Intro to Neural Nets

Week 2: Mathematical Building Blocks & Working with Keras API

Today’s Agenda

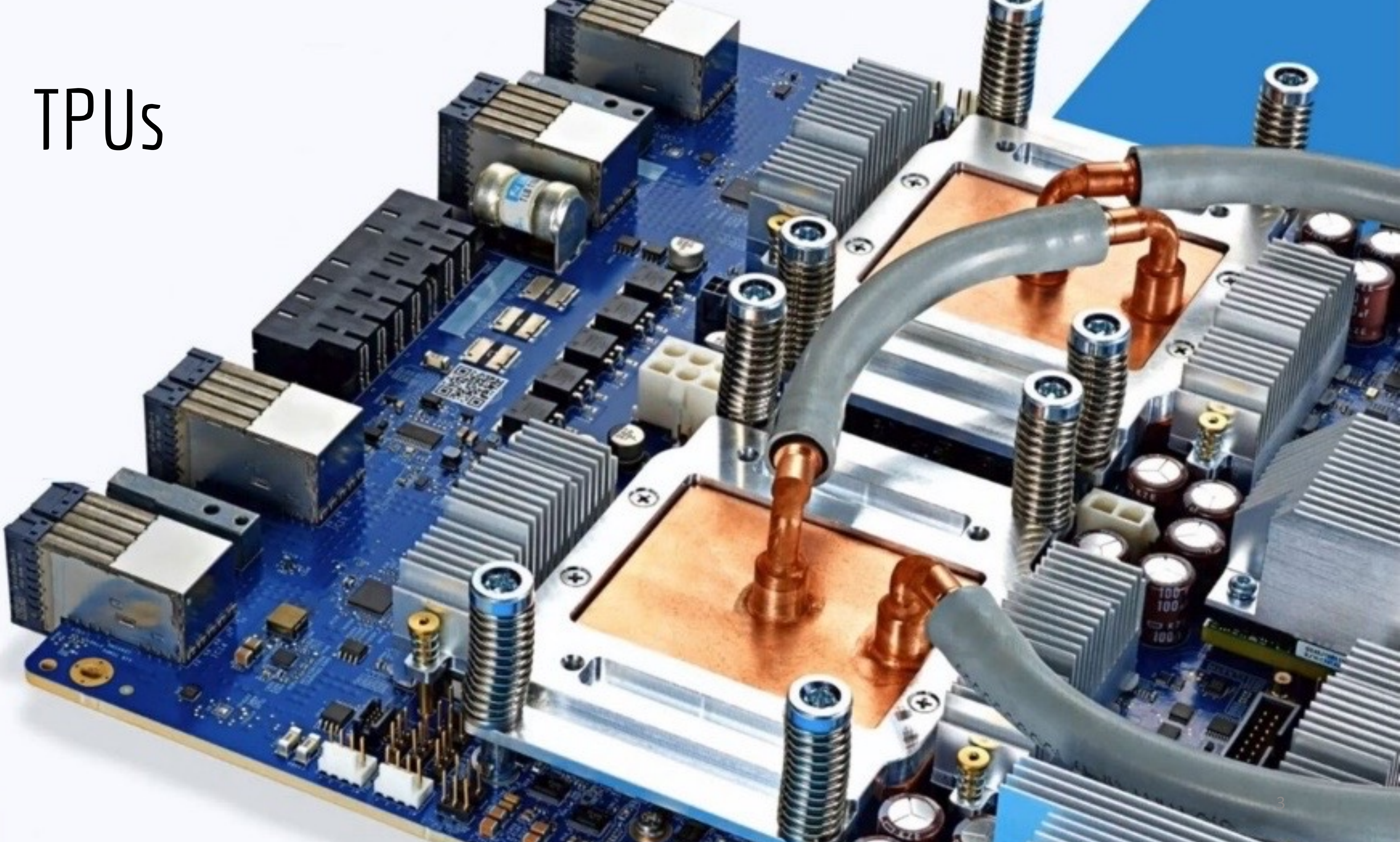
1. Building Blocks of NNs

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

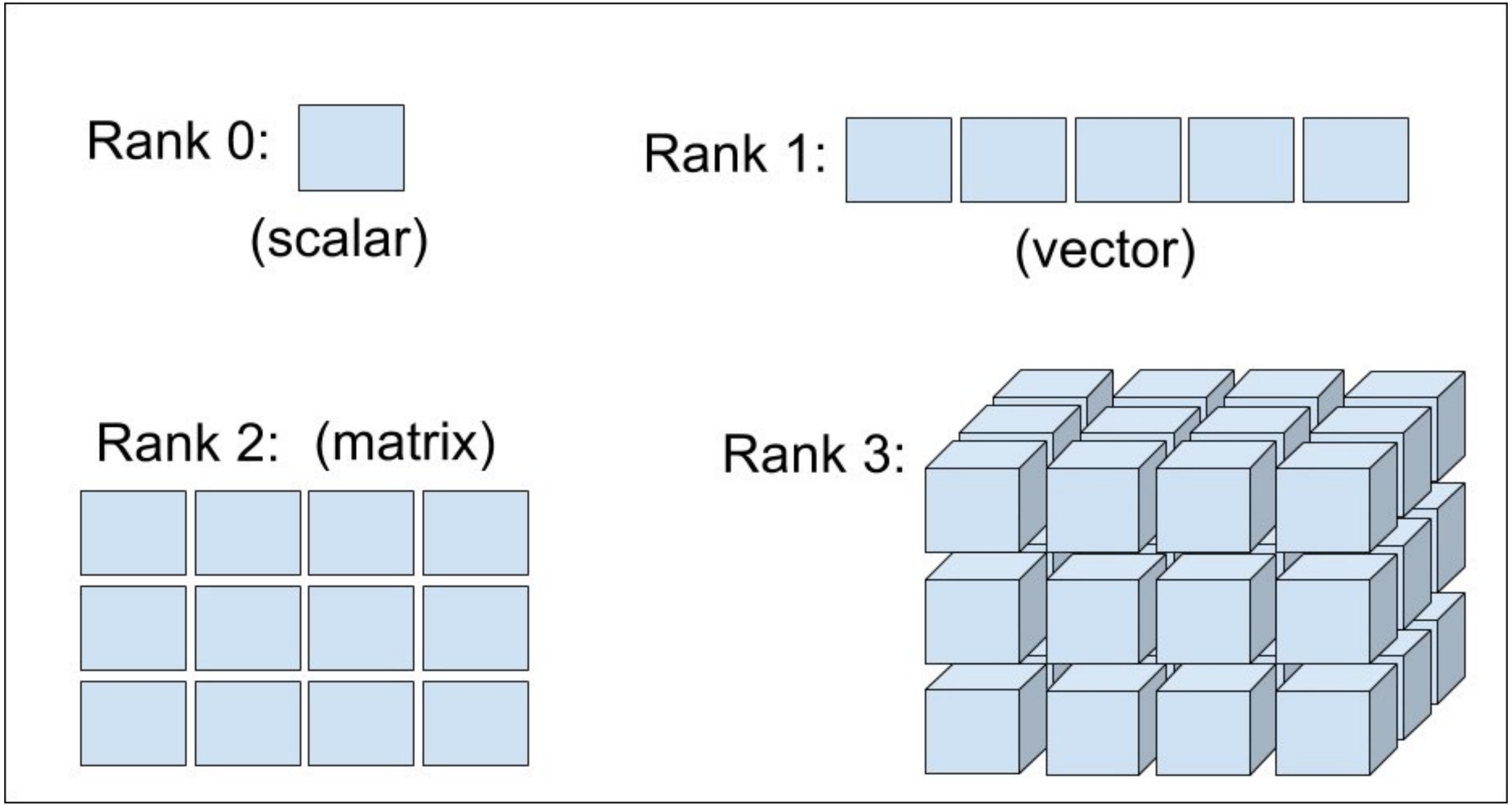
2. Building a Linear Classifier

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

TPUs



Tensors



Neuron / Network Components

X and Y are data

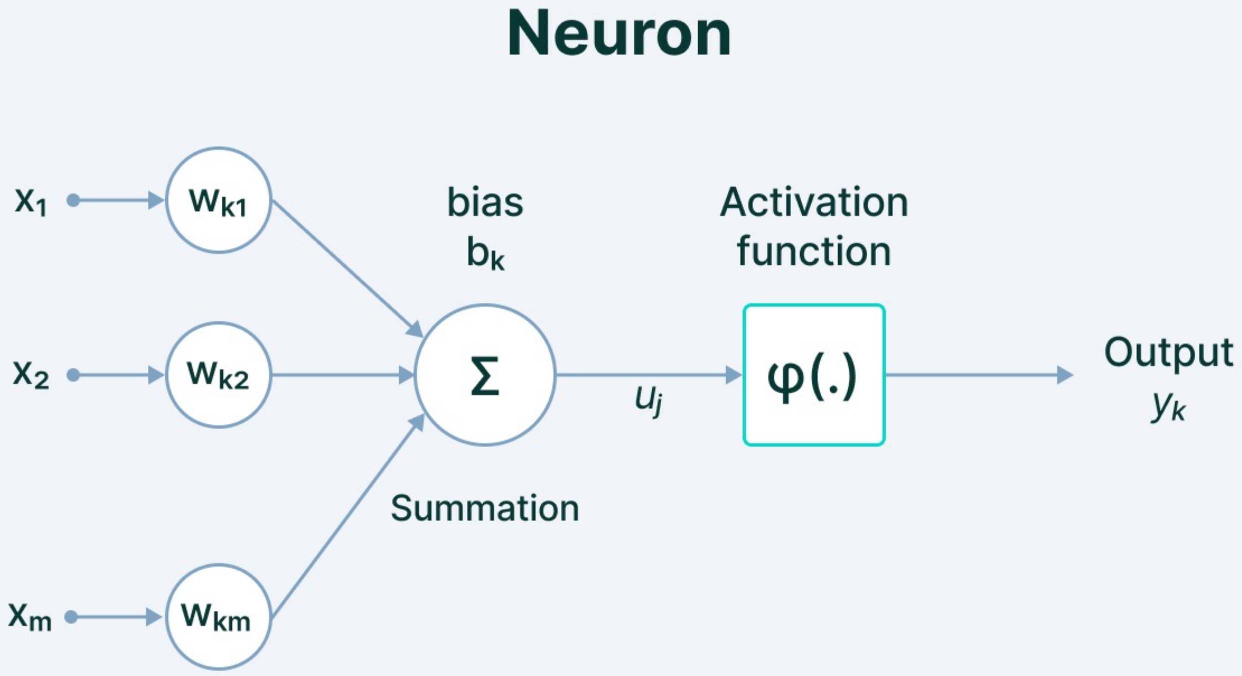
- These are input values and labels.

W and b are parameters

- These are values we 'learn' through the optimization process.

$\varphi(.)$ is a function we choose

- This is a hyper-parameter.



Neuron / Network Components

***x* and *w* are vectors for a node**

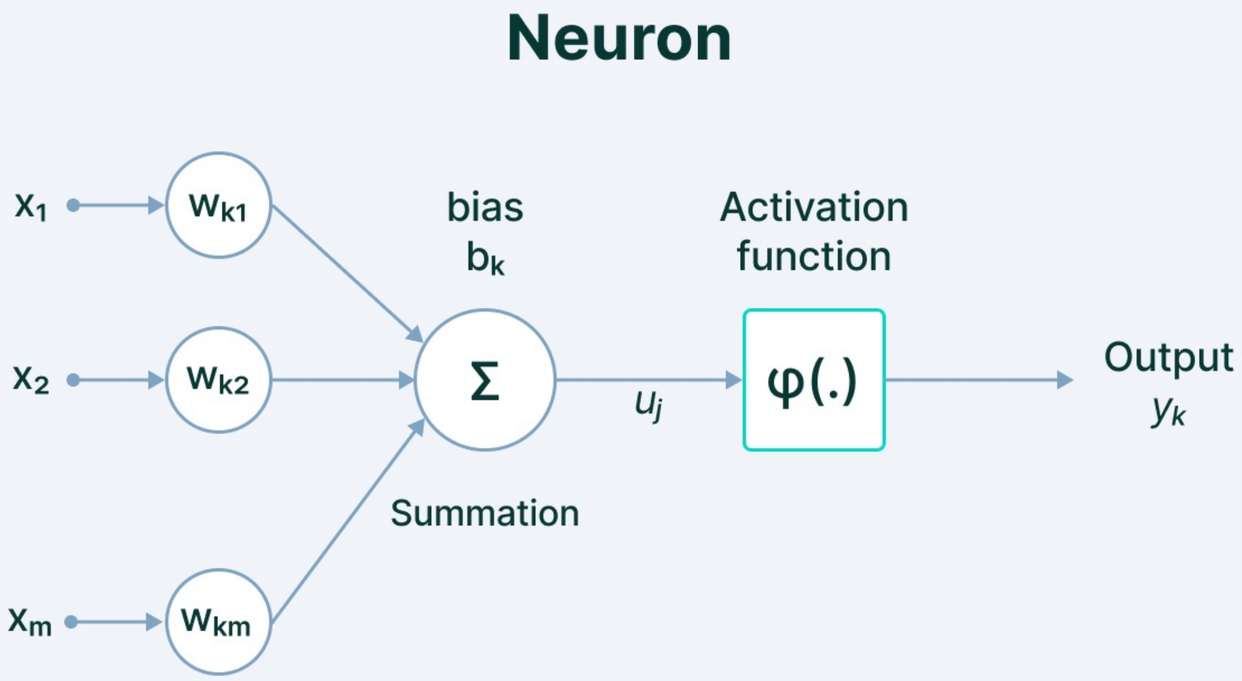
- These vectors comprise matrices that represent a layer of nodes in the network.

***b* and *y* are scalars for a node**

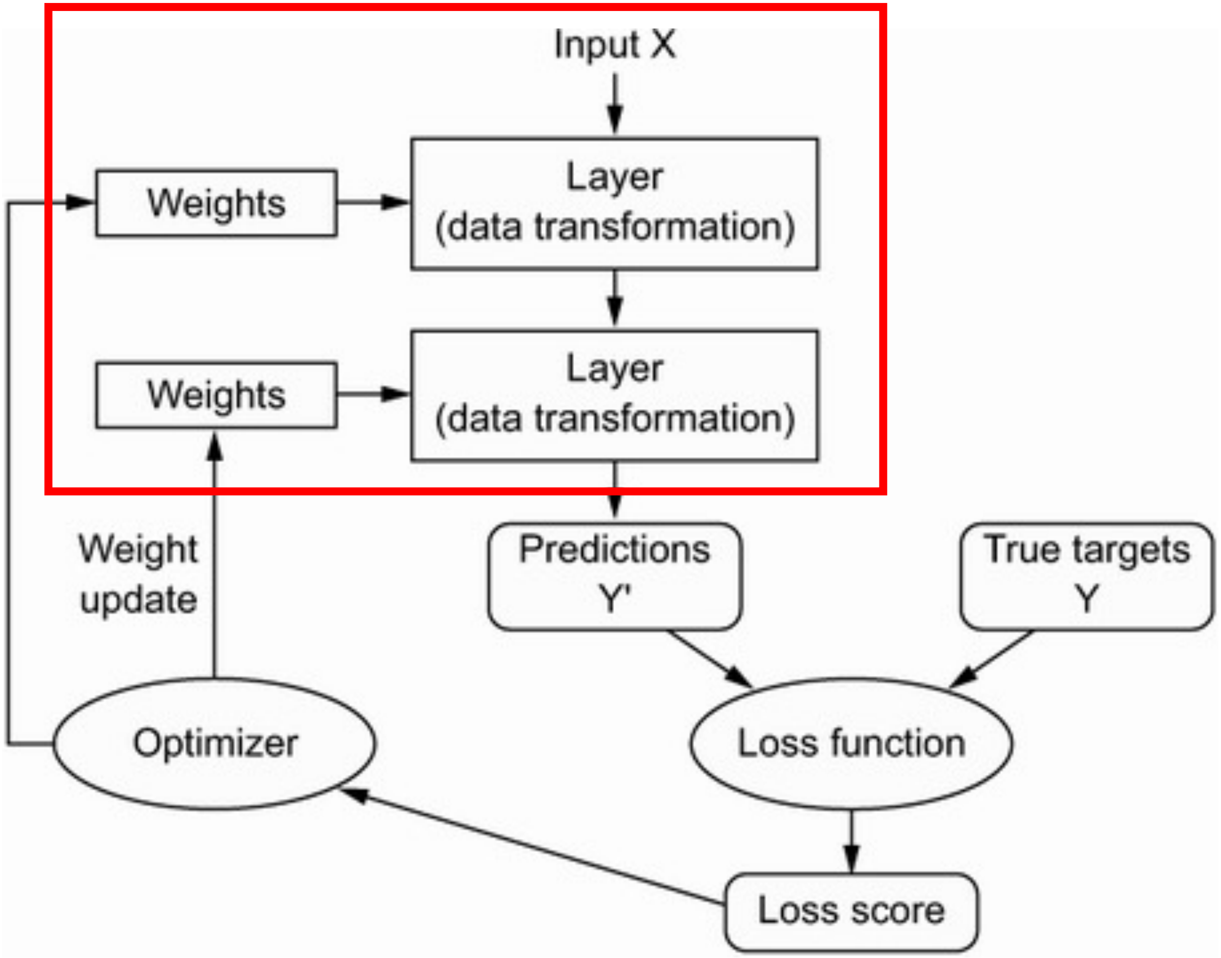
- The set of all b's in a layer becomes a vector.

Nature of output, i.e., *y*

- Depends on position in the network, and what we are predicting



Forward Pass



Multiplication

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

Conformity of Shapes

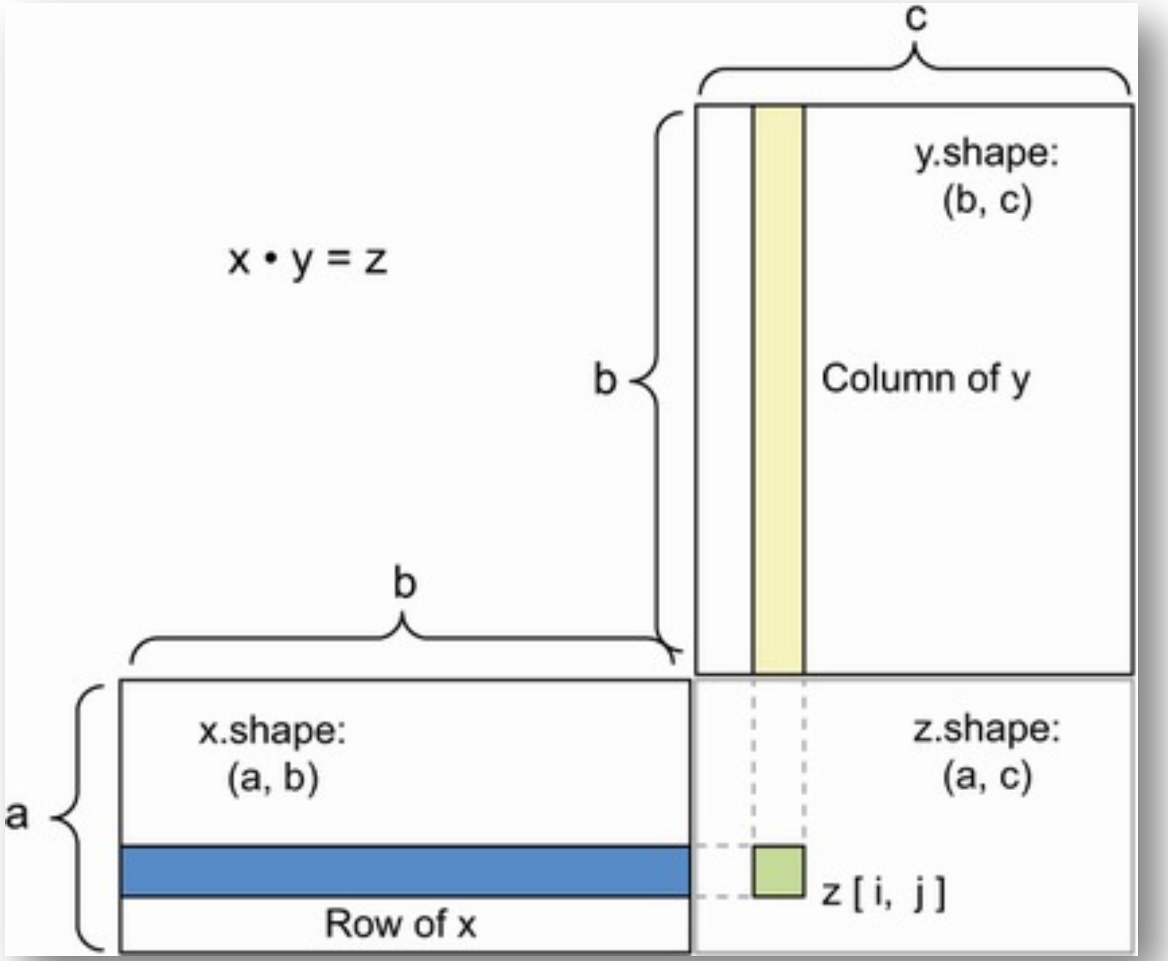
- NCOL(X) == NROW(W)

Elements of Resulting Tensor are the Dot Product of X's Rows and Y's Columns

- Z[2,2] = X[2,:] · Y[:,2]

We Use This for Multiplication Step

- x*w calculations.



Addition + Broadcast

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

Shape of the Two Tensors Needs to Conform

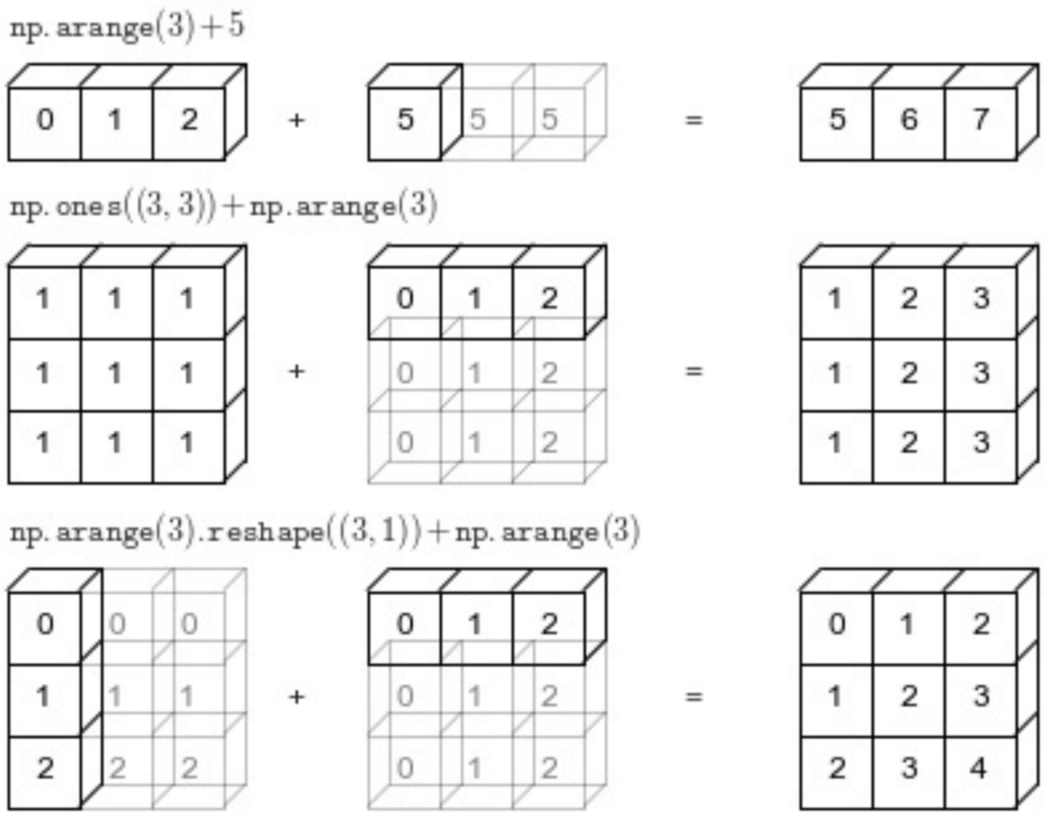
- A + B will only work if A is cleanly divisible by B (or vice versa)

Sum the Element-wise Products

- Replicate B until it matches A's dimensions, then element-wise addition.

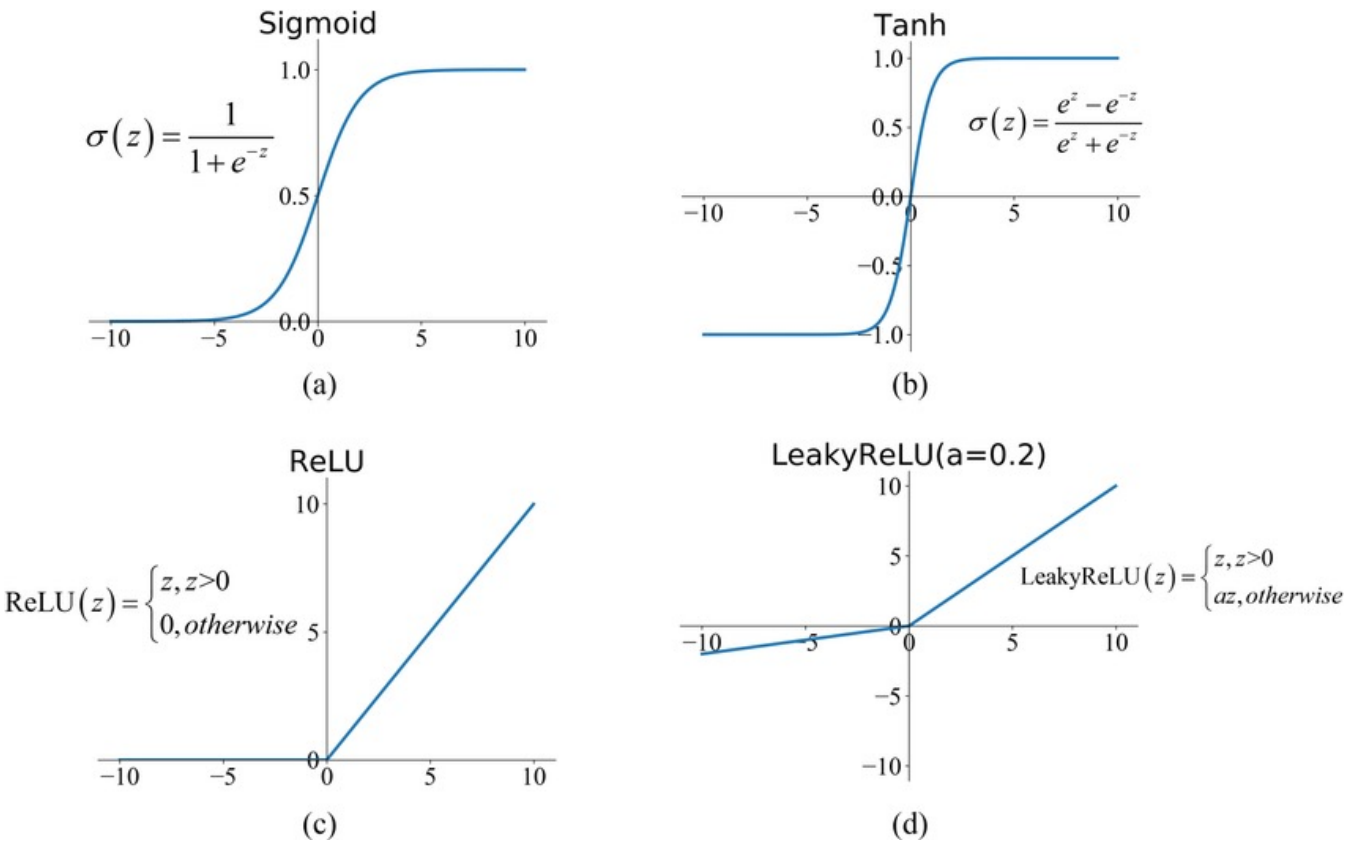
We Use This for the Addition Step

- Add x*w and b (bias)



Activation Functions

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



We Know Enough for a Forward Pass

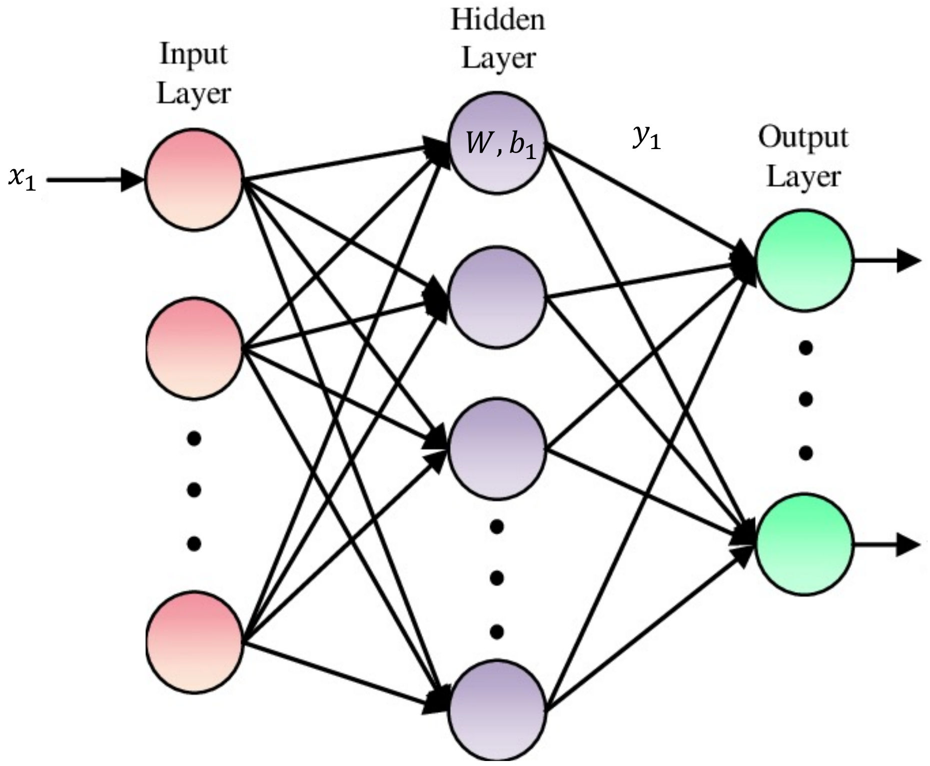
Calculate Output of Each Node Sequentially

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

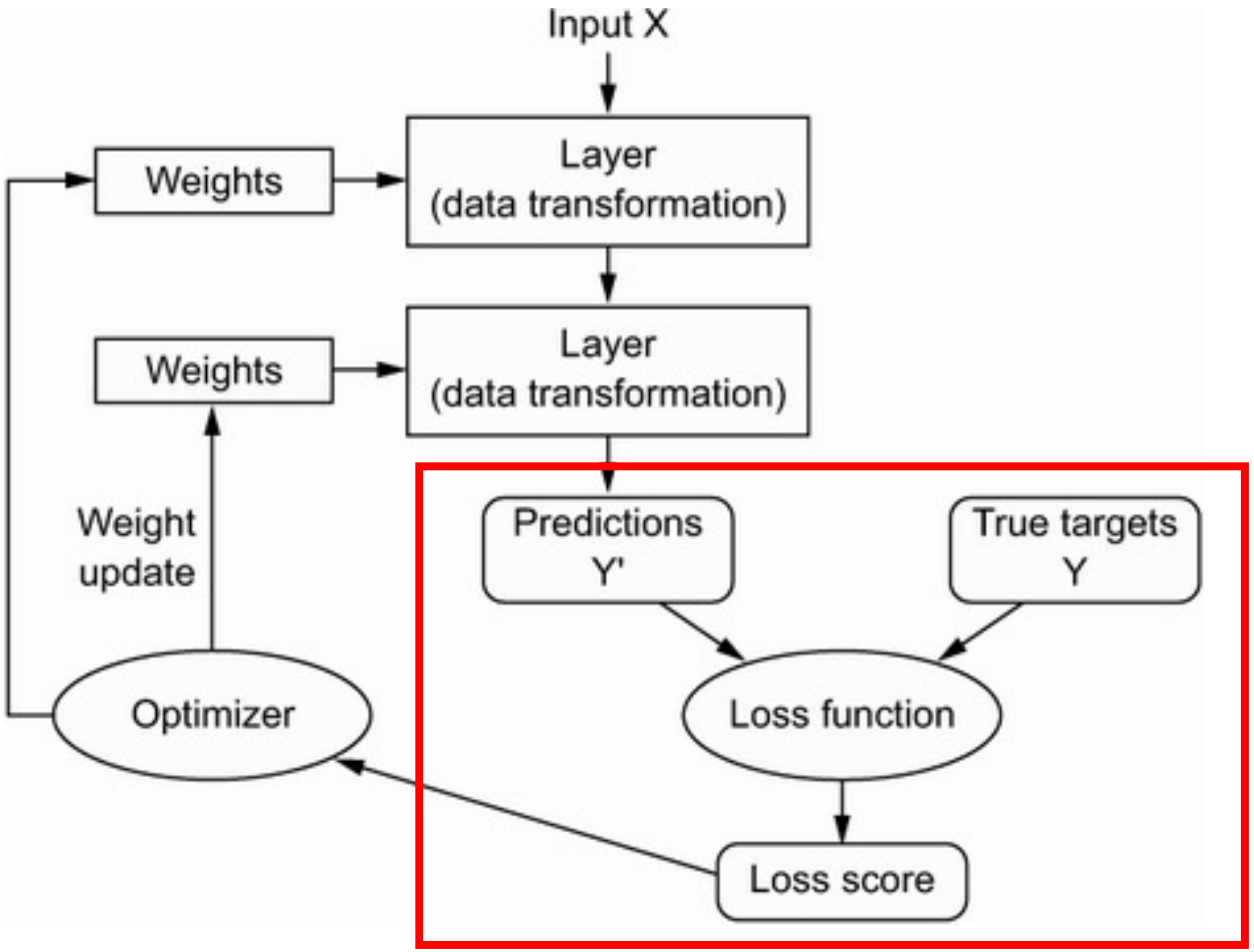
$$y_2 = \varphi\left(x_1 \cdot w_{2,1} + x_2 \cdot w_{2,2} + \cdots + b_2\right)$$

…

Eventually We Obtain Model's Predictions



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 multi-class cross-entropy.

MAE / L1 Loss

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

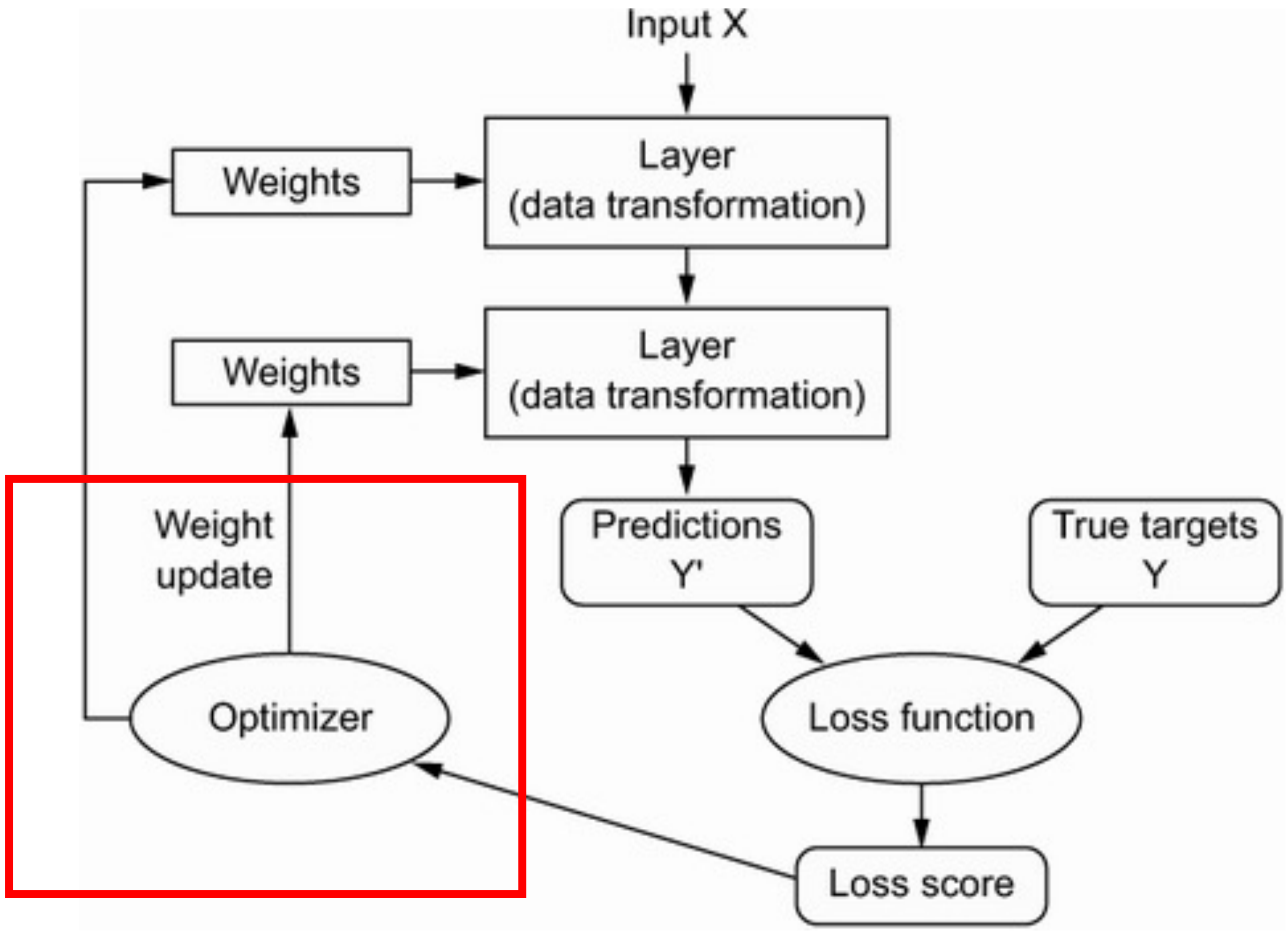
- Typical for continuous outcomes. Errors are penalized homogenously, in magnitude and direction. This should look familiar!

MSE / Quadratic / L2 Loss

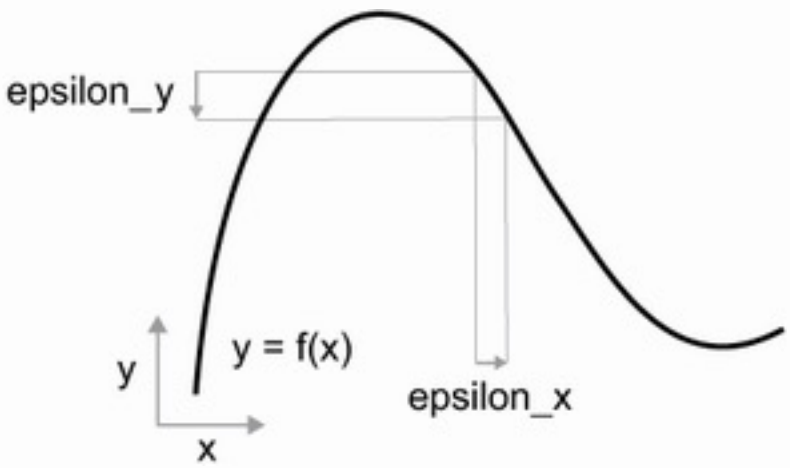
$$MSE = \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}$$

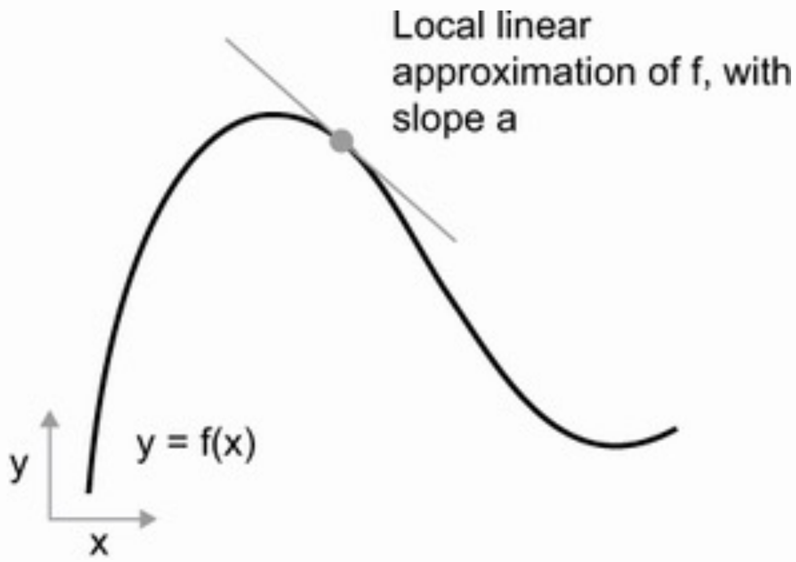
- Typical for continuous outcomes, larger errors penalized exponentially more. This should look familiar!

Backpropagation

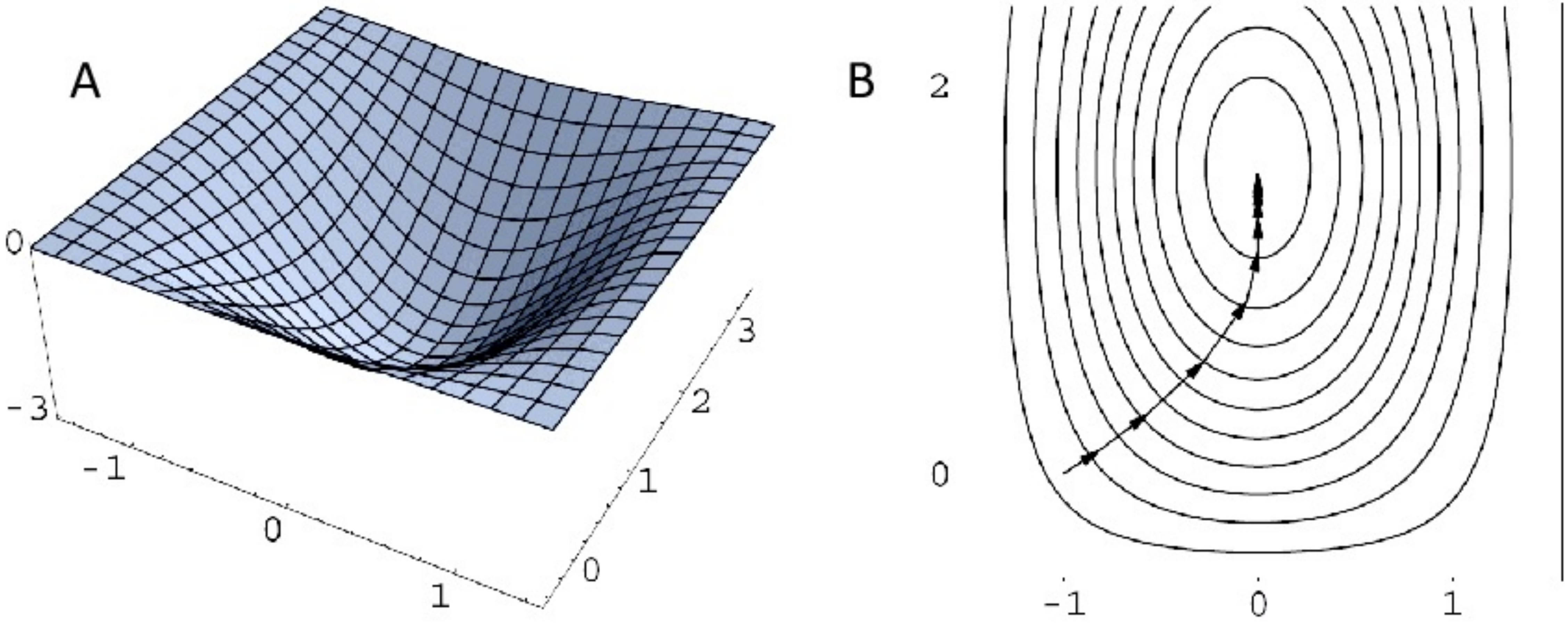


Derivative = “Rate” of Change

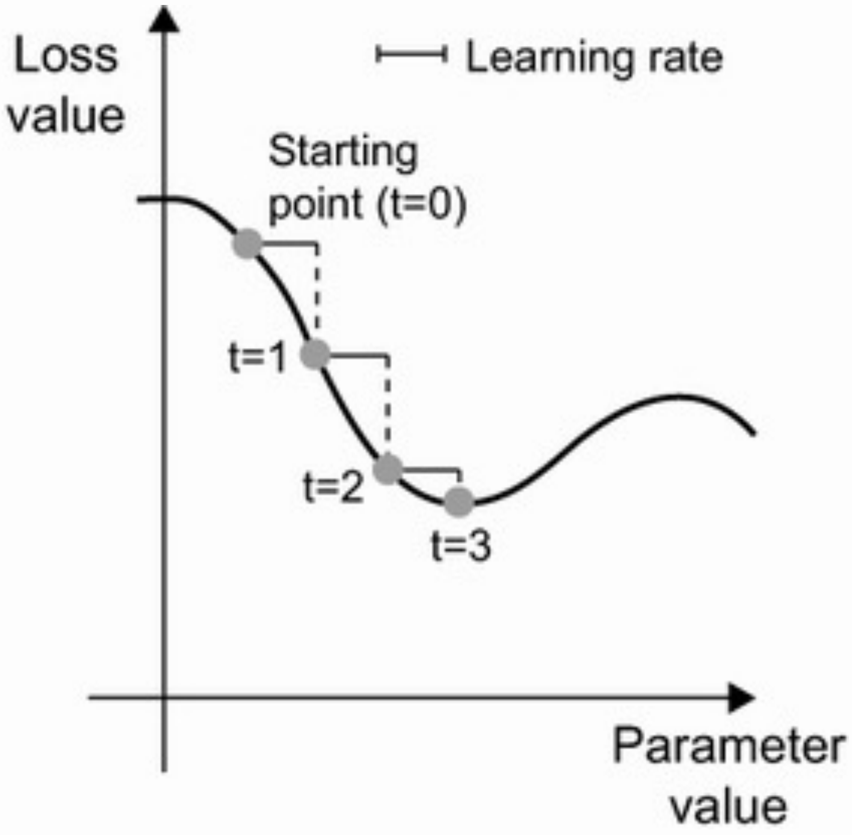




Gradient = Derivative in Multiple Dimensions



Gradient Descent



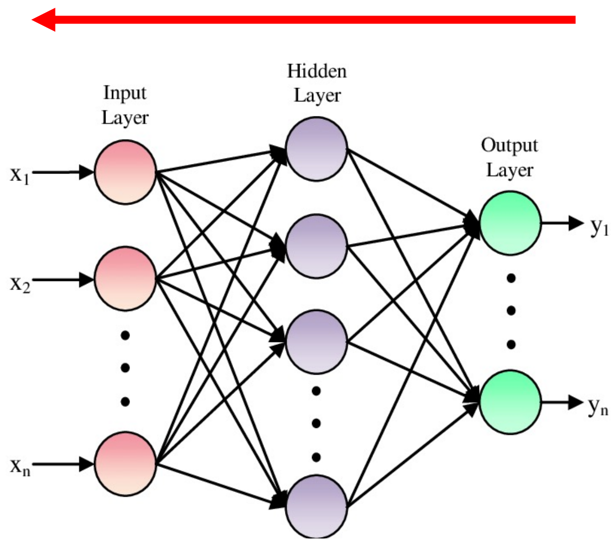
Derivatives of Loss w.r.t All Parameters

Recall that Each Node's Output Can be Expressed as a Function of the Prior Nodes' Outputs

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

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

…

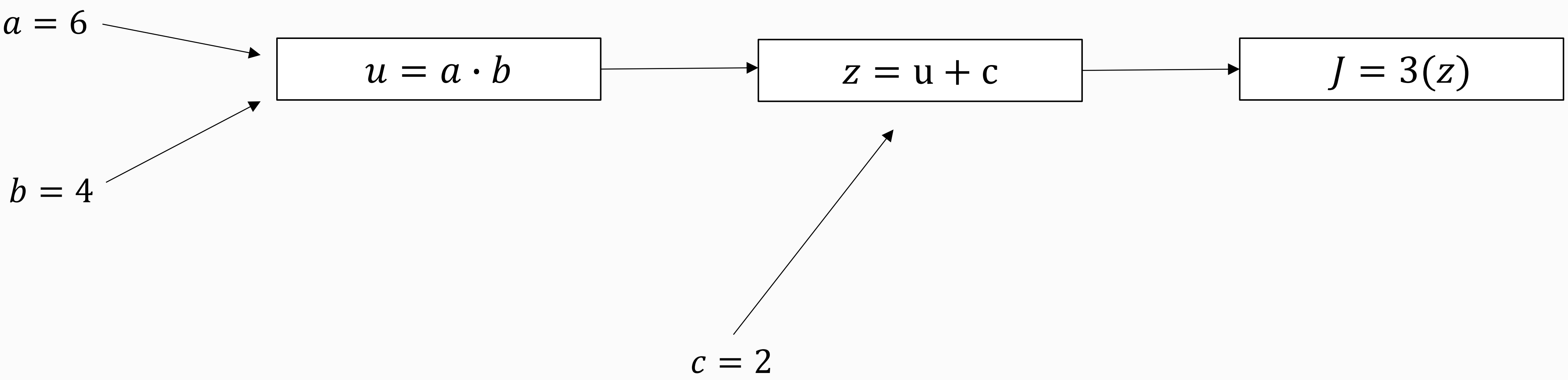


Start at the final nodes in the network and work backwards

- We calculate partial derivatives w.r.t. their inputs / weights.
- Then, use those partial derivatives and work backward into earlier layers to get partial derivatives w.r.t. *their* inputs / weights, and so on.

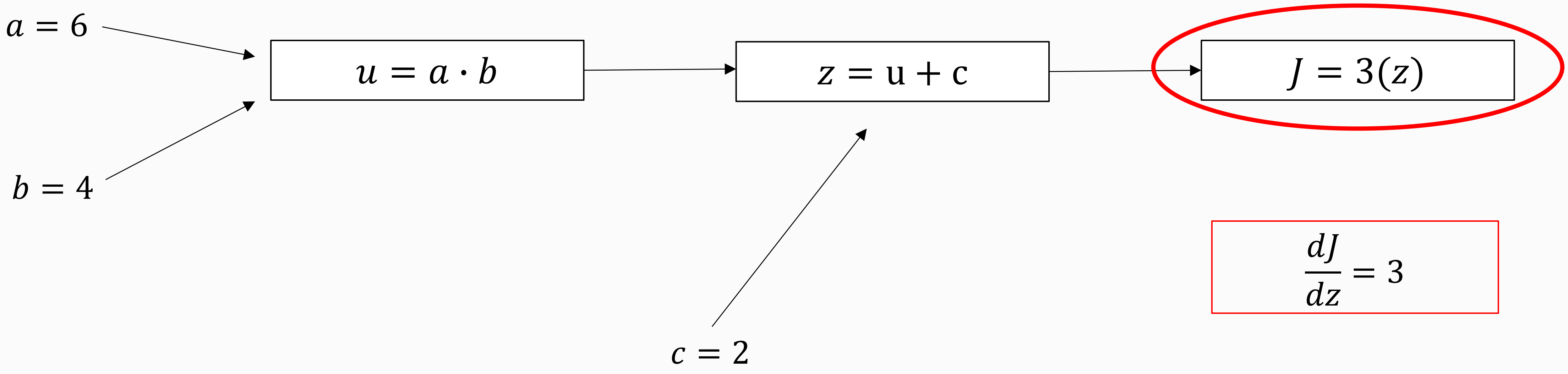
Computation Graphs

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



Backpropagation = Work Backwards

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



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

Backpropagation = Work Backwards

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

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

$$\begin{tikzcd}
a = 6 \arrow[dr] & & & \\
& u = a \cdot b \arrow[r] & z = \mathrm{u} + \mathrm{c} \arrow[r] & J = 3(z) \\
b = 4 \arrow[ur] & c = 2 \arrow[ur] & &
\end{tikzcd}$$

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

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

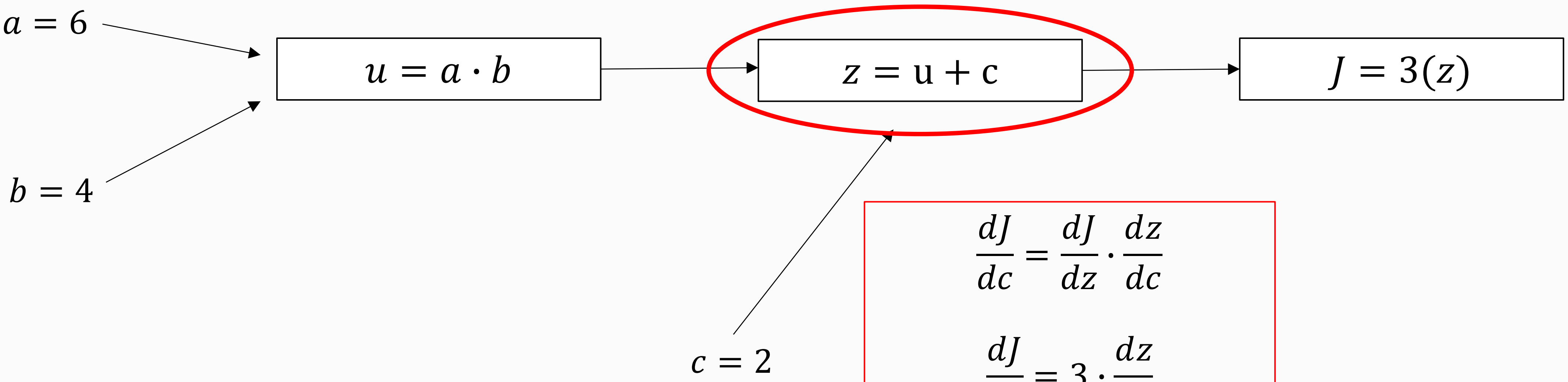
$$\frac{dJ}{du} = 3 \cdot 1 = 3$$

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

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

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

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

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

$a = 6$

$b = 4$

$u = a \cdot b$

$z = \mathrm{u} + \mathrm{c}$

$J = 3(z)$

$c = 2$

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

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

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

Backpropagation = Work Backwards

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

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

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

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

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

$a = 6$

$b = 4$

$c = 2$

$$\boxed{u = a \cdot b} \rightarrow \boxed{z = \mathrm{u} + \mathrm{c}} \rightarrow \boxed{J = 3(z)}$$

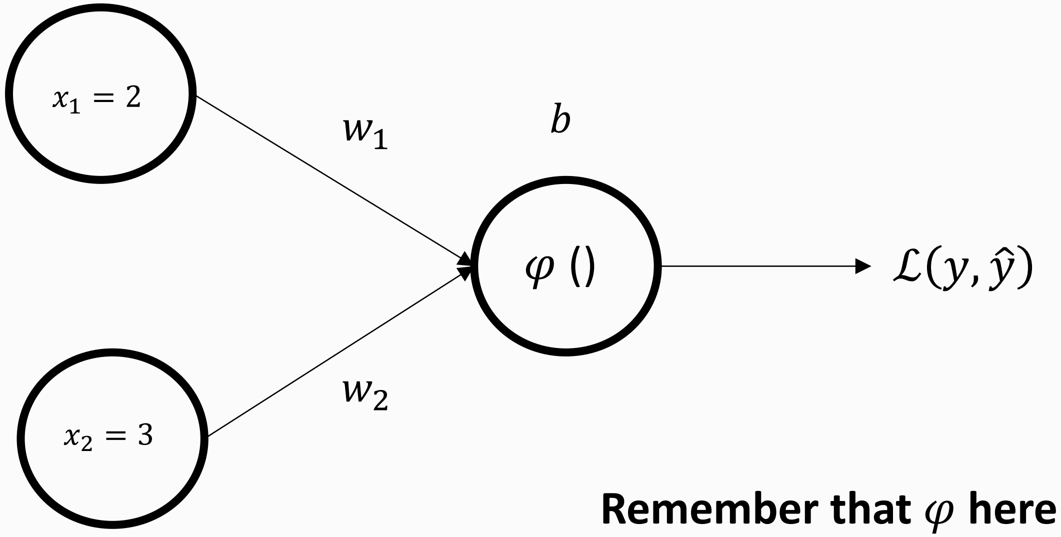
$$\frac{dJ}{db} = \frac{dJ}{du} \cdot \frac{du}{db}$$

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

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

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)



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

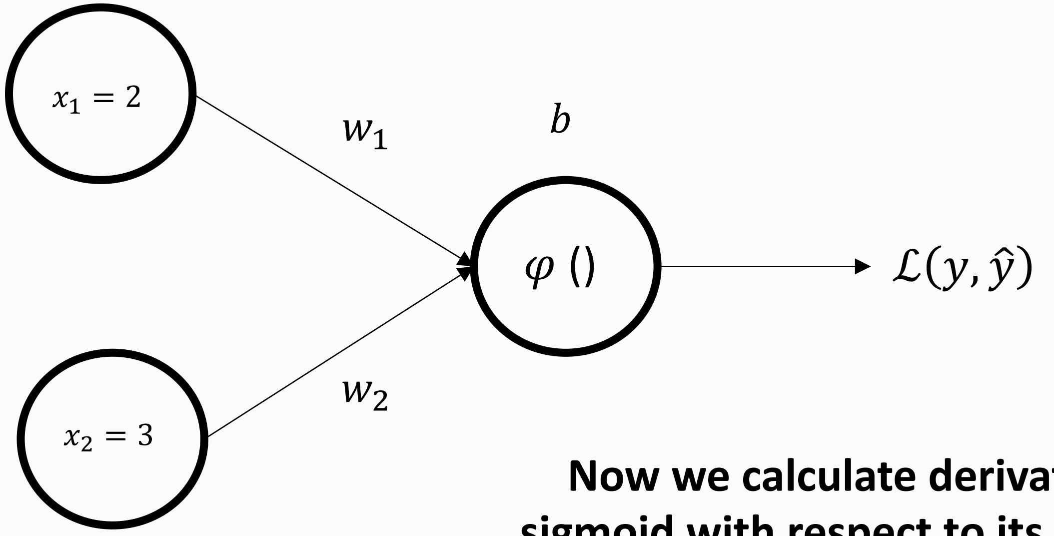
$$\frac{d\mathcal{L}}{d\varphi} = \frac{\varphi(1-y) - y(1-\varphi)}{\varphi(1-\varphi)}$$

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

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

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.

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



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

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

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

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

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

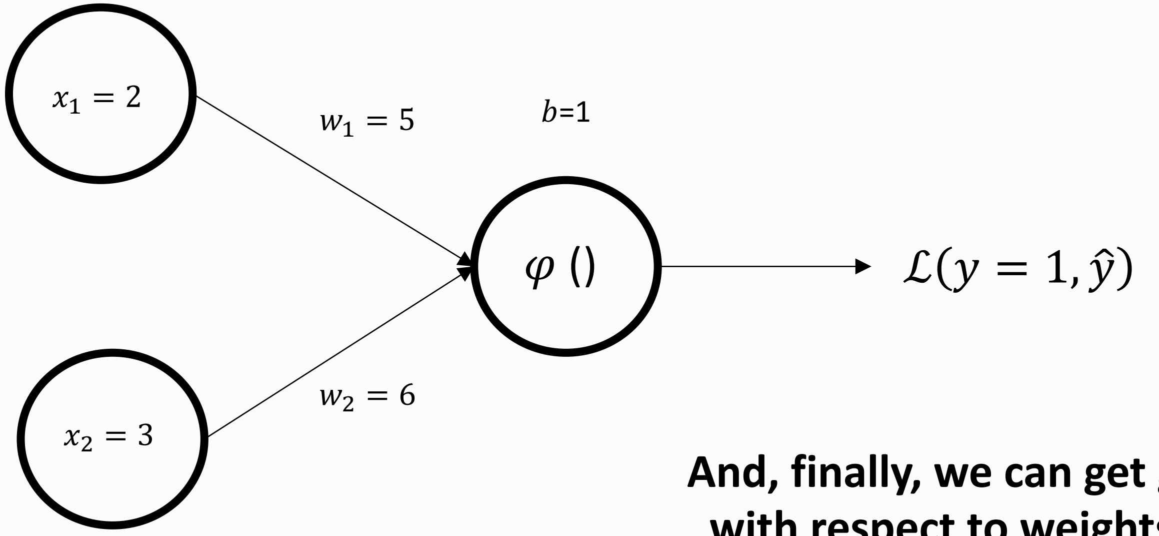
$$\frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{d\varphi} \cdot \frac{d\varphi}{dz}$$

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

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

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

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



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

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

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

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…

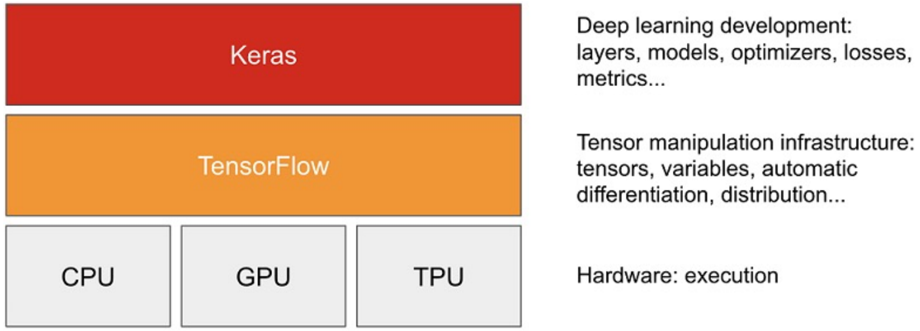
Keras and Tensorflow

1. Tensorflow

- A Python platform for working with tensors, implementing automatic differentiation, providing access to repositories of (well-known) pre-trained models.

2. Keras

- A higher-level API that wraps common usage patterns with Tensorflow functions, pre-defined loss functions, optimization algorithms, etc.
- Keras simplifies data scientists' interaction with Tensorflow.



Tensorflow GradientTape

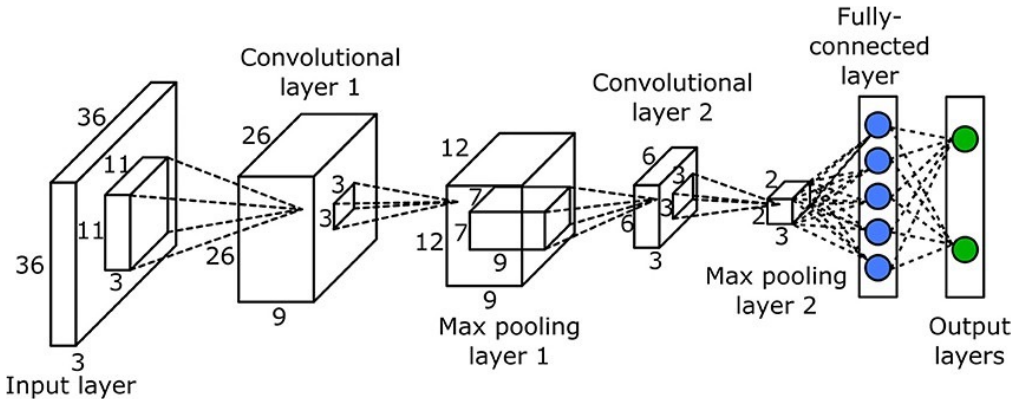
1. Gradient Tape

- 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.

The Layer

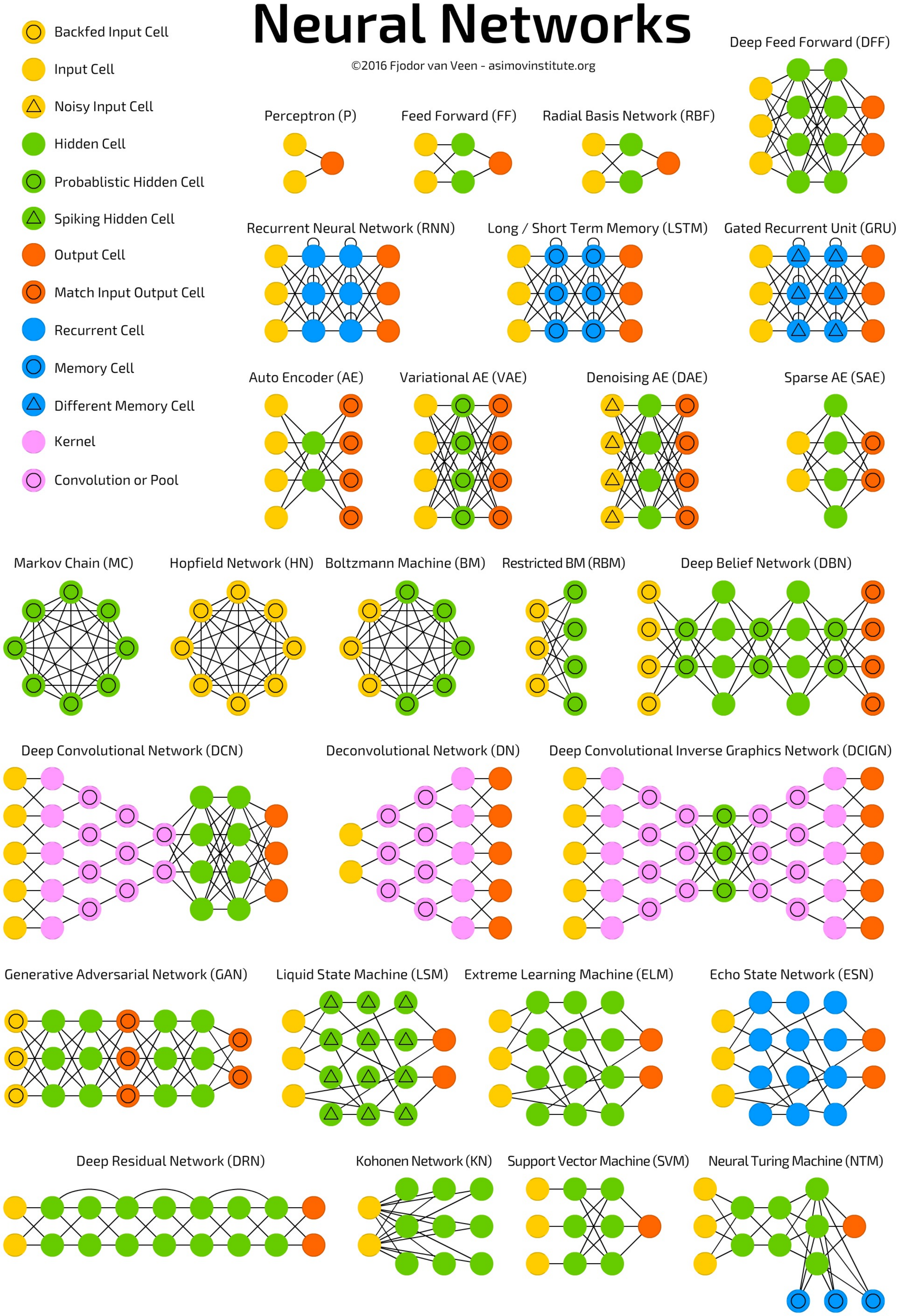
Layers are the Key Building Block of NNs in Keras

- There are a few subclasses of the Layers class: e.g., Dense is the one we have seen so far – layers.Dense(), but we also have convolutional layers, max-pooling layers, recurrent layers, and so on. There are many pre-defined layers in Keras. See: https://keras.io/api/layers/.
- These are different architectural components that can be mixed and matched in different ways to create different network topologies.
- It is also possible to construct custom layers.



A mostly complete chart of

Neural Networks



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.