MNIST Digit Classification with Neural Net

Computing Science

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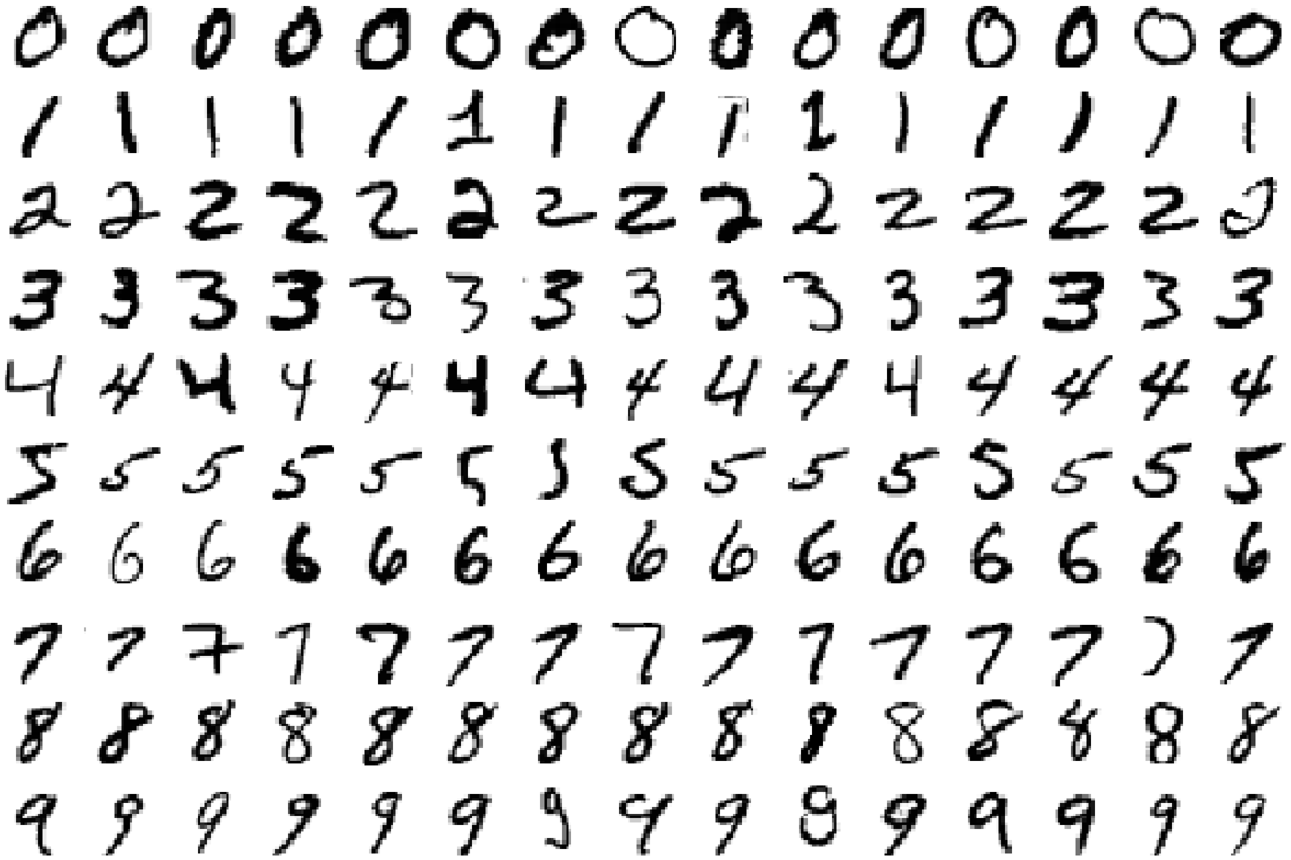
Agenda

- Building a neural net with PyTorch for MNIST digit recognition
- How does backpropagation work?
- Softmax function
- Cross-entropy loss

MNIST dataset



Classify images into digits

Each image is **28x28**

10 labels

55,000 training images

5,000 validation images

10,000 test images.

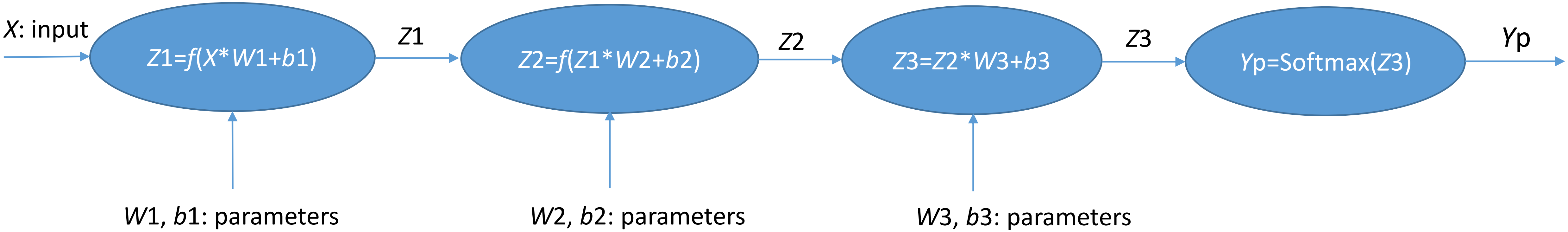
MNIST classification problem

Small 28 pixels-by-28 pixels images of hand written digits

The visual recognition problem definition:
to recognize the digit from an image

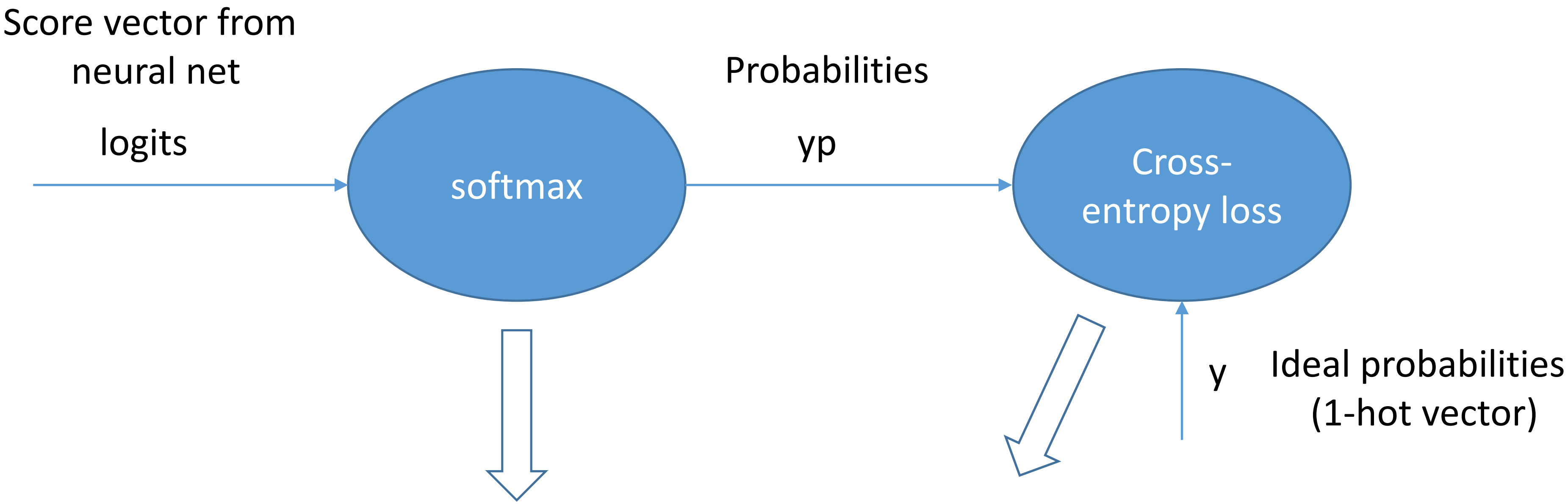
Pixel values (feature)				Digit: 1-hot vector		
x_1	x_2	…	x_{784}	y_1	…	y_{10}
0.1	0.3	…	0.0	0	…	1
0.2	0.1	…	0.5	1		0
…	…	…	…	…	…	…
…	…	…	…	…	…	…
0.0	0.98	…	0.8	0	…	1
0.5	0.25	…	0.36	?	…	?
0.1	0.95	…	0.1	?	…	?

NN Architecture for MNIST Classification



Activation function, *f* is ReLU in our implementation

Softmax and cross-entropy loss



Score vector from neural net

logits

softmax

Probabilities

yp

Cross-entropy loss

y

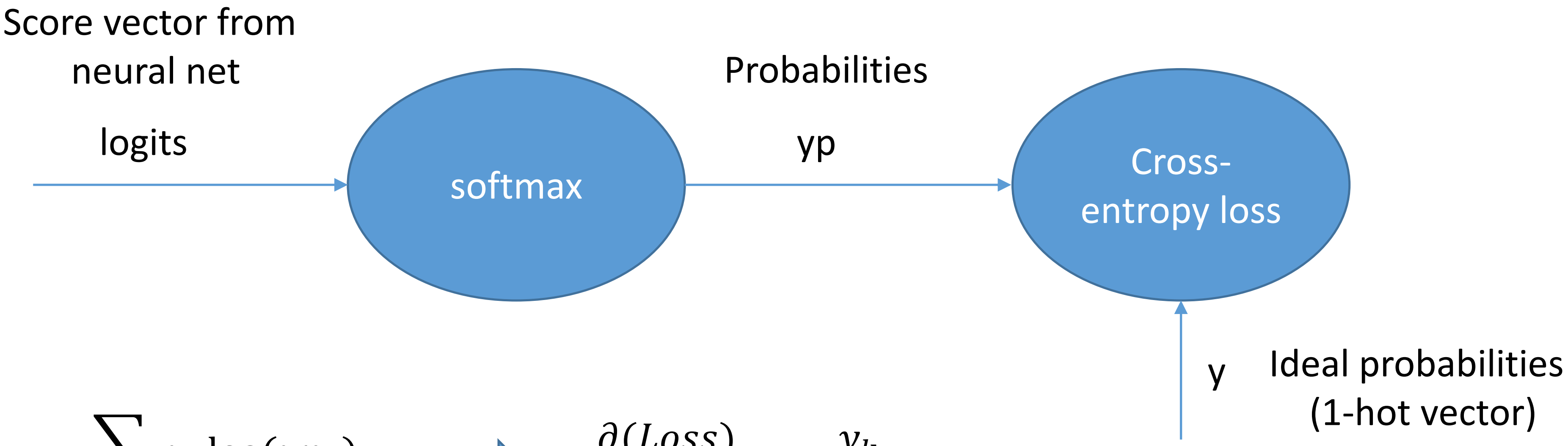
Ideal probabilities (1-hot vector)

$$yp_i = \frac{\exp(logits_i)}{\sum_k \exp(logits_k)}$$

$$Loss = -\sum_k y_k \log(yp_k)$$

To backpropagate error, we need to compute: $\delta(logits)_i \equiv \frac{\partial(Loss)}{\partial(logits)_i}$

Softmax and cross-entropy loss: backprop


Score vector from neural net
logits
softmax
Probabilities
yp
Cross-entropy loss
y
Ideal probabilities (1-hot vector)

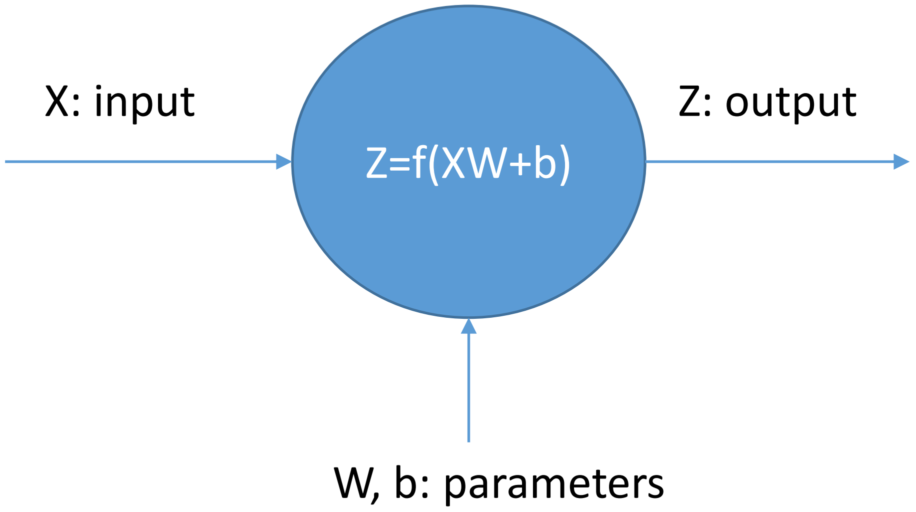
$$Loss = -\sum_k y_k \log(yp_k) \Longrightarrow \frac{\partial(Loss)}{\partial(yp)_k} = -\frac{y_k}{yp_k}$$

$$yp_i = \frac{\exp(logits_i)}{\sum_k \exp(logits_k)} \Longrightarrow \frac{\partial(yp)_k}{\partial(logits)_i} = \begin{cases} yp_i(1 - yp_i), & \text{if } i = k, \\ -yp_i yp_k, & \text{otherwise.} \end{cases}$$

Using the above two results in the chain rule, $\delta(logits)_i \equiv \frac{\partial(Loss)}{\partial(logits)_i} = \sum_k \frac{\partial(yp)_k}{\partial(logits)_i} \frac{\partial(Loss)}{\partial(yp)_k} = yp_i - y_i$

What if, instead of cross-entropy, we used L2 loss along with softmax?

Backprop across a neural net layer



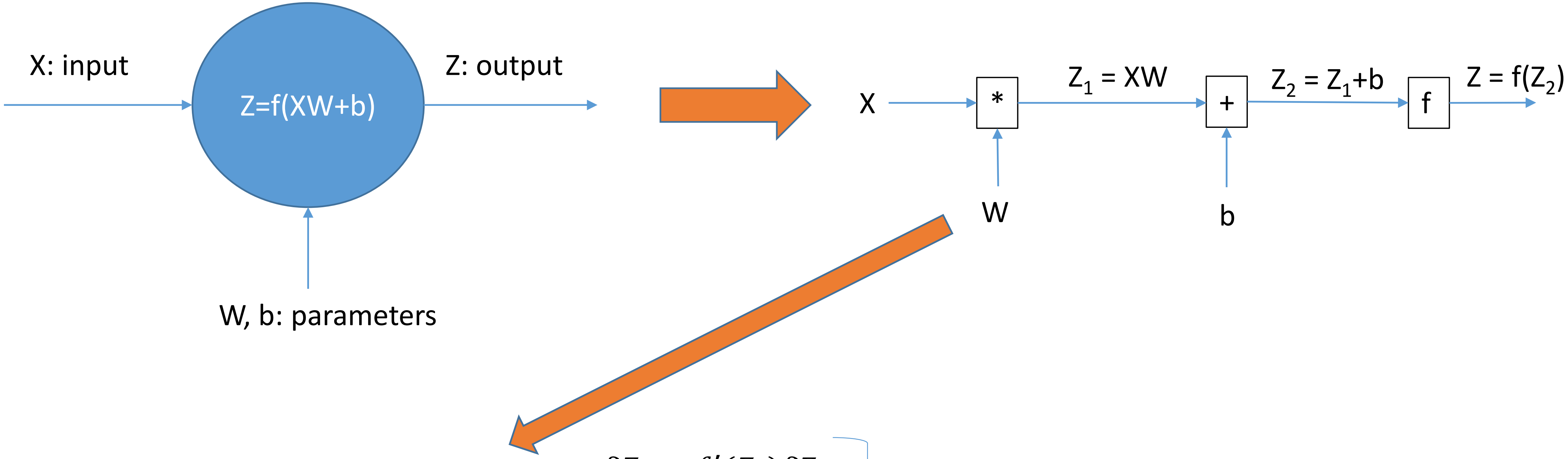
Pointwise multiplication

Backprop rules:

$$\delta X = [f'(XW + b) \cdot \delta Z] * W^T \qquad \delta W = X^T * [f'(XW + b) \cdot \delta Z] \qquad \delta b = \sum_l [f'(XW + b) \cdot \delta Z]_{l,:}$$

Matrix multiplication

Backprop across a neural net layer: derivation

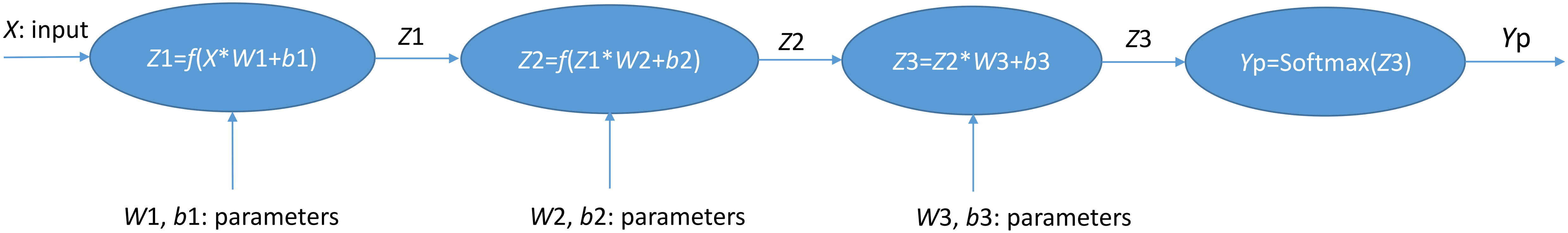


Apply chain rule to computational nodes:

$$\left.\begin{aligned} \delta Z_2 &= f'(Z_2)\delta Z \\ \delta Z_1 &= \delta Z_2 \\ \delta X &= \delta Z_1 W^T \end{aligned}\right\} \Rightarrow \delta X = [f'(XW+b)\cdot\delta Z] * W^T$$

Similarly, we can derive backprop rules for δW and δb

NN for MNIST Classification: Gradients



X: input

$Z1=f(X*W1+b1)$

$Z1$

$Z2=f(Z1*W2+b2)$

$Z2$

$Z3=Z2*W3+b3$

$Z3$

$Yp=\text{Softmax}(Z3)$

Yp

$W1$, $b1$: parameters

$W2$, $b2$: parameters

$W3$, $b3$: parameters

Backprop:

$\delta Z3 = Yp\text{-}Y$

$\delta Z2 = \delta Z3 * W3^T$

$\delta Z1 = [f'(Z1*W2+b2).\delta Z2] * W2^T$

$$\delta W3 = Z2^T * \delta Z3$$

$$\delta W2 = Z1^T * [f'(Z1 * W2 + b2) \cdot \delta Z2]$$

$$\delta W1 = X^T * [f'(X * W1 + b1) \cdot \delta Z1]$$

$$\delta b3 = \sum_l [\delta Z3]_{l,:}$$

$$\delta b2 = \sum_l [f'(Z1 * W2 + b2) \cdot \delta Z2]_{l,:}$$

$$\delta b1 = \sum_l [f'(X * W1 + b1) \cdot \delta Z1]_{l,:}$$

Learning MNIST NN with Backprop and SGD

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

Iterate:

(Load Data): Get training data batch *X*

(Forward pass): Compute *Z*1, *Z*2, Z3, *Y*p

(Backward pass): Compute gradients $\delta Z3$, $\delta Z2$, $\delta Z1$, $\delta W3$, $\delta W2$, $\delta W1$, $\delta b3$, $\delta b2$, $\delta b1$

(Gradient descent to update parameters): $W3 \leftarrow W3 - lr * \delta W3, \quad b3 \leftarrow b3 - lr * \delta b3, \ldots,$

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