Backpropagation in Neural Nets

Materials from

- Intel Deep Learning https://www.intel.com/content/www/us/en/developer/learn/course-deep-learning.html

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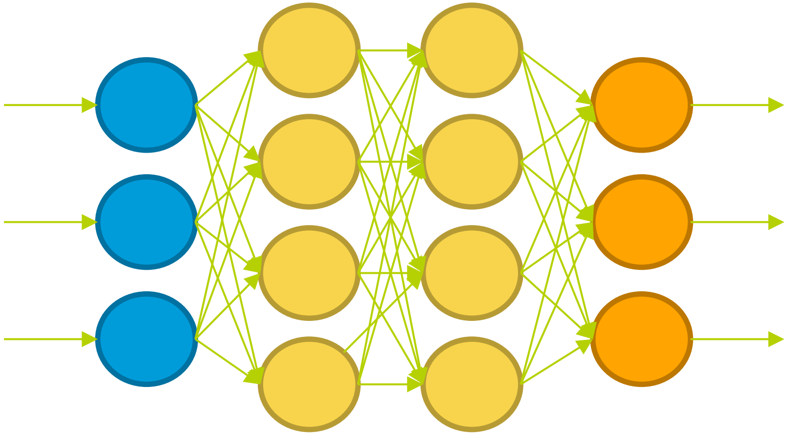
How to Train a Neural Net?

Input
(Feature Vector)



Output
(Label)

- Put in Training inputs, get the output
- Compare output to correct answers: Look at loss function J
- Adjust and repeat!
- Backpropagation tells us how to make a single adjustment using calculus.

How have we trained before?

- Gradient Descent!

1. Make prediction
2. Calculate Loss
3. Calculate gradient of the loss function w.r.t. parameters
4. Update parameters by taking a step in the opposite direction
5. Iterate

How have we trained before?

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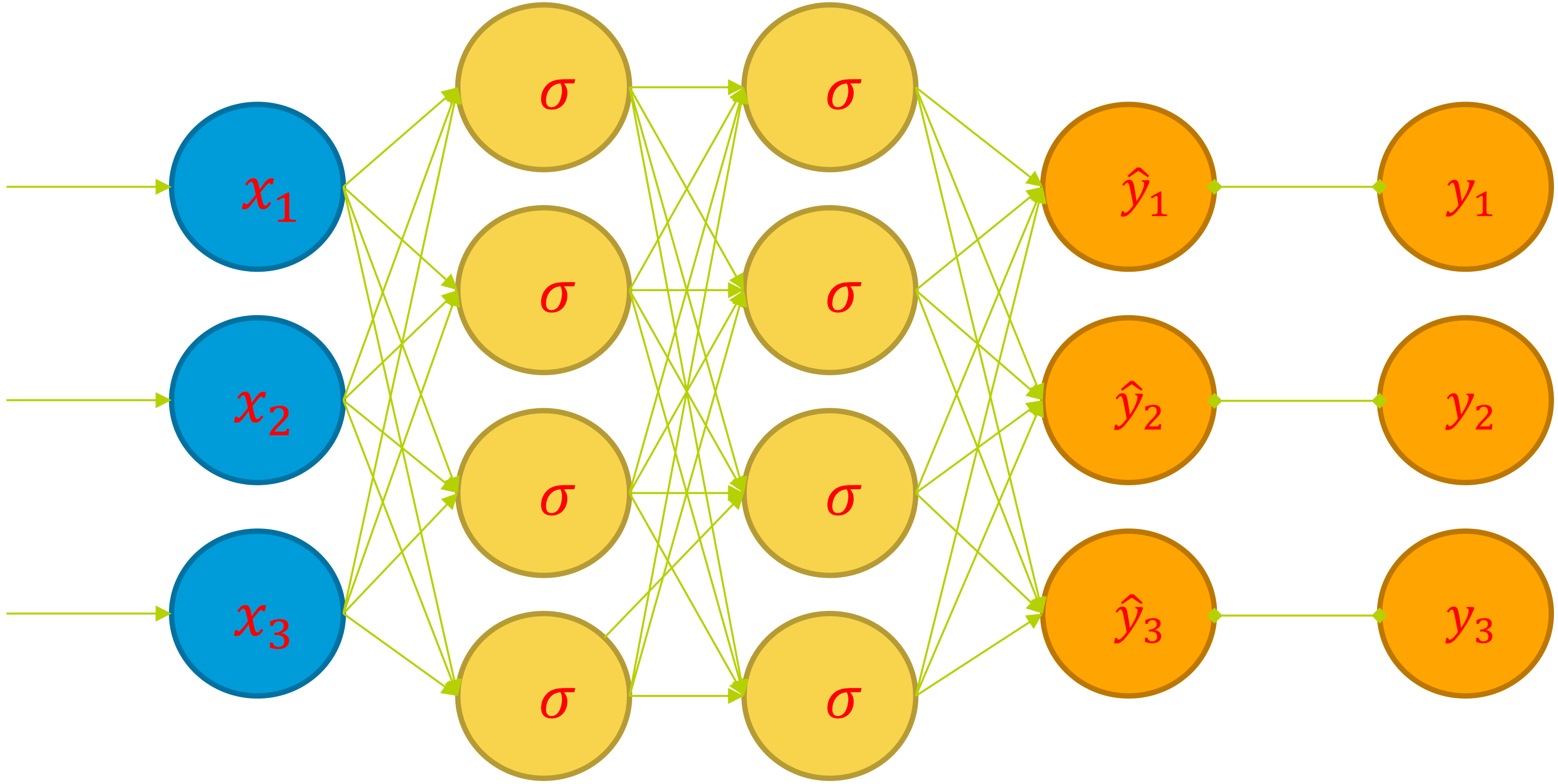
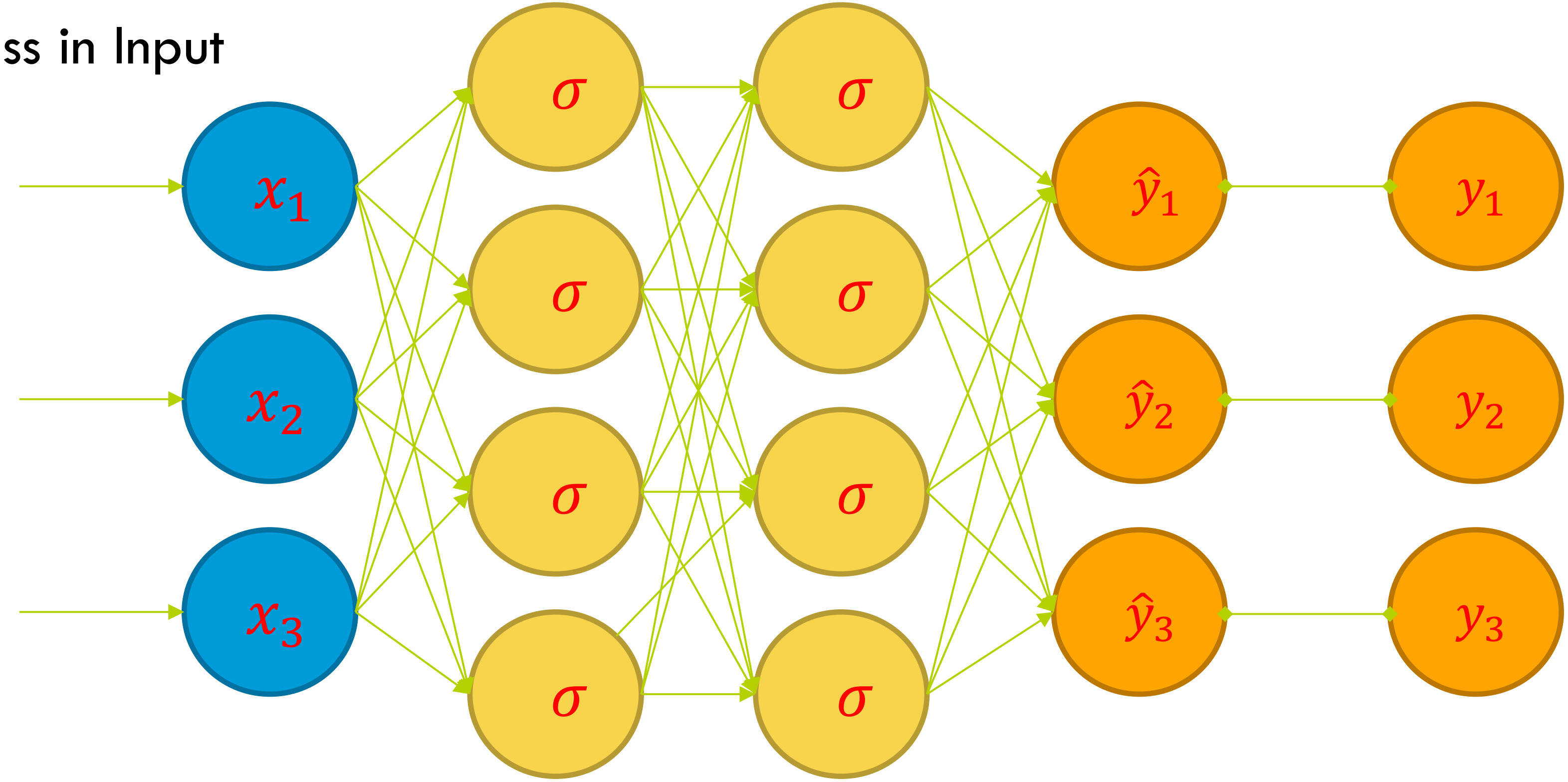
Feedforward Neural Network

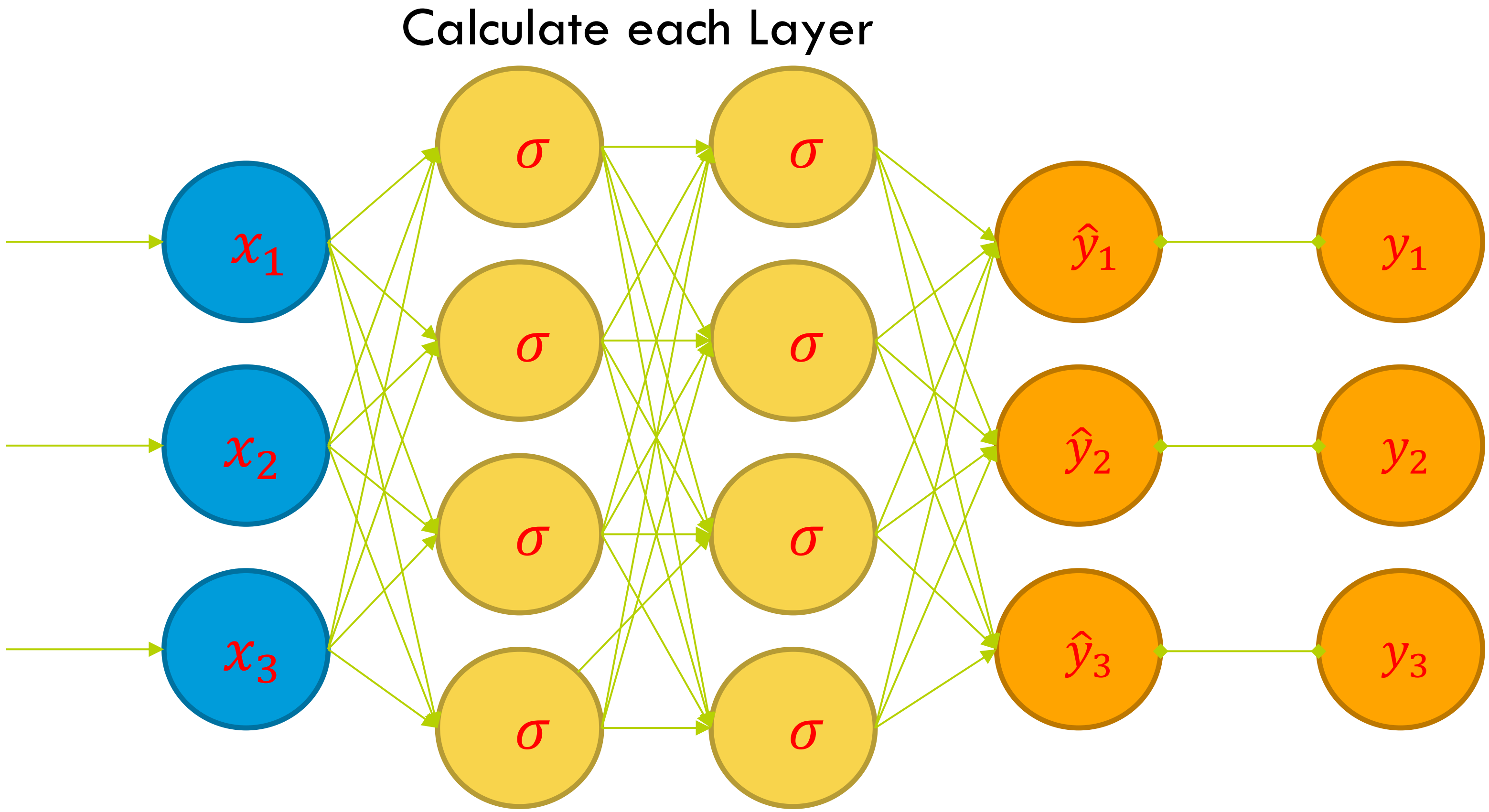


Forward Propagation

Pass in Input

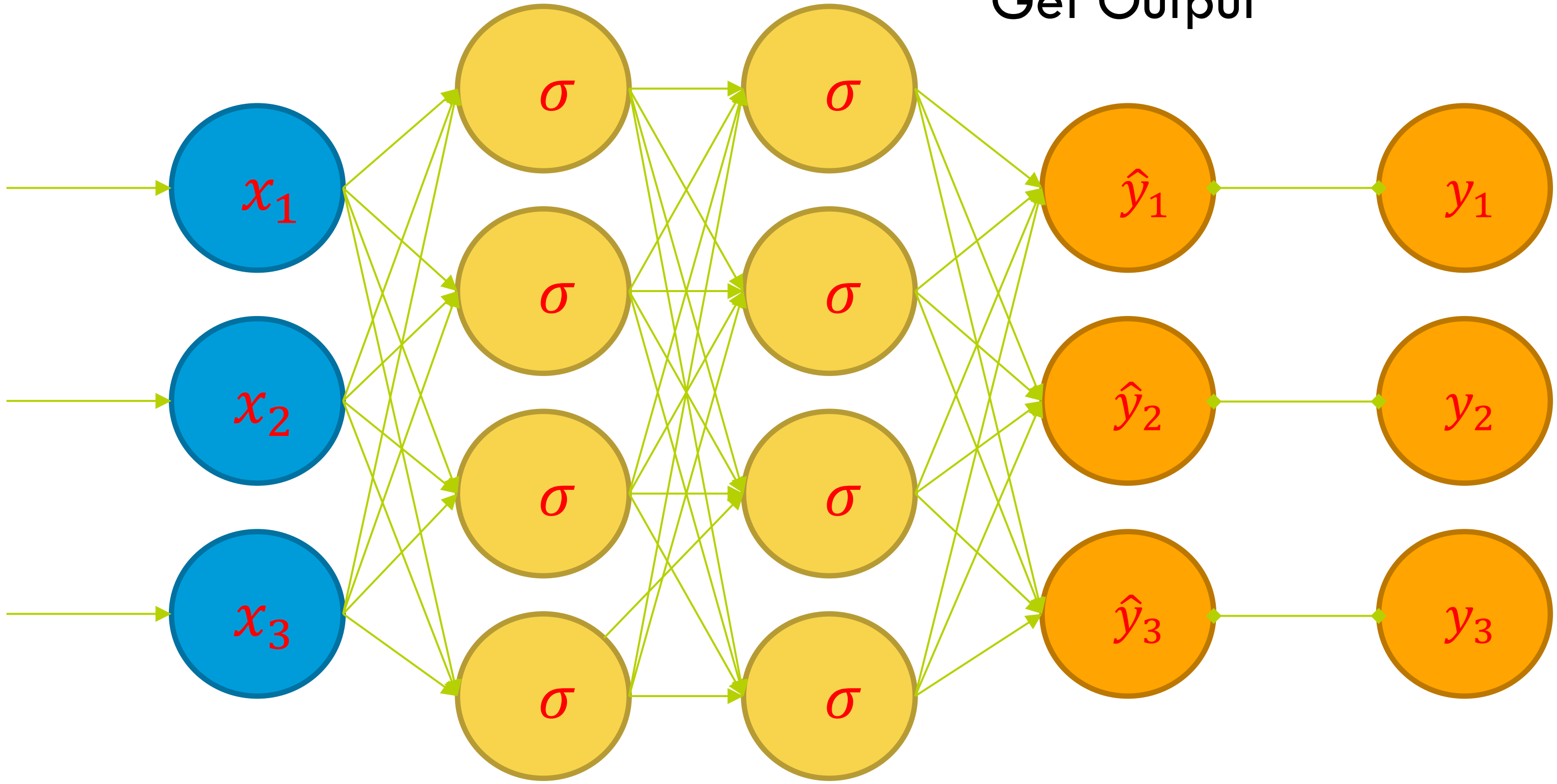


Forward Propagation

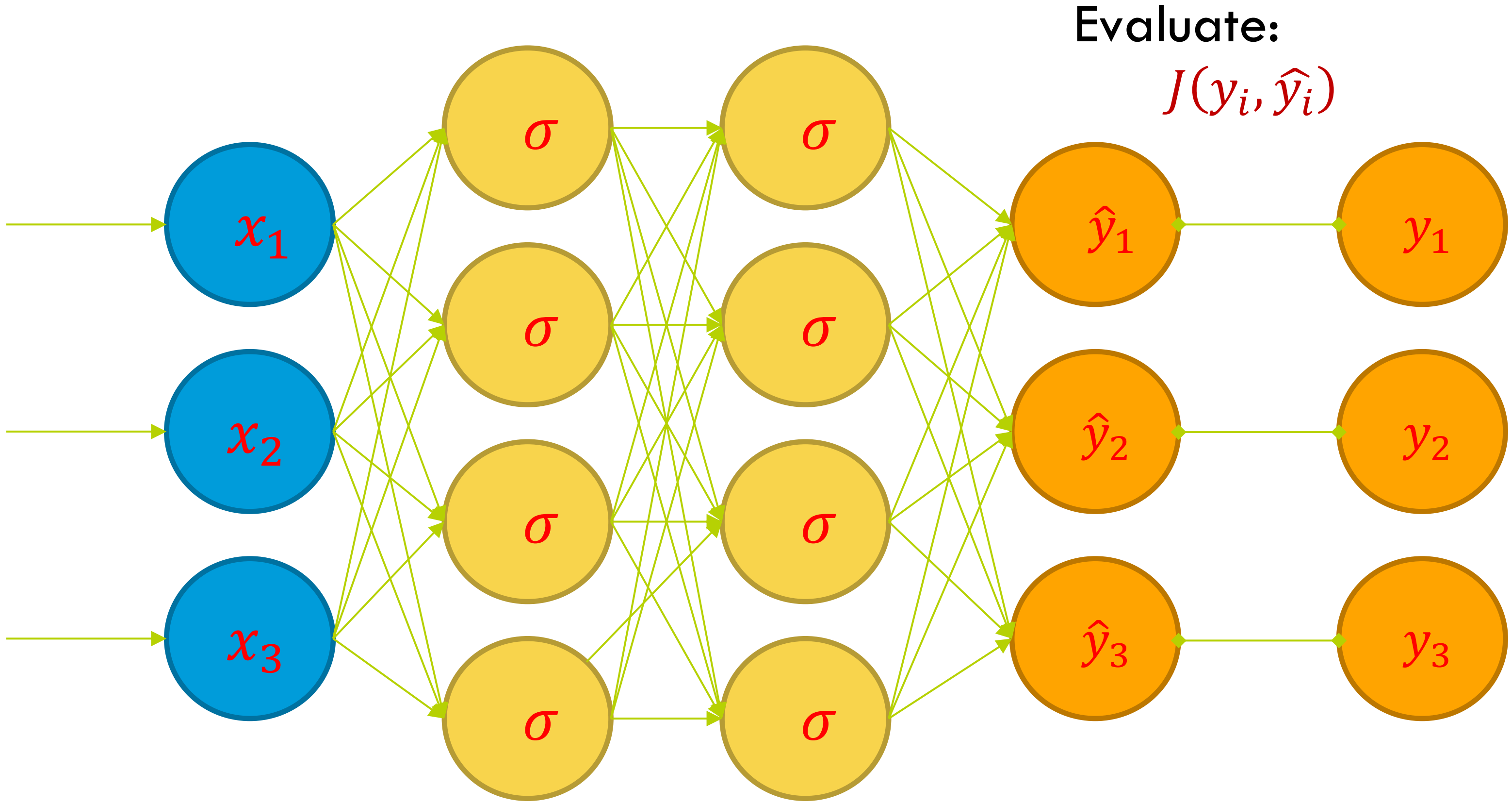


Forward Propagation

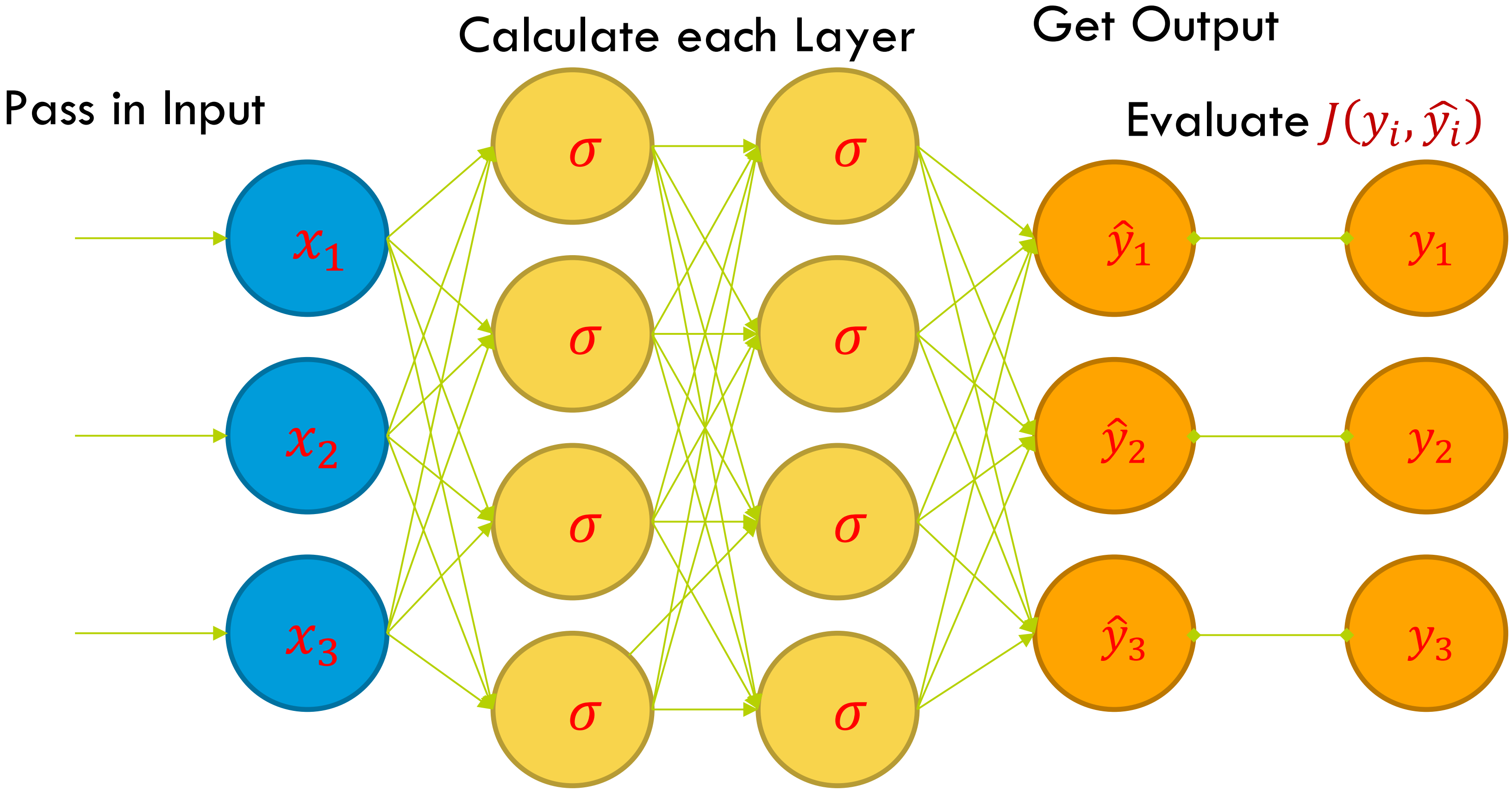
Get Output



Loss Calculation



Loss Calculation



How have we trained before?

- Gradient Descent!

1. Make prediction
2. Calculate Loss
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5. Iterate

How to calculate gradient?

- Chain rule

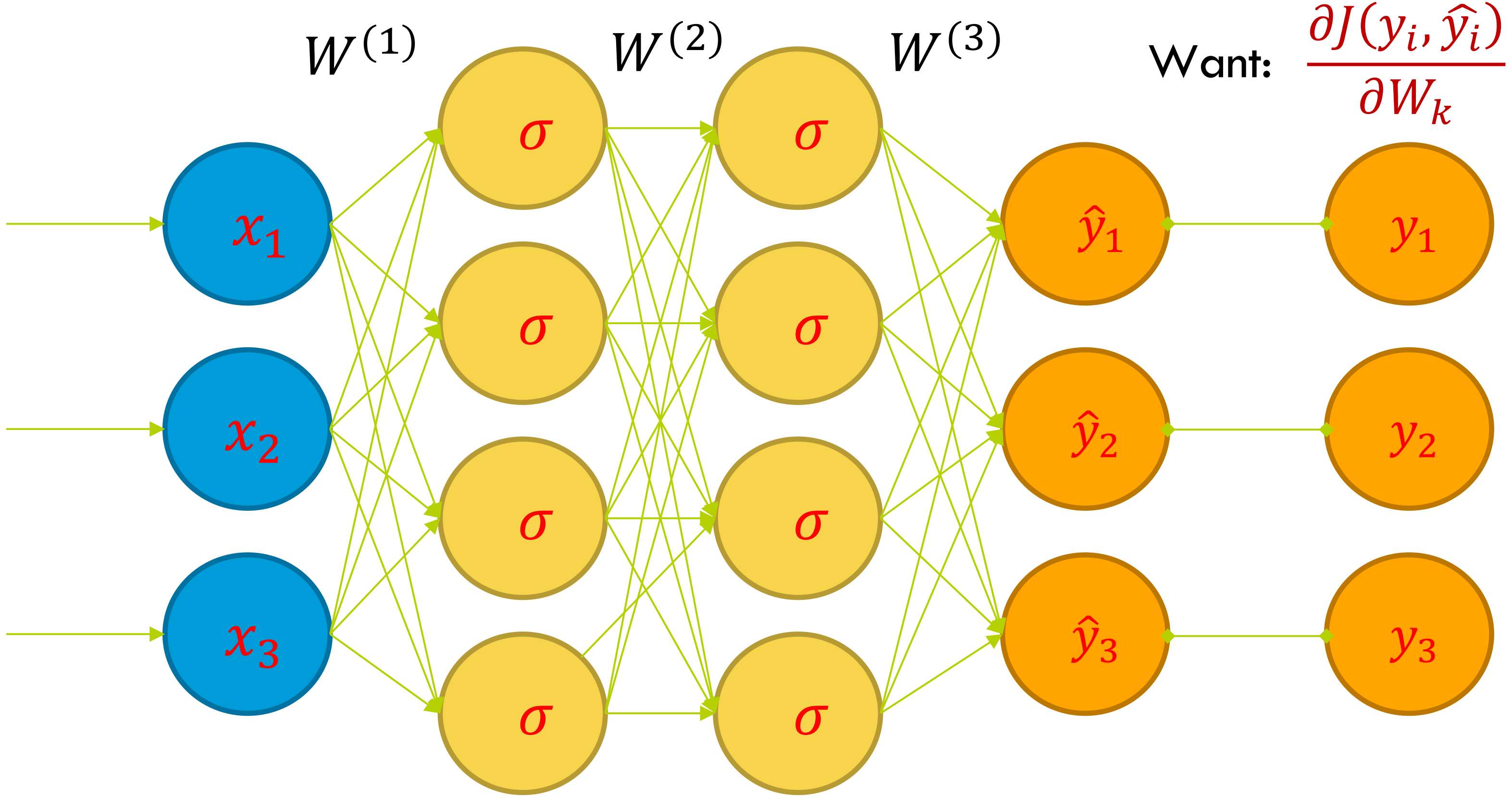
How to Train a Neural Net?

- How could we change the weights to make our Loss Function lower?
- Think of neural net as a function $F: X \rightarrow Y$
- F is a complex computation involving many weights W_k
- Given the structure, the weights "define" the function F (and therefore define our model)
- Loss Function is $J(y, F(x))$

How to Train a Neural Net?

- Get $\frac{\partial J}{\partial W_k}$ for every weight in the network.
- This tells us what direction to adjust each W_k if we want to lower our loss function.
- Make an adjustment and repeat!

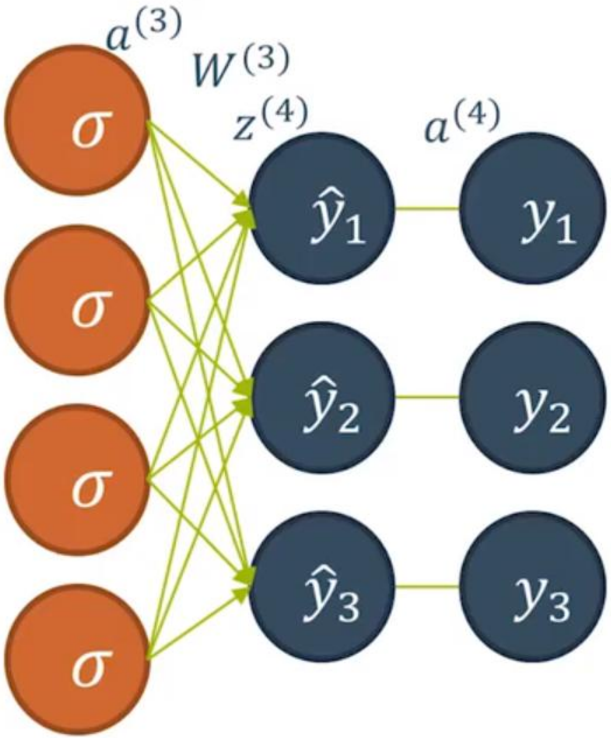
Feedforward Neural Network



Calculus to the Rescue

- Use calculus, chain rule, etc.
- Functions are chosen to have “nice” derivatives
- Numerical issues to be considered

How to calculate gradient



Calculate $\frac{\partial J}{\partial W^{(3)}}$

Where:

$$\frac{\partial J}{\partial W^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial W^{(3)}}$$

How to calculate gradient

Ex. of regression task

Need to Calculate three pieces for $\dfrac{\partial J}{\partial W^{(3)}}$

1. $J = (1/2)\,(a^{(4)} - y)^2$

$$\Rightarrow \frac{\partial J}{\partial a^{(4)}} = 2 * (1/2)(a^{(4)} - y) * 1$$

2. $a^{(4)} = z^{(4)} \quad \Rightarrow. \quad \dfrac{\partial a^{(4)}}{\partial z^{(4)}} = 1$

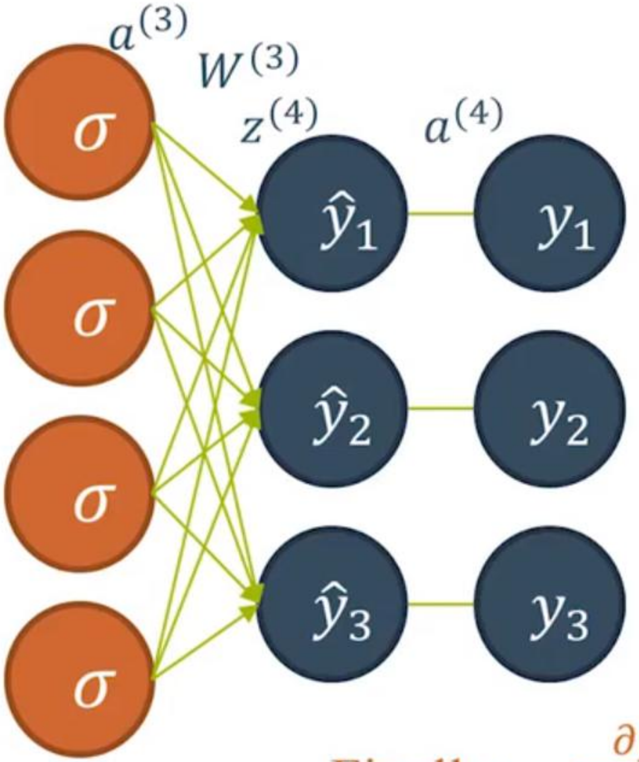
3. $z^{(4)} = a^{(3)} W^{(3)} \quad \Rightarrow \quad \dfrac{\partial z^{(4)}}{\partial W^{(3)}} = a^{(3)}$

Calculate $\dfrac{\partial J}{\partial W^{(3)}}$

Where:

$$\frac{\partial J}{\partial W^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial W^{(3)}}$$

How to calculate gradient



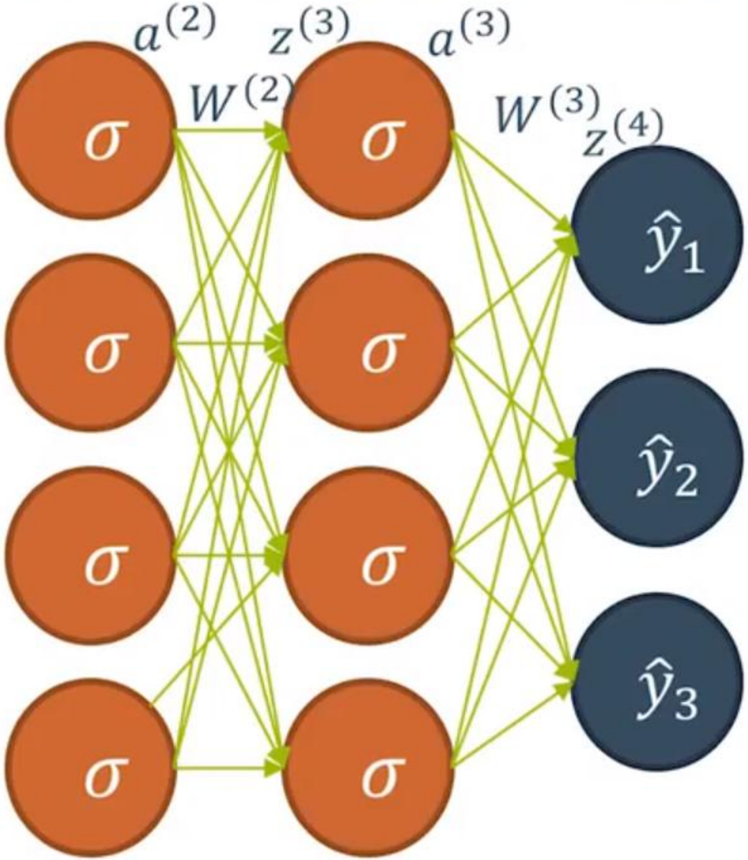
Calculate $\frac{\partial J}{\partial W^{(3)}}$

Where:

$$\frac{\partial J}{\partial W^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial W^{(3)}}$$

Finally: $\frac{\partial J}{\partial W^{(3)}} = (a^{(4)} - y) * a^{(3)}$

How to calculate gradient



Calculate $\frac{\partial J}{\partial W^{(2)}}$

Where:

$$\frac{\partial J}{\partial W^{(2)}} = \frac{\partial J}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial W^{(2)}}$$

and

$$\frac{\partial J}{\partial a^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial a^{(3)}}$$

How to calculate gradient

Need to calculate three new pieces for $\dfrac{\partial J}{\partial W^{(2)}}$

1. $z^{(3)} = a^{(2)} W^{(2)} \quad \Longrightarrow \quad \dfrac{\partial z^{(3)}}{\partial W^{(2)}} = a^{(2)}$

2. $a^{(3)} = \dfrac{1}{1+e^{-z^{(3)}}}$

Sigmoid function

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

$$\Longrightarrow \frac{\partial a^{(3)}}{\partial z^{(3)}} = \sigma'(z^{(3)}) = \sigma(z^{(3)})(1-\sigma(z^{(3)}))$$

3. $z^{(4)} = a^{(3)} W^{(3)} \quad \Longrightarrow. \quad \dfrac{\partial z^{(4)}}{\partial a^{(3)}} = W^{(3)}$

Calculate $\dfrac{\partial J}{\partial W^{(2)}}$

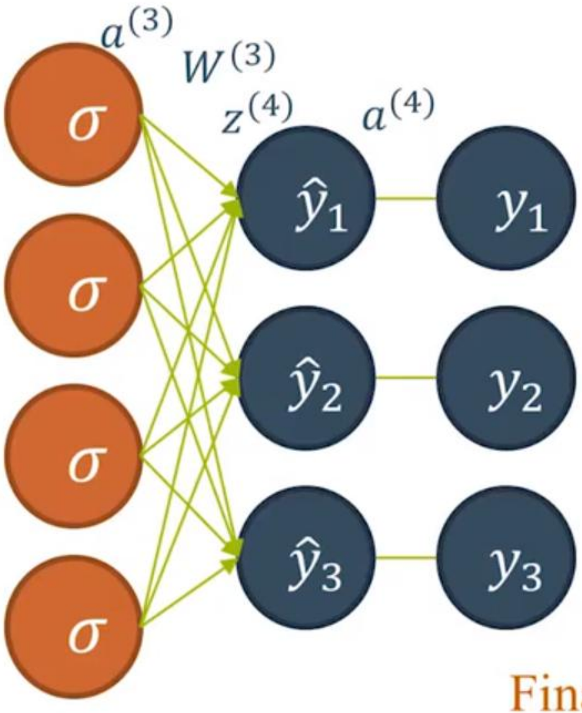
Where:

$$\frac{\partial J}{\partial W^{(2)}} = \frac{\partial J}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial W^{(2)}}$$

and

$$\frac{\partial J}{\partial a^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial a^{(3)}}$$

How to calculate gradient



Calculate $\frac{\partial J}{\partial W^{(2)}}$

Where:

$$\frac{\partial J}{\partial W^{(2)}} = \frac{\partial J}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial W^{(2)}}$$

and

$$\frac{\partial J}{\partial a^{(3)}} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \frac{\partial z^{(4)}}{\partial a^{(3)}}$$

Finally:

$$\frac{\partial J}{\partial W^{(2)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma\left(z^{(3)}\right)\left(1 - \sigma\left(z^{(3)}\right)\right) \cdot a^{(2)}$$

Punchline

$$\frac{\partial J}{\partial W^{(3)}} = (\hat{y} - y) \cdot a^{(3)}$$

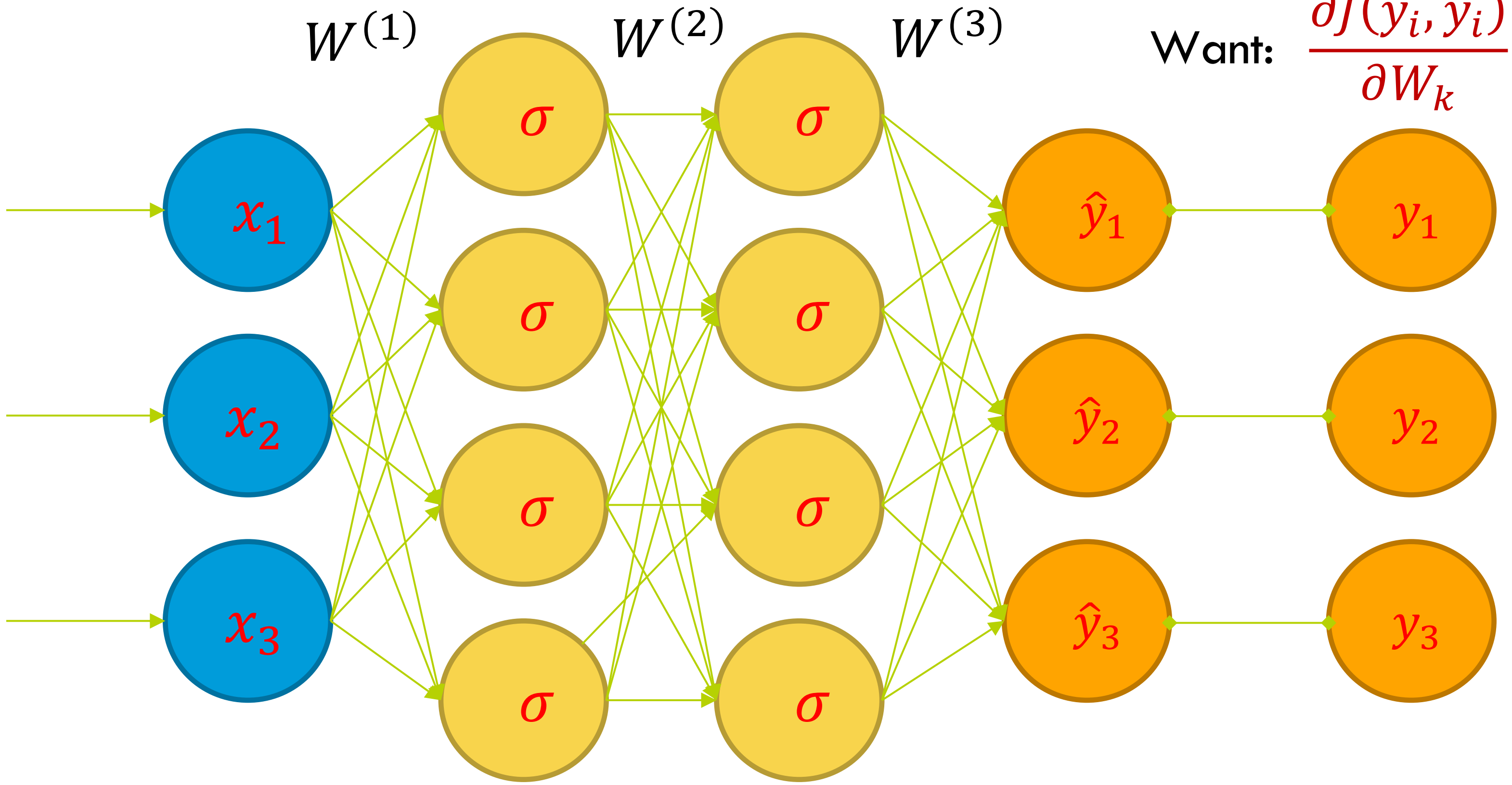
$$\frac{\partial J}{\partial W^{(2)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot a^{(2)}$$

$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot W^{(2)} \cdot \sigma'\left(z^{(2)}\right) \cdot X$$

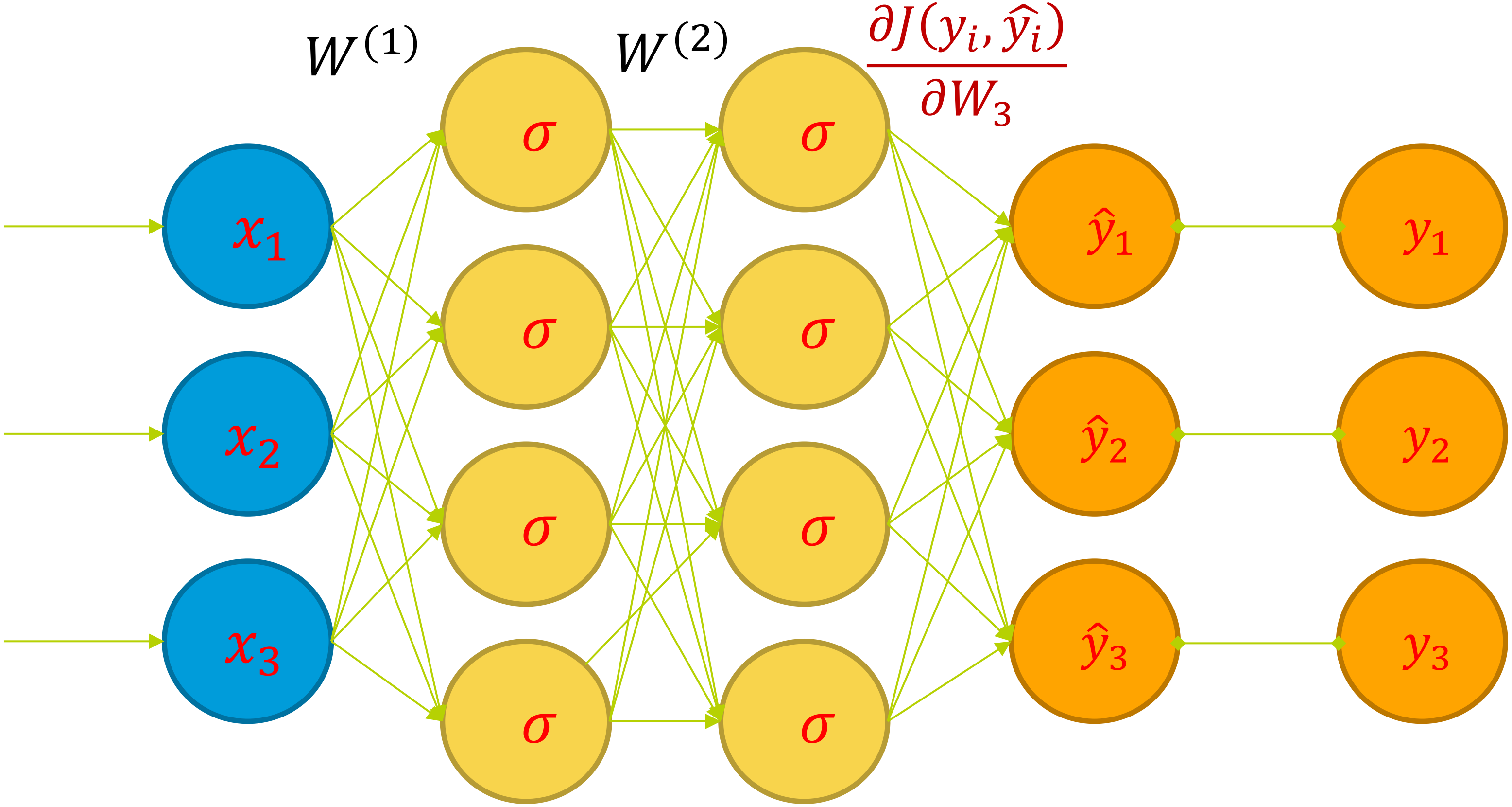
- Recall that: $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
- Though they appear complex, above are easy to compute!

Backpropagation

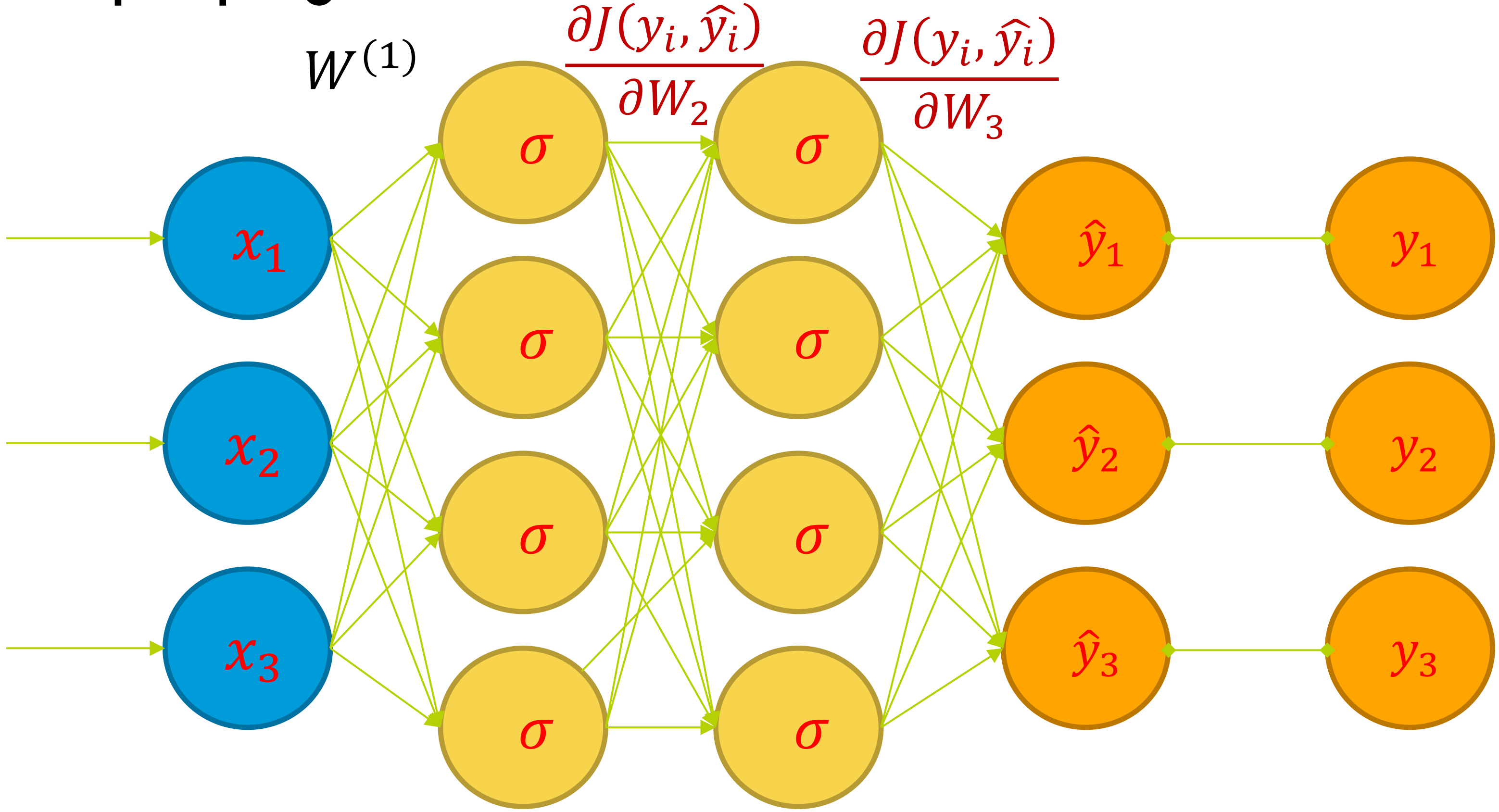
Want: $\frac{\partial J(y_i, \hat{y_i})}{\partial W_k}$



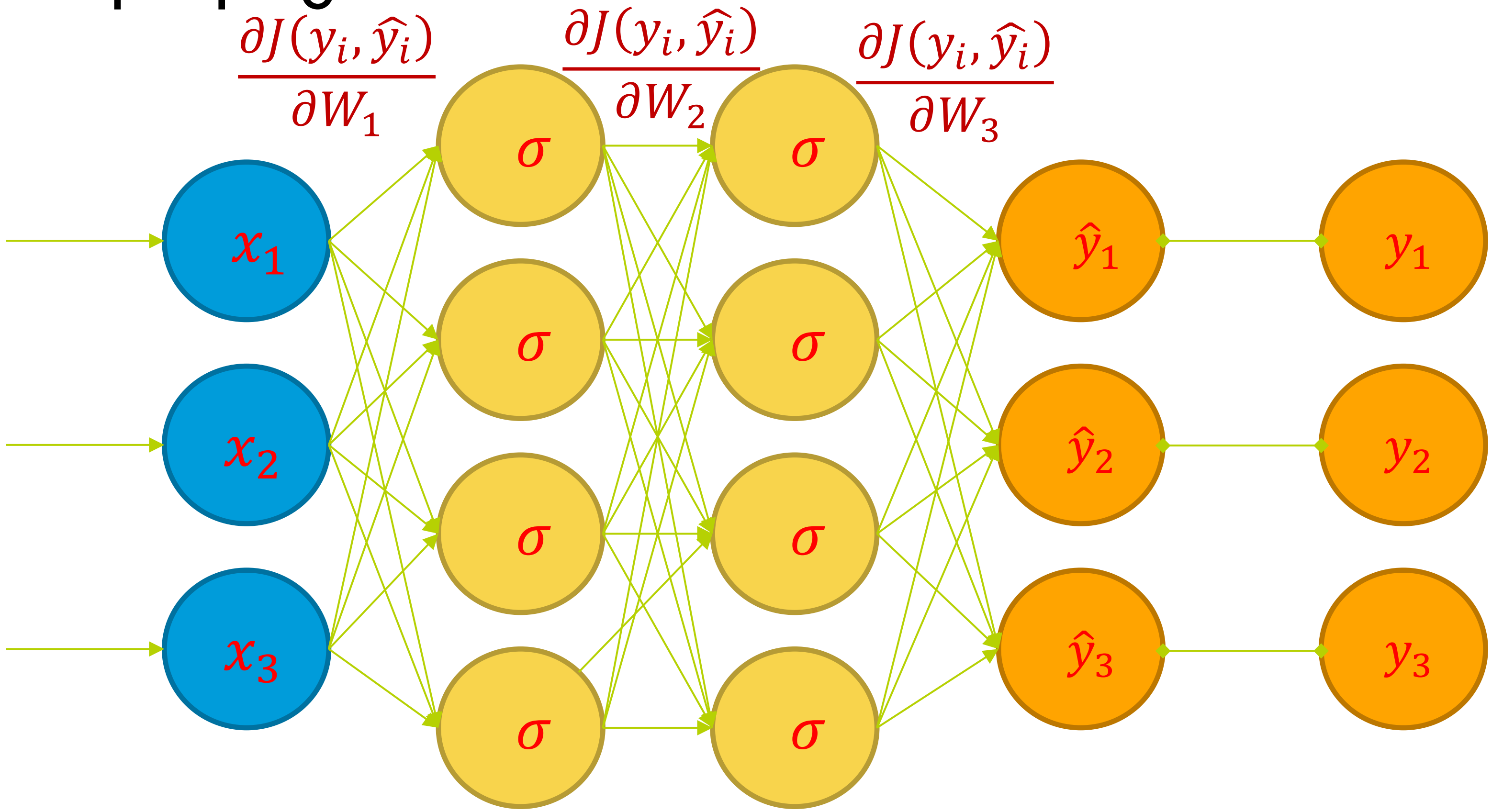
Backpropagation



Backpropagation



Backpropagation



How have we trained before?

- Gradient Descent!

1. Make prediction
2. Calculate Loss
3. Calculate gradient of the loss function w.r.t. parameters
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5. Iterate

Vanishing Gradients

Recall that:

$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot W^{(2)} \cdot \sigma'\left(z^{(2)}\right) \cdot X$$

- Remember: $\sigma'(z) = \sigma(z)\big(1 - \sigma(z)\big) \leq .25$
- As we have more layers, the gradient gets very small at the early layers.
- This is known as the “vanishing gradient” problem.
- For this reason, other activations (such as ReLU) have become more common.

Other Activation Functions

Hyperbolic Tangent Function

- Hyperbolic tangent function
- Pronounced “tanch”

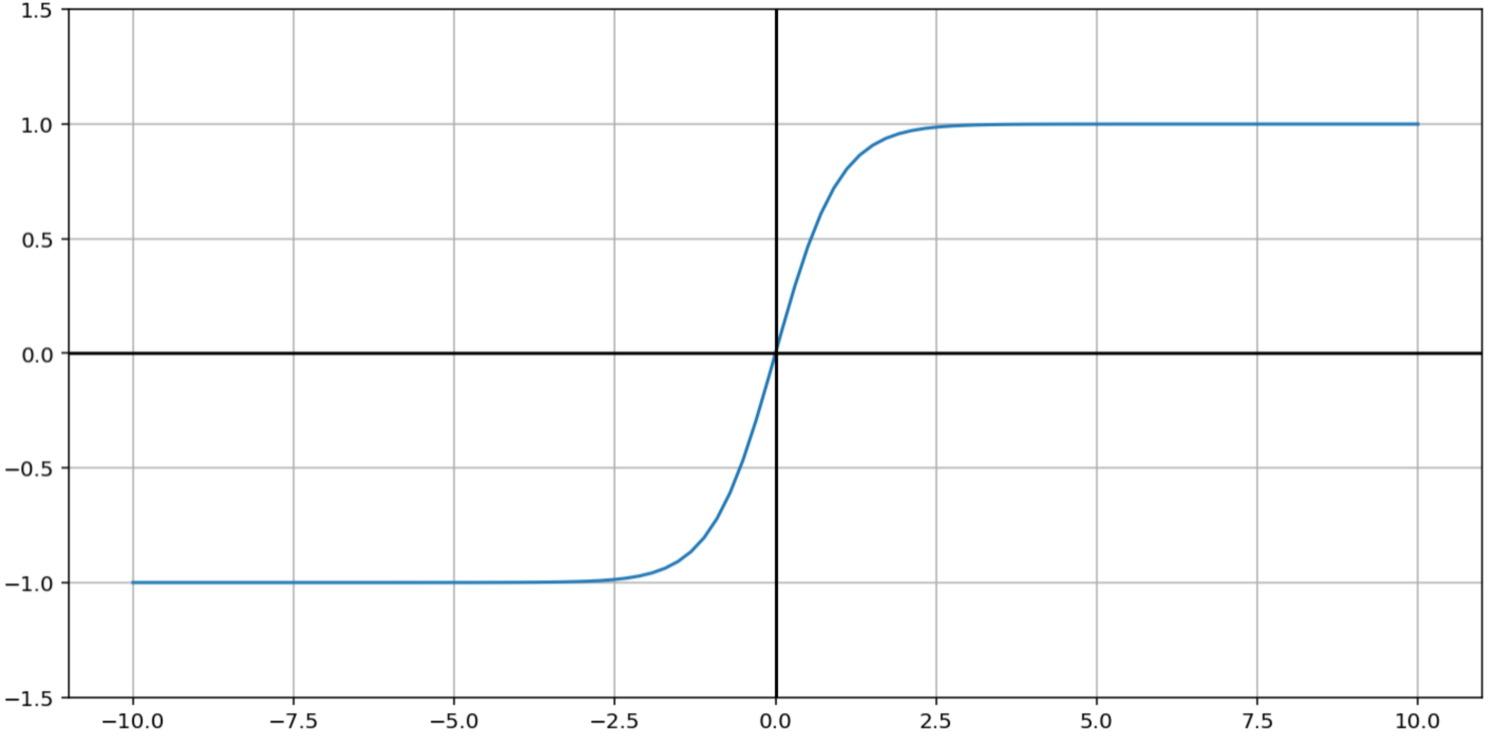
$$tanh(z) = \frac{\sinh(z)}{\cosh(z)} = \frac{e^{2x} - 1}{e^{2x} + 1}$$

$$tanh(0) = 0$$

$$tanh(\infty) = 1$$

$$tanh(-\infty) = -1$$

Hyperbolic Tangent Function



Rectified Linear Unit (ReLU)

$$ReLU(z) = \begin{cases} 0, & z < 0 \\ z, & z \geq 0 \end{cases}$$

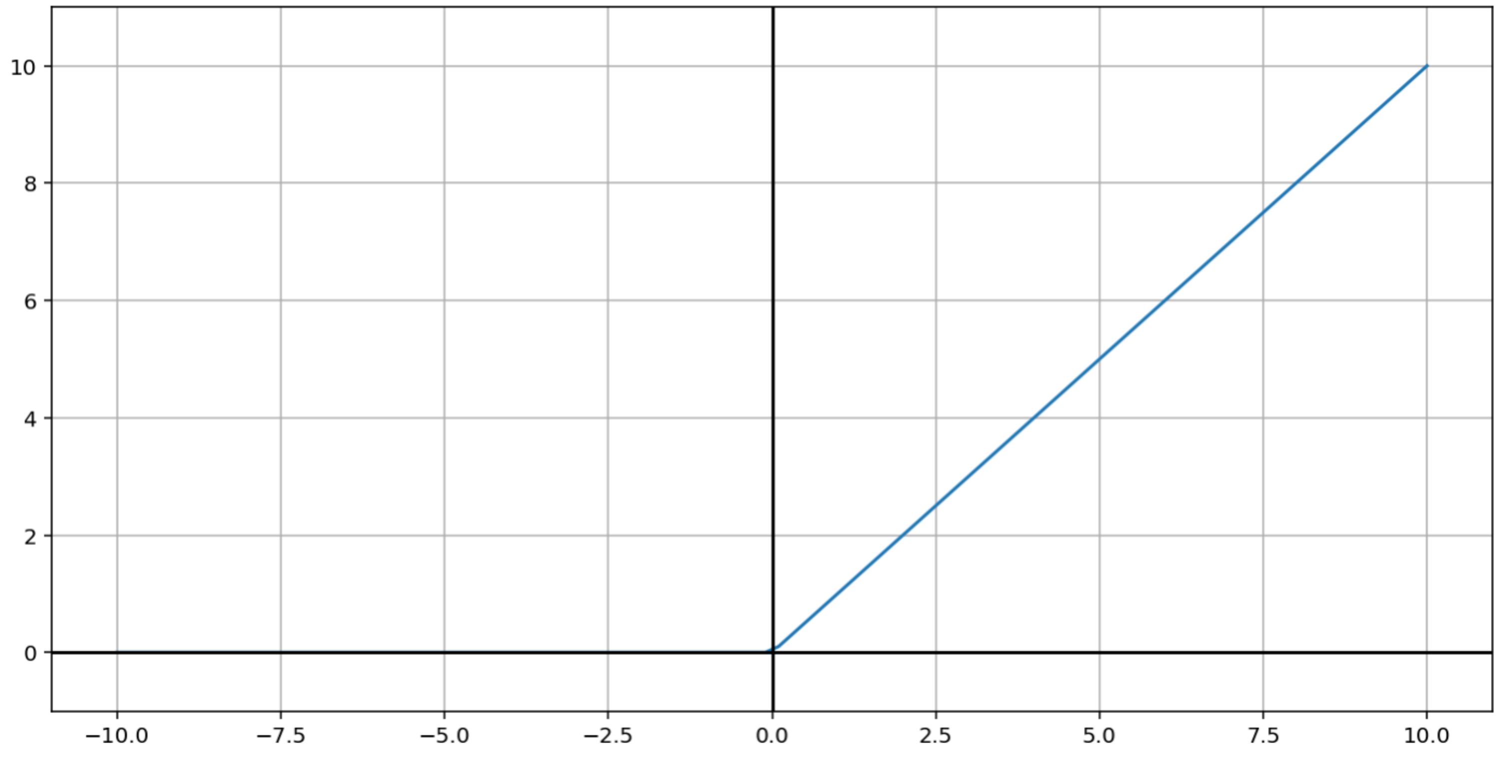
$$= \max(0, z)$$

$$ReLU(0) = 0$$

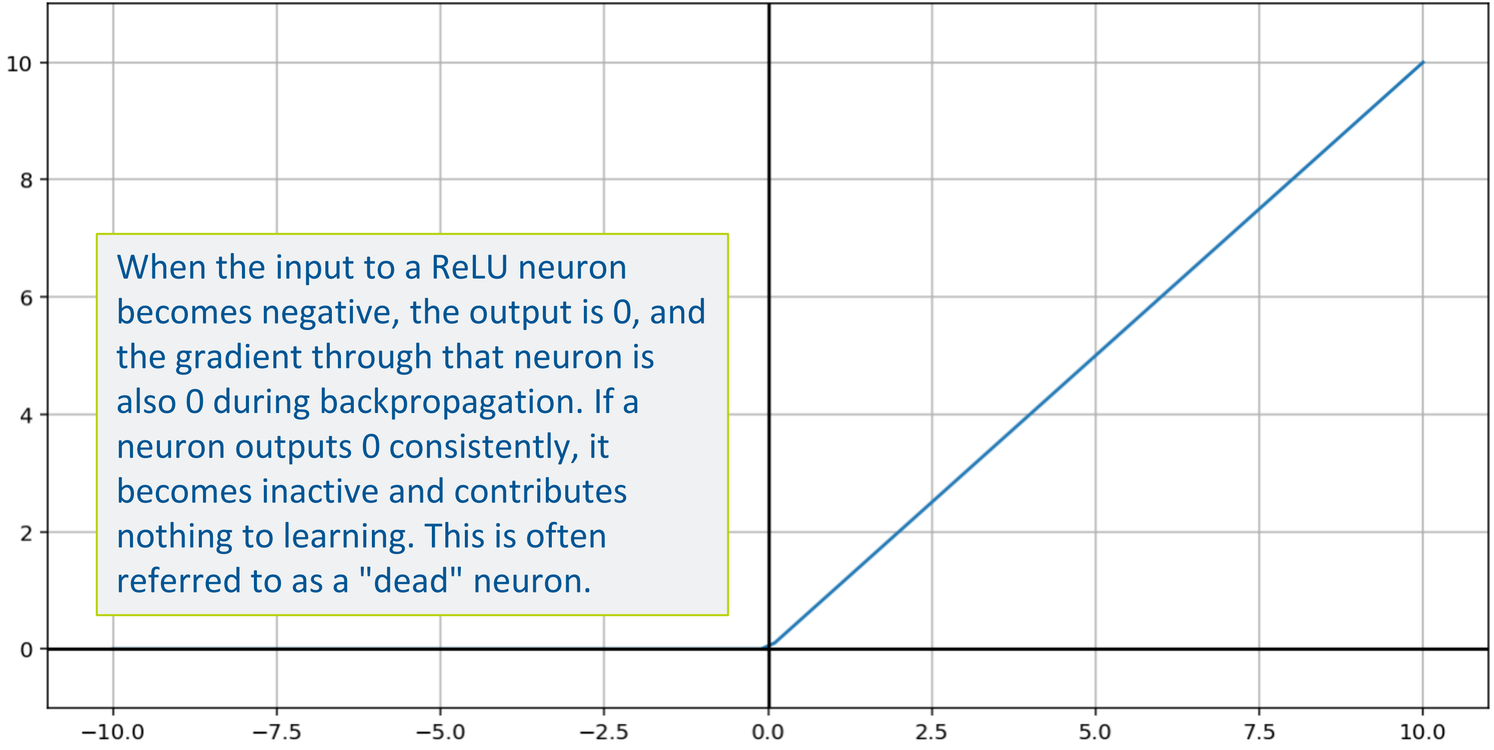
$$ReLU(z) = z \qquad \text{for } (z \gg 0)$$

$$ReLU(-z) = 0$$

Rectified Linear Unit (ReLU)



Dying ReLU Problem



When the input to a ReLU neuron becomes negative, the output is 0, and the gradient through that neuron is also 0 during backpropagation. If a neuron outputs 0 consistently, it becomes inactive and contributes nothing to learning. This is often referred to as a "dead" neuron.

“Leaky” Rectified Linear Unit (ReLU)

$$LReLU(z) = \begin{cases} \alpha z, & z < 0 \\ z, & z \geq 0 \end{cases}$$

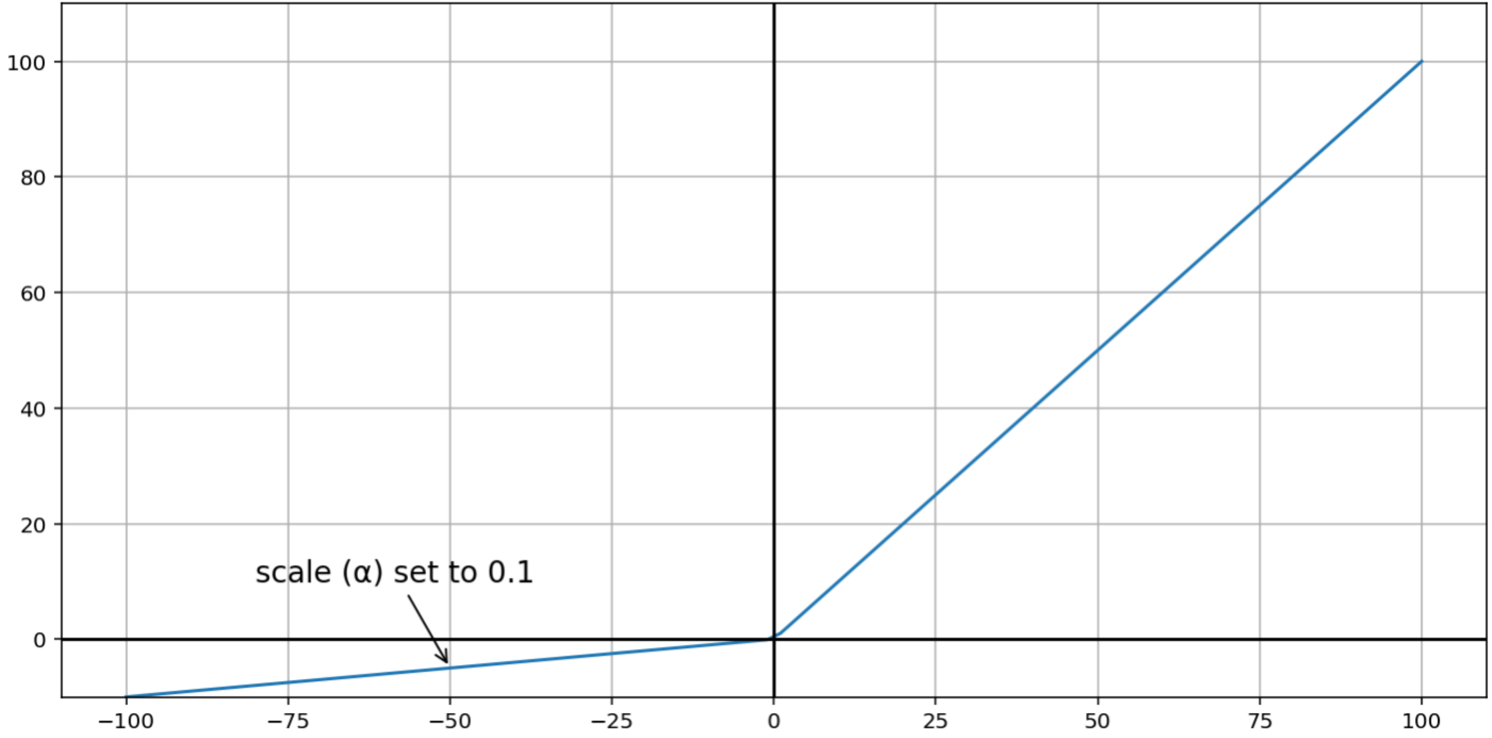
$$= \max(\alpha z, z) \quad \text{for } (\alpha < 1)$$

$$LReLU(0) = 0$$

$$LReLU(z) = z \quad \text{for } (z \gg 0)$$

$$LReLU(-z) = -\alpha z$$

"Leaky" Rectified Linear Unit (ReLU)



Softmax Activation Function

- For multiclass classification problems, let the final layer be a vector with length equal to the number of possible classes.
- Extension of sigmoid to multiclass is the softmax function.
- Yields a vector with entries that are between 0 and 1, and sum to 1

$$softmax(z_i) = \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}$$

Comparison and Guidelines

Function	Range	Use Case	Pros	Cons
ReLU	$[0, \infty)$	Hidden layers	Simple, efficient; reduces vanishing gradients	Dying neurons (zero gradients for $x < 0$)
Leaky ReLU	$(-\infty, \infty)$	Hidden layers (fix Dying ReLU)	Avoids zero gradients for $x < 0$	Requires tuning of α (leak factor)
Sigmoid	$(0, 1)$	Binary classification output	Outputs probabilities	Vanishing gradients for extreme inputs
Tanh	$(-1, 1)$	Hidden layers	Zero-centered output, better than sigmoid for some cases	Vanishing gradients for large inputs
Softmax	$(0, 1)$	Multiclass classification output	Outputs probabilities summing to 1	Computationally expensive; not suitable for hidden layers
Linear	$(-\infty, \infty)$	Regression tasks	Simple; suitable for outputs in regression tasks	No non-linearity; limited learning capacity

What next?

- We now know how to make a single update to a model given some data.
- But how do we do the full training?
- We will dive into these details in the next lecture.

Software