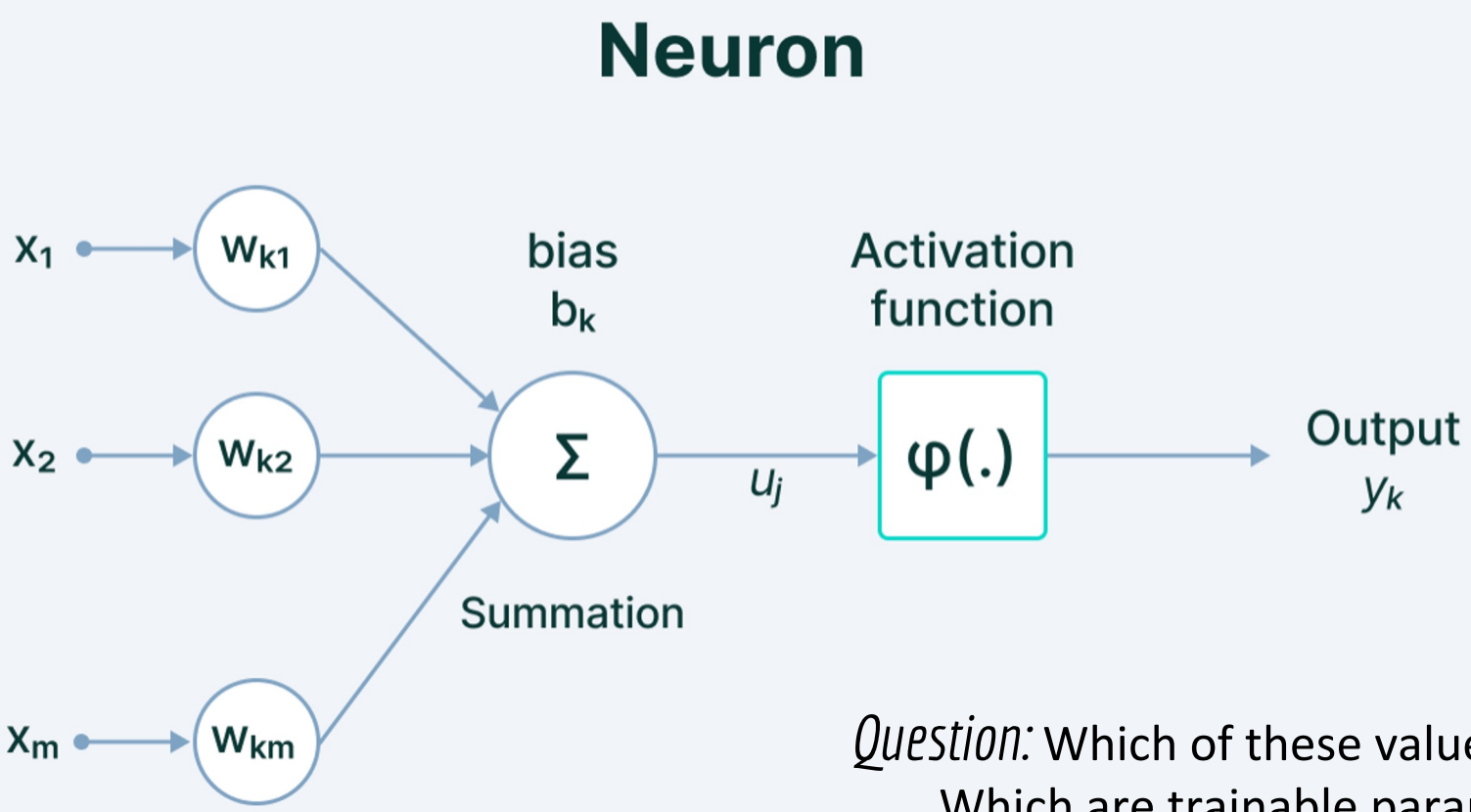


Question: What sort of data (give an example) would be stored in a rank-3 tensor? How about a rank-4 tensor?

Forward Pass

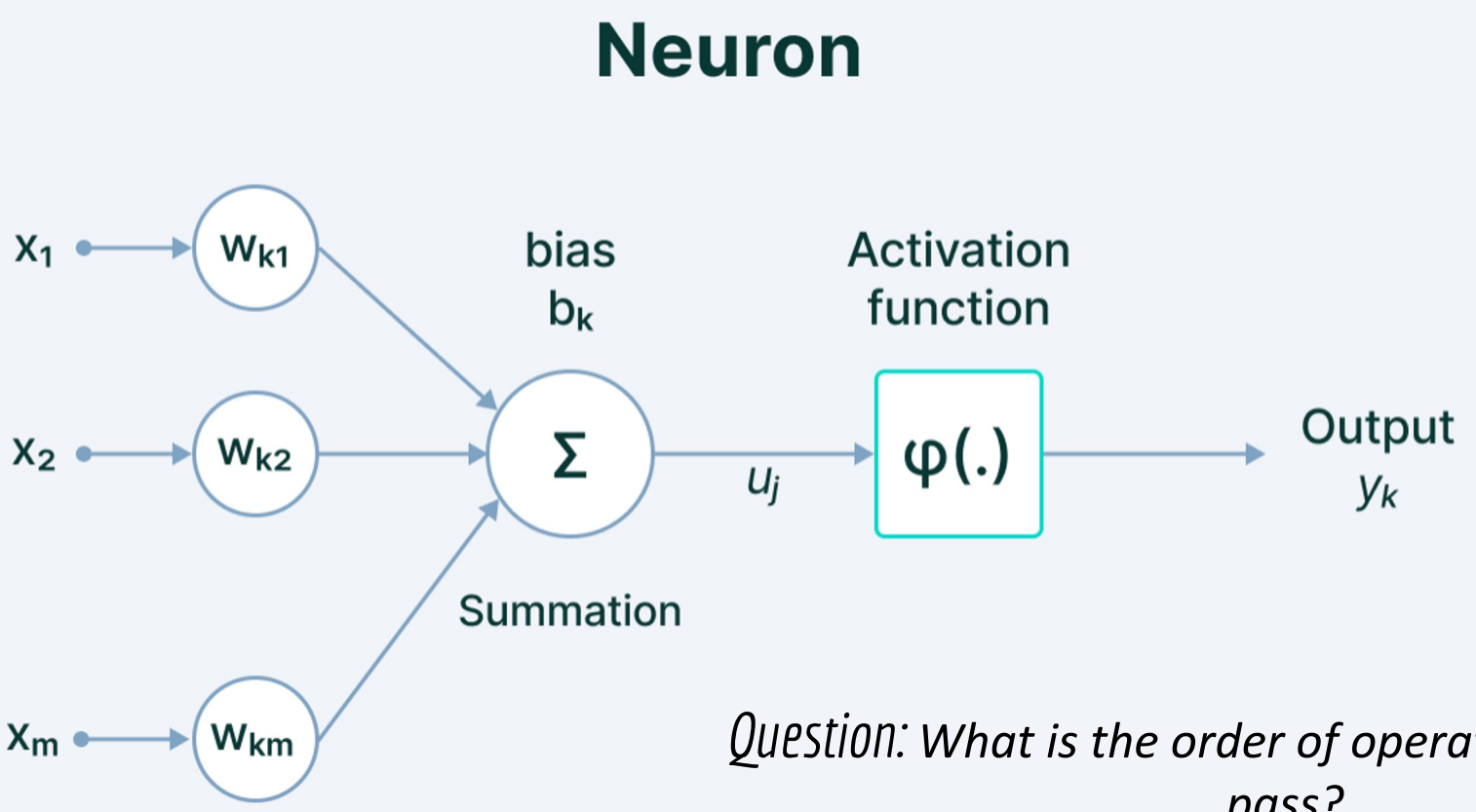


Neuron / Network Components



Question: Which of these values are fixed?
Which are trainable parameters?

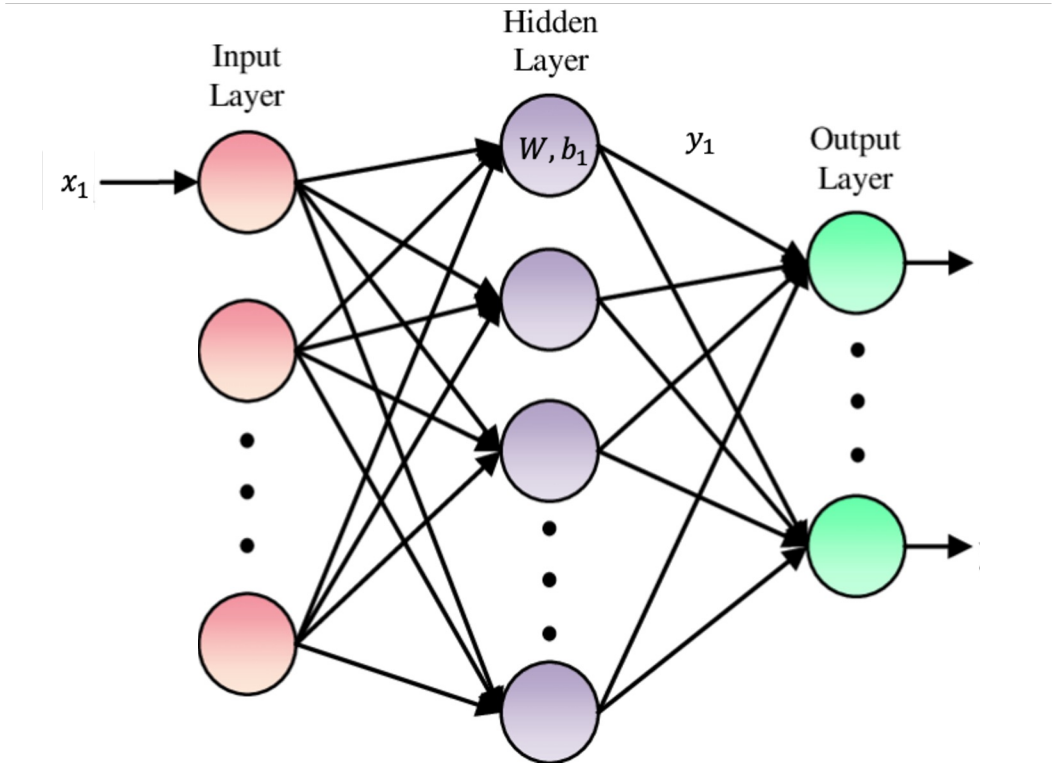
Neuron / Network Components



Question: What is the order of operations in a forward pass?

Multiple Neurons Execute in Parallel

- Recall… x is our flattened digit image, a vector of 784 elements. Matrix X, which contains our 60,000 images, is thus 784 x 60,000.
- For each hidden node, we need 784 weights (one weight per input value). We have 512 nodes, so matrix W is 784 x 512.
- We have 512 bias terms, one per hidden node, in vector B.



Matrix (Tensor) Multiplication

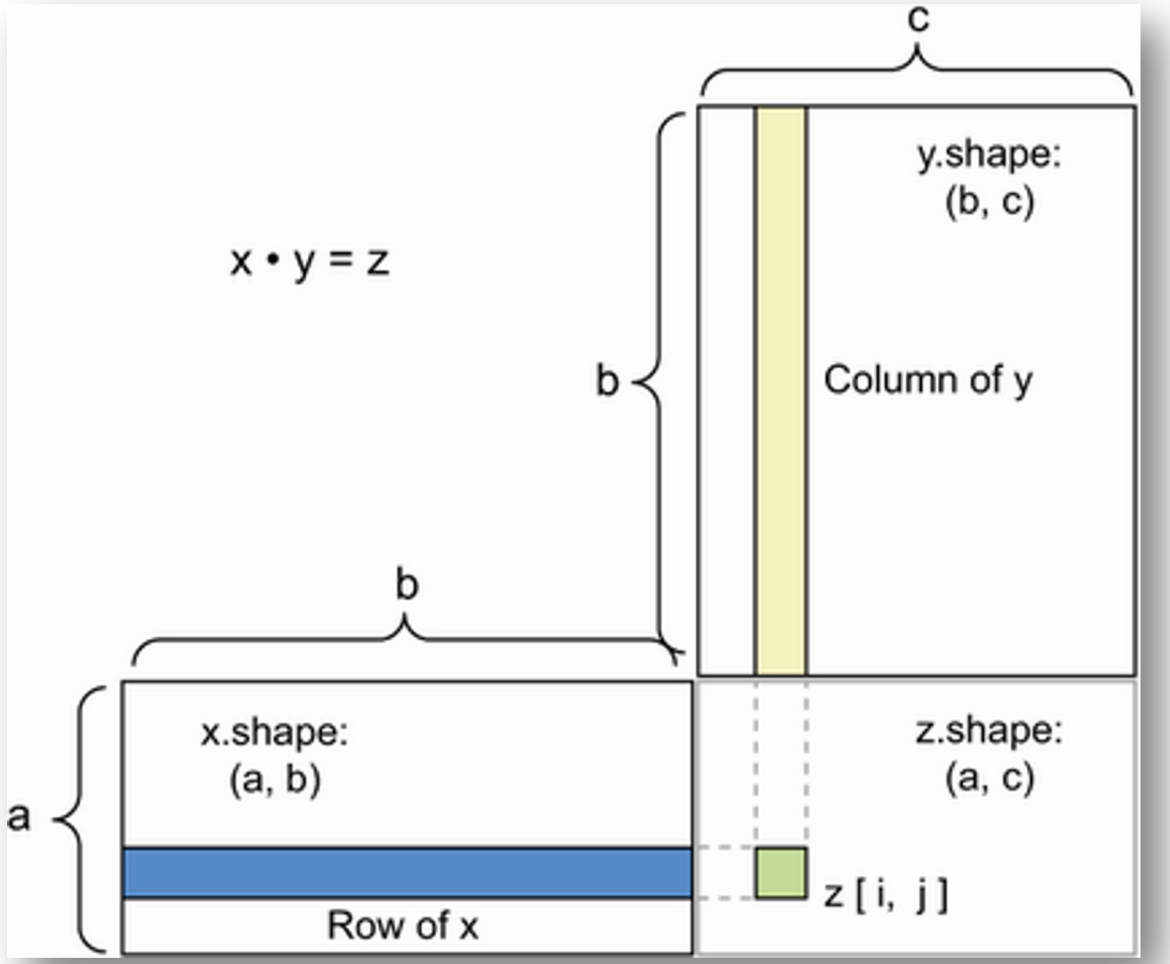
$$y_1 = \varphi\,(x_1 \cdot w_1 + b_1)$$

We calculate all x's * w's at once via matrix multiplication, i.e., W^T*X

Elements of the Resulting Matrix are the Dot Products of X's Rows and Y's Columns

- Y[2,2] = W^T[2,:] · X[:,2]

If you get a cryptic error message about shapes not conforming, it is referring to this.



Parallel Addition Requires Broadcasting

$$y_1 = \varphi\,(x_1 \cdot w_1 + b_1)$$

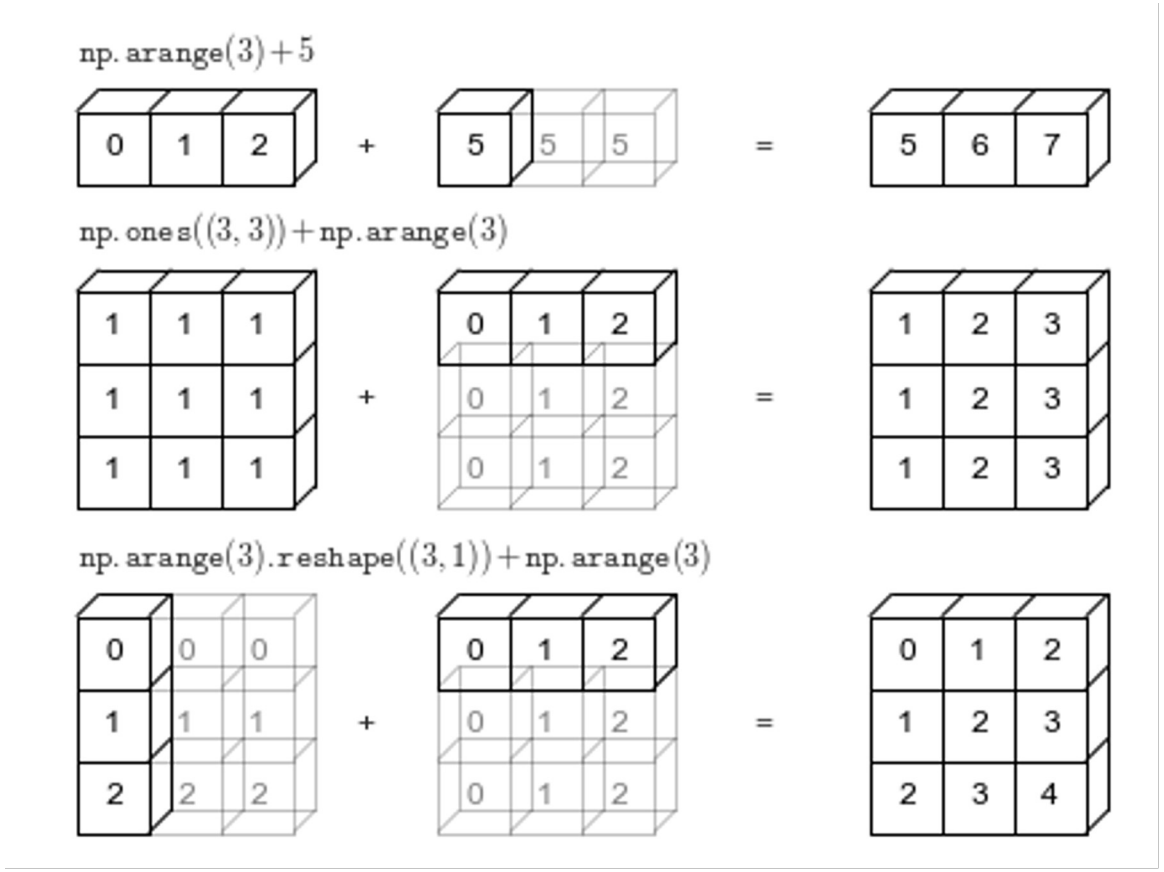
Shape of the Two Tensors Needs to Conform

- A + B will only work if len(A) is cleanly divisible by len(B).

Broadcasting

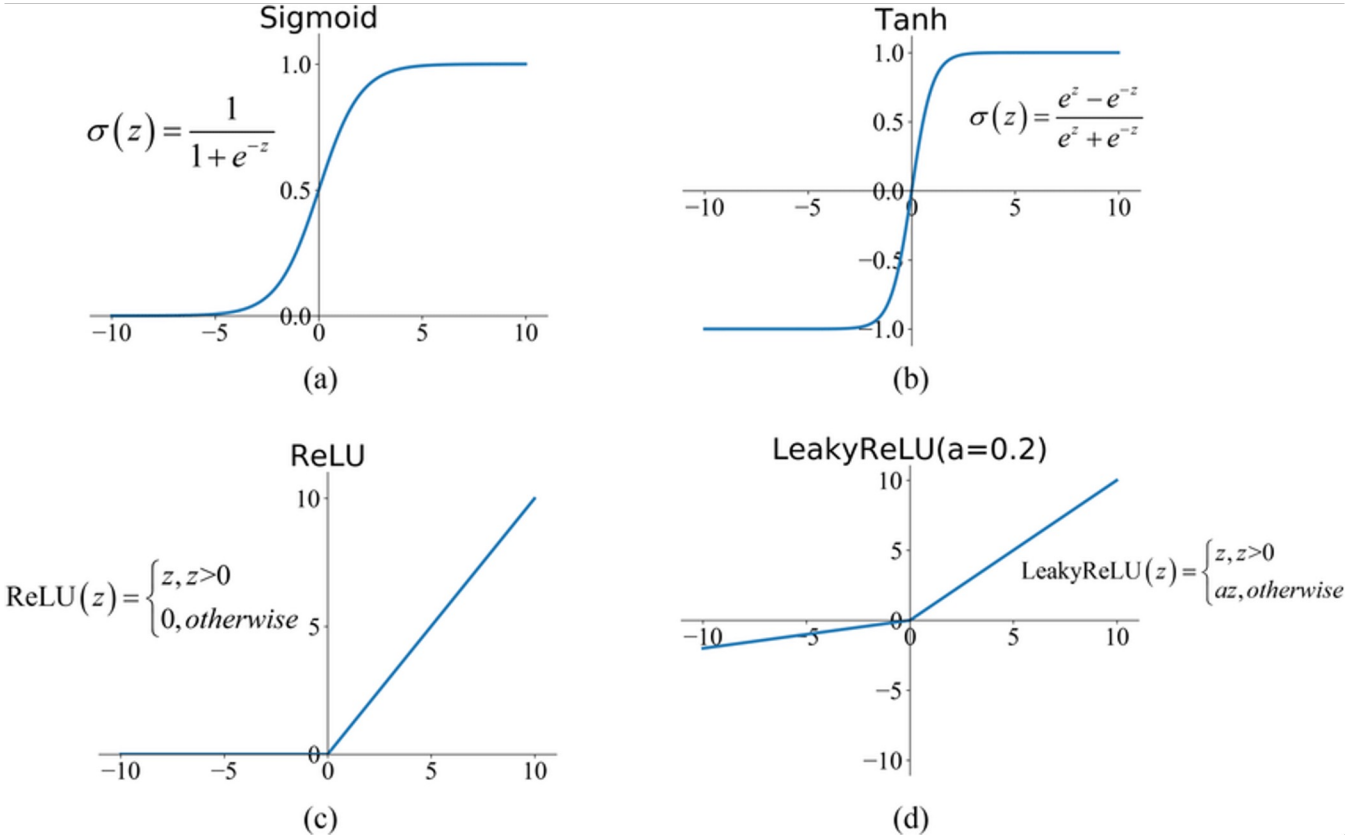
- Duplicates B until it matches A's dimensions, then performs element-wise operation.

Code might run but broadcast in a different direction than you expect, yielding a wrong answer!



Activation Applied Element-wise

$y_1 = \varphi\,(x_1 \cdot w_1 + b_1)$



Softmax Activation

$$y_1 = \varphi\,(x_1 \cdot w_1 + b_1)$$

Multi-class, Single Label:

This is a generalization of sigmoid activation. Whereas sigmoid (logit) is for a single binary outcome (e.g., fraud vs. not), softmax (multinomial logit) deals with a single multi-class outcome (e.g., red vs. green vs. blue).

We only use softmax activation in the output layer.

```
[ ]  predictions = model.predict(test_images)
     predictions[1:5]
```

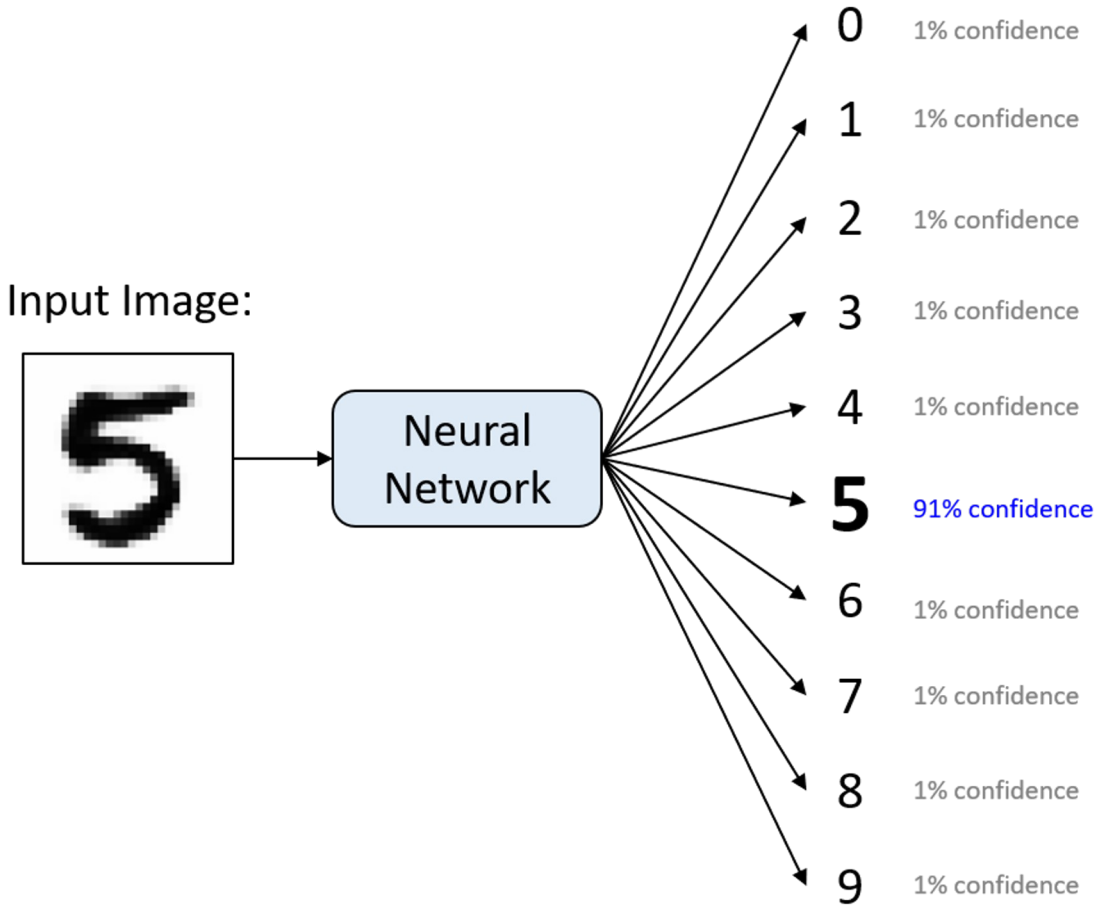
```
array([[3.6144251e-11, 1.9087817e-07, 9.9999964e-01, 7.4062939e-08,
        1.8678016e-17, 4.8710058e-09, 1.2722286e-11, 7.0804596e-17,
        1.8209119e-09, 1.5724455e-16],
       [1.4256794e-07, 9.9912840e-01, 1.6355875e-04, 1.5004550e-05,
        7.7388759e-06, 3.4624031e-06, 4.7226295e-06, 1.8777854e-04,
        4.8707443e-04, 2.1639225e-06],
       [9.9995363e-01, 8.8815255e-10, 2.9017941e-05, 1.2894120e-07,
        1.0134034e-08, 2.1255494e-06, 1.3782760e-06, 3.7380698e-06,
        5.5121645e-09, 9.9050267e-06],
       [9.0073827e-06, 4.1446402e-09, 8.8214925e-05, 6.3586896e-07,
        9.4997090e-01, 6.3517414e-06, 2.1397573e-06, 4.1880834e-04,
        4.4119348e-05, 4.9459830e-02]], dtype=float32)
```

$$y_1 = \varphi\,(x_1 \cdot w_1 + b_1)$$

Multi-Class, Single-Label

Multi-class, Single Label:

As with sigmoid, we can loosely interpret the values output by softmax activation as probabilities.

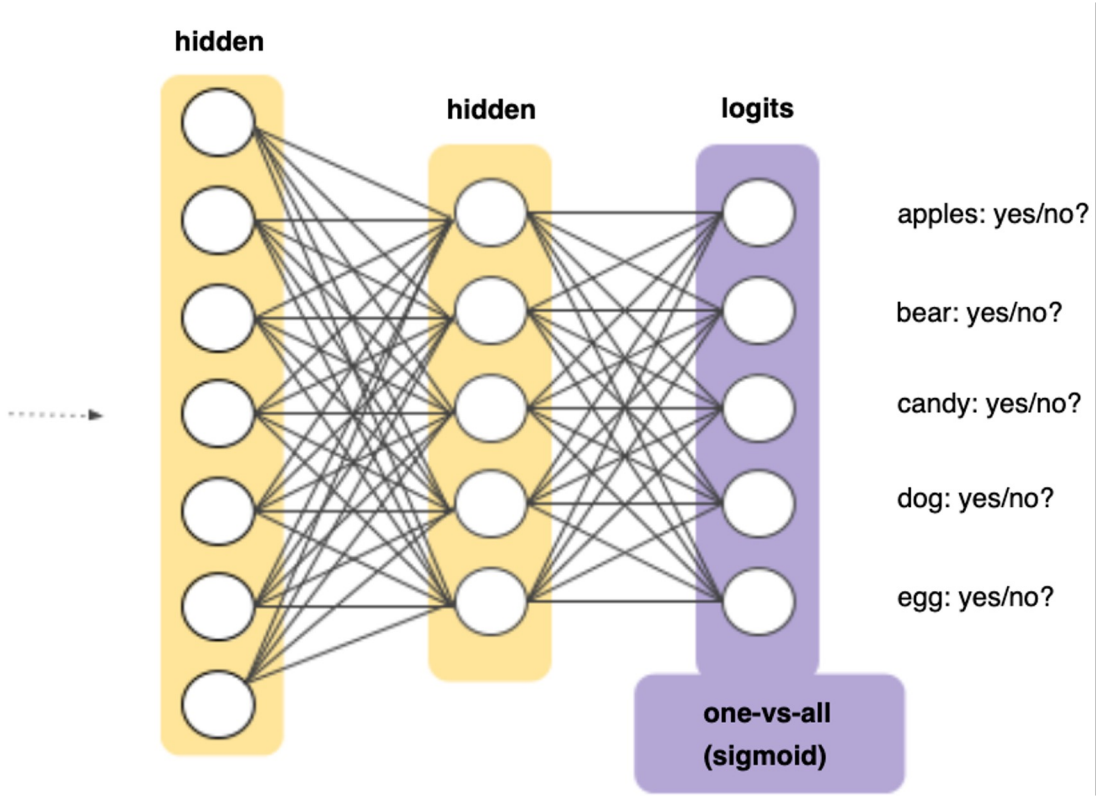


Aside: Multi-Class, Multi-Label

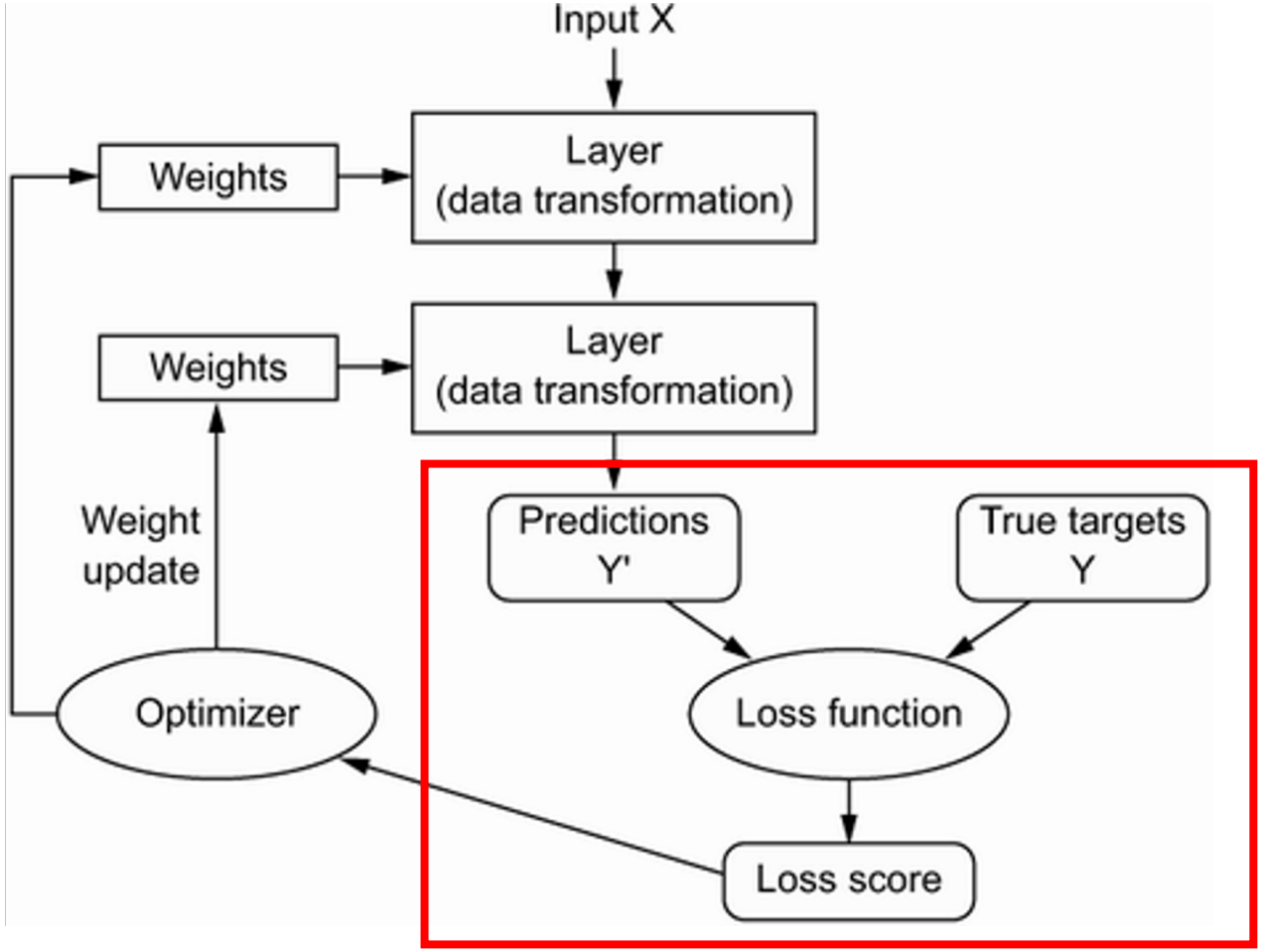
Many Binary Choices vs.
One Multi-category Choice

- We might also have an output layer comprised of many binary labels in some cases (e.g., a cat, a guitar, and a tree may be present in a photo all at the same time).

Many sigmoids versus one softmax depends on whether labels are mutually exclusive or not.



Calculate Loss



Loss Functions

Cross-Entropy / Log-Loss

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

- Typical for binary outcomes. Value grows exponentially larger as the predicted probability moves away from the true 0,1 label.
- Multi-category outcomes have an analogous loss function known as categorical cross-entropy.

$$CE = -\sum_{i}^{C} t_i log(s_i)$$

MAE / L1 Loss

$$MAE = \frac{\sum_{i=1}^{n} | y_i - \hat{y}_i |}{n}$$

- Typical for continuous outcomes. Errors are penalized homogenously, in magnitude and direction. This should look familiar!

MSE / Quadratic / L2 Loss

$$MSE = \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}$$

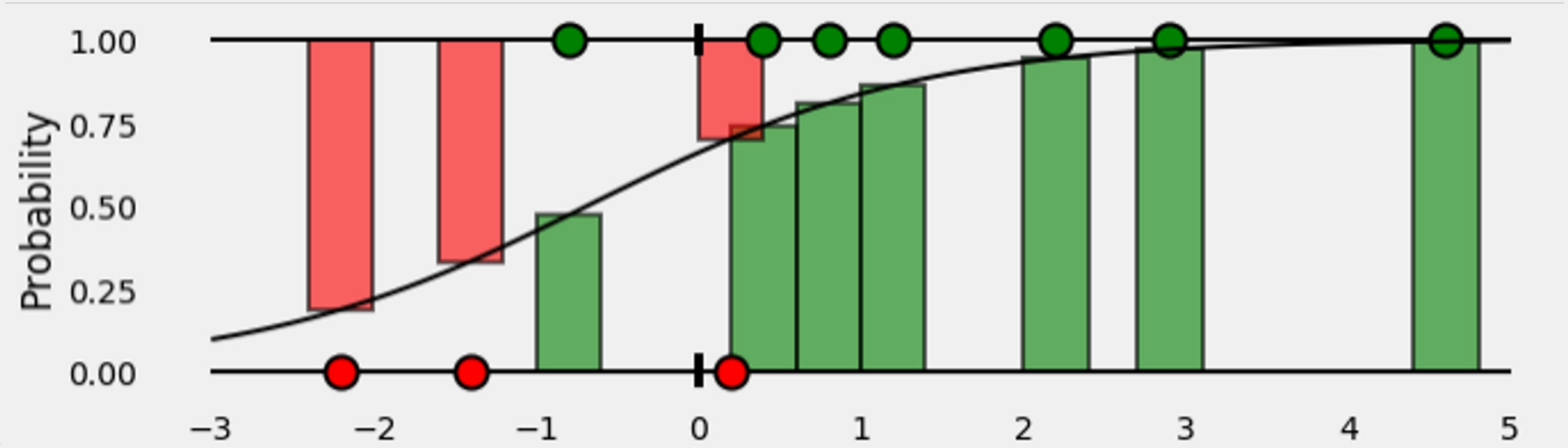
- Typical for continuous outcomes, larger errors penalized exponentially more. This should look familiar!

Binary Cross-Entropy Loss

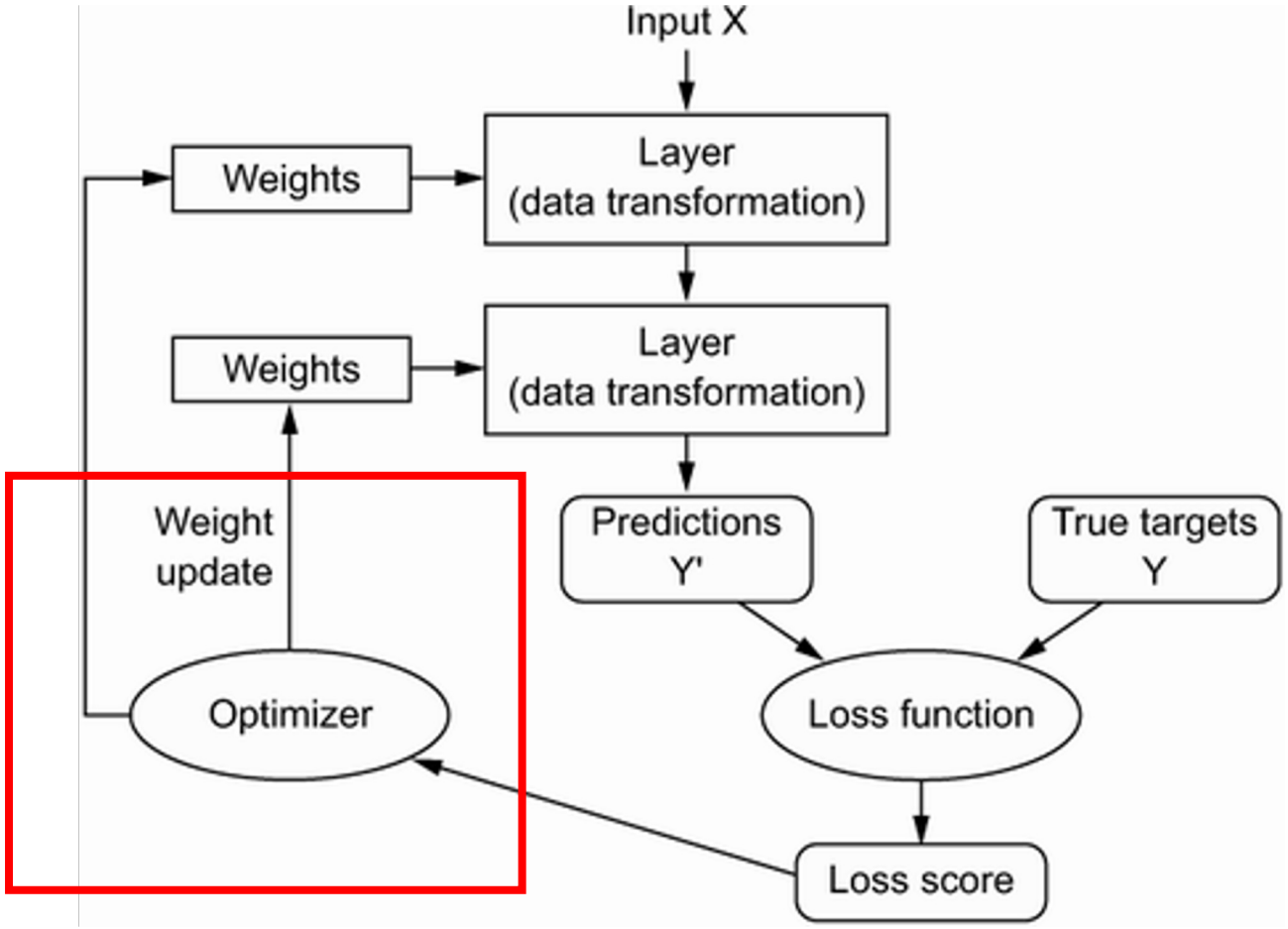
$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

Piecemeal Function:

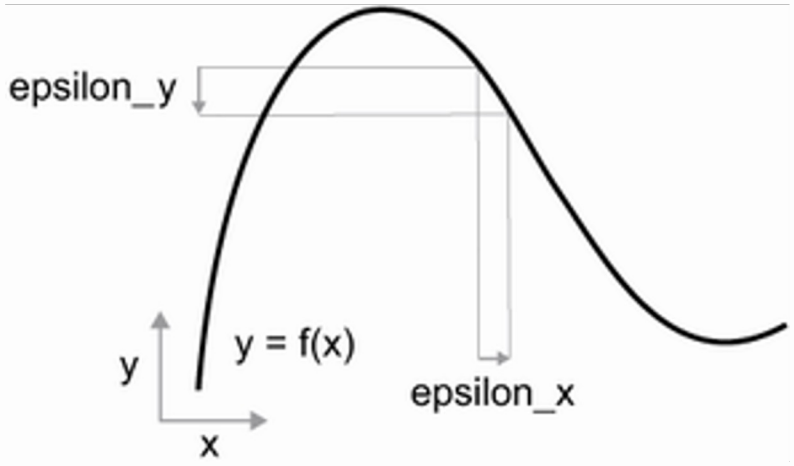
- If ground truth is 1, then loss is -1*log(ρ). As prediction approaches 1, loss approaches 0. As prediction approaches 0, loss grows exponentially.
- If ground truth is 0, then loss is -1*log(1-ρ). As prediction approaches 1, loss rises exponentially. As prediction approaches 0, loss approaches 0.

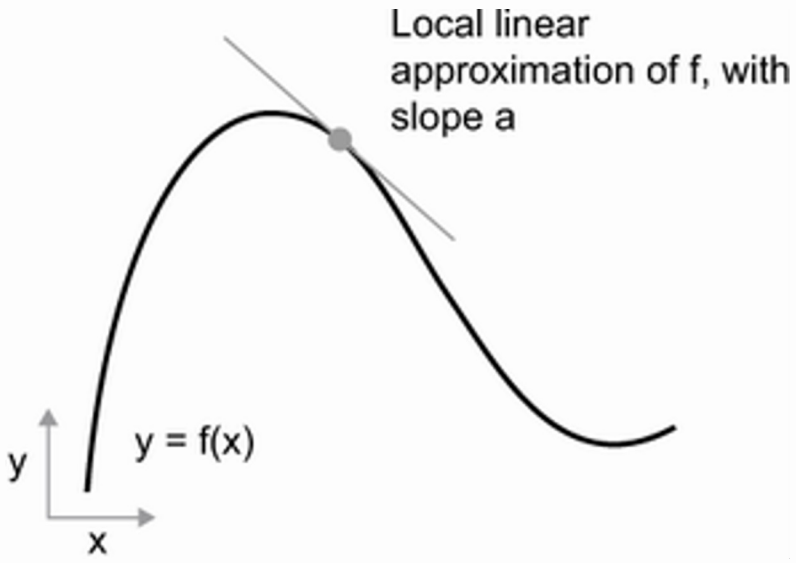


Backpropagation



Derivative = Rate of Change



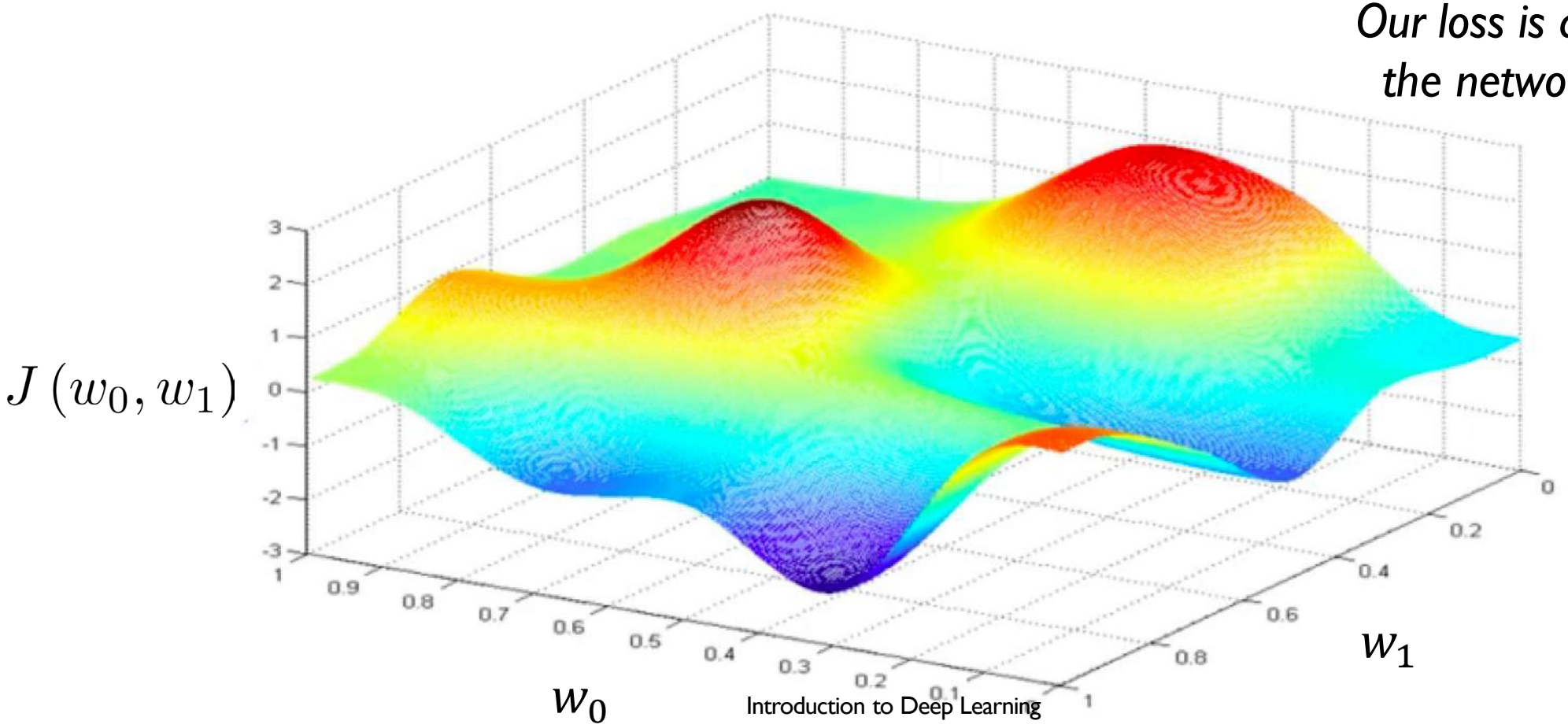


Loss Optimization

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

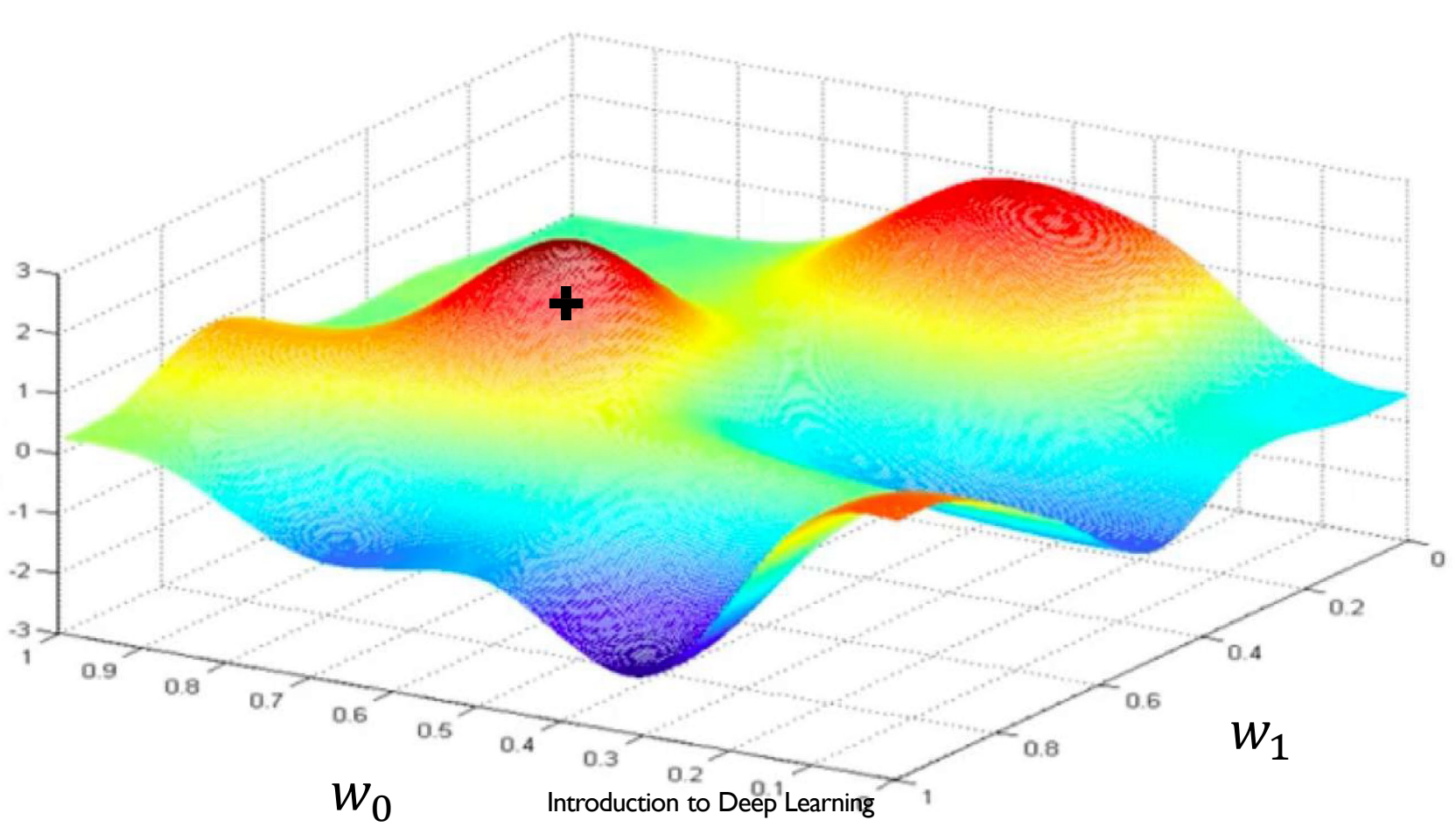
Remember:

Our loss is a function of the network weights!



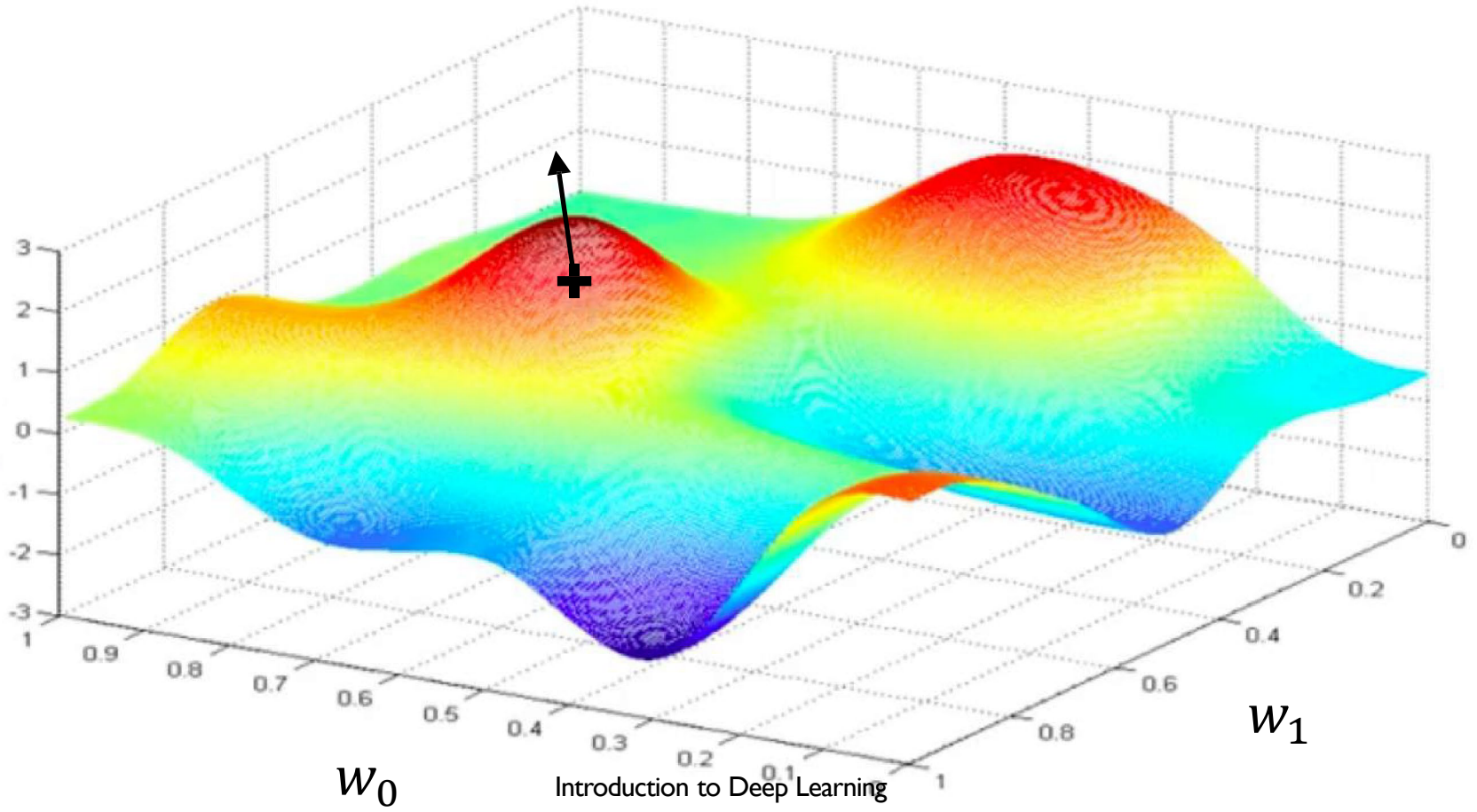
Loss Optimization

Randomly pick an initial (w_0, w_1)



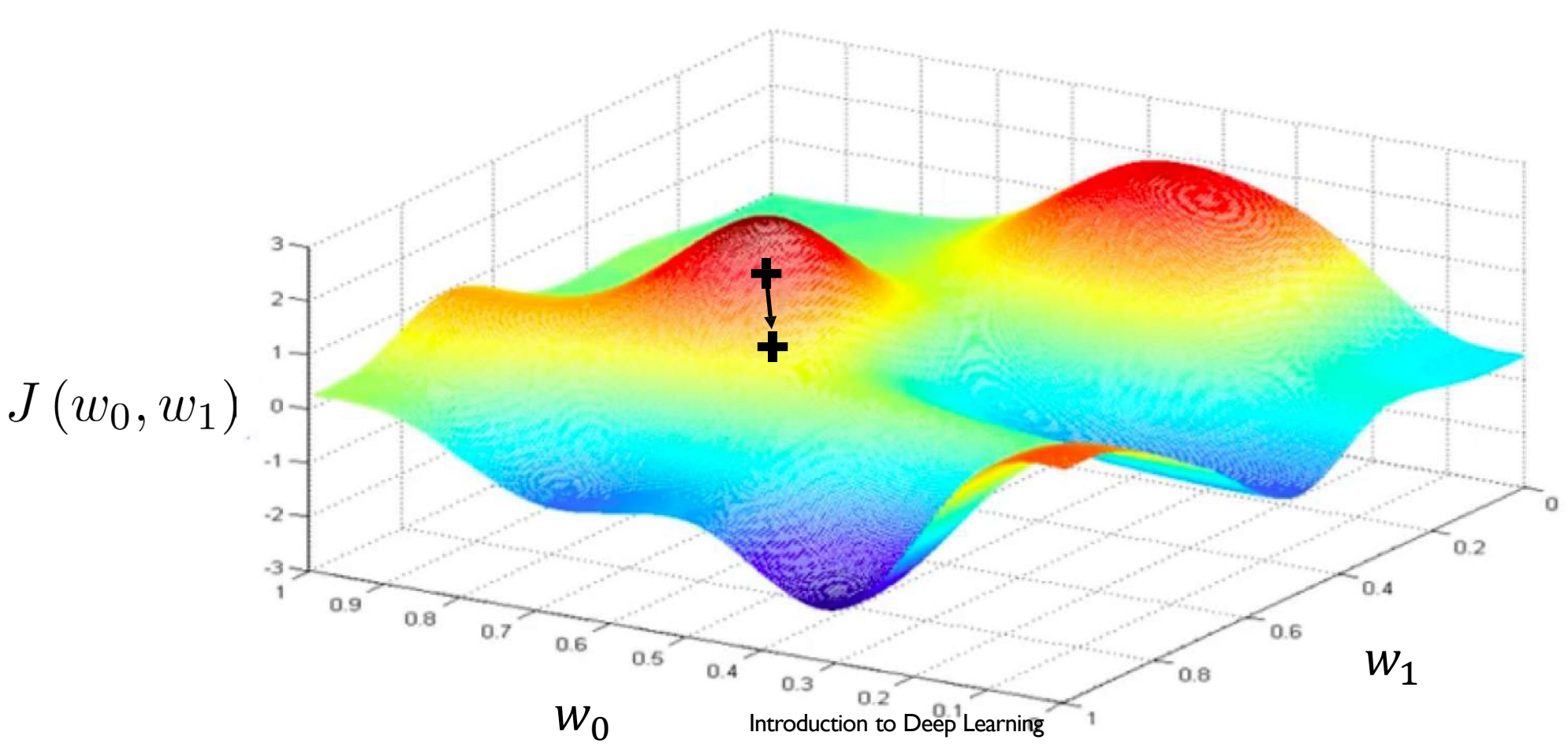
Loss Optimization

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



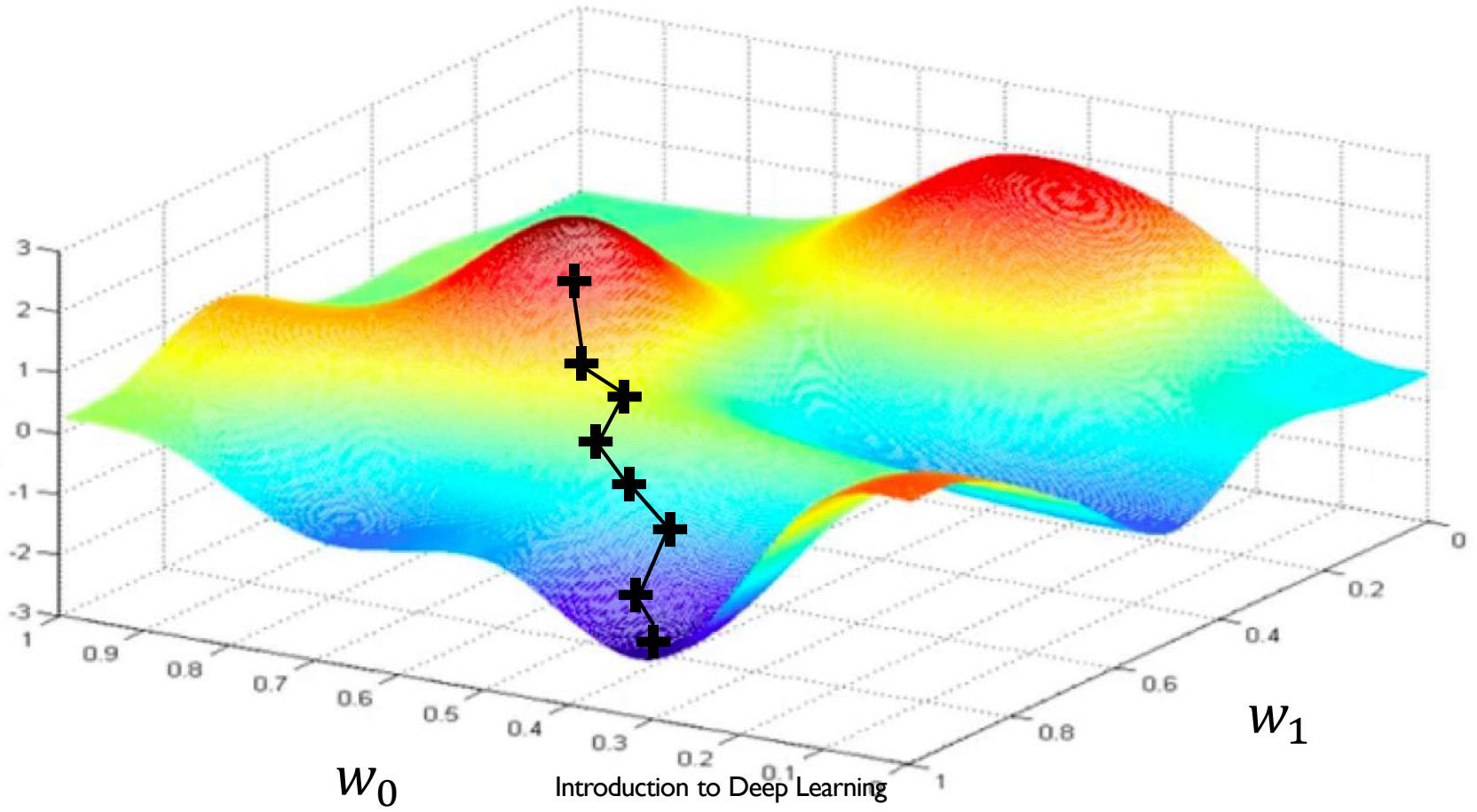
Loss Optimization

Take small step in opposite direction of gradient



Gradient Descent

Repeat until convergence



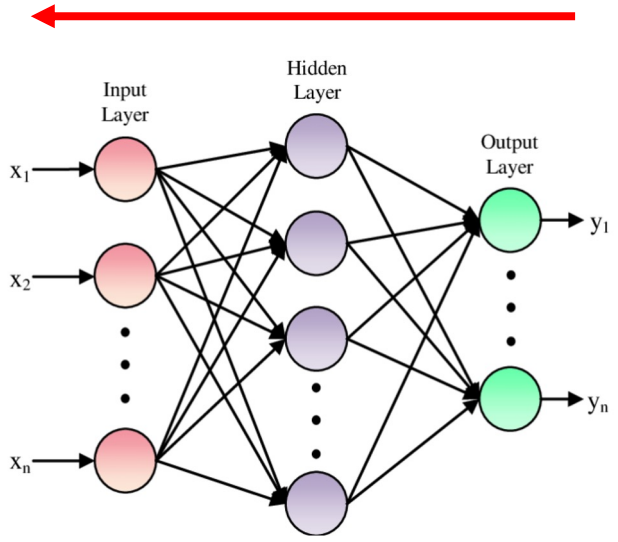
Derivatives of Loss w.r.t **ALL** Model Parameters

Each Node's Output Can be Expressed as a Function of all Prior Nodes' Outputs

$$y_1 = \varphi\left(x_1 \cdot w_{1,1} + x_2 \cdot w_{1,2} + \cdots + b_1\right)$$

$$y_2 = \varphi\left(x_1 \cdot w_{2,1} + x_2 \cdot w_{2,2} + \cdots + b_2\right)$$

...

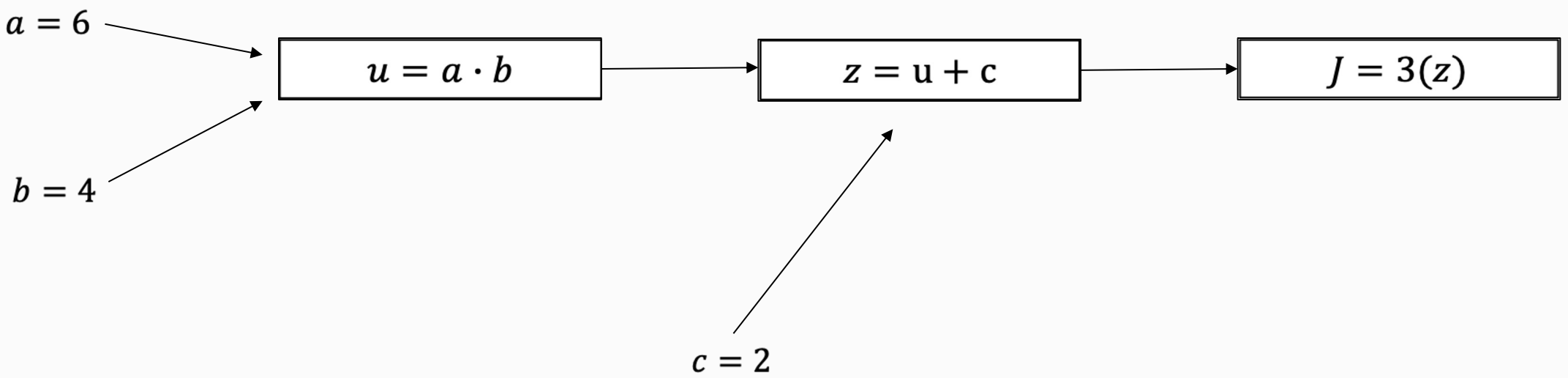


Start at the final nodes in the network and work backwards

- We calculate partial derivatives that explain how Loss will change if we modify a particular weight.
- We use that understanding to decide how we modify each weight for the next iteration.
- So, how can we figure out the derivative of Loss w.r.t. a particular weight in the neural network? **Backpropagation!**

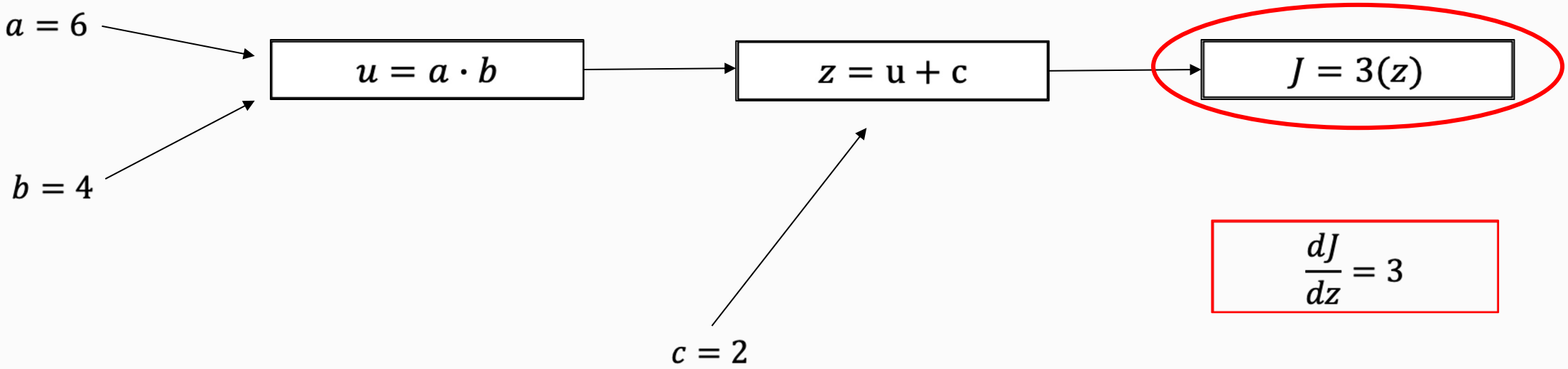
Simplifying Gradients: Computation Graph

$$J = 3(a \cdot b + c)$$



Backpropagation = Working Backwards

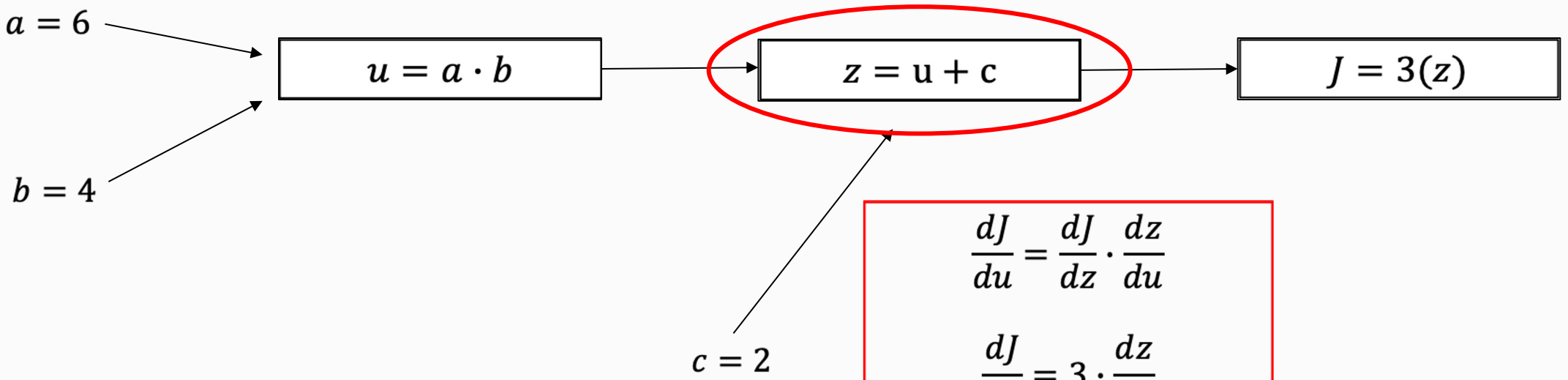
$$J = 3(a \cdot b + c)$$



Backpropagation = Work Backwards

$\frac{dJ}{dz} = 3$

$J = 3(a \cdot b + c)$



$$\frac{dJ}{du} = \frac{dJ}{dz} \cdot \frac{dz}{du}$$

$$\frac{dJ}{du} = 3 \cdot \frac{dz}{du}$$

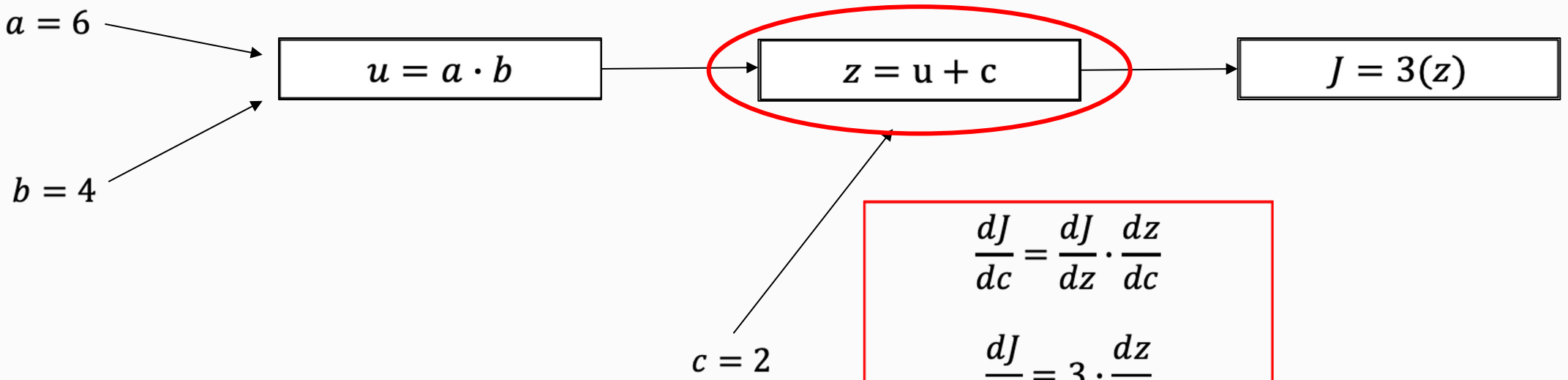
$$\frac{dJ}{du} = 3 \cdot 1 = 3$$

Backpropagation = Work Backwards

$$\frac{dJ}{dz} = 3$$

$$\frac{dJ}{du} = 3$$

$$J = 3(a \cdot b + c)$$



$$\frac{dJ}{dc} = \frac{dJ}{dz} \cdot \frac{dz}{dc}$$

$$\frac{dJ}{dc} = 3 \cdot \frac{dz}{dc}$$

$$\frac{dJ}{dc} = 3 \cdot 1 = 3$$

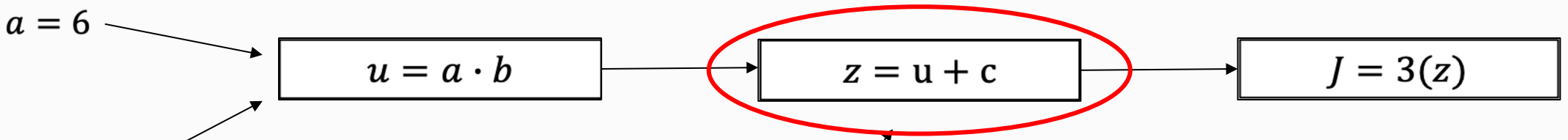
Backpropagation = Work Backwards

$$\frac{dJ}{dz} = 3$$

$$\frac{dJ}{du} = 3$$

$$\frac{dJ}{dc} = 3$$

$$J = 3(a \cdot b + c)$$



$$\frac{dJ}{da} = \frac{dJ}{du} \cdot \frac{du}{da}$$

$$\frac{dJ}{da} = 3 \cdot b$$

$$\frac{dJ}{da} = 3 \cdot 4 = 12$$

Backpropagation = Work Backwards

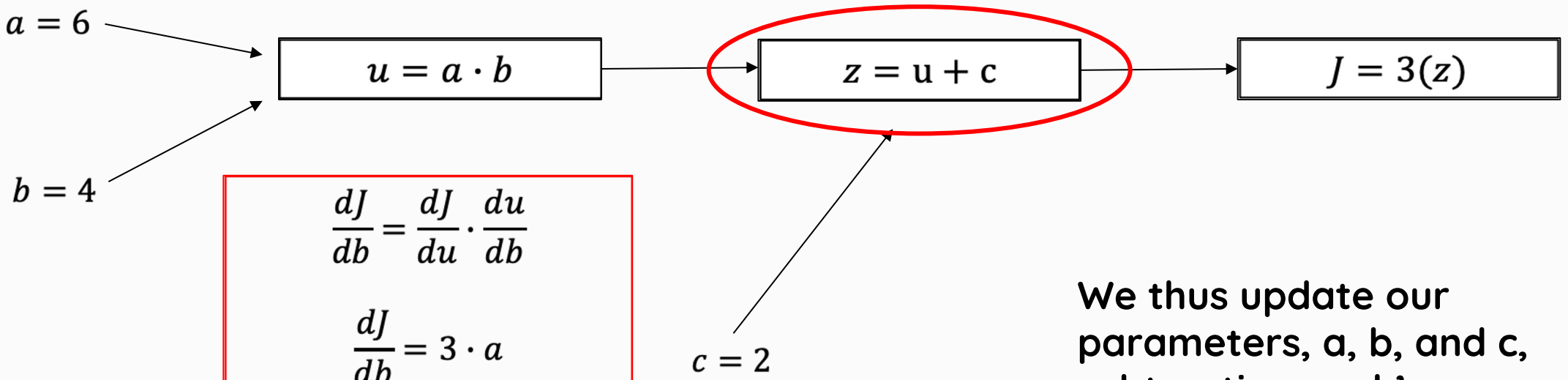
$$\frac{dJ}{dz} = 3$$

$$\frac{dJ}{du} = 3$$

$$\frac{dJ}{dc} = 3$$

$$J = 3(a \cdot b + c)$$

$$\frac{dJ}{da} = 12$$



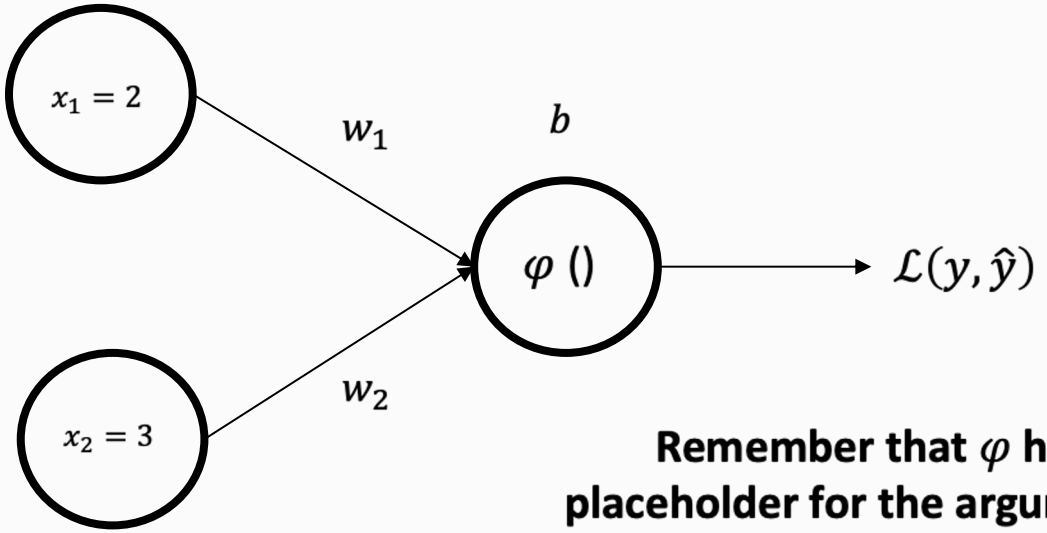
$$\frac{dJ}{db} = \frac{dJ}{du} \cdot \frac{du}{db}$$

$$\frac{dJ}{db} = 3 \cdot a$$

$$\frac{dJ}{da} = 3 \cdot 6 = 18$$

We thus update our parameters, a, b, and c, subtracting each's gradients*epsilon from its current value. Epsilon is the learning rate.

Single Node with Sigmoid & Cross-Entropy Loss (i.e., Logistic Regression)



Remember that φ here is just a placeholder for the argument to the loss function. It happens to be a sigmoid transformation of 'something', i.e., φ(wx+b), but it doesn't really matter. We just represent it with some variable name and calculate an expression for the derivative.

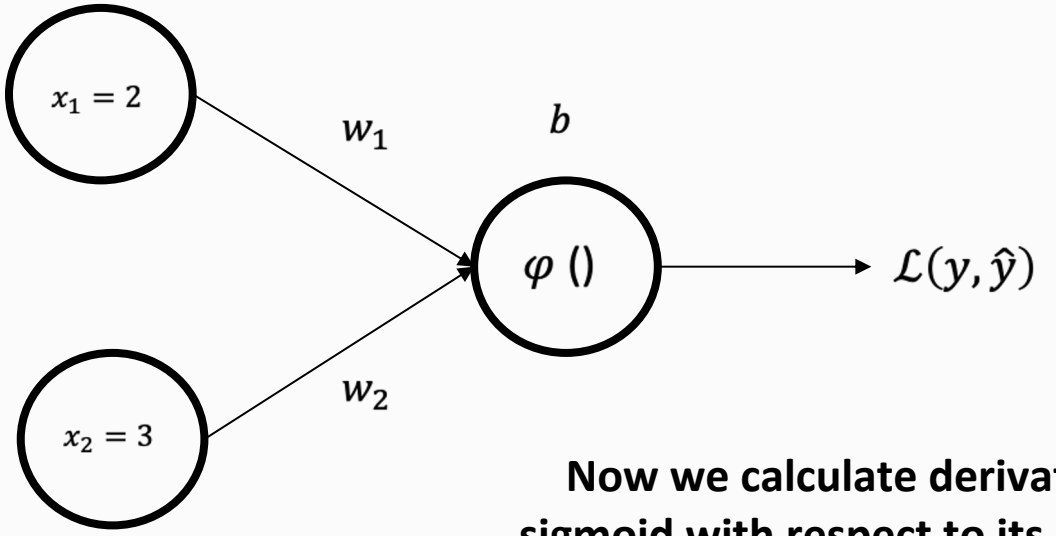
$$\frac{d\mathcal{L}}{d\varphi} = -\frac{y}{\varphi} + \frac{1-y}{1-\varphi}$$

$$\frac{d\mathcal{L}}{d\varphi} = \frac{\varphi(1-y) - y(1-\varphi)}{\varphi(1-\varphi)}$$

$$\frac{d\mathcal{L}}{d\varphi} = \frac{\varphi - \varphi y - y + \varphi y}{\varphi(1-\varphi)}$$

$$\frac{d\mathcal{L}}{d\varphi} = \frac{\varphi - y}{\varphi(1-\varphi)}$$

Single Node with Sigmoid & Cross-Entropy Loss (i.e., Logistic Regression)



Now we calculate derivative of the sigmoid with respect to its argument, z.

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

$$\varphi'(z) = -1 \cdot (1 + e^{-z})^{-2} \cdot (0 + e^{-z} \cdot -1)$$

$$\varphi'(z) = (1 + e^{-z})^{-2} \cdot e^{-z}$$

$$\varphi'(z) = \varphi(z) \cdot (1 - \varphi(z))$$

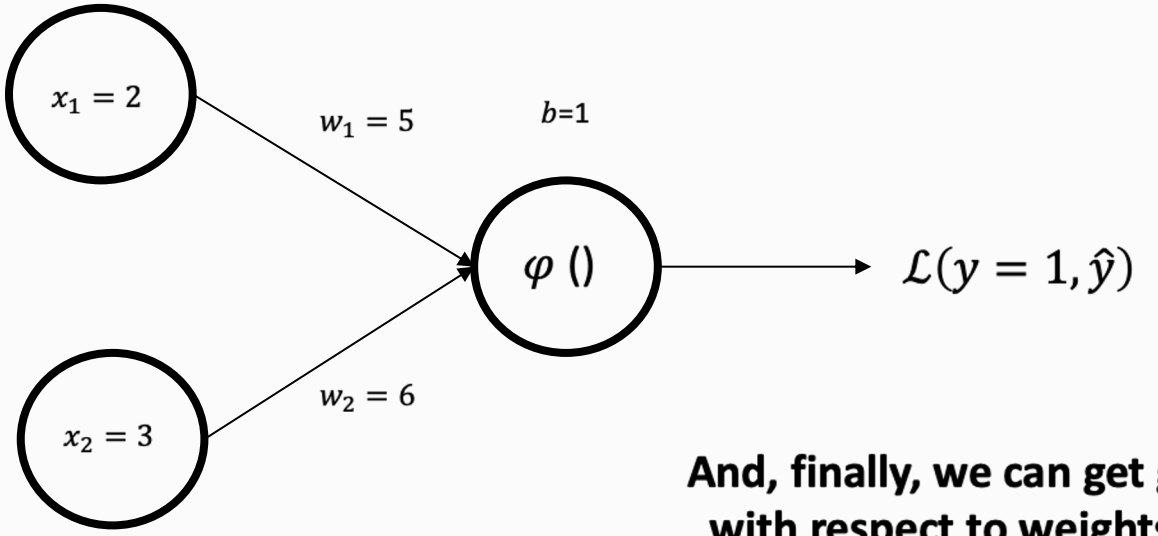
$$\frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{d\varphi} \cdot \frac{d\varphi}{dz}$$

$$\frac{d\mathcal{L}}{dz} = \frac{\varphi - y}{\varphi(1 - y)} \cdot \frac{d\varphi}{dz}$$

$$\frac{d\mathcal{L}}{dz} = \frac{\varphi - y}{\varphi(1 - y)} \cdot \varphi(1 - \varphi)$$

$$\frac{d\mathcal{L}}{dz} = \varphi - y$$

Single Node with Sigmoid & Cross-Entropy Loss (i.e., Logistic Regression)



And, finally, we can get gradient of loss with respect to weights and bias. For example, for the first weight…

Evaluate φ based on current values of parameters and the data.

Finally, update the weights…

$$\frac{d\mathcal{L}}{dw_1} = \frac{d\mathcal{L}}{dz} \cdot \frac{dz}{dw_1}$$

$$\frac{d\mathcal{L}}{dw_1} = (\varphi - y) \cdot x_1$$

$$w_{1,new} = w_{1,old} - (\frac{d\mathcal{L}}{dw_{1,old}} \cdot \varepsilon)$$

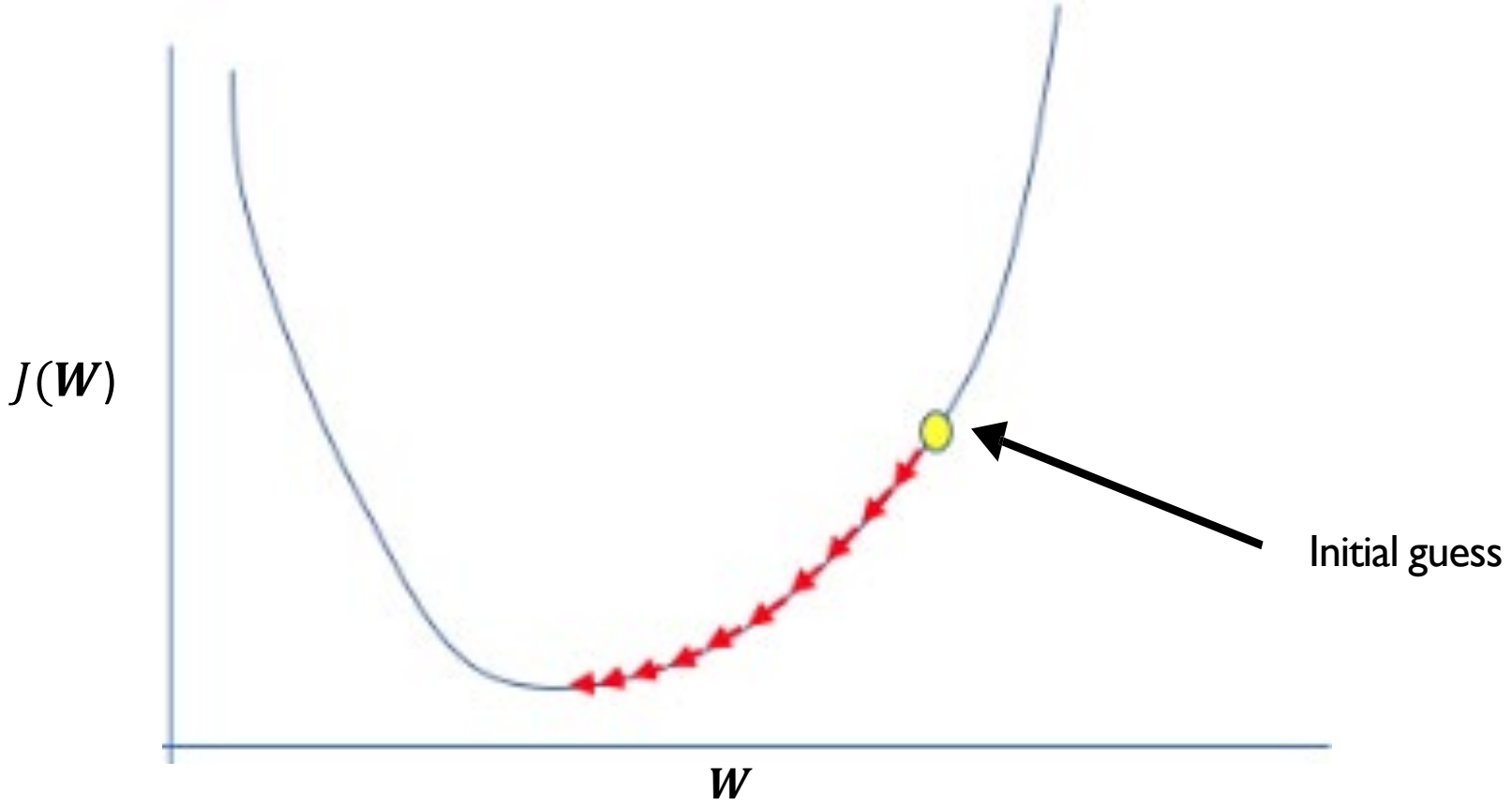
Tensorflow GradientTape: AutoDiff

1. Gradient Tape

- A Tensorflow function that automates the calculation of derivatives.
- It constructs a computation graph in the background and implements codified rules for calculating derivatives of functions.
- You could technically use gradient tape to implement a gradient descent algorithm for many optimization problems.

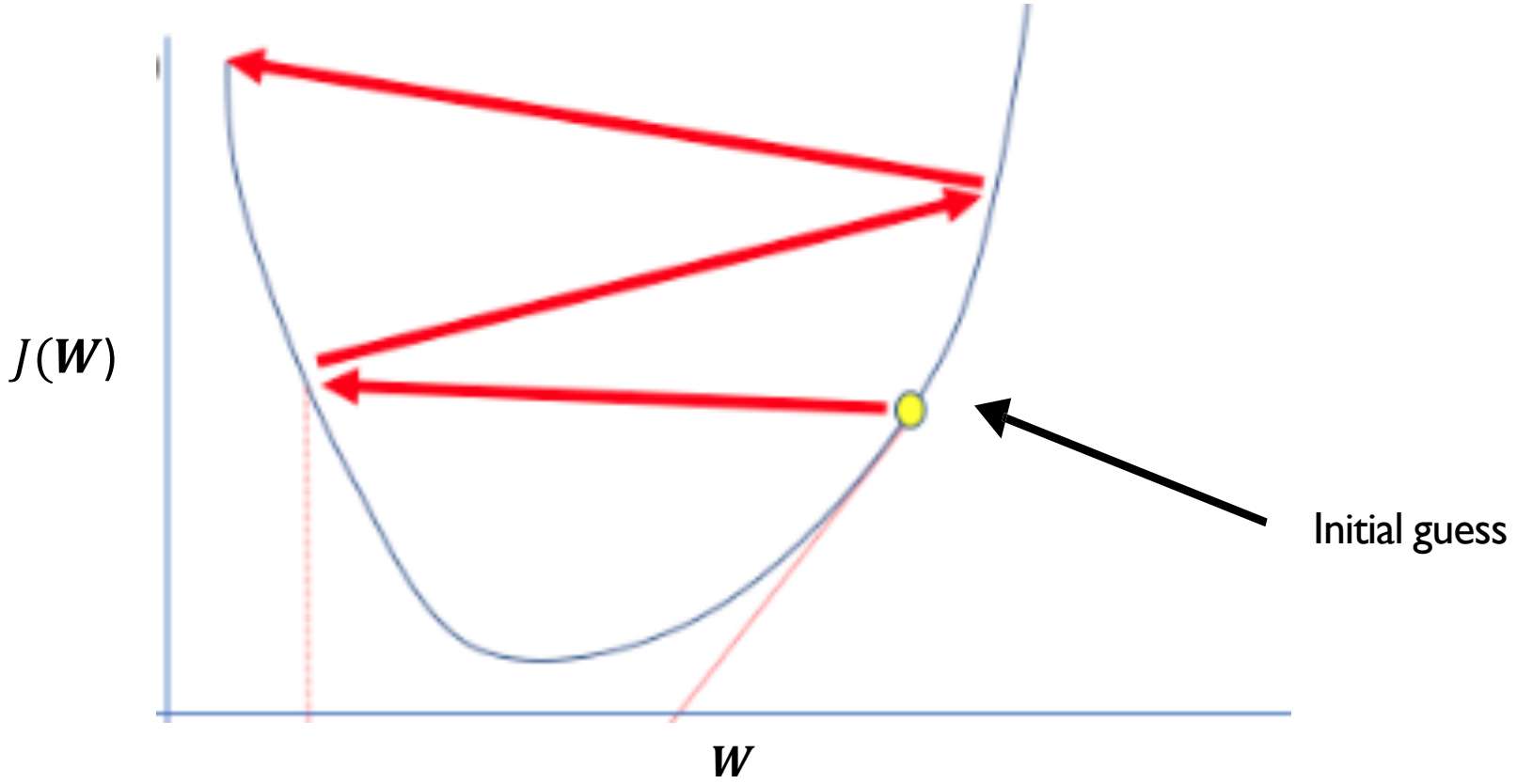
Setting the Learning Rate

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

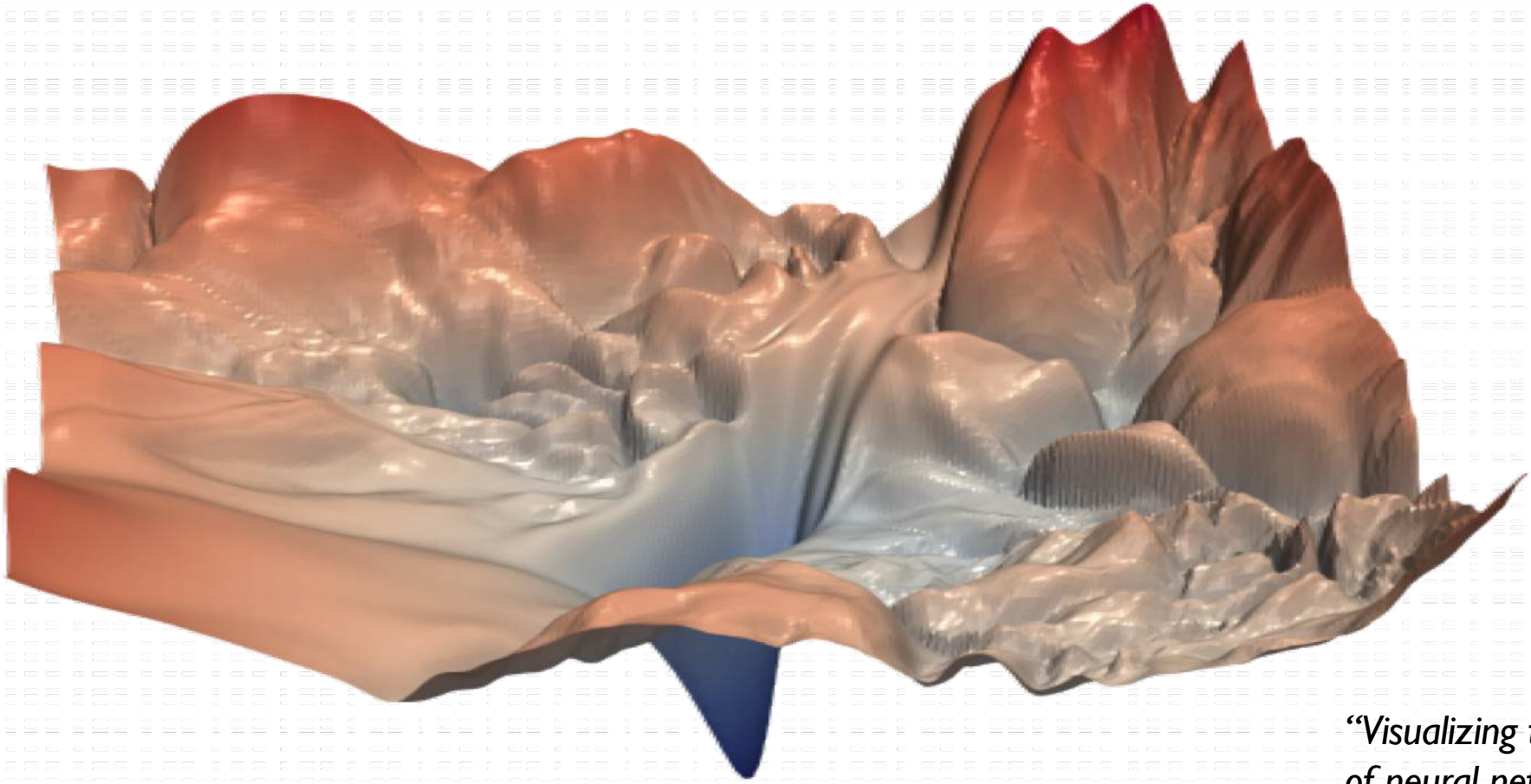


Setting the Learning Rate

Large learning rates overshoot, become unstable and diverge



Training neural networks (tuning learning rate) is difficult: complex loss landscape

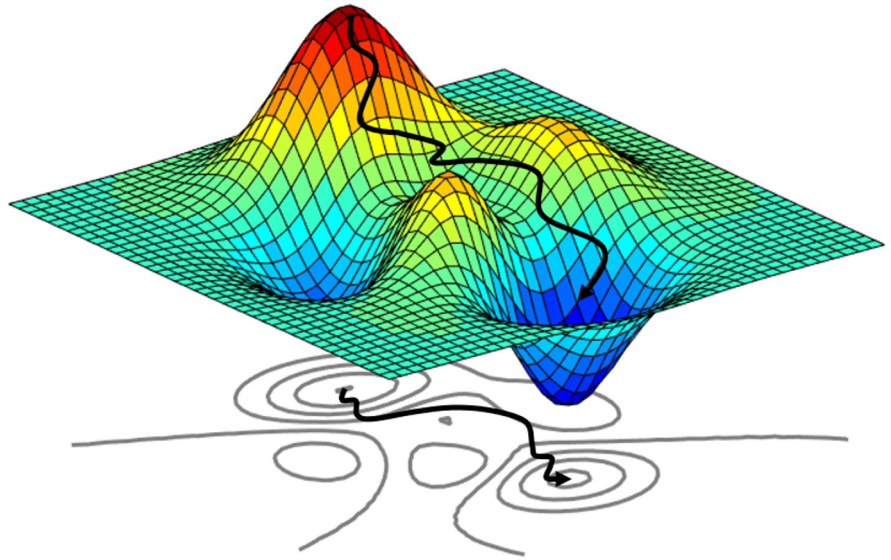


"Visualizing the loss landscape of neural nets". Dec 2017.

Optimizers

Keras Supports 8 Optimizers

- SGD = Stochastic Gradient Descent
- Momentum
- Ftrl (2010) = Follow the Regularized Leader
- Adagrad and Adadelta (2012) = Adaptive Gradient Des
- RMSprop (~2012) = Root Mean Squared propagation
- Adam (2015) = Adadelta / RMSProp with Momentum.
    - Adamax, Nadam are extensions to Adam.



SGD: Gradient Descent

Types of GD

- Batch GD = Use all the available training data in each pass.
  - Works well if the loss surface is smooth and lacks any saddle points / valleys.
  - Computationally expensive!
- Stochastic GD = Mini-batch with batch size = 1.
  - If troughs / saddles exist, we move past them as our exploration of gradients for the model will vary with a given observation that we are considering in an iteration.
  - Learns quite slowly but performs well on non-linear problems (eventually).
- Mini-batch GD = Happy medium and what we have been doing so far – more than 1 observation per batch, less than total sample..

Role of Batch Size

- Empirically has been observed that smaller batches yield less overfitting (because of implicit noise in the training process – variance of the gradients obtained will go up though).

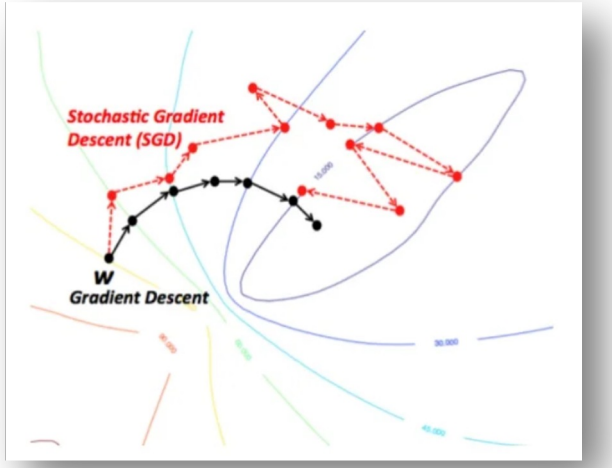
Batch (All) vs. Stochastic (1)

Same Convergence

- If you have a convex surface, either approach will converge to the global optimum. Always converges at least to a local minimum.

Tradeoffs

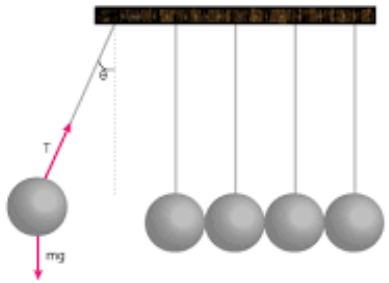
- Batch, each step is slower, more computationally burdensome, but convergence with fewer iterations; Need to be able to hold the entire dataset in memory.
- SGD makes noisier updates, and requires more iterations to converge, but a single iteration is quick. Only need one observation in memory at a time.



Momentum

Getting Past Local Minima

- SGD gets stuck in local minima; the idea of momentum is to make updates be a function of current gradient*learning rate, as well as some fraction (decay) of the update you made last iteration.
- This reduces updates to parameters where the gradients are flipping sign and amplifies updates to gradients that are going in a consistent direction (steeply descending).



Adagrad & Adadelta (RMS Prop)

Adaptive Gradient Descent (Variable Learning Rate)

- We implicitly apply a high learning rate for features we have been updating very little so far (speed up movement through saddle points, for example).
- We implicitly apply a low learning rate for features we have been updating a lot so far.
- Technically learning rate is removed from the process, every update is a function of past updates.

Adadelta

- Same idea but we use a sliding window of previous updates to determine magnitude of current updates (rather than all prior updates).
- RMSProp is conceptually very similar but was independently developed (around the same time).

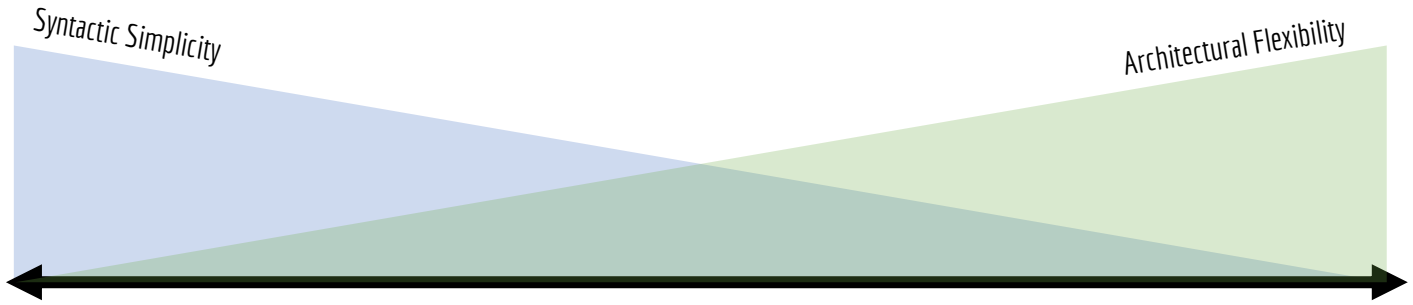
Note: Sequential vs. Functional API

We Have Only Seen Sequential API So Far

- Sequential is easy to work with but is also very inflexible. Can only really handle basic feed-forward networks. It automatically figures out the shape of each layer's output tensor and specifies the next layer's input shape accordingly.

Functional API Let's You Construct Any Topology You Want

- We will see the difference in how each API is used, syntactically.



Recap

Building Blocks of NNs

- Tensors and Tensor Operations
- Activation Functions
- Loss Functions
- Backpropagation: Derivatives, Gradients & the Chain Rule

Procedure of Minibatch Stochastic Gradient Descent

- Grab a batch of observations (samples)
- Predict their labels using current weights / bias terms.
- Calculate loss value.
- Calculate gradient of loss w.r.t. all weight / bias terms.
- Update each weight by subtracting its gradient*learning rate
- Cycle over the whole training dataset (each cycle is an epoch) repeatedly, until loss is small.