Intro to Neural Nets

Week 2: Mathematical Building Blocks & Working with Keras API

Today’s Agenda

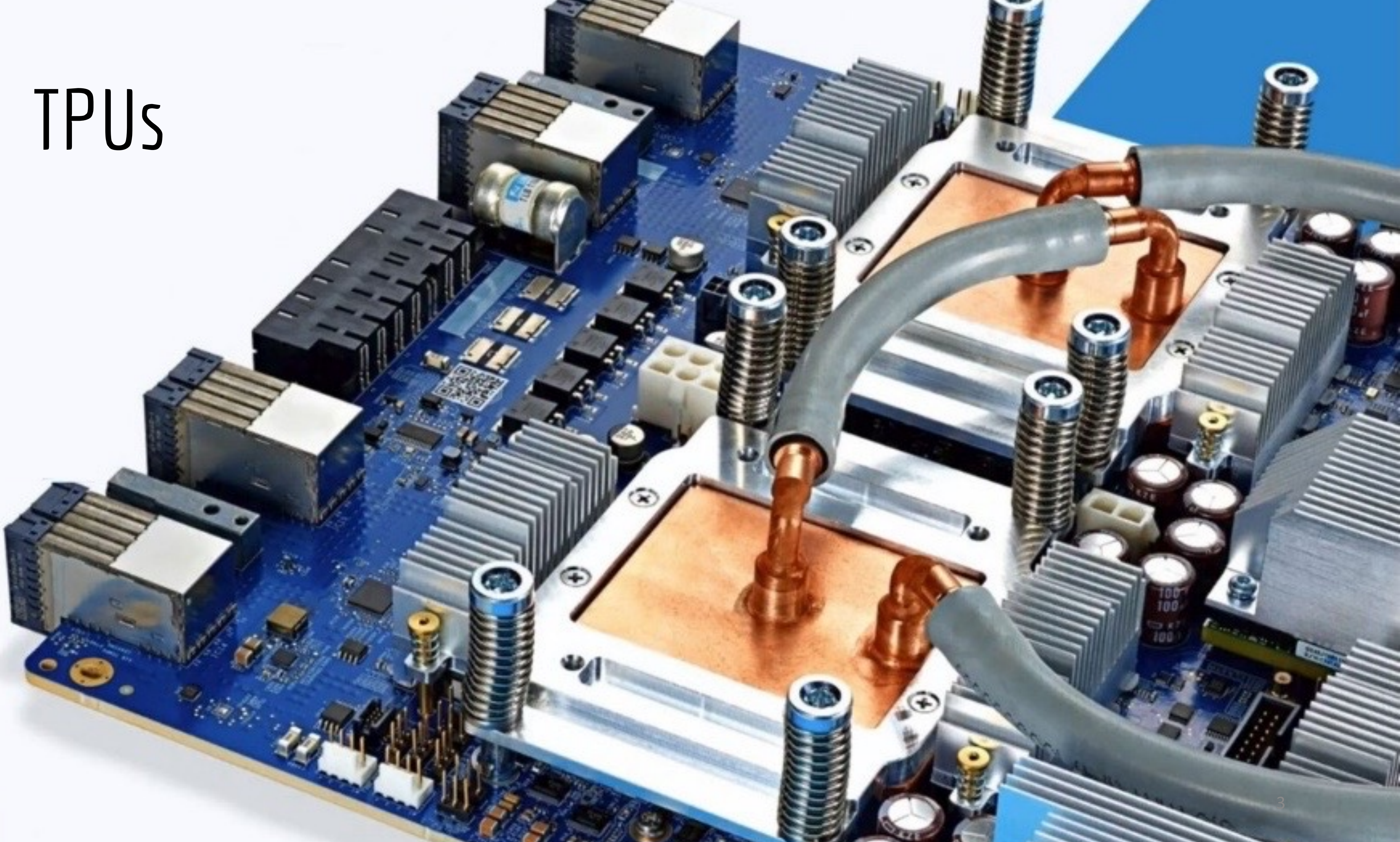
1. Building Blocks of NNs

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

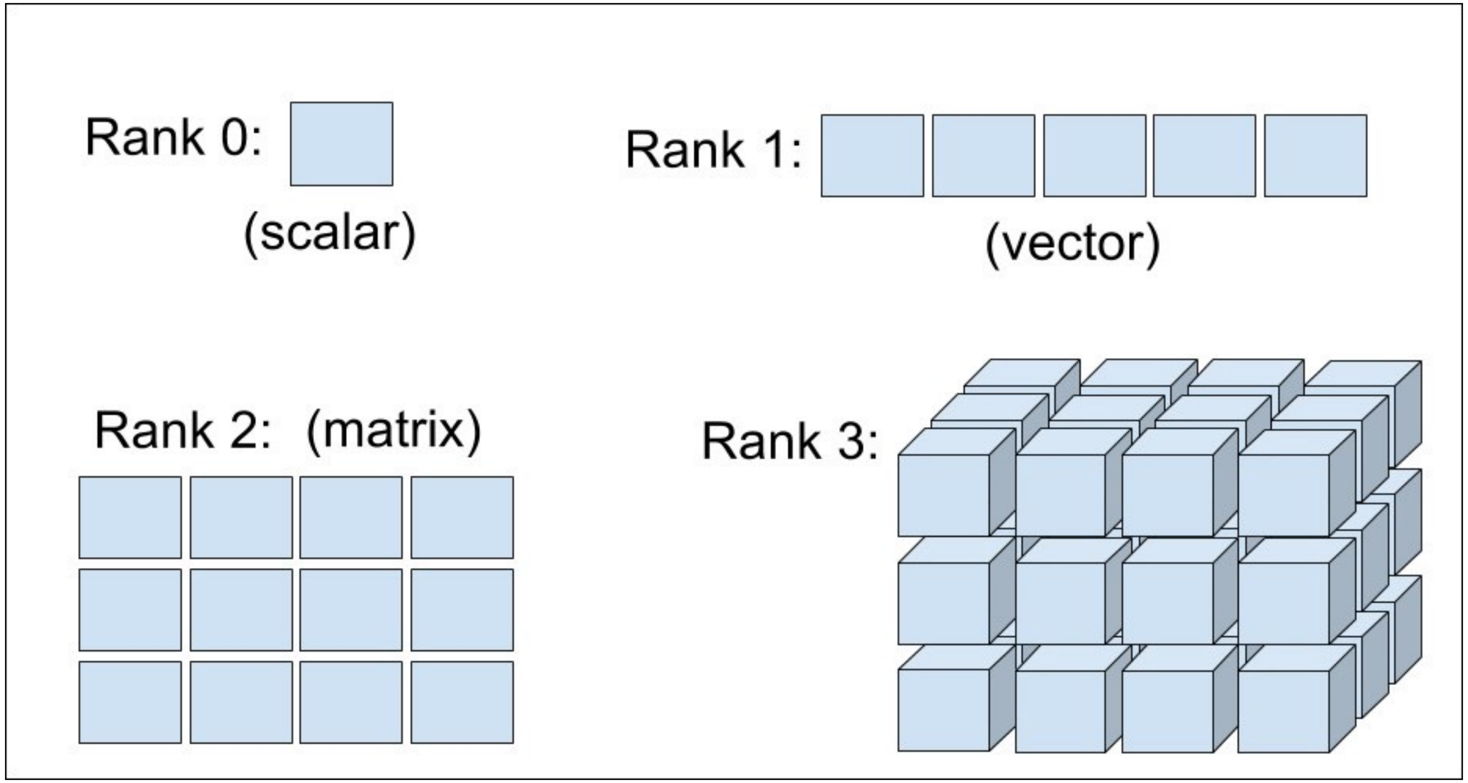
2. Building a Linear Classifier

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

TPUs

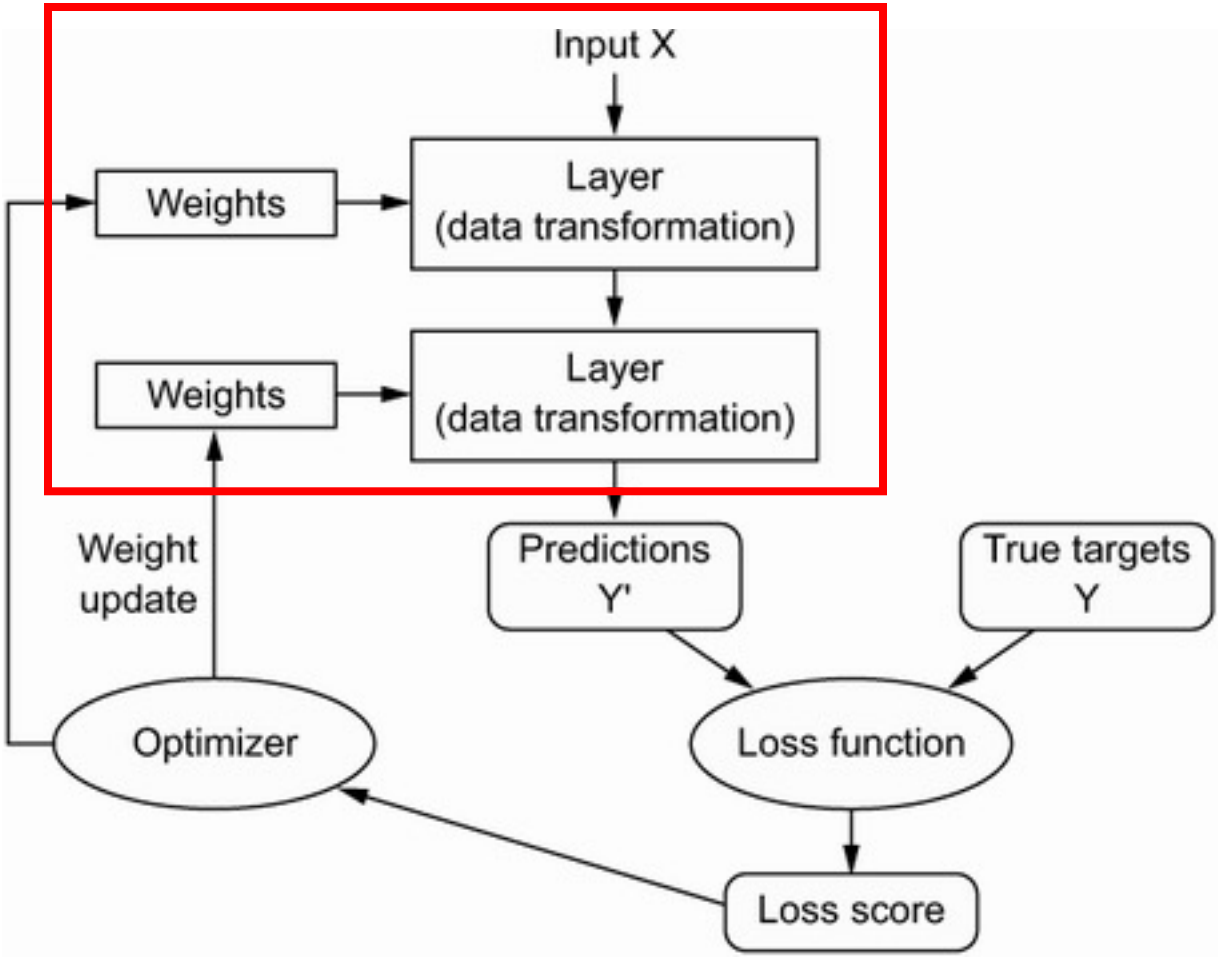


Tensors

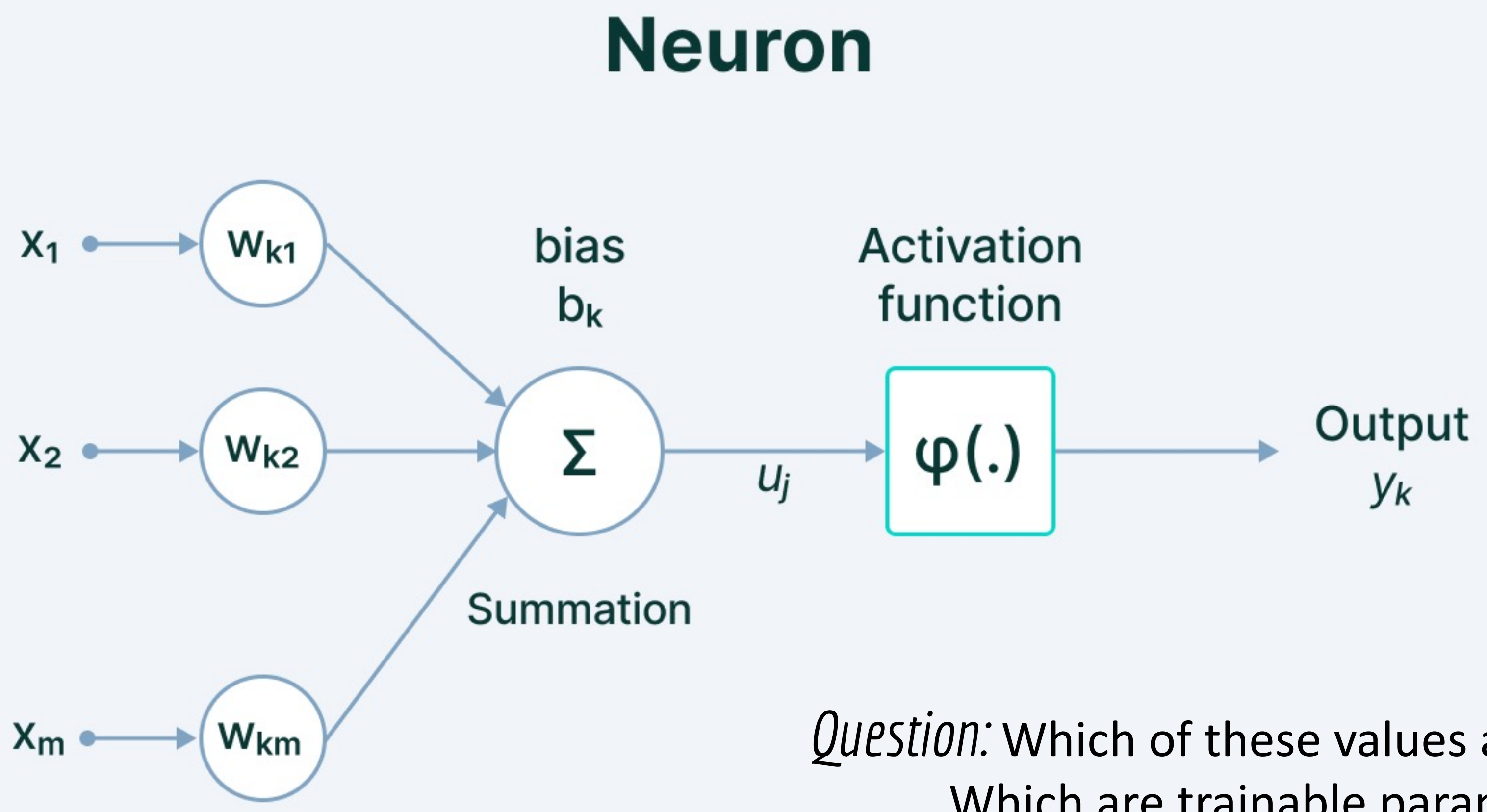


Question: What sort of data (give an example) would be stored in a rank-3 tensor? How about a rank-4 tensor?

Forward Pass

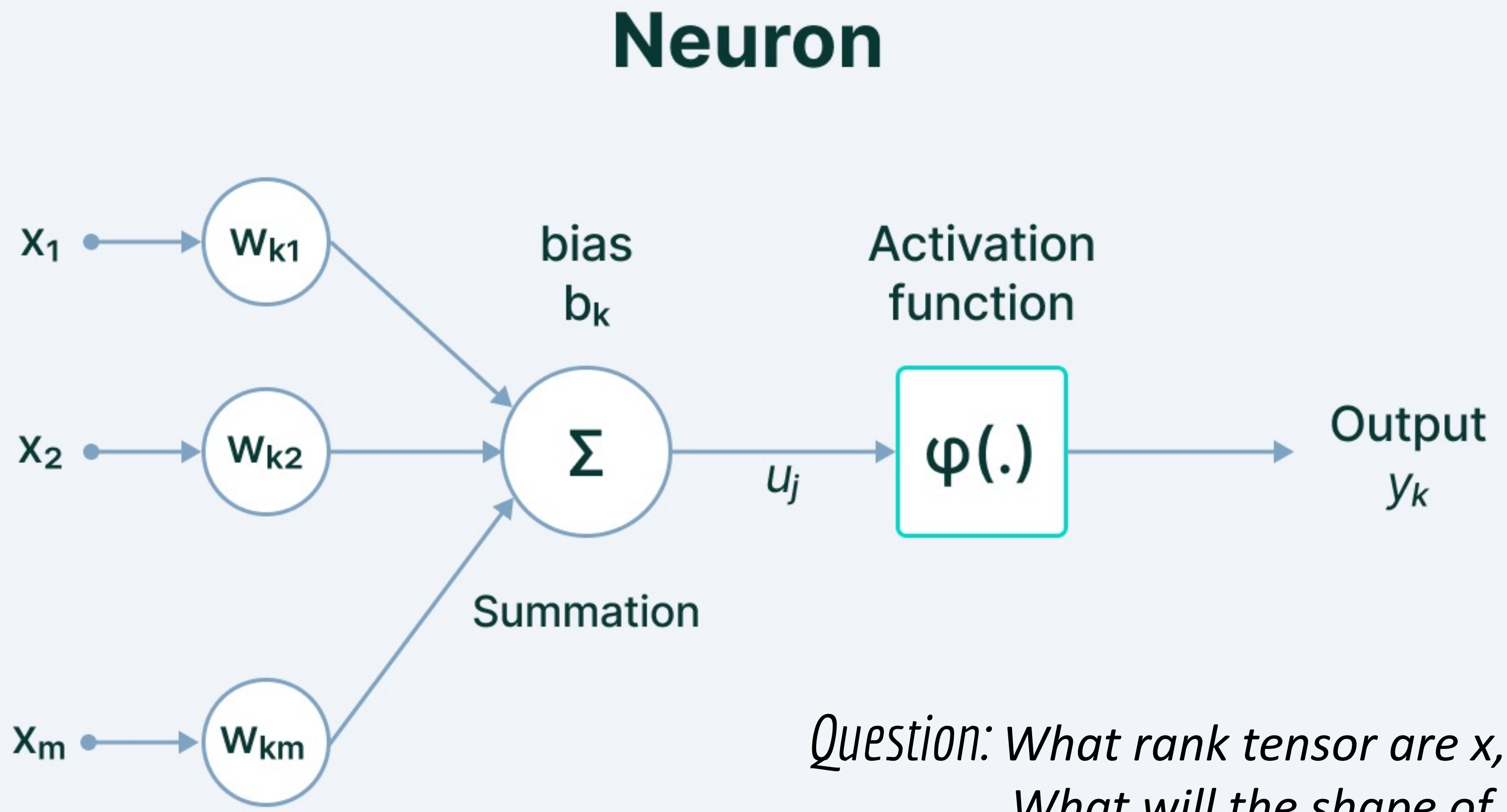


Neuron / Network Components



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

Neuron / Network Components



Question: What rank tensor are x, w and b here?
What will the shape of y be?
What is the order of operations in a forward pass?

Multiplication

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

Conformity of Shapes

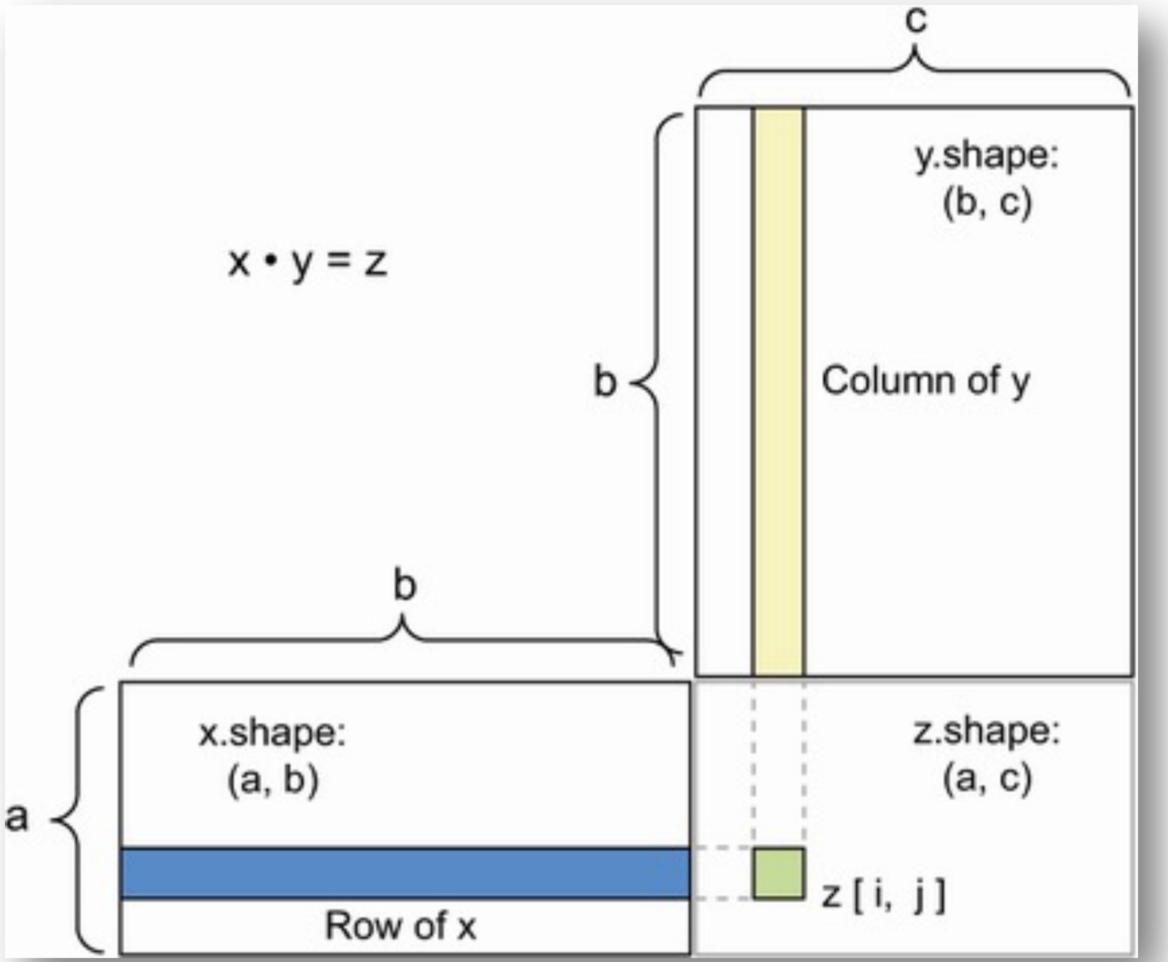
- NCOL(X) == NROW(W)

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.



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

Matrix Addition (Broadcast)

Shape of the Two Tensors Needs to Conform

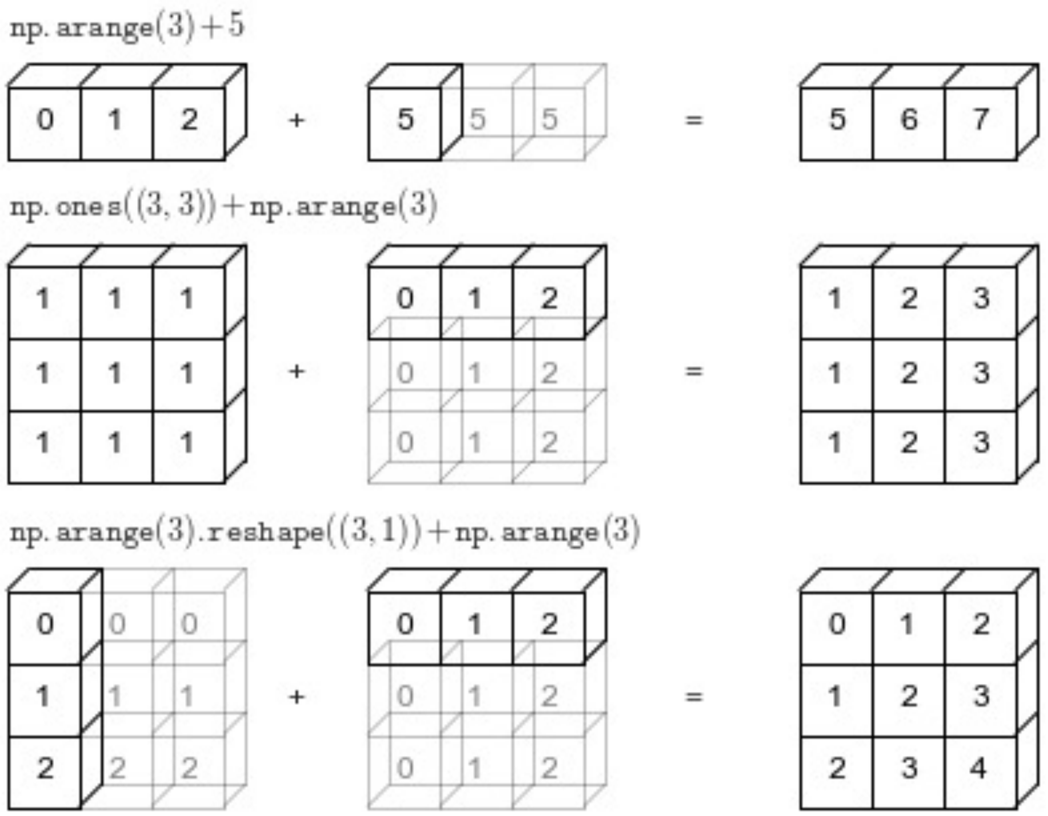
- A + B will only work if A is cleanly divisible by B (or vice versa)

Sum Element-wise

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

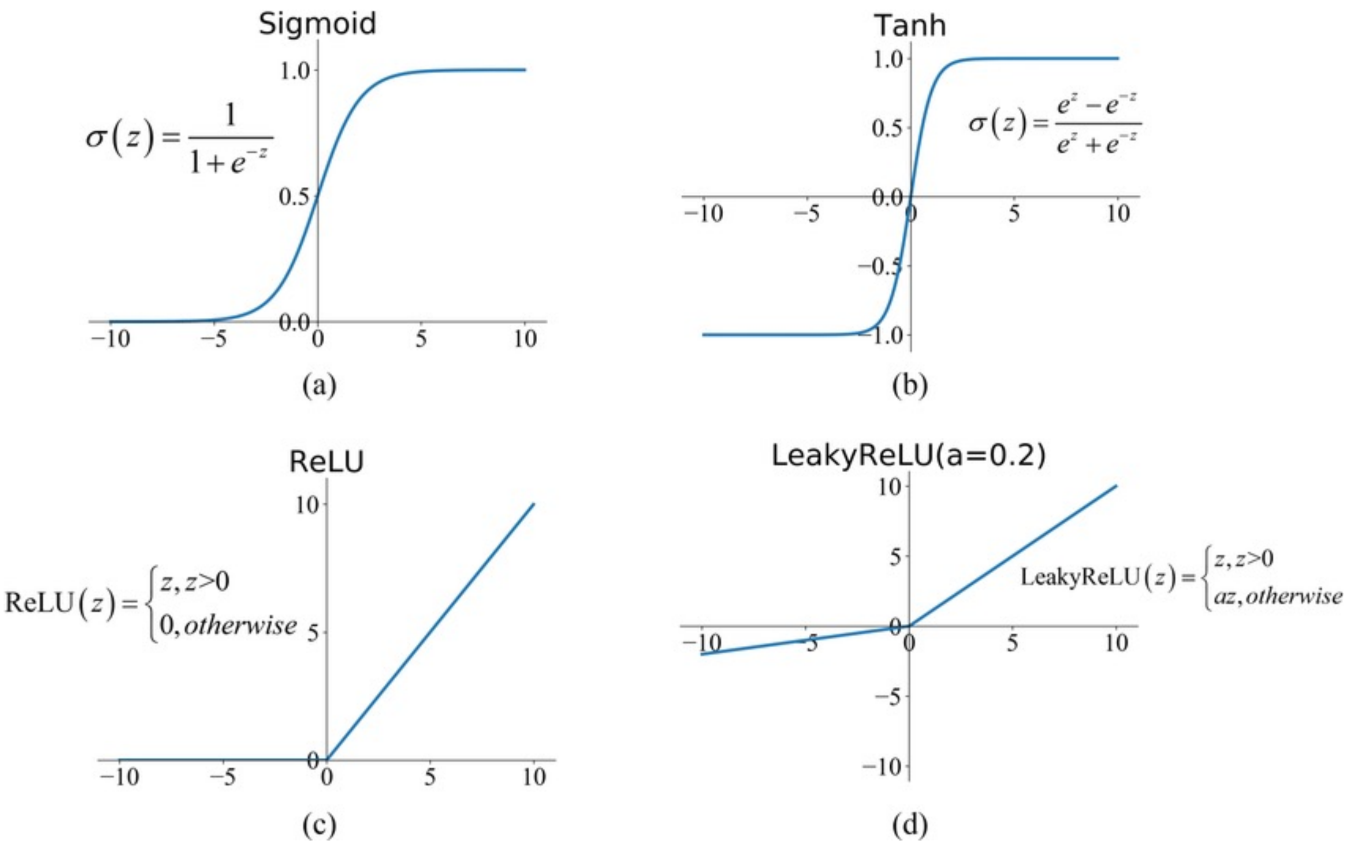
We Use This for the Addition Step

- Add x*w and b (bias)



Activation Functions

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



Multi-Class, Single-Label

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

Softmax (MLOGIT):

We have D inputs (x's).
We have k outputs (classes).

So, W is a (D,k) matrix and X is a (D,1) matrix.

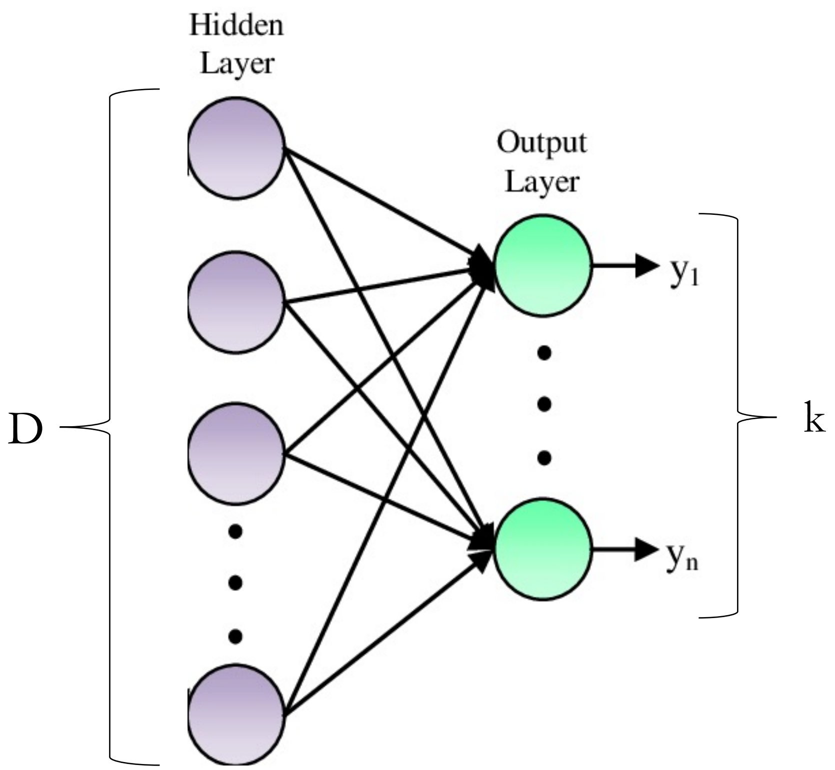
That means, A is a (k,1) matrix.

That means Y is also a (k,1) matrix.

$$A = W^T X,$$

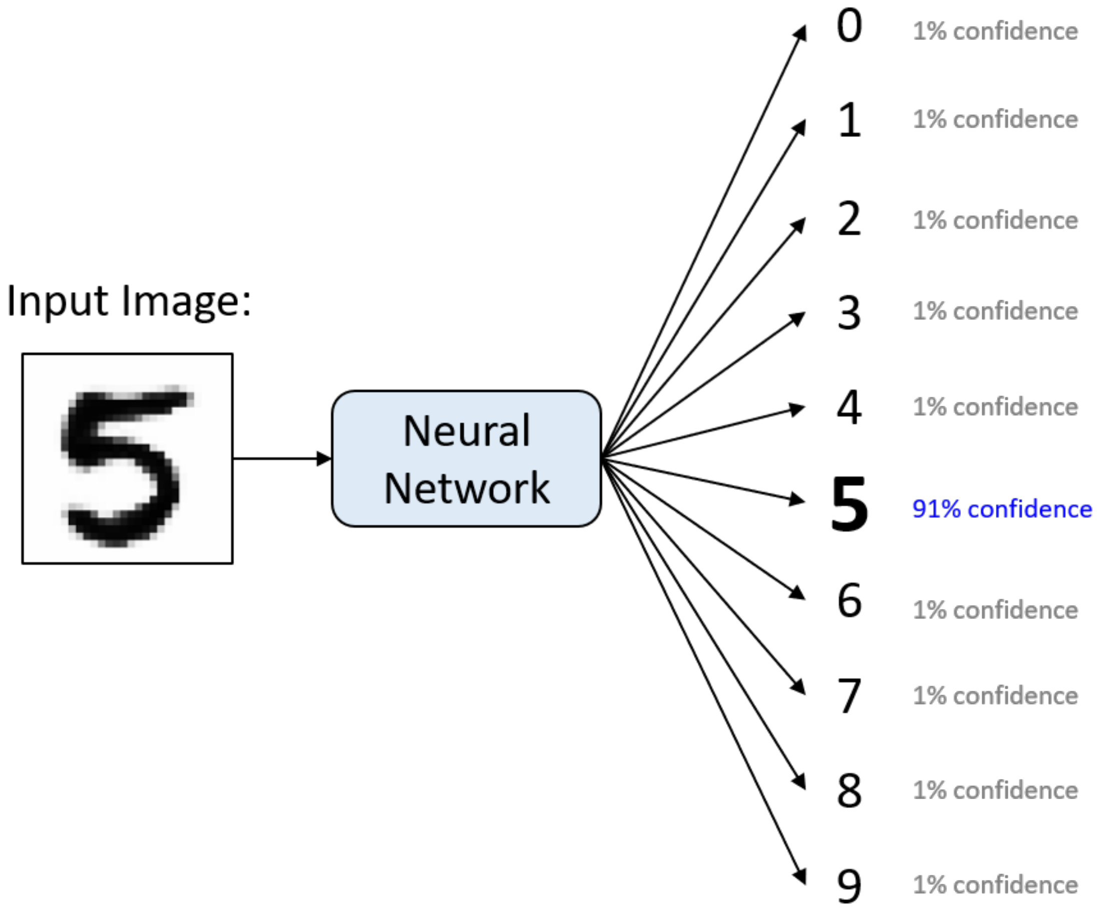
$$Y = \text{softmax}(A),$$

$$Y_i = \frac{e^{A_i}}{\sum_{j=1}^{k} e^{A_j}}.$$



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

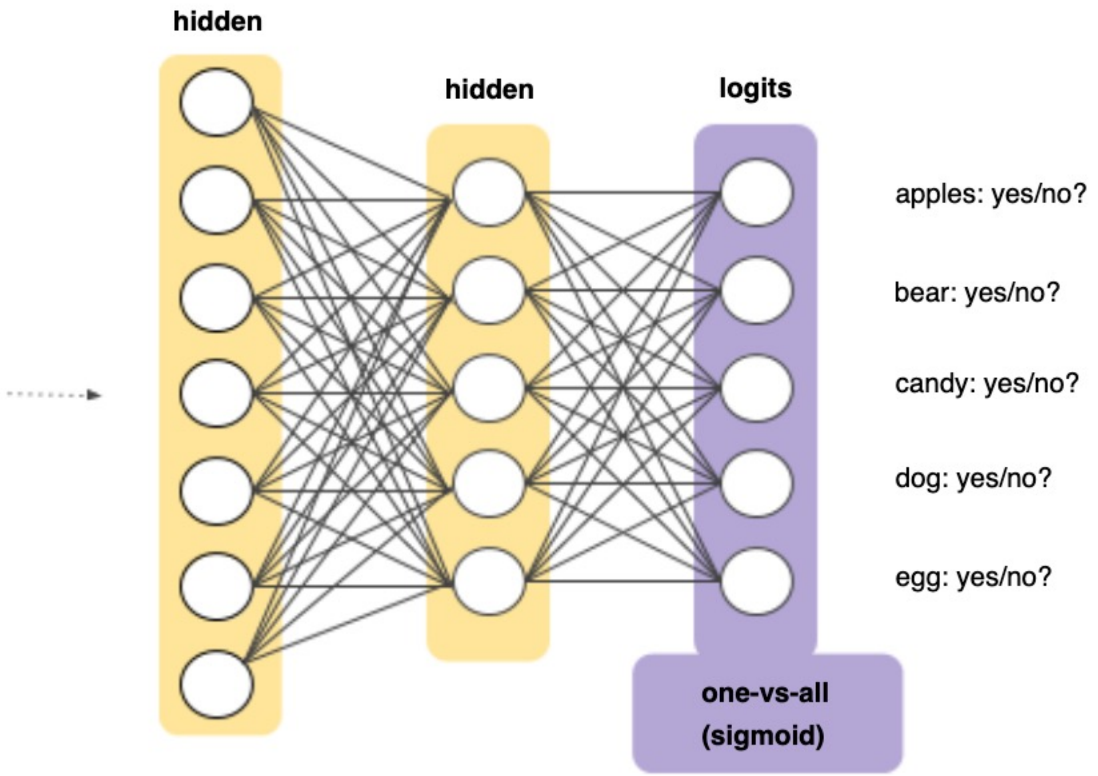
Multi-Class, Single-Label



Multi-Class, Multi-Label

Many Non-Exclusive Labels

- We would create a sigmoid output layer with one output for each class we are predicting.
- Train on all labels together.



We Know Enough for a Forward Pass

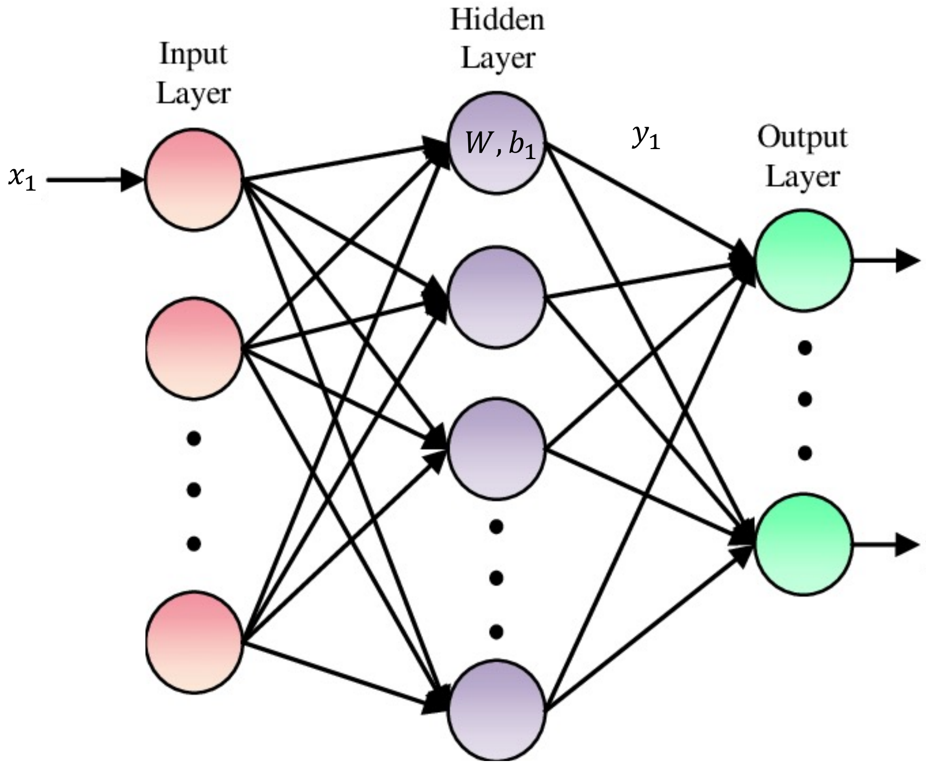
Calculate Output of Each Node Sequentially

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

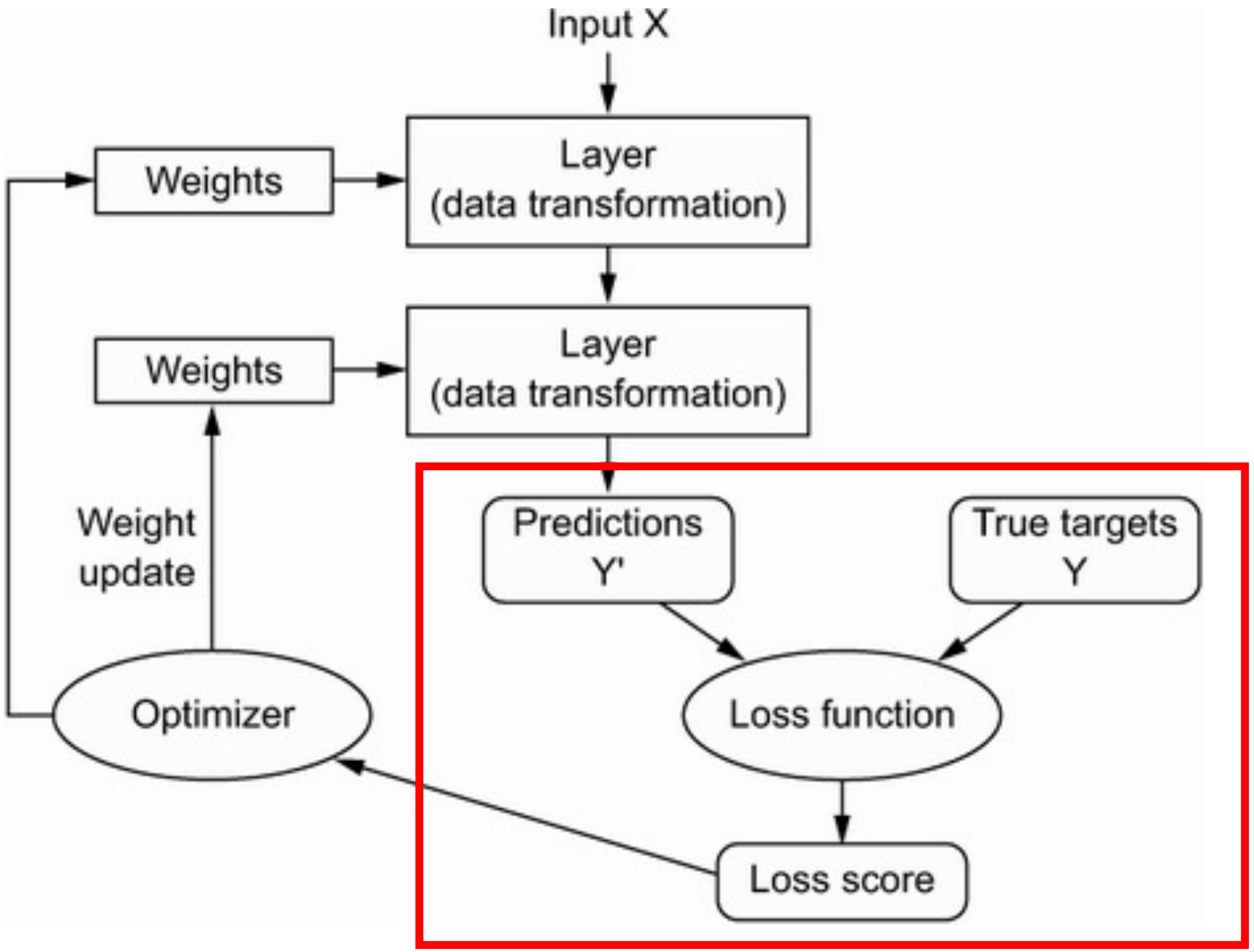
$$y_2 = \varphi\left(x_1 \cdot w_{2,1} + x_2 \cdot w_{2,2} + \cdots + b_2\right)$$

…

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 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

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

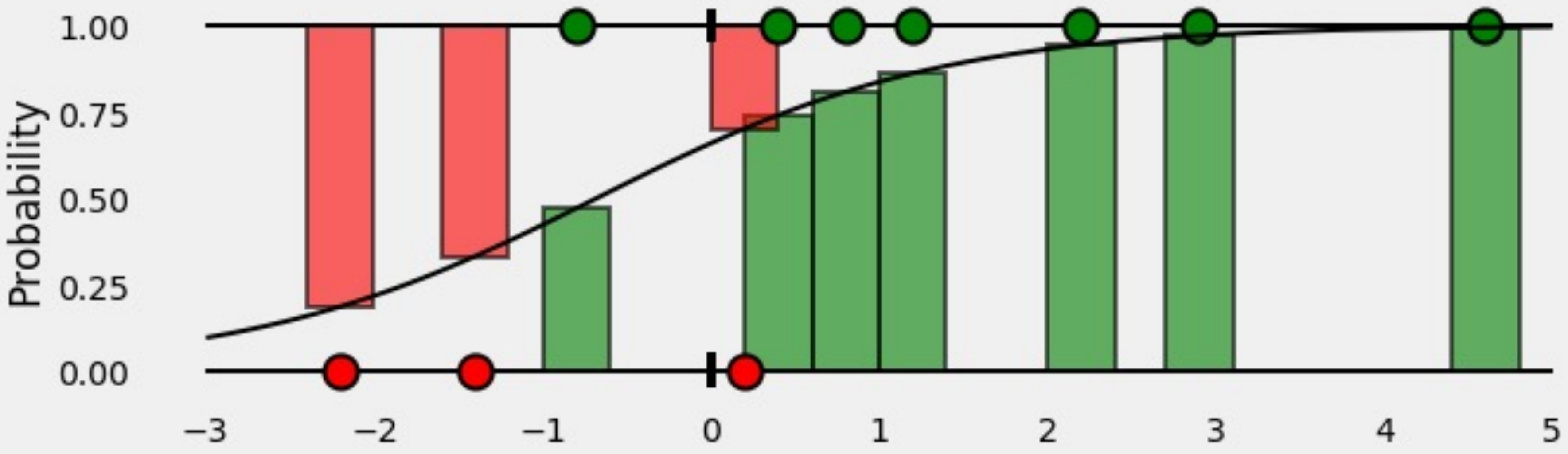
- Typical for continuous outcomes, larger errors penalized exponentially more. This should look familiar!

Binary Cross-Entropy Loss

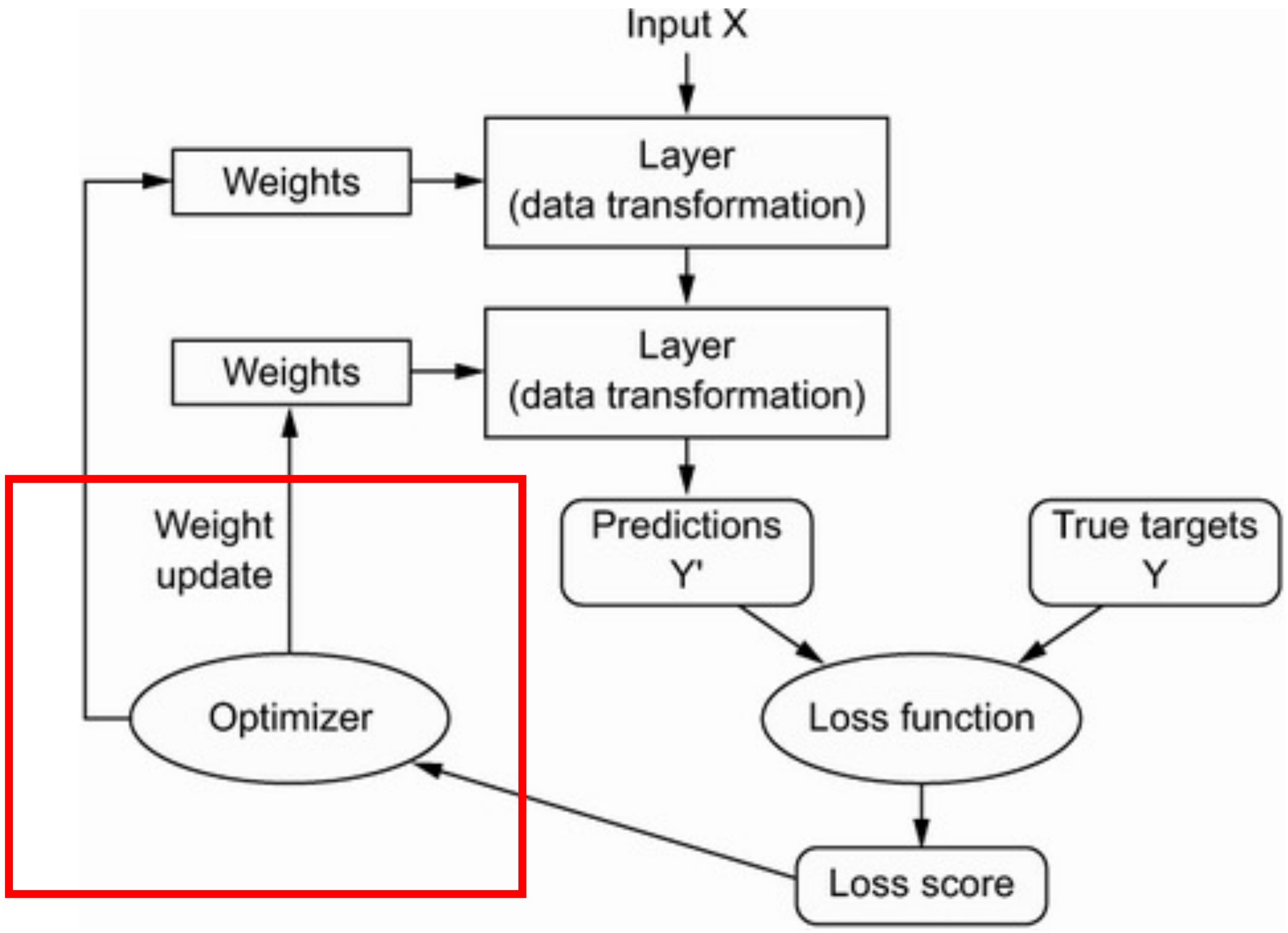
$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1-y_i) \cdot log(1-p(y_i))$$

Piecemeal Function:

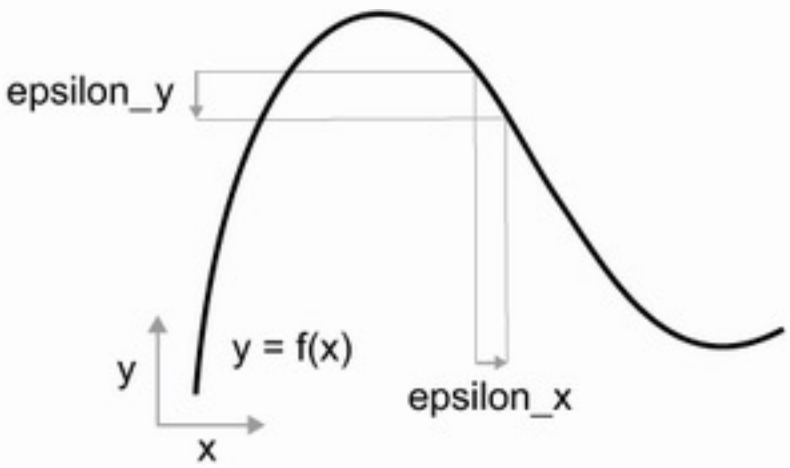
- If ground truth is 1, then loss is -1*log(*p*). As prediction approaches 1, loss approaches 0. As prediction approaches 0, loss grows exponentially.
- If ground truth is 0, then loss is -1*log(1-*p*). As prediction approaches 1, loss rises exponentially. As prediction approaches 0, loss approaches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

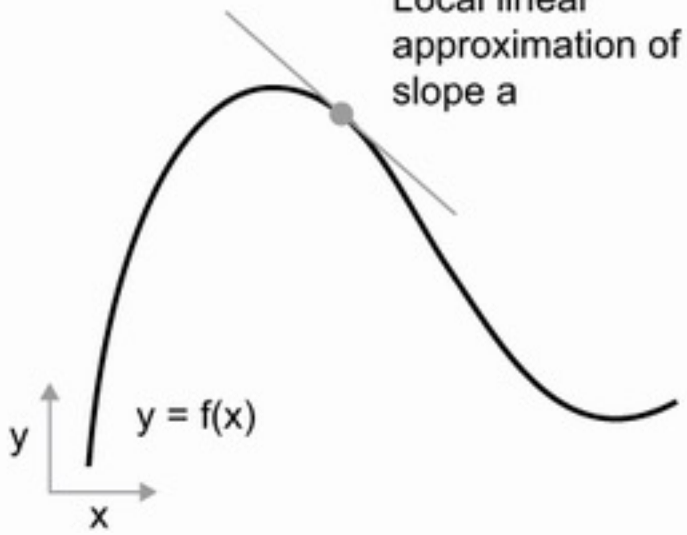


Backpropagation

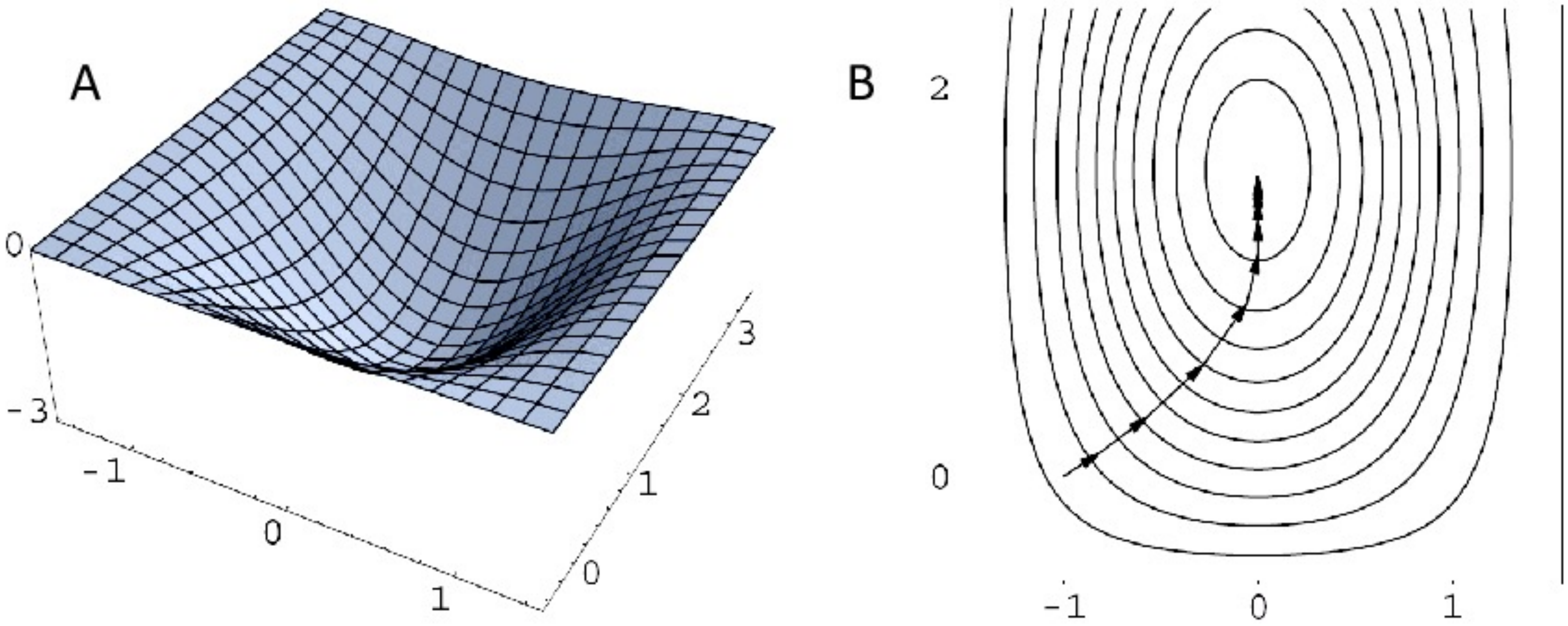


Derivative = “Rate” of Change

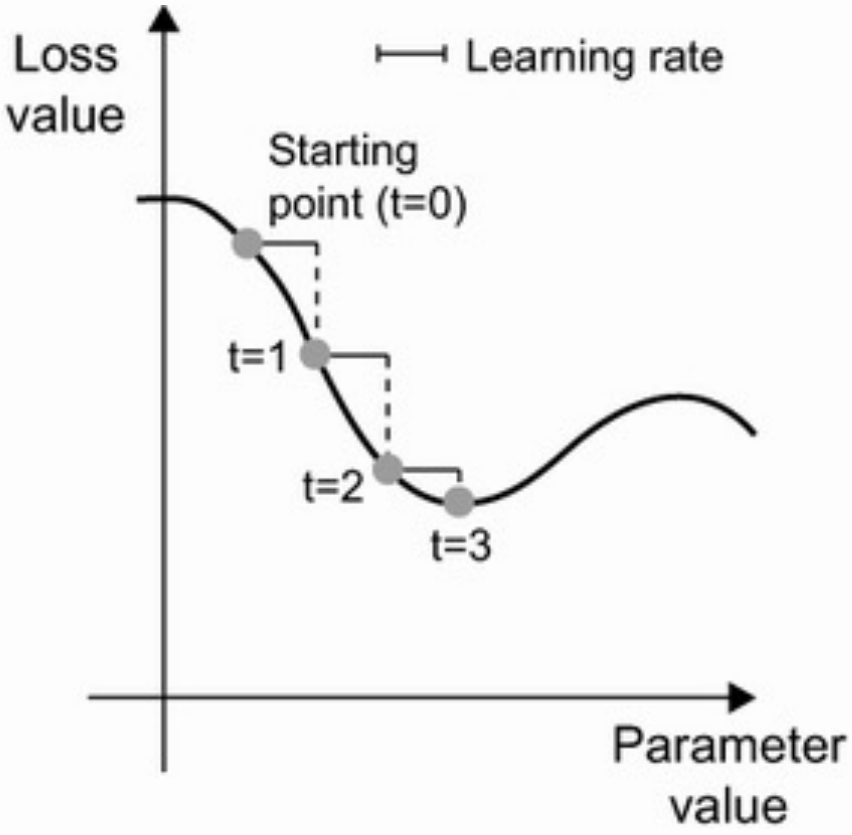




Gradient = Derivative in Multiple Dimensions



Gradient Descent



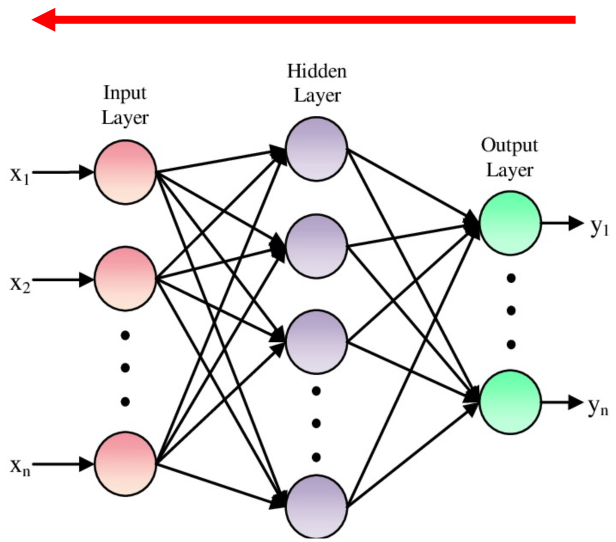
Derivatives of Loss w.r.t All Parameters

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

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

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

…

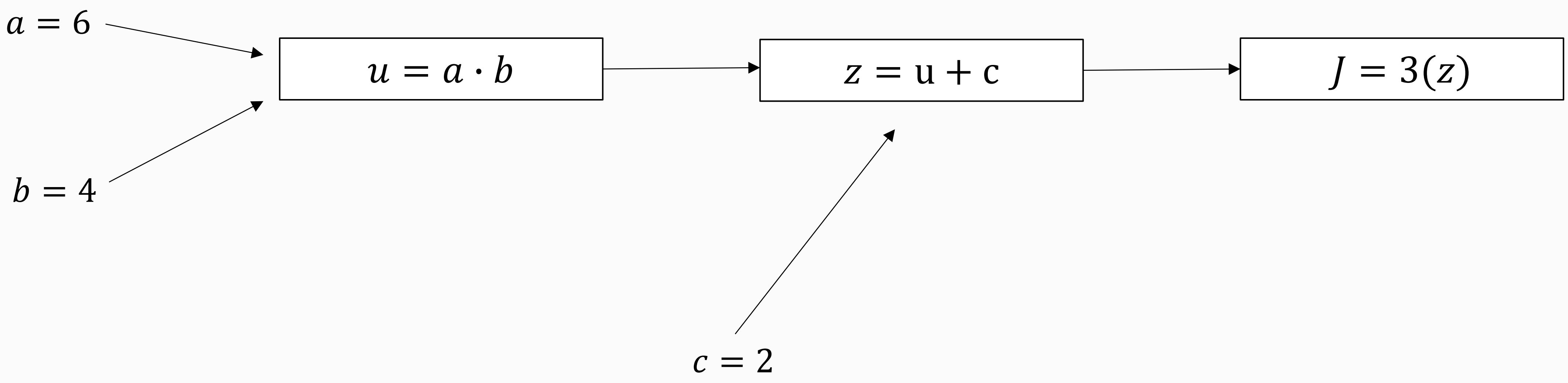


Start at the final nodes in the network and work backwards

- 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.

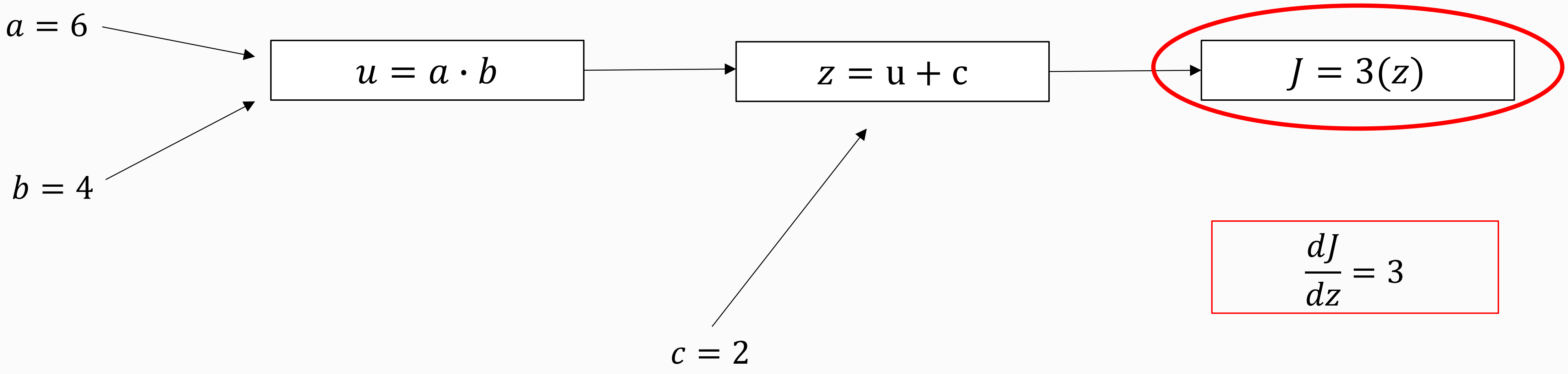
Simplifying Gradients: Computation Graph

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



Backpropagation = Working Backwards

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



Backpropagation = Work Backwards

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

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

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

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

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

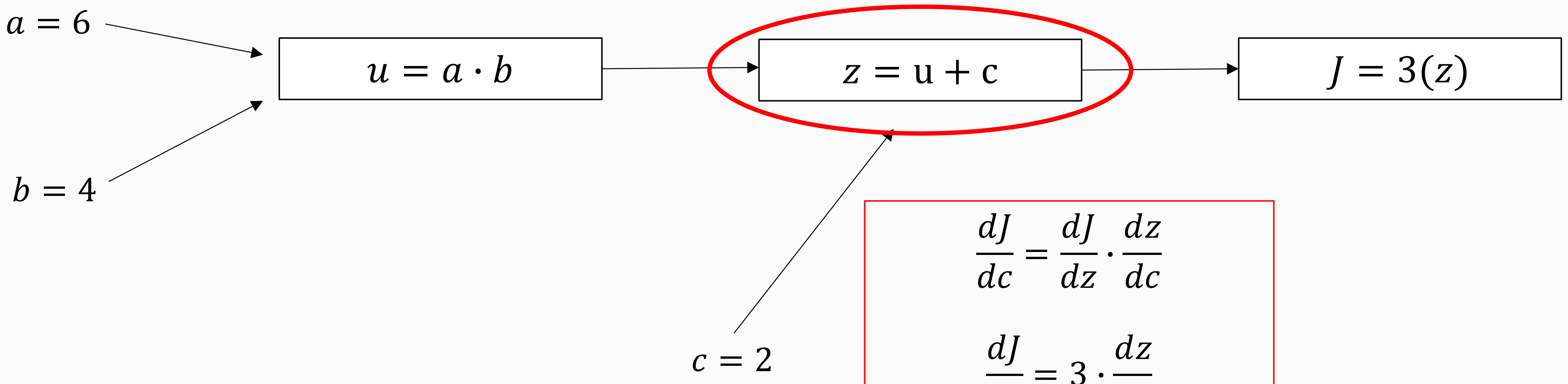
$$\frac{dJ}{du} = 3 \cdot 1 = 3$$

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

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

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

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

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

$$\begin{array}{ccccccc} a = 6 & \searrow & & & & & \\ & & \boxed{u = a \cdot b} & \rightarrow & \boxed{z = \mathrm{u} + \mathrm{c}} & \rightarrow & \boxed{J = 3(z)} \\ b = 4 & \nearrow & & & \uparrow & & \\ & & & & c = 2 & & \end{array}$$

$$\boxed{\begin{gathered} \frac{dJ}{da} = \frac{dJ}{du} \cdot \frac{du}{da} \\[2ex] \frac{dJ}{da} = 3 \cdot b \\[2ex] \frac{dJ}{da} = 3 \cdot 4 = 12 \end{gathered}}$$

Backpropagation = Work Backwards

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

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

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

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

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

$a = 6$

$b = 4$

$c = 2$

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

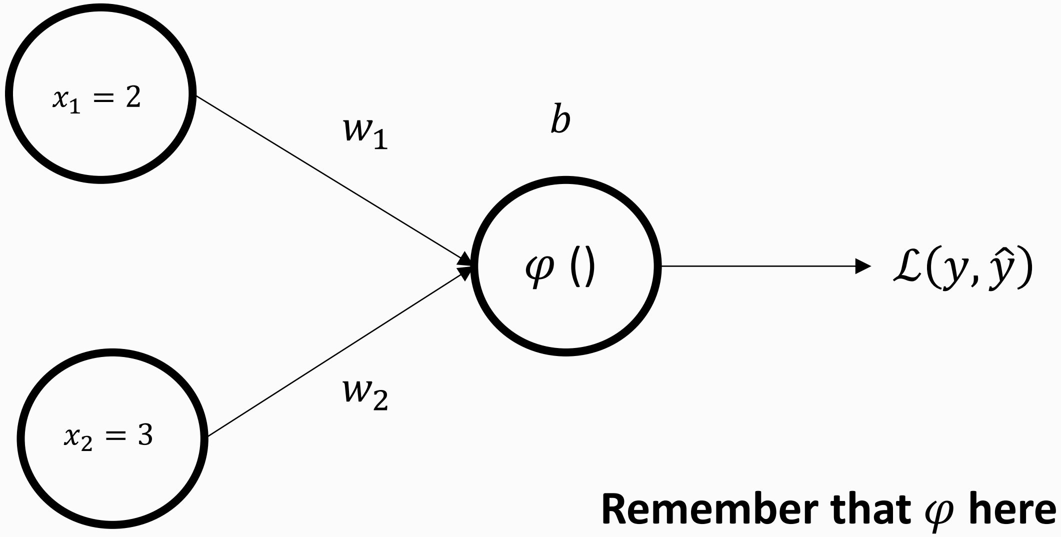
$$\frac{dJ}{db} = \frac{dJ}{du} \cdot \frac{du}{db}$$

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

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

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)



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

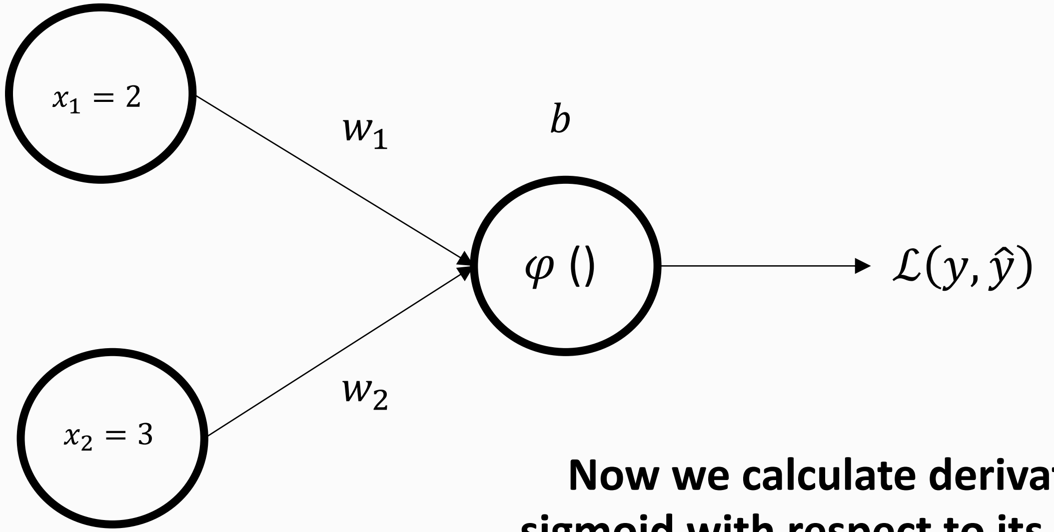
$$\frac{d\mathcal{L}}{d\varphi} = \frac{\varphi(1-y) - y(1-\varphi)}{\varphi(1-\varphi)}$$

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

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

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., $\boldsymbol{\varphi}$(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.

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

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

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

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

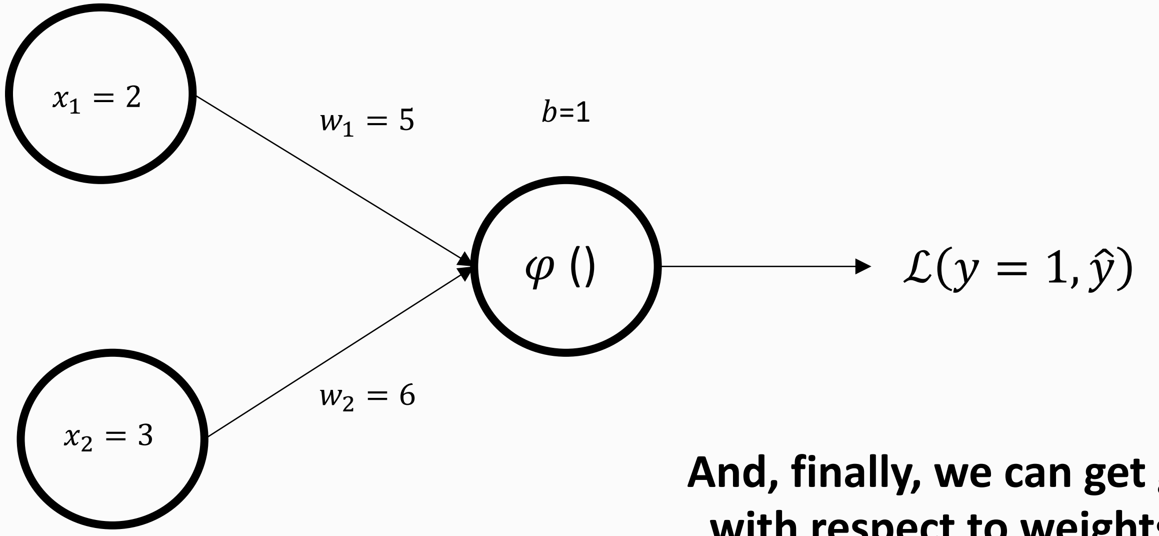
$$\frac{d\mathcal{L}}{dz} = \frac{d\mathcal{L}}{d\varphi} \cdot \frac{d\varphi}{dz}$$

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

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

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

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



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

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

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

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…

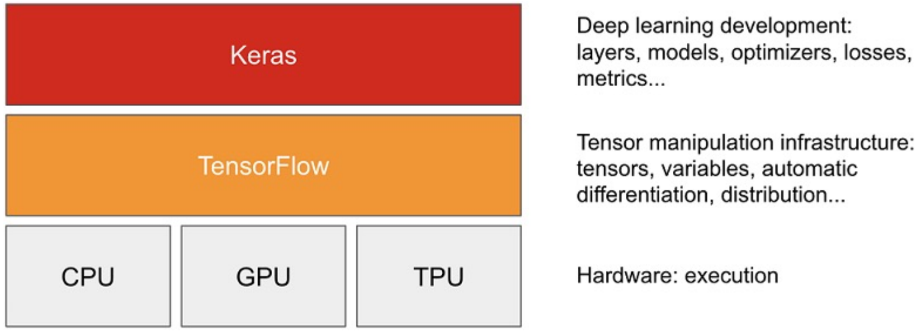
Keras and Tensorflow

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: AutoDiff

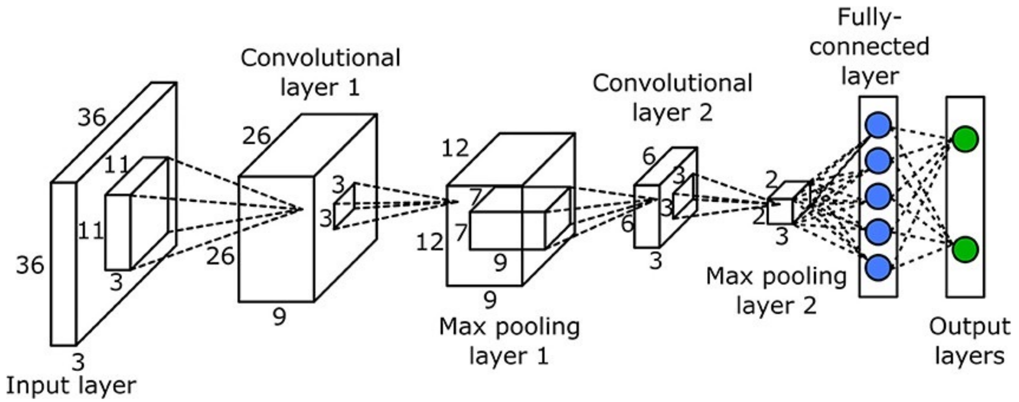
1. Gradient Tape

- 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.

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.



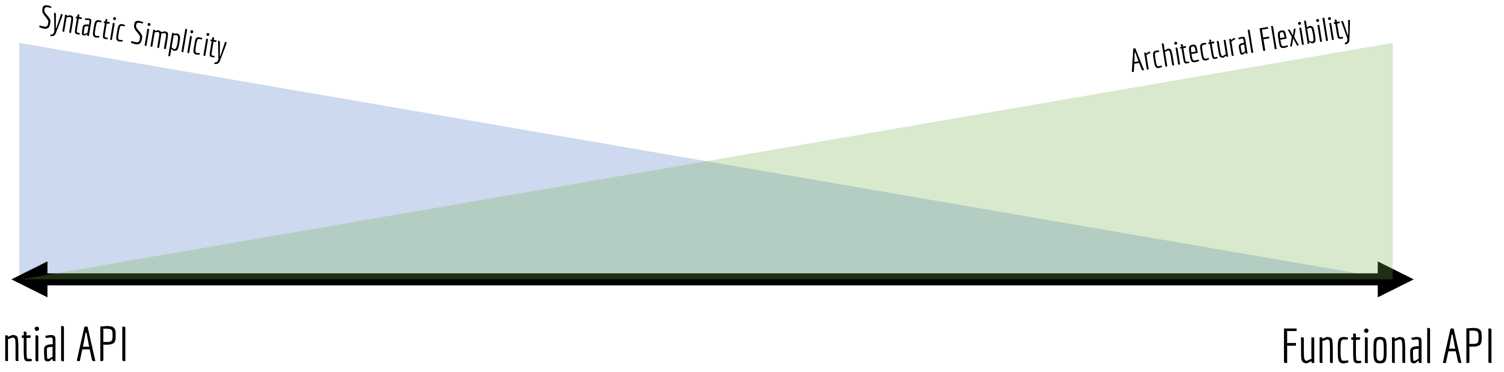
Sequential vs. Functional API

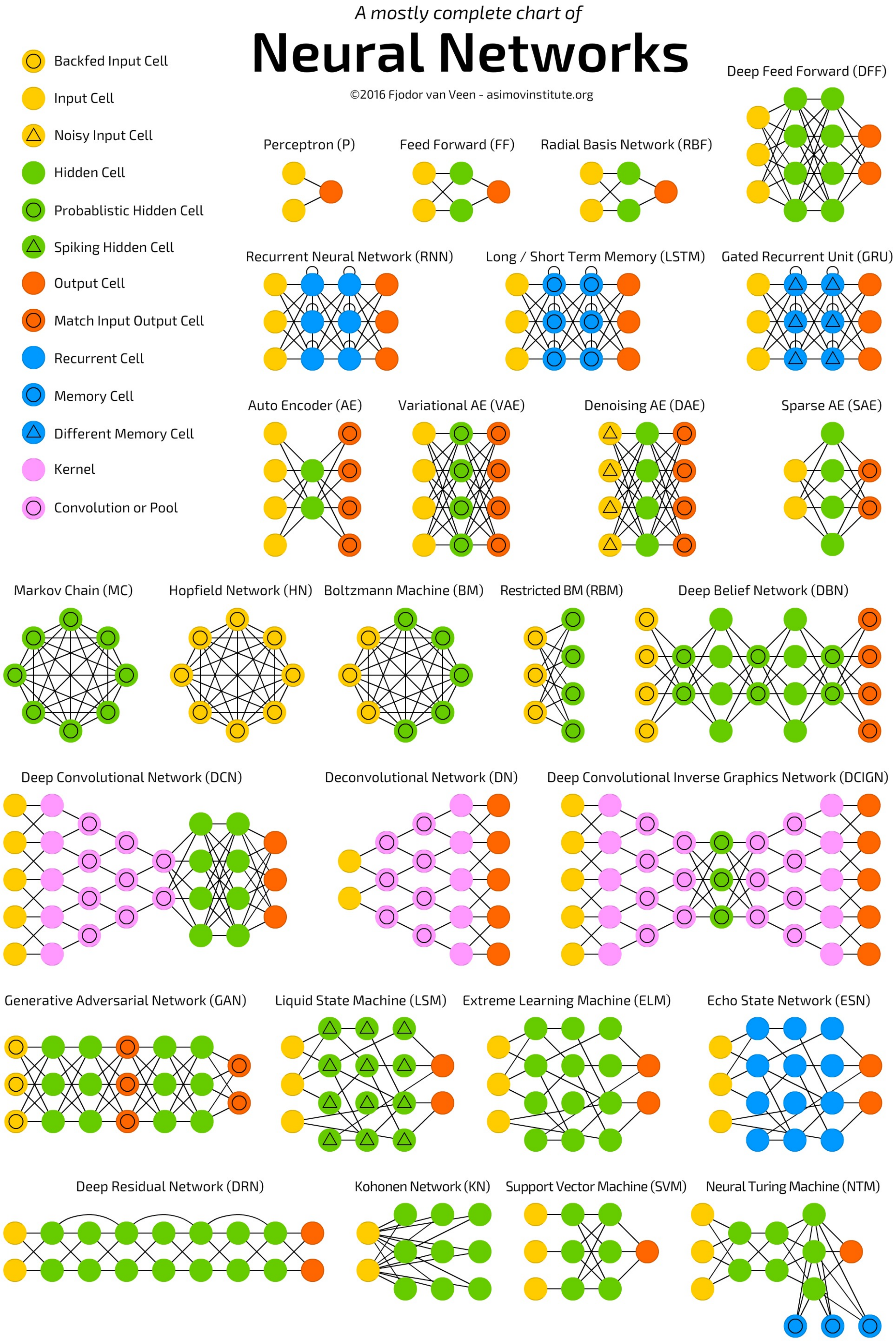
We Have Only Used Sequential API So Far

- 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

- But – we will look at the difference in how each API is used, syntactically.




A mostly complete chart of
Neural Networks
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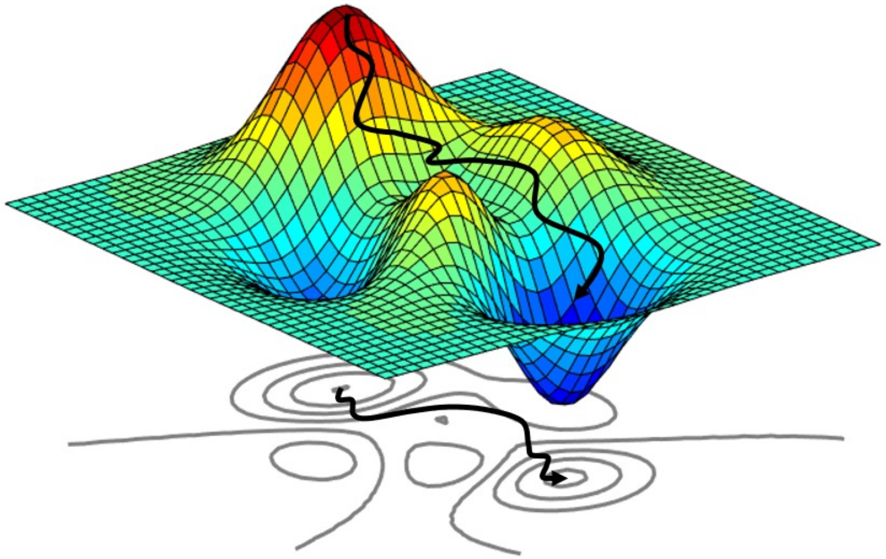
Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)
Markov Chain (MC)
Hopfield Network (HN)
Boltzmann Machine (BM)
Restricted BM (RBM)
Deep Belief Network (DBN)
Deep Convolutional Network (DCN)
Deconvolutional Network (DN)
Deep Convolutional Inverse Graphics Network (DCIGN)
Generative Adversarial Network (GAN)
Liquid State Machine (LSM)
Extreme Learning Machine (ELM)
Echo State Network (ESN)
Deep Residual Network (DRN)
Kohonen Network (KN)
Support Vector Machine (SVM)
Neural Turing Machine (NTM)

Optimizers

Keras Supports 8 Optimizers

- SGD = Stochastic Gradient Descent
- Momentum
- Ftrl (2010) = Follow the Regularized Leader
- Adagrad and Adadelta (2012) = Adaptive Gradient Descent
- 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.
- 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 withe a given observation that we are considering in an iteration.
    - Computationally quite burdensome but performs well on non-linear problems (eventually).
- Mini-batch GD = What we have been doing so far (randomly split the data in each epoch, into folds, and then cycle over the folds for training).
    - This is a happy-medium between batch and stochastic GD.

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).

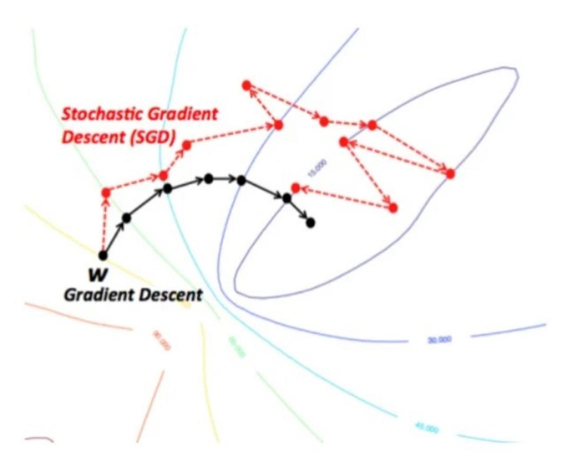
Batch (All) vs. Stochastic (1)

Same Convergence

- If you have a convex surface, either approach will converge to the global optimum (no guarantee your problem is convex of course). 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).

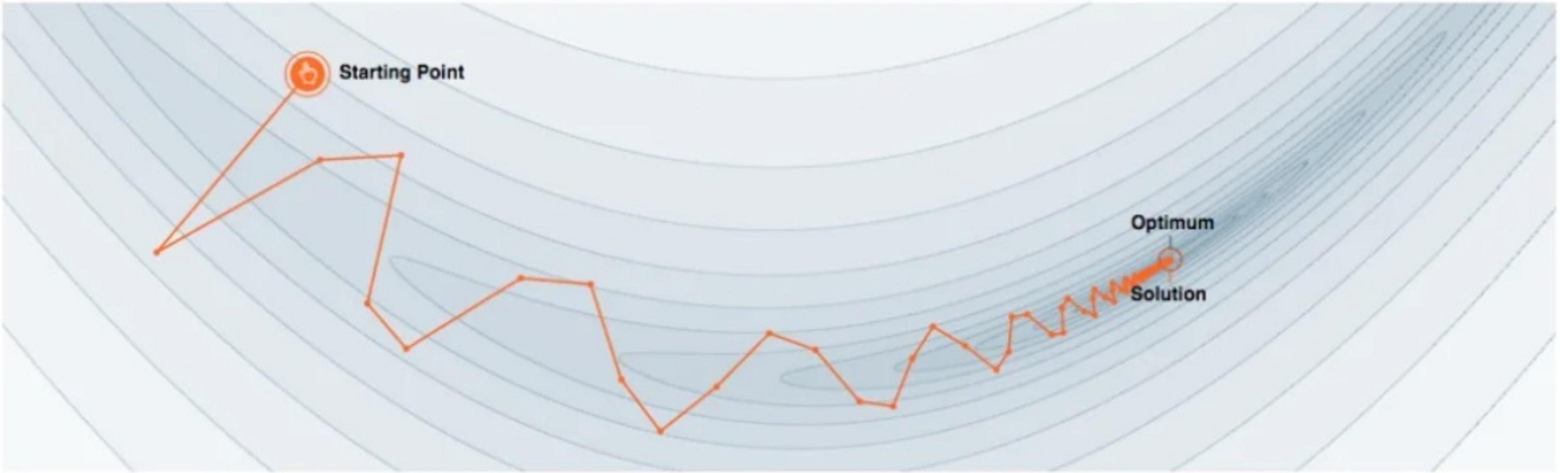


Figure: Optimization with momentum (Source: distill.pub)

FTRL

Google Developed in 2010…

- This is an optimization technique that is used in “online” learning; it’s typically used in situations where your model training is happening continuously as new data arrives, and where drift might therefore happen.
- It works well in situations where you have a ton of sparse features.
- Was originally used for predicting conversion in online advertising systems.

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).

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.