Introduction to Neural Networks

Computing Science

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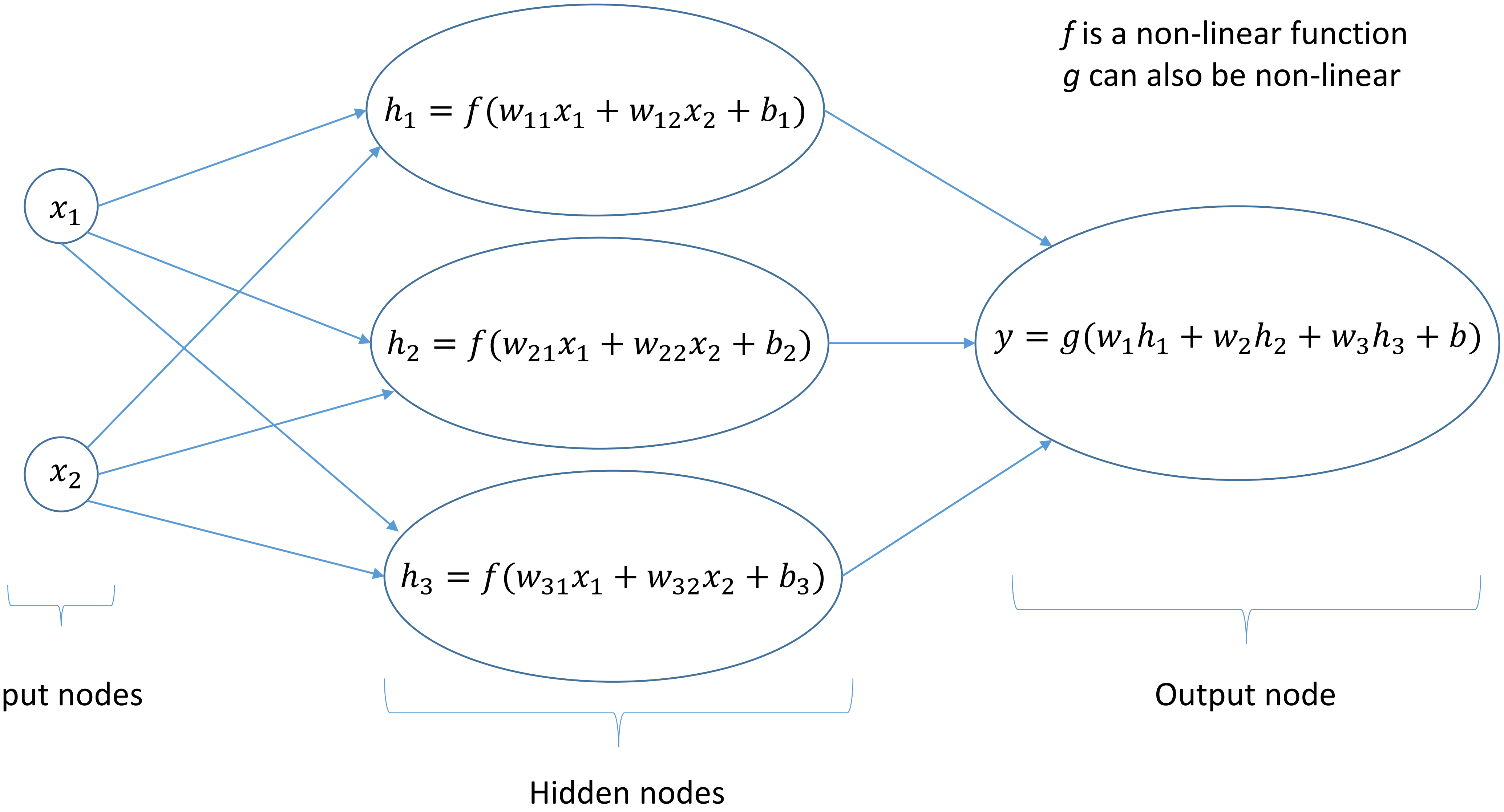
Agenda

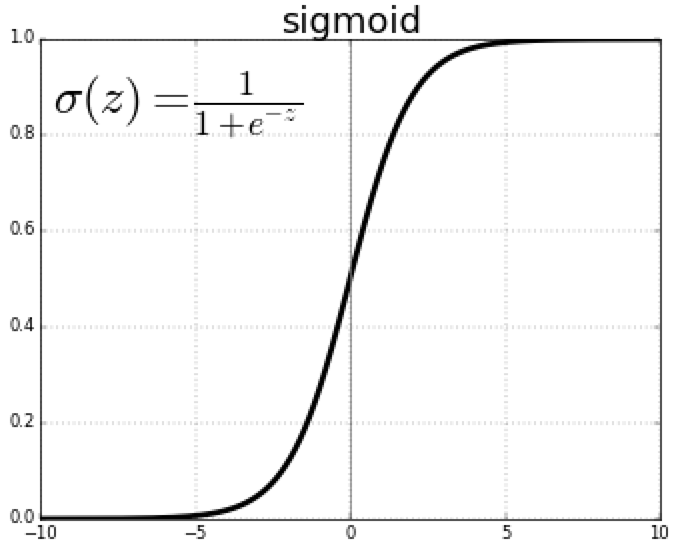
- What is a Neural Net?
  - Neural net as a computational graph
- Approximating “XOR” function with neural net
- Understanding backpropagation
- Universal function approximation by a neural net

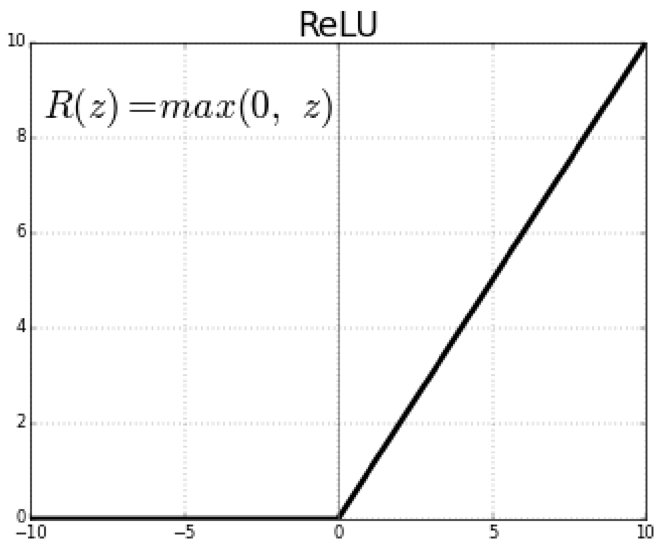
Feed forward neural network



Feed forward net: non-linear functions

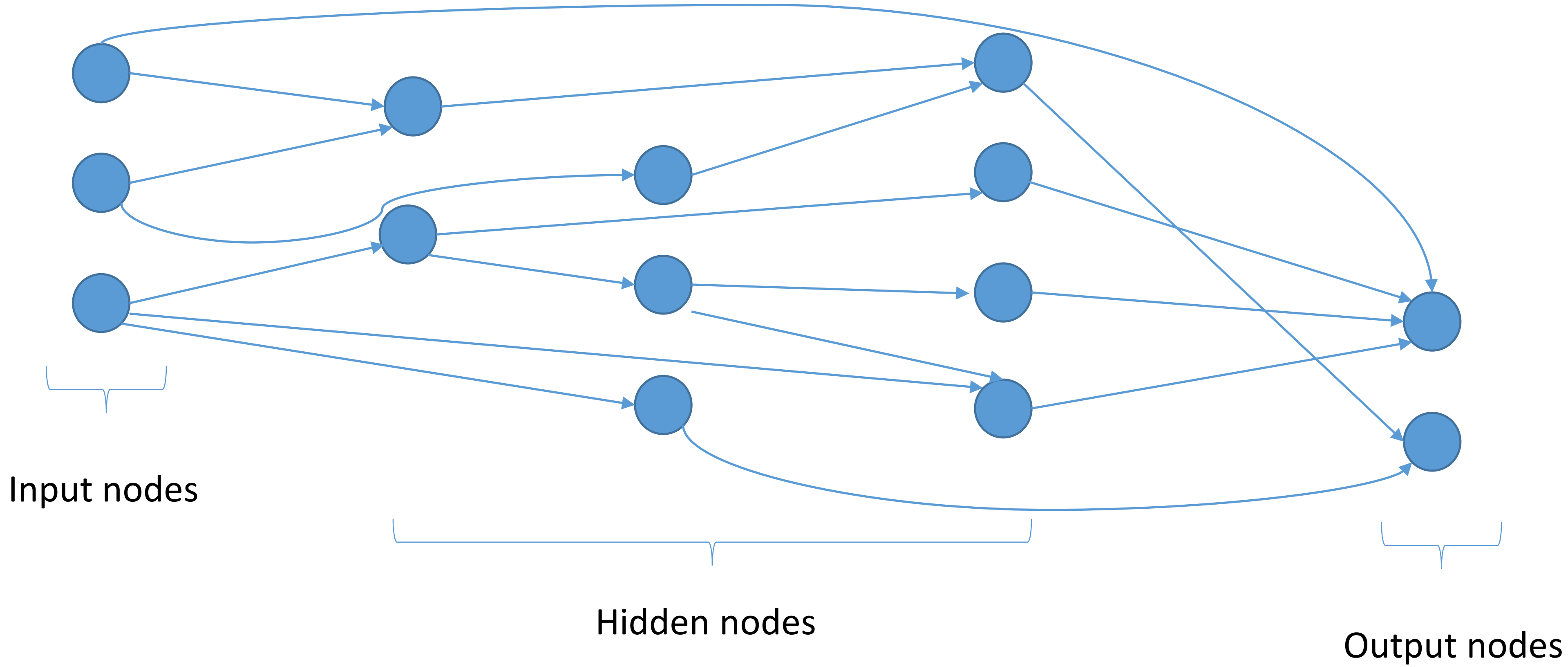
- Non-linear functions at hidden nodes are known as “activation function”
  - Sigmoid, ReLU, ELU, ….





Why activation functions are non-linear?

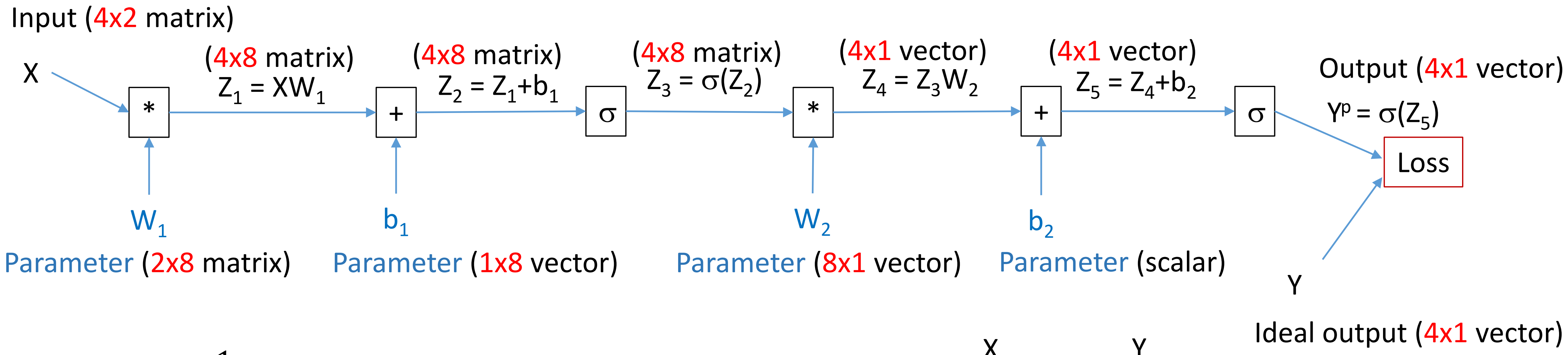
Feedforward net in general: Directed acyclic graph



What’s the big deal about neural net?

- Mathematically very rich: it can approximate any function
- It is biologically inspired: (loosely) resembles brain connections
- Computationally:
  - Simple: matrix-vector multiplication and point-wise non-linear function
  - Highly paralleizable: cuBLAS, GEMM, Batched GEMM!
- Excellent empirical results on “generalization capability” over variety of applications!

Neural network as a computational graph



$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

Sigmoid function; applied pointwise to a vector or matrix input

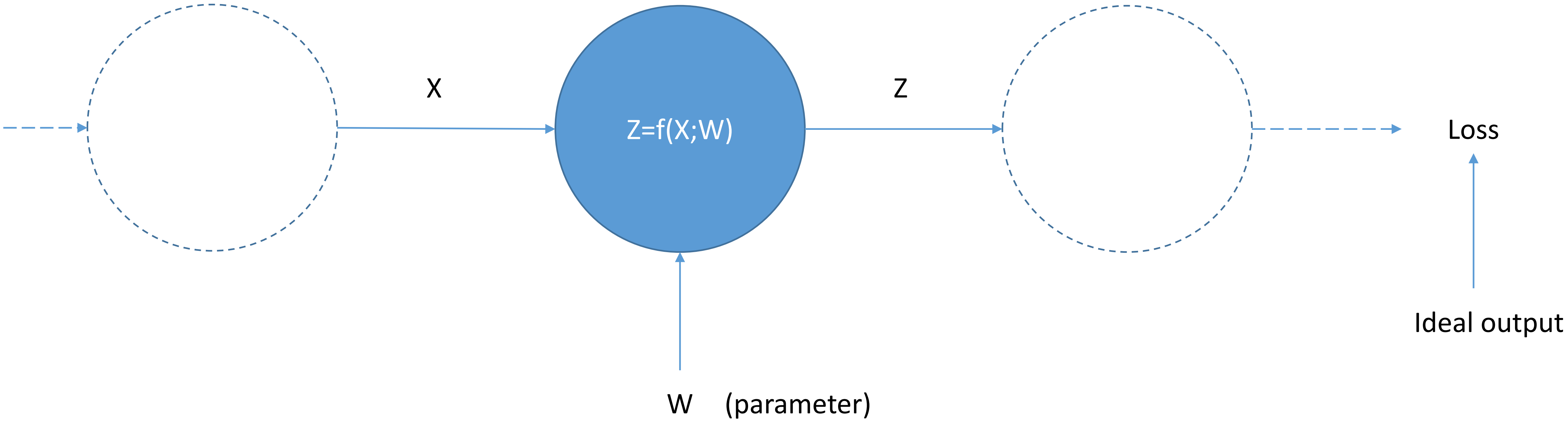
This network is trying to learn XOR function

X		Y
1	0	1
0	0	0
0	1	1
1	1	0

How does PyTorch optimize parameters?

- By gradient descent PyTorch adjusts network parameters to reduce the value of the loss function.
- But how?
  - Answer: Backpropagation
- Let us learn how to do backpropagation on a computational graph!

Chain rule of derivative for a computational node

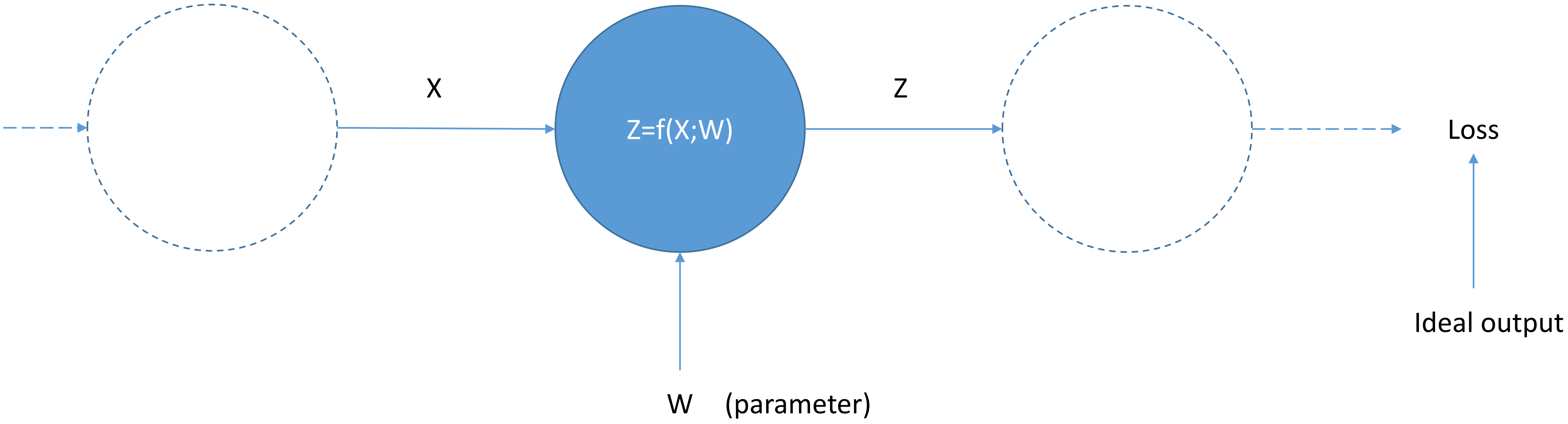


If X, Z, W are all scalars, then usual chain rule of derivative applies:

$$\frac{\partial(\mathrm{Loss})}{\partial X} = \frac{\partial Z}{\partial X}\frac{\partial(\mathrm{Loss})}{\partial Z}$$

$$\frac{\partial(\mathrm{Loss})}{\partial W} = \frac{\partial Z}{\partial W}\frac{\partial(\mathrm{Loss})}{\partial Z}$$

Chain rule of derivative...



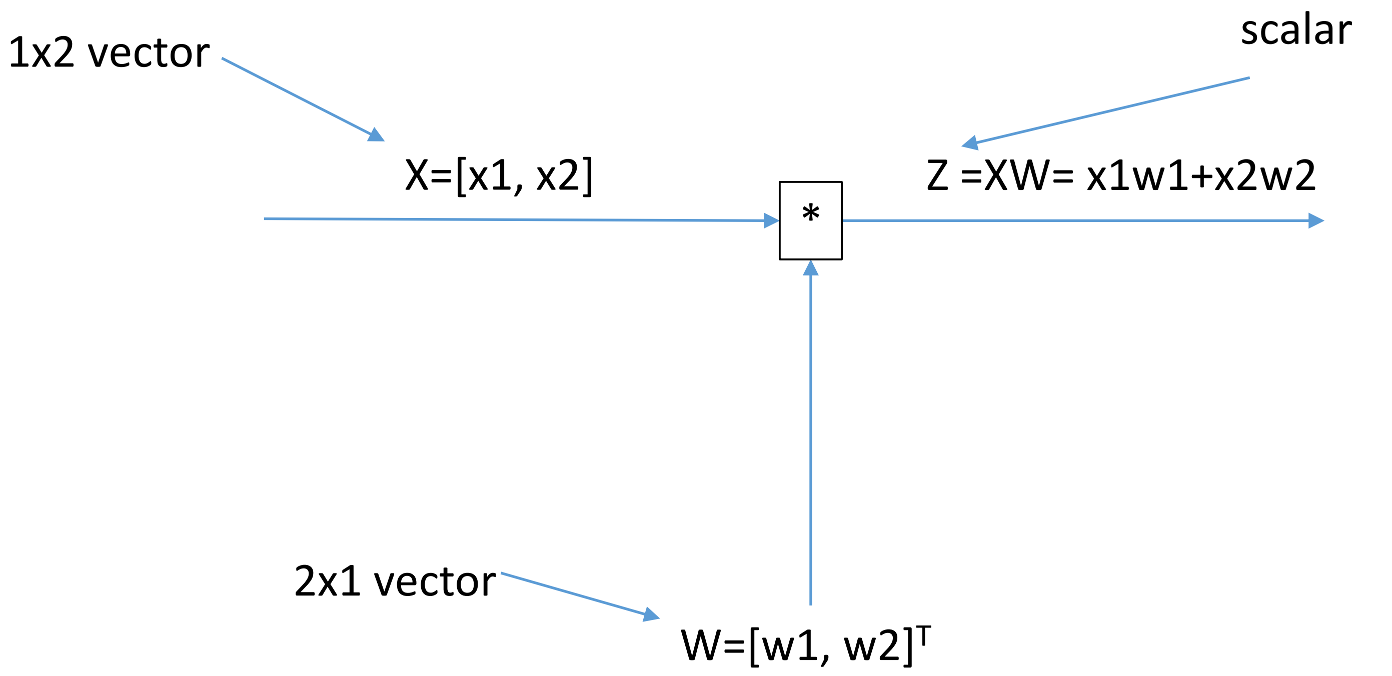
If X, Z, W are matrices or vectors, then :

$$\nabla_X(\text{Loss}) = \left(\frac{\partial Z}{\partial X}\right) * \nabla_Z(\text{Loss})$$

$$\nabla_W(\text{Loss}) = \left(\frac{\partial Z}{\partial W}\right) * \nabla_Z(\text{Loss})$$

"*" refers to matrix vector multiplication

Example 1



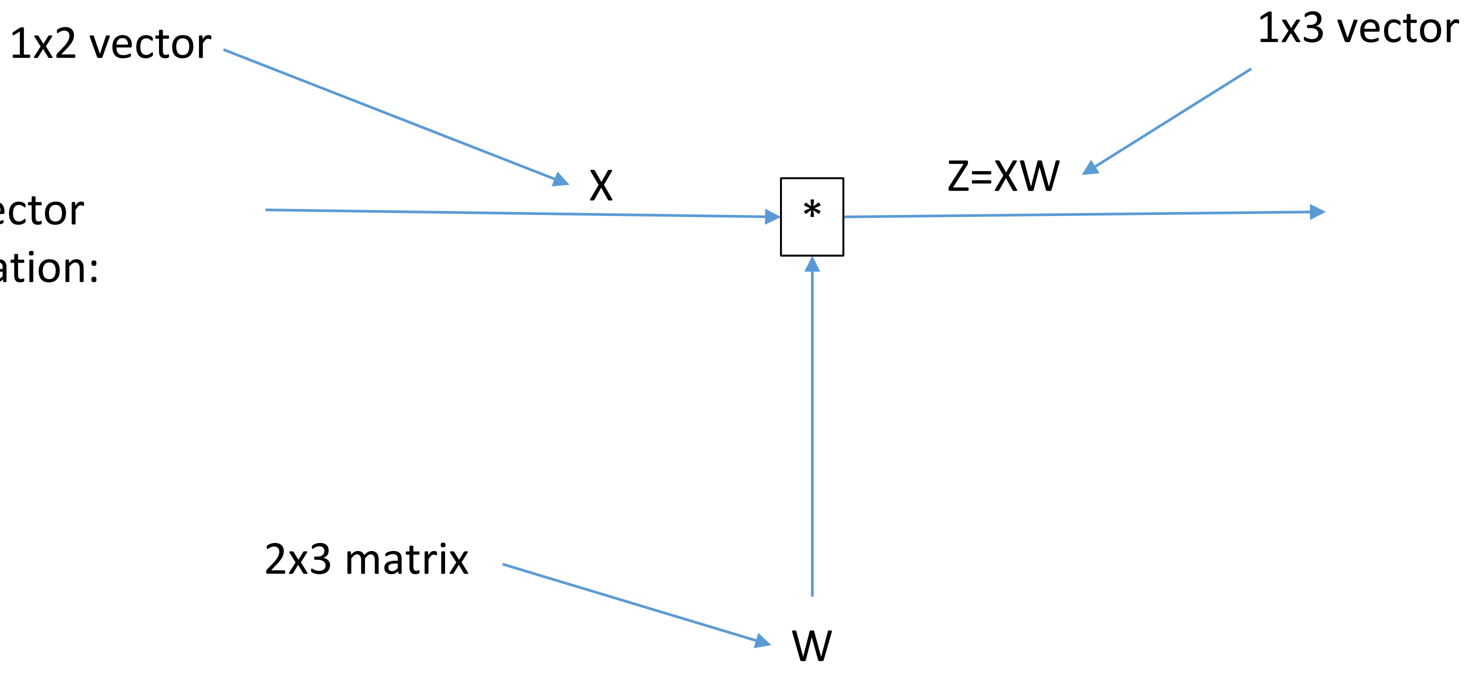
Chain rules: $$\nabla_X(\text{Loss}) = W^T \frac{\partial(\text{Loss})}{\partial Z} = [w1 \quad w2] \frac{\partial(\text{Loss})}{\partial Z}$$

Why?

$$\nabla_W(\text{Loss}) = X^T \frac{\partial(\text{Loss})}{\partial Z} = \begin{bmatrix} x1 \\ x2 \end{bmatrix} \frac{\partial(\text{Loss})}{\partial Z}$$

Example 2

Matrix-vector multiplication:



Chain rules:

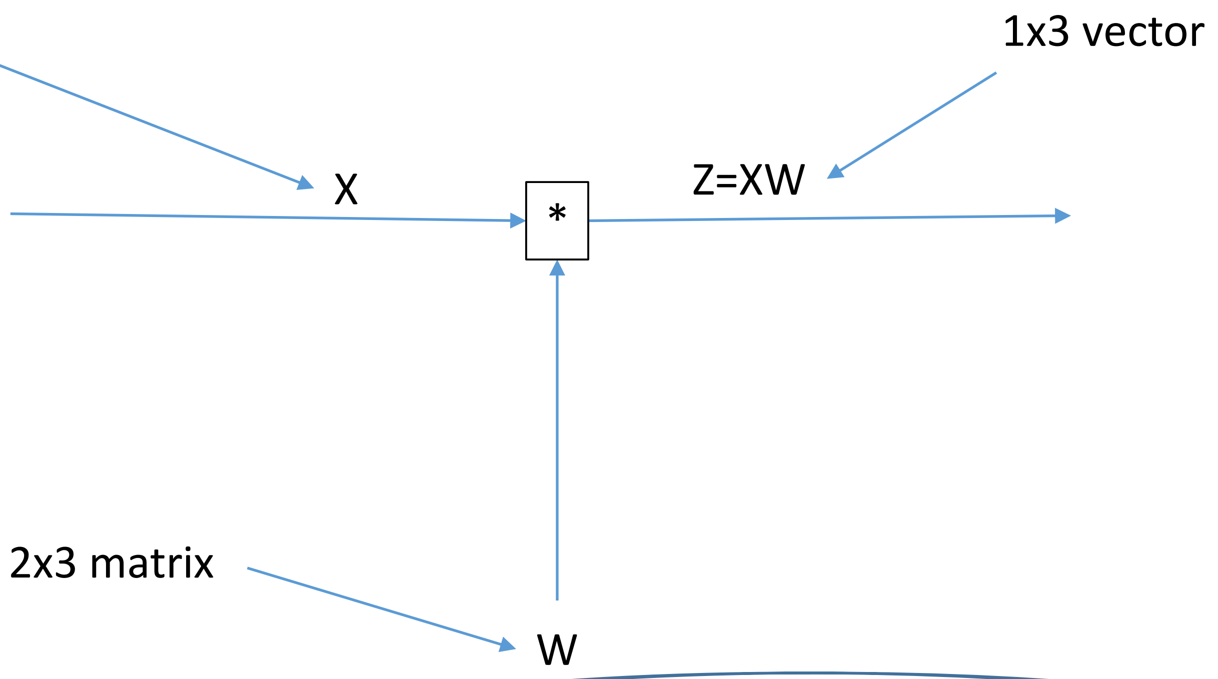
$$\nabla_X(\text{Loss}) = \nabla_Z(\text{Loss})W^T$$

Why?

$$\nabla_W(\text{Loss}) = X^T\nabla_Z(\text{Loss})$$

Backprop derivation

Matrix-vector multiplication:



Chain rules:

$$\nabla_X(\text{Loss}) = \nabla_Z(\text{Loss})W^T$$

$$\nabla_W(\text{Loss}) = X^T\nabla_Z(\text{Loss})$$

Using short notation for gradients:

$$\delta S \equiv \nabla_S(\text{Loss})$$

$$\delta X = \delta Z W^T$$

$$\delta W = X^T \delta Z$$

Backprop derivation…

$$\delta X_i = \underbrace{\sum_k \frac{\partial Z_k}{\partial X_i}\frac{\partial(\text{Loss})}{\partial Z_k}}_{\text{Chain rule of derivative}} = \sum_k \frac{\partial}{\partial X_i}\underbrace{\left[\sum_j X_j W_{jk}\right]}_{\text{Substitute } Z_k}\delta Z_k = \sum_k W_{ik}\,\delta Z_k \Longrightarrow \delta X = \delta Z W^T$$

i^{th} component of δX vector

k^{th} component of δZ vector

Because,

$$\frac{\partial}{\partial X_i}\left[\sum_j X_j W_{jk}\right] = W_{ik}$$

Writing in matrix-vector multiplication form

Backprop derivation…

$$\delta W_{ij} = \underbrace{\sum_k \frac{\partial Z_k}{\partial W_{ij}} \frac{\partial(\text{Loss})}{\partial Z_k}}_{\text{Chain rule of derivative}} = \sum_k \frac{\partial}{\partial W_{ij}} \underbrace{\left[\sum_m X_m W_{mk}\right]}_{\text{Substitute } Z_k} \delta Z_k = X_i \delta Z_j \quad \Longrightarrow \quad \delta W = X^T \delta Z$$

Writing in matrix-vector multiplication form

*(i,j)*th component of δW matrix

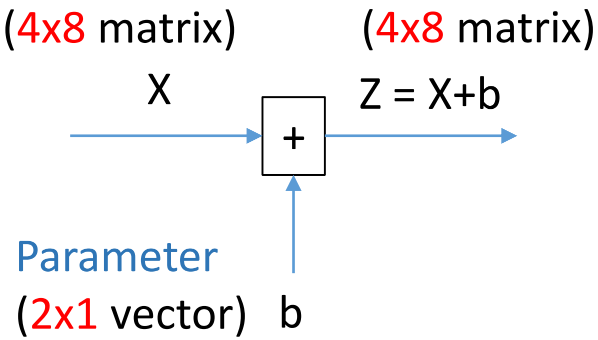
Because,

$$\frac{\partial}{\partial W_{ij}}\left[\sum_m X_m W_{mk}\right] = \begin{cases} X_i, & \text{if } i = m \text{ and } j = k, \\ 0, & \text{otherwise.} \end{cases}$$

kth component of δZ vector

Backprop derivation…

"Broadcast" addition:



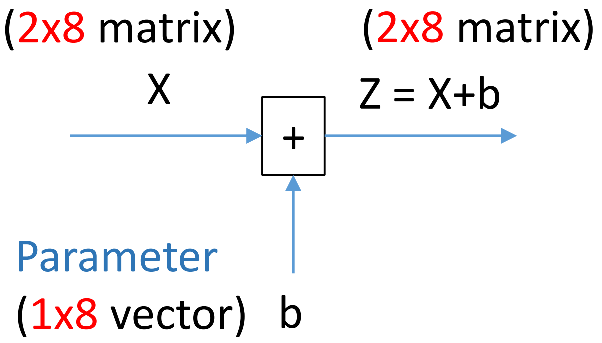
$$\delta X_{i,j} = \underbrace{\sum_k \sum_l \frac{\partial Z_{k,l}}{\partial X_{i,j}}}_{\text{Chain rule}} \delta Z_{k,l} = \sum_k \sum_l \frac{\partial}{\partial X_{i,j}} \underbrace{\left[X_{k,l} + b_k\right]}_{\text{Substitute } Z_{k,l}} \delta Z_{k,l} = \delta Z_{i,j} \quad \Longrightarrow \quad \delta X = \delta Z$$

Because,

$$\frac{\partial}{\partial X_{i,j}}\left[X_{k,l} + b_k\right] = \begin{cases} 1, \text{if } i = k \text{ and } j = l, \\ 0, \text{otherwise.} \end{cases}$$

Backprop derivation for broadcast addition

"Broadcast" addition:



$$\delta b_i = \underbrace{\sum_k \sum_l \frac{\partial Z_{k,l}}{\partial b_i} \delta Z_{k,l}}_{\text{Chain rule}} = \sum_k \sum_l \frac{\partial}{\partial b_i} \underbrace{[X_{k,l} + b_l]}_{\text{Substitute } Z_{k,l}} \delta Z_{k,l} = \sum_k \delta Z_{k,i} \Longrightarrow \delta b = \sum_k \delta Z_{k,:}$$

Because,

$$\frac{\partial}{\partial b_i}[X_{k,l} + b_l] = \begin{cases} 1, \text{if } i = l, \\ 0, \text{otherwise.} \end{cases}$$

Backprop derivation for activation function

Non-linear function:
(applied pointwise)

$$\xrightarrow{X} \boxed{\sigma} \xrightarrow{Z = \sigma(X)}$$

Using chain rule: $\delta X_{i,j} = \frac{dZ_{i,j}}{dX_{i,j}} \delta Z_{i,j} = \frac{d\sigma(X_{i,j})}{dX_{i,j}} \delta Z_{i,j}$

If the non-linear function is sigmoid, $\sigma(a) = \frac{1}{1 + \exp(-a)}$

$$\frac{d\sigma}{da} = \frac{\exp(-a)}{(1 + \exp(-a))^2} = \frac{1}{1 + \exp(-a)}\left(1 - \frac{1}{1 + \exp(-a)}\right) = \sigma(a)(1 - \sigma(a))$$

$$\delta X_{i,j} = \sigma(X_{i,j})(1 - \sigma(X_{i,j}))\delta Z_{i,j}$$

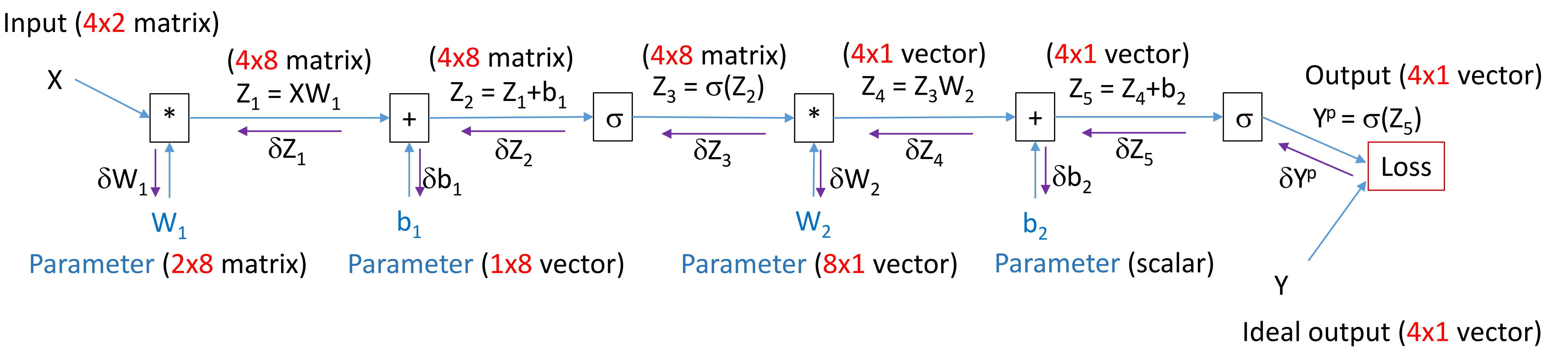
Backprop derivation for loss function

Euclidean loss function: $Loss(Y^p, Y) = \frac{1}{2}\|Y^p - Y\|^2 = \frac{1}{2}\sum_i \left(Y_i^p - Y_i\right)^2$

i^{th} component of δY^p vector: $\delta Y_i^p = \frac{\partial}{\partial Y_i^p} Loss(Y^p, Y) = \frac{\partial}{\partial Y_i^p}\frac{1}{2}\sum_i \left(Y_i^p - Y_i\right)^2 = Y_i^p - Y_i$

Using vector notation: $\delta Y^p = Y^p - Y$

Apply chain rule to XOR neural network



Chain rule of derivatives:

$$\delta Y^p = Y^p - Y$$

$$\delta Z_5 = \sigma(Z_5)(1-\sigma(Z_5))\delta Y^p$$

$$\delta Z_4 = \delta Z_5$$

$$\delta Z_3 = \delta Z_4 W_2^T$$

$$\delta Z_2 = \sigma(Z_2)(1-\sigma(Z_2))\delta Z_3$$

$$\delta Z_1 = \delta Z_2$$

Gradient of "Loss" with respect to input signals

Propagates backward

$$\delta W_2 = Z_3^T \delta Z_4$$

$$\delta b_2 = \sum_k (\delta Z_5)_k$$

$$\delta W_1 = X^T \delta Z_1$$

$$\delta b_1 = \sum_k (\delta Z_2)_{k,:}$$

Gradient of "Loss" with respect to parameters

New notation:

$\delta S \equiv \nabla_S(\text{Loss})$

Backprop to train a neural net

Initialize all parameters of the neural network
Initialize learning rate variable *lr*

Iterate:

If loading the whole training data, do it once outside the "Iterate" loop, to be efficient

(Load Data): Get training data batch

(Forward pass): Compute Z_1, Z_2,…,Y^p

(Backward pass): Compute gradients δY^p, δZ_5,…, δZ_1, δW_2, δW_1, δb_2, δb_1

(Gradient descent to update parameters): $W_2 \leftarrow W_2 - lr * \delta W_2$, $b_2 \leftarrow b_2 - lr * \delta b_2, \dots,$

(Diagnostics): Compute "Loss" from time to time to check if it is decreasing

"Learn_XOR_manualBP.ipnyb" implements this learning algorithm

PyTorch magic!

- Fortunately, PyTorch can automatically compute derivatives by chain rules!
- Also, it has several optimizers that can use these derivatives in the gradient descent optimization method.
- Look at “Learn_XOR.ipnyb” and “Learn_XOR_with_LBFGS.ipnyb”

Universal function approximation

- A neural network with a single hidden layer can approximate “any” function!
  - Wikipedia has a clear statement: https://en.wikipedia.org/wiki/Universal_approximation_theorem
- A non-technical explanation of universality theorem:
  - http://neuralnetworksanddeeplearning.com/chap4.html

Why do we then even need multiple layers and why even deep nets?