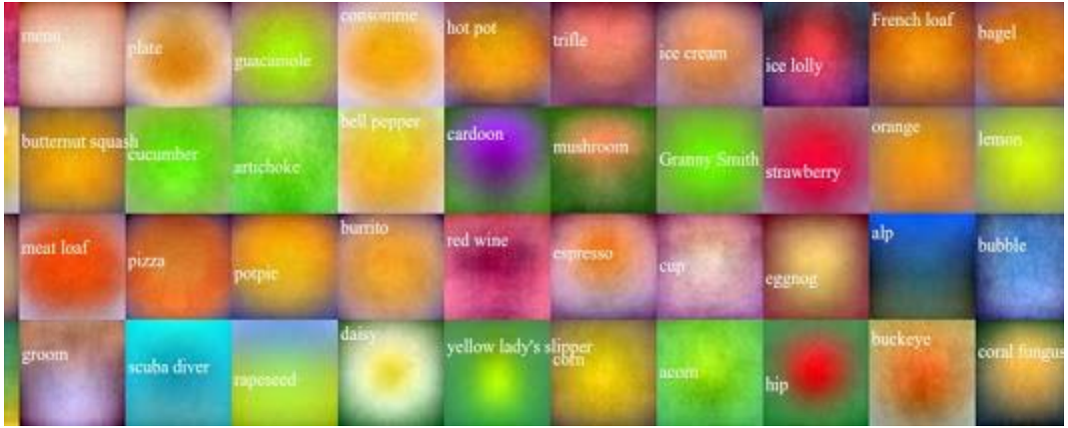
Optimization and Backpropagation

Lecture 3 Recap

Neural Network

- Linear score function $\boldsymbol{f} = \boldsymbol{W}\boldsymbol{x}$

On CIFAR-10



On ImageNet

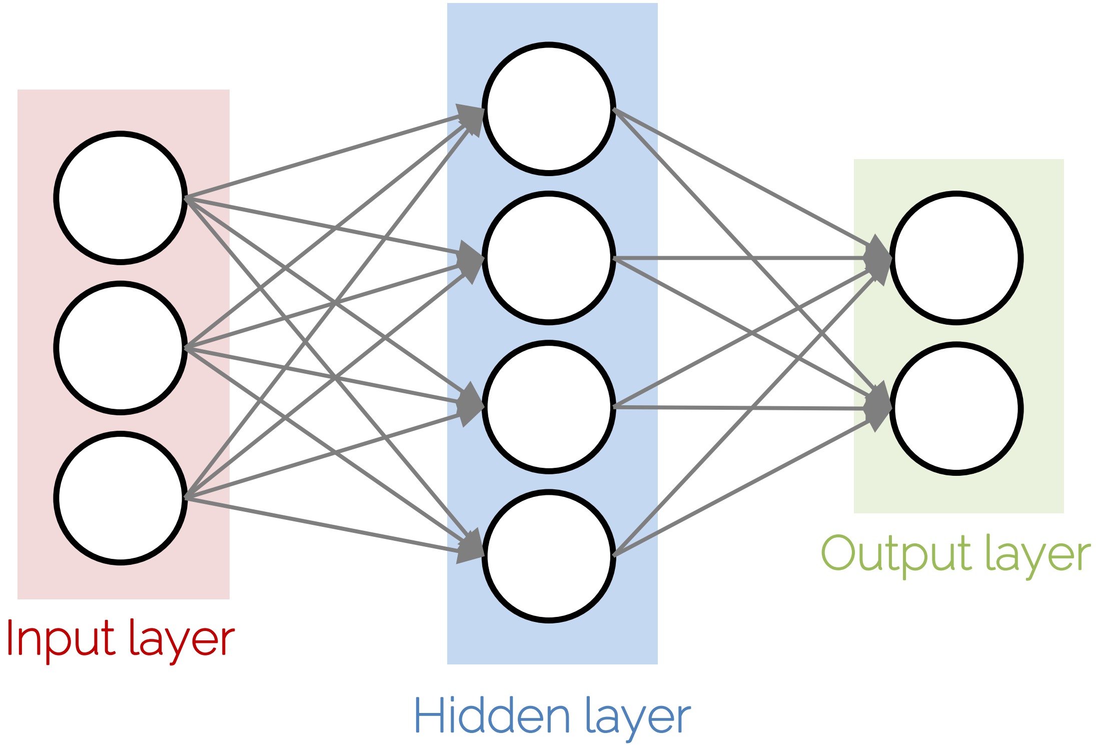
Credit: Li/Karpathy/Johnson

Neural Network

- Linear score function $\boldsymbol{f} = \boldsymbol{W}\boldsymbol{x}$

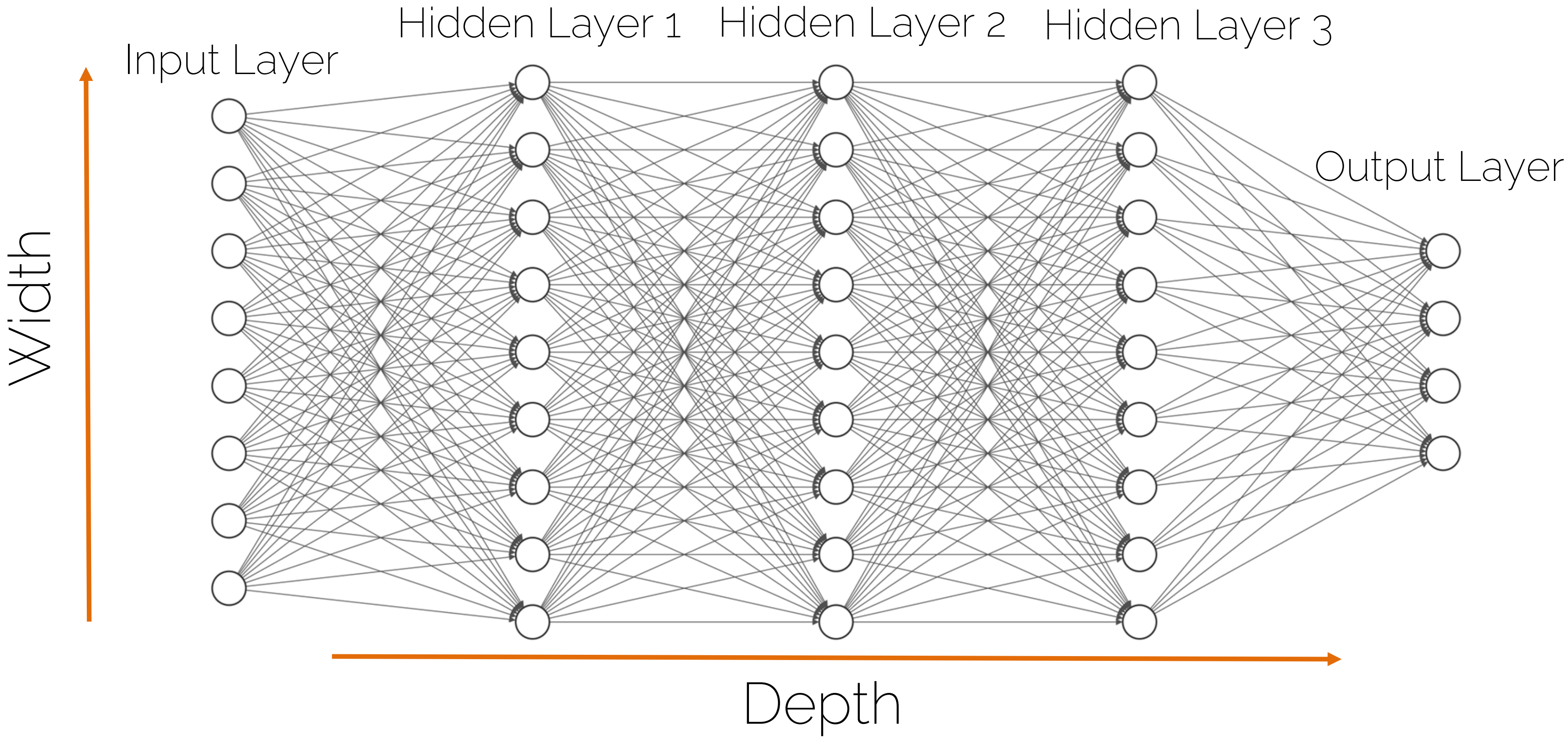
- Neural network is a nesting of 'functions'
  - 2-layers: $\boldsymbol{f} = \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1\boldsymbol{x})$
  - 3-layers: $\boldsymbol{f} = \boldsymbol{W}_3 \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1\boldsymbol{x}))$
  - 4-layers: $\boldsymbol{f} = \boldsymbol{W}_4 \tanh\left(\boldsymbol{W}_3, \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1\boldsymbol{x}))\right)$
  - 5-layers: $\boldsymbol{f} =$ $\boldsymbol{W}_5\sigma(\boldsymbol{W}_4 \tanh(\boldsymbol{W}_3, \max(\boldsymbol{0}, \boldsymbol{W}_2 \max(\boldsymbol{0}, \boldsymbol{W}_1\boldsymbol{x}))))$
  - ... up to hundreds of layers

Neural Network



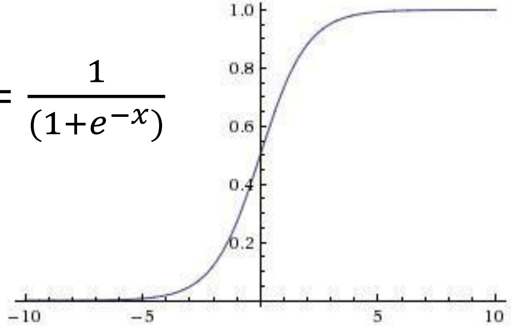
Credit: Li/Karpathy/Johnson

Neural Network

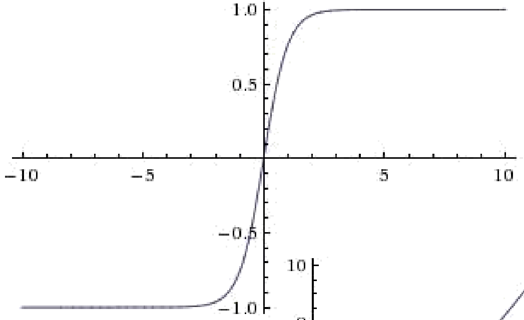


Activation Functions

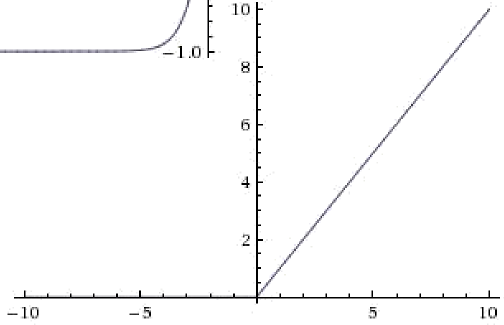
Sigmoid: $\sigma(x) = \frac{1}{(1+e^{-x})}$



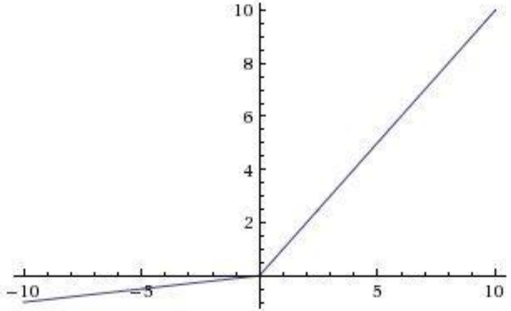
tanh: $\tanh(x)$



ReLU: $\max(0, x)$



Leaky ReLU: $\max(0.1x, x)$



Parametric ReLU: $\max(\alpha x, x)$

Maxout $\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU $f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases}$

Loss Functions

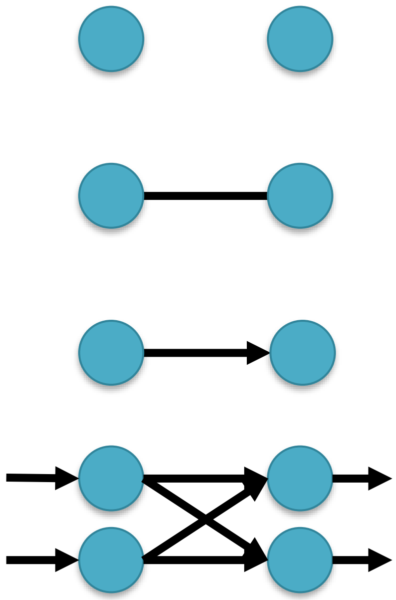
- Measure the goodness of the predictions (or equivalently, the network's performance)

- Regression loss
  - L1 loss $\boldsymbol{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n \|y_i - \hat{y}_i\|_1$
  - MSE loss $\boldsymbol{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}; \boldsymbol{\theta}) = \frac{1}{n} \sum_i^n \|y_i - \hat{y}_i\|_2^2$

- Classification loss (for multi-class classification)
  - Cross Entropy loss $E(y, \hat{y}; \theta) = -\sum_{i=1}^n \sum_{k=1}^K (y_{ik} \cdot \log \hat{y}_{ik})$

Computational Graphs

- Neural network is a computational graph
  - It has compute nodes
  - It has edges that connect nodes
  - It is directional
  - It is organized in 'layers'



Backprop

The Importance of Gradients

- Our optimization schemes are based on computing gradients

$$\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

- One can compute gradients analytically but what if our function is too complex?

- Break down gradient computation

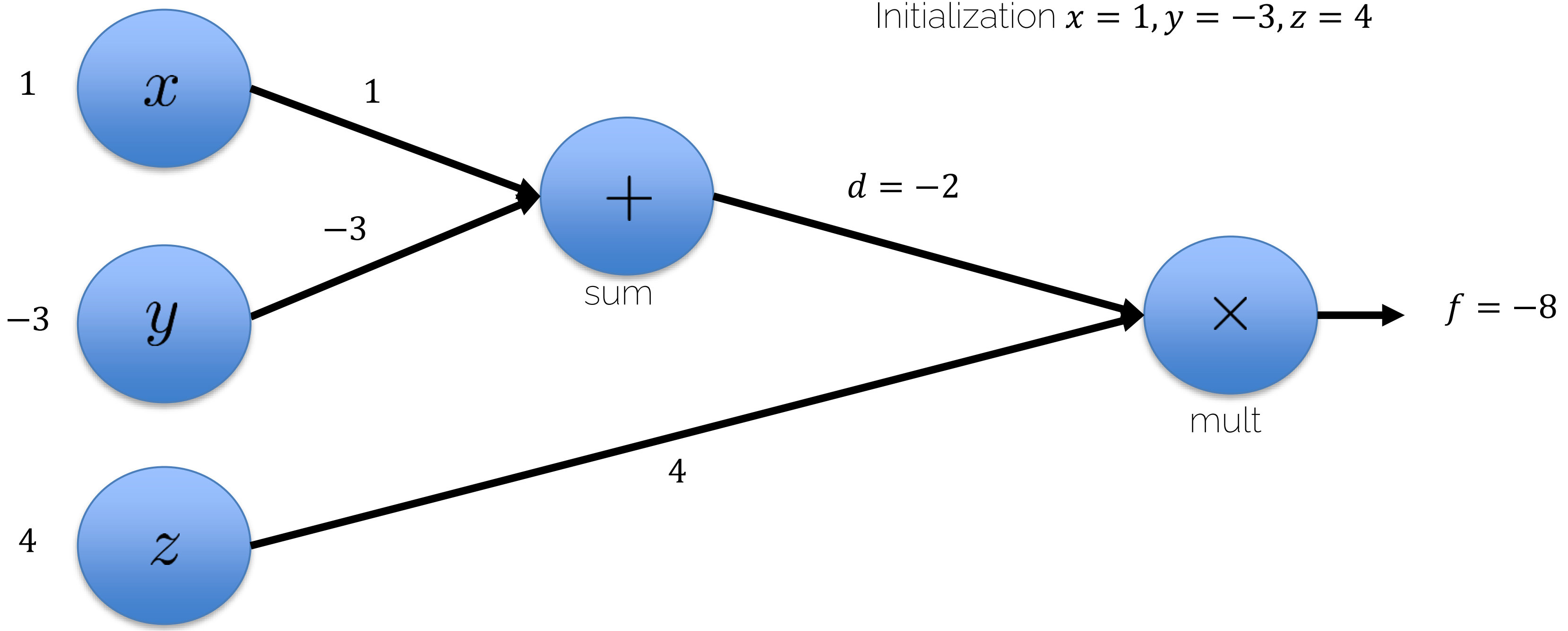
Backpropagation

Done by many people before, but often credited to Rumelhart 1986

Backprop: Forward Pass

- $f(x, y, z) = (x + y) \cdot z$

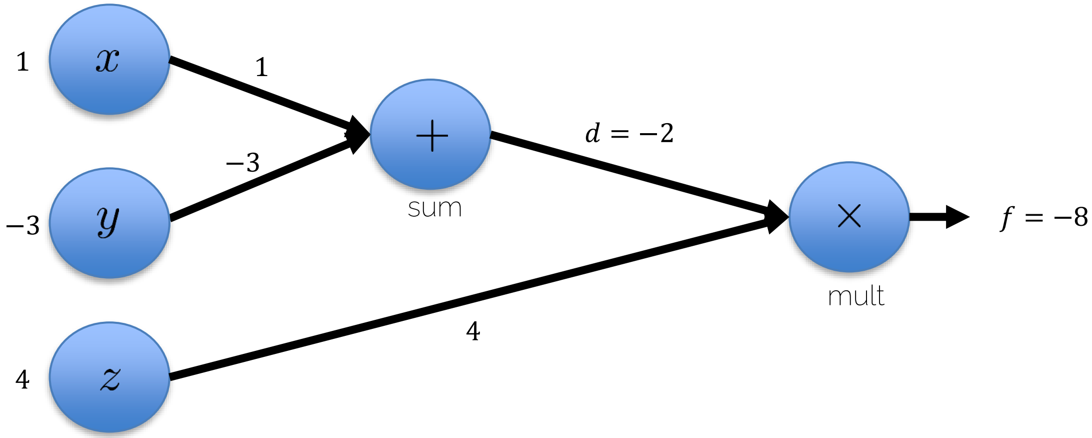
Initialization $x = 1, y = -3, z = 4$



Backprop: Backward Pass

$$f(x, y, z) = (x + y) \cdot z$$

with $x = 1, y = -3, z = 4$



$d = x + y$ $\qquad \dfrac{\partial d}{\partial x} = 1, \dfrac{\partial d}{\partial y} = 1$

$f = d \cdot z$ $\qquad \dfrac{\partial f}{\partial d} = z, \dfrac{\partial f}{\partial z} = d$

What is $\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}, \dfrac{\partial f}{\partial z}$?

Backprop: Backward Pass

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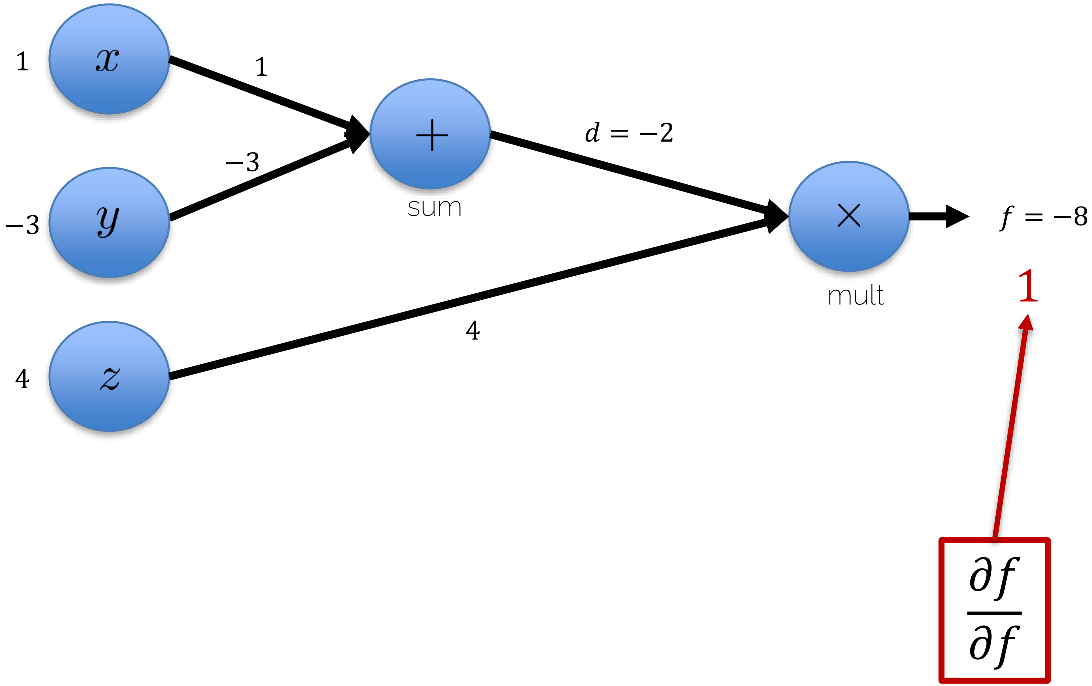
with $x = 1, y = -3, z = 4$



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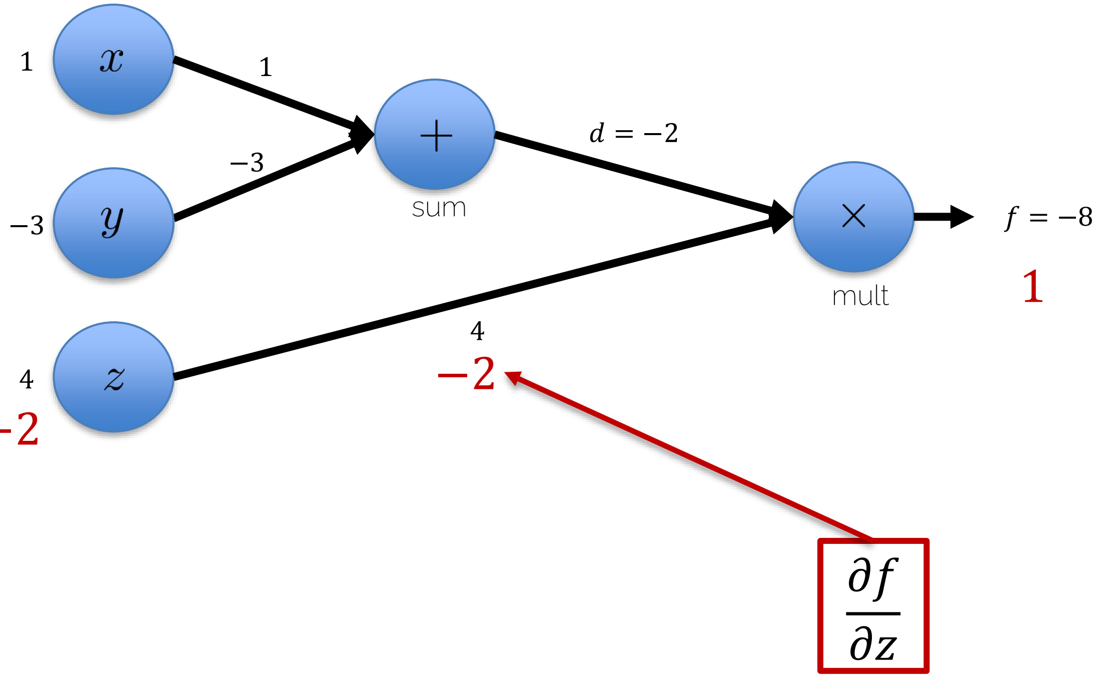

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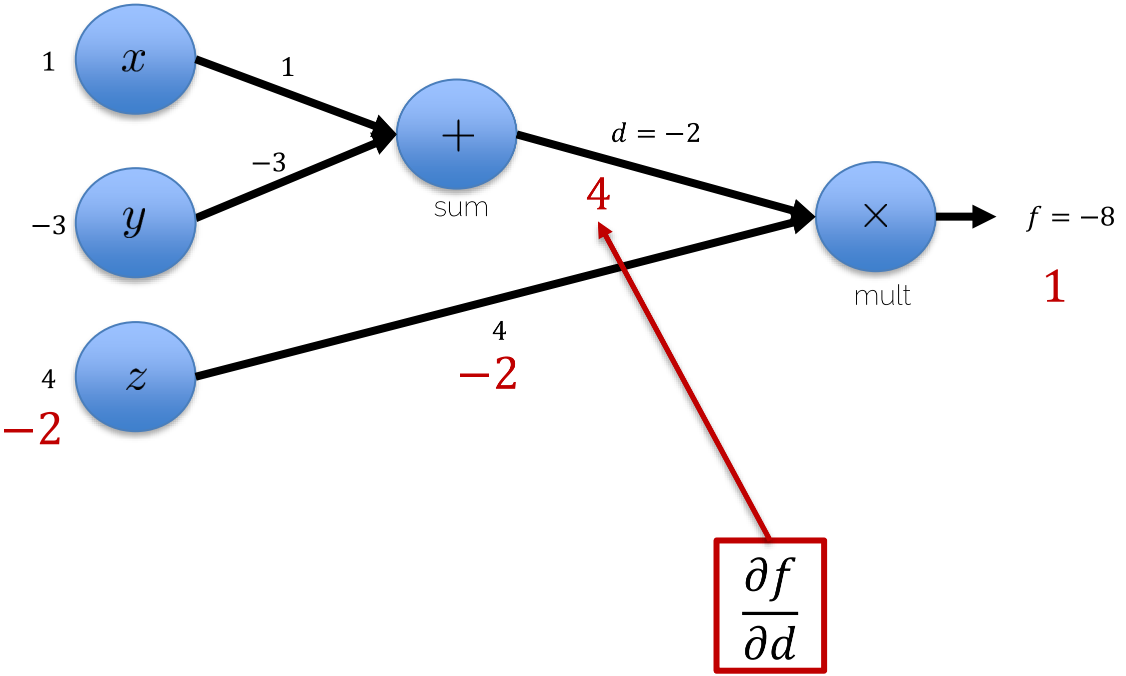

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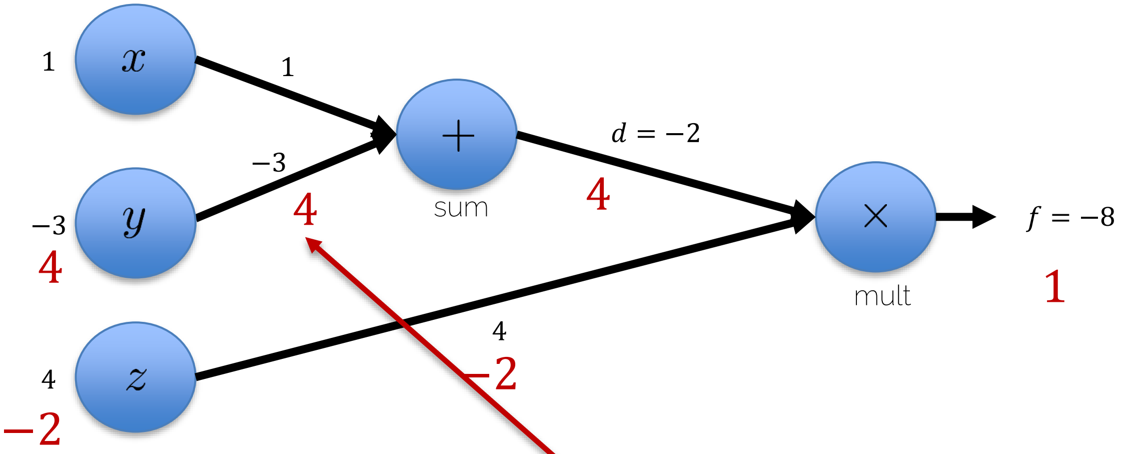

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Chain Rule:

$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial f}{\partial d} \cdot \frac{\partial d}{\partial y}}$$

$$\to \frac{\partial f}{\partial y} = 4 \cdot 1 = 4$$

$$\boxed{\frac{\partial f}{\partial y}}$$

What is $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$?

Backprop: Backward Pass

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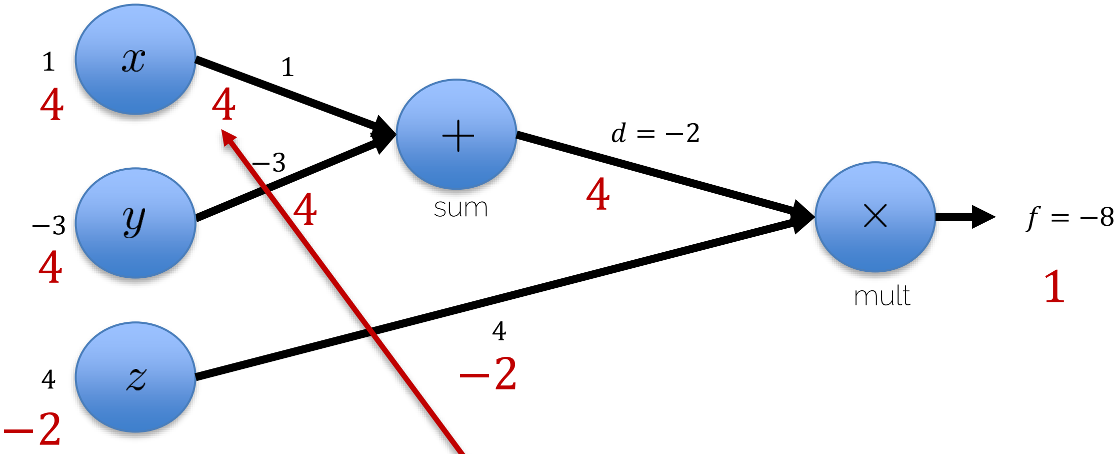


$$\boxed{\frac{\partial f}{\partial x}}$$

Chain Rule:

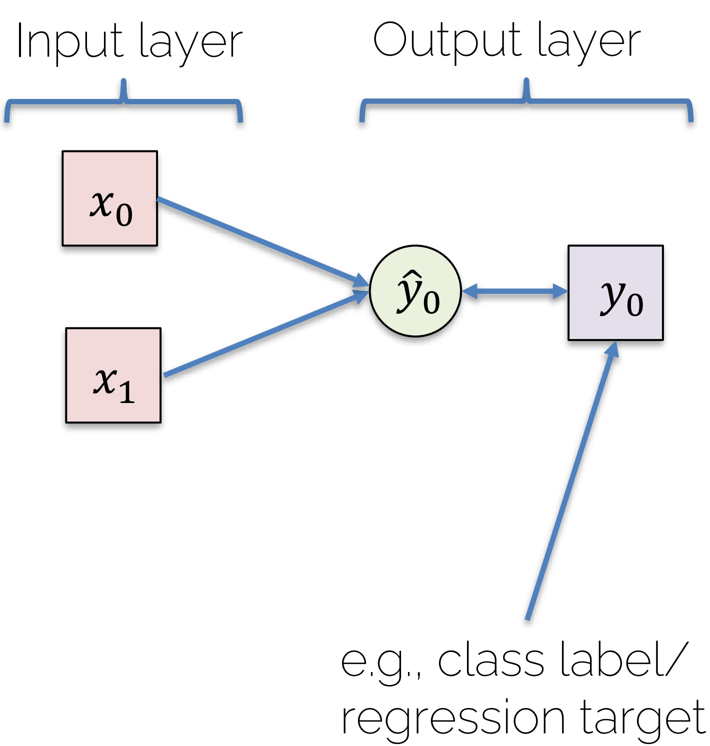
$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial f}{\partial d} \cdot \frac{\partial d}{\partial y}}$$

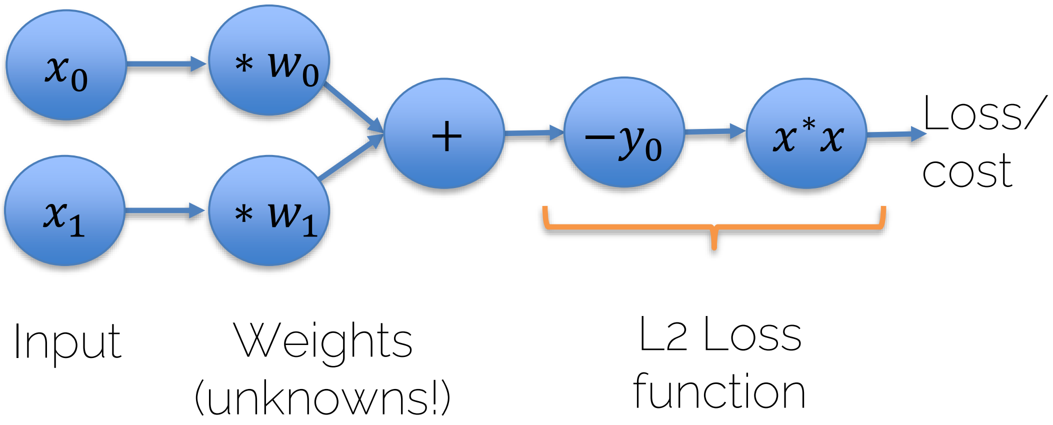
$$\rightarrow \frac{\partial f}{\partial x} = 4 \cdot 1 = 4$$

Compute Graphs -> Neural Networks

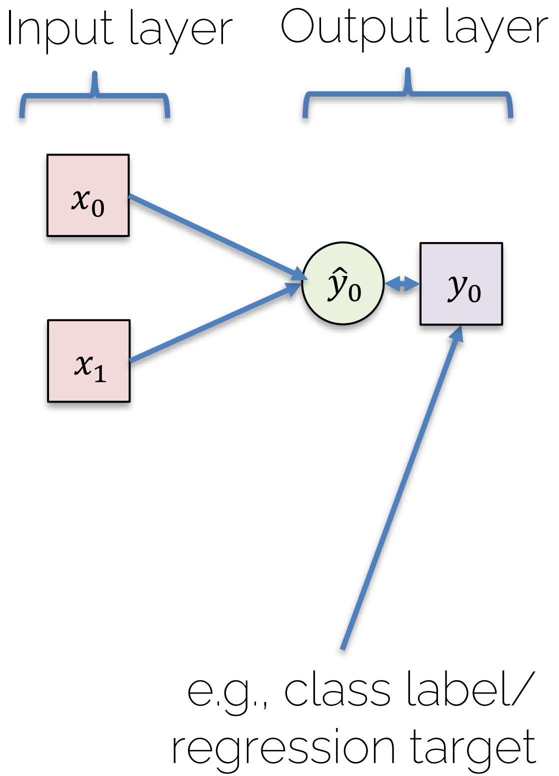
- x_k input variables
- $w_{l,m,n}$ network weights (note 3 indices)
  - l which layer
  - m which neuron in layer
  - n which weight in neuron
- $\hat{y}_i$ computed output (i output dim; n_{out})
- y_i ground truth targets
- L loss function

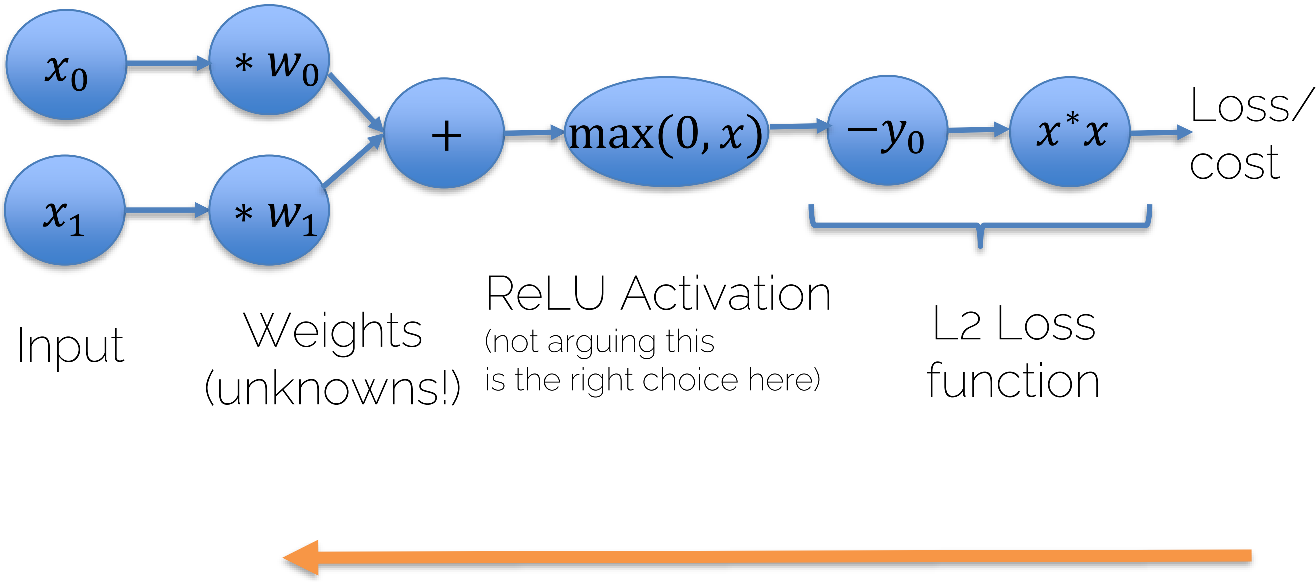
Compute Graphs -> Neural Networks





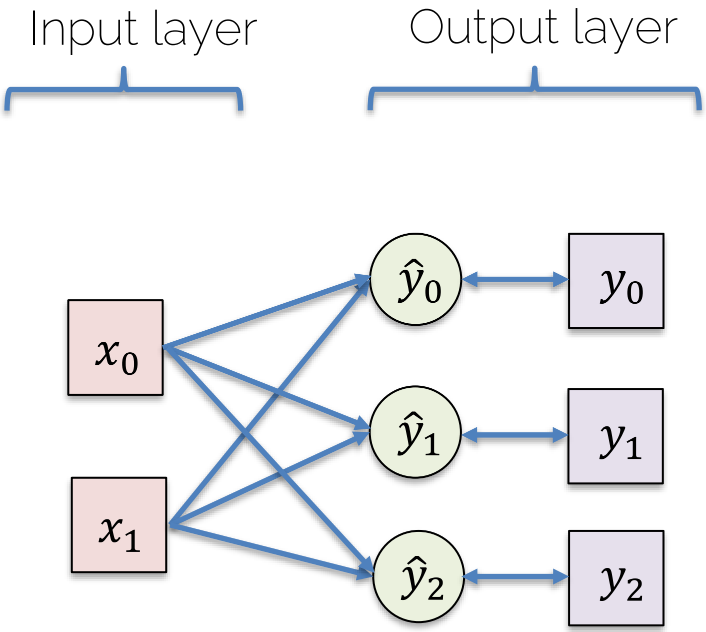
Compute Graphs -> Neural Networks

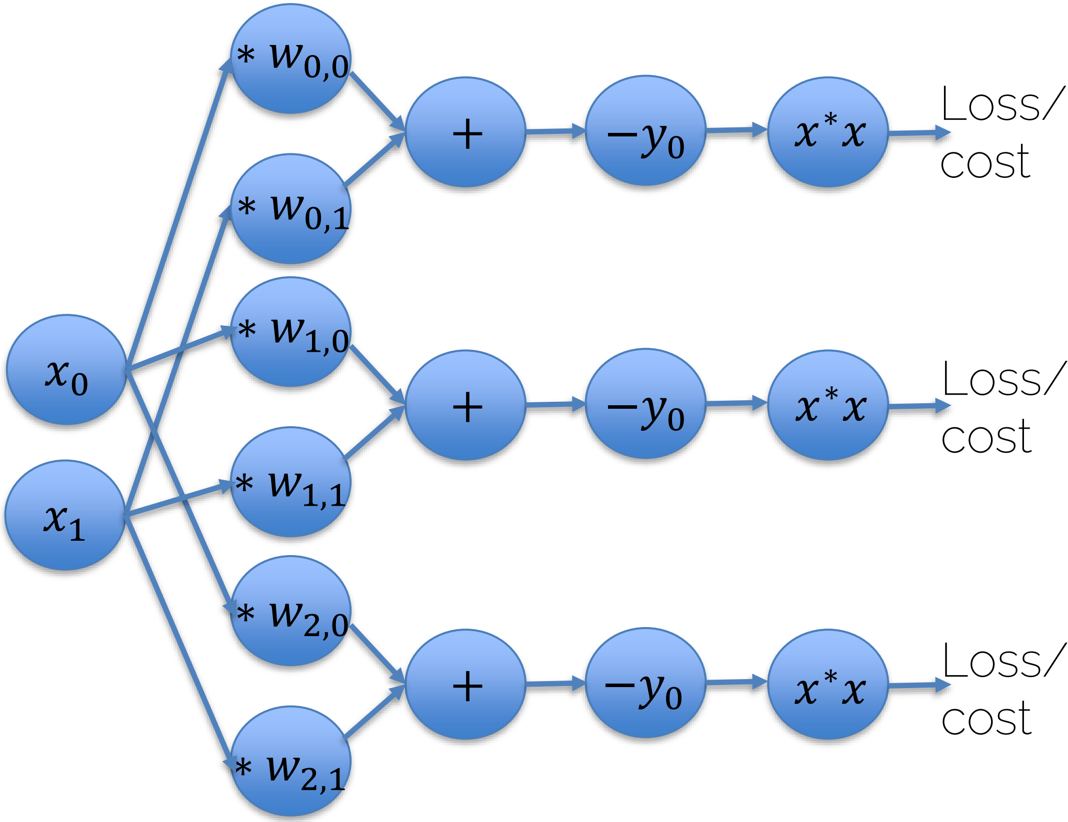




We want to compute gradients w.r.t. all weights $\boldsymbol{W}$

Compute Graphs -> Neural Networks





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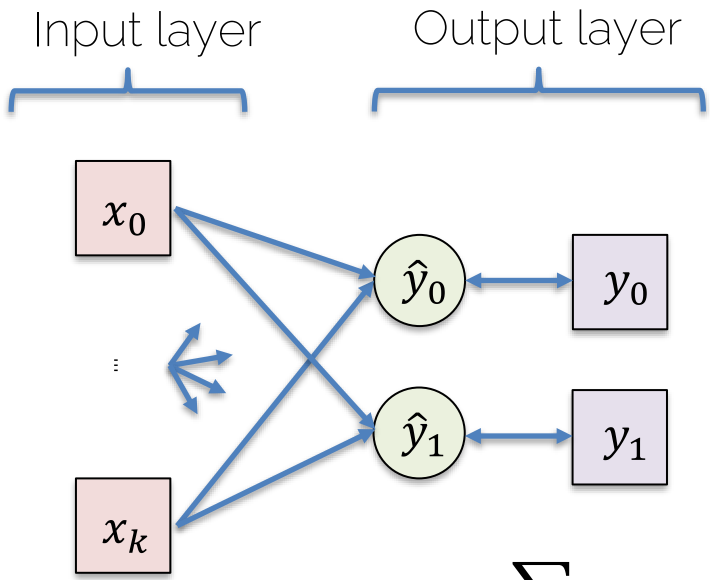
Compute Graphs -> Neural Networks



$$\hat{y}_i = A(b_i + \sum_k x_k w_{i,k})$$

Activation function

bias

Goal: We want to compute gradients of the loss function $\boldsymbol{L}$ w.r.t. all weights $\boldsymbol{W}$

$$L = \sum_i L_i$$

$\boldsymbol{L}$: sum over loss per sample, e.g.
L2 loss $\longrightarrow$ simply sum up squares:

$$L_i = (\hat{y}_i - y_i)^2$$

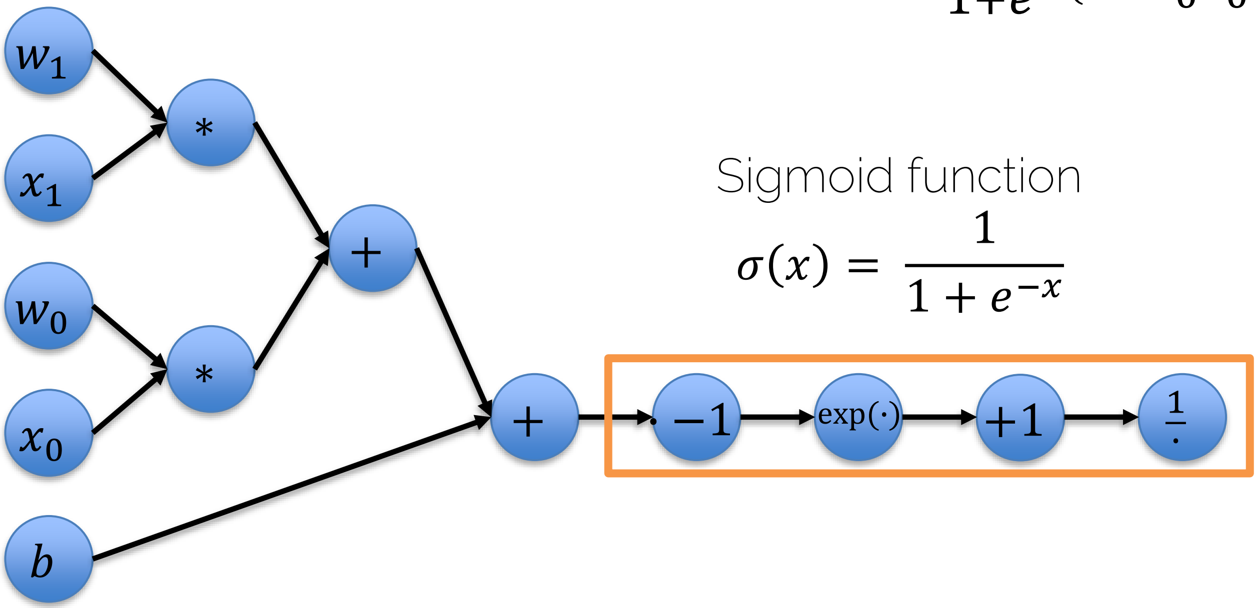
$\longrightarrow$ use chain rule to compute partials

$$\frac{\partial L}{\partial w_{i,k}} = \frac{\partial L}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial w_{i,k}}$$

We want to compute gradients w.r.t. all weights $\boldsymbol{W}$ AND all biases $\boldsymbol{b}$

NNs as Computational Graphs

- We can express any kind of functions in a computational graph, e.g. $f(\mathbf{w}, \mathbf{x}) = \frac{1}{1+e^{-(b+w_0 x_0 + w_1 x_1)}}$



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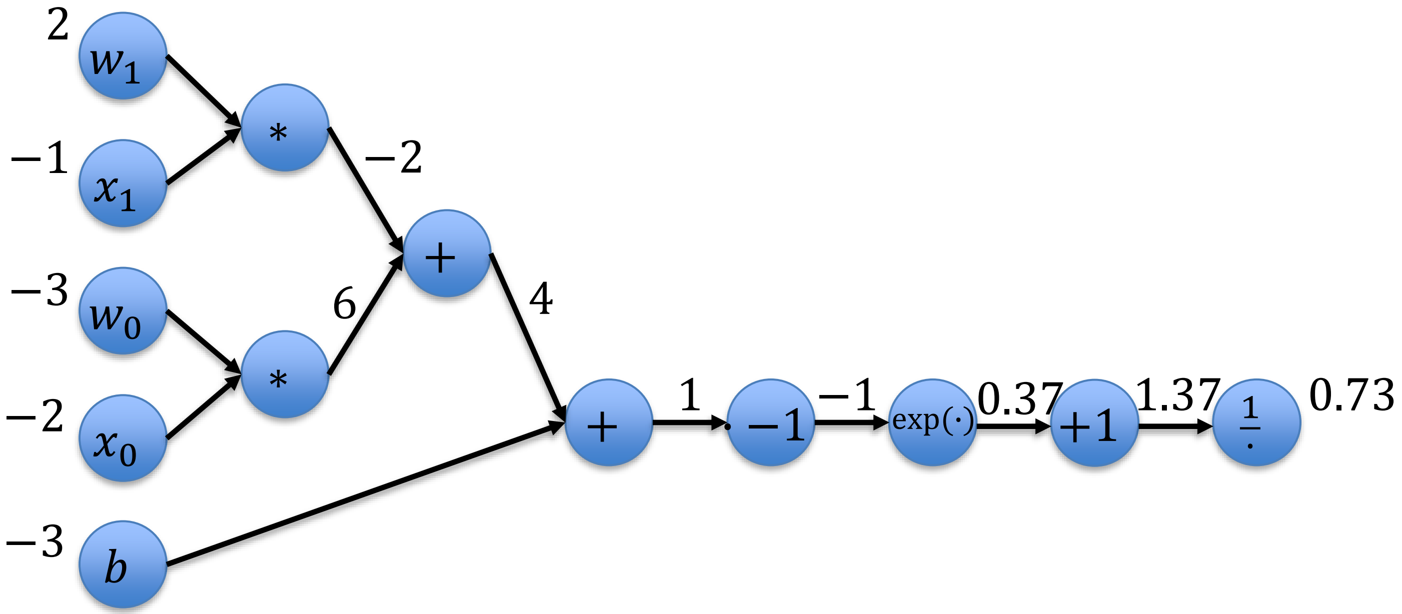


NNs as Computational Graphs

- $f(\boldsymbol{w}, \boldsymbol{x}) = \frac{1}{1+e^{-(b+w_0x_0+w_1x_1)}}$

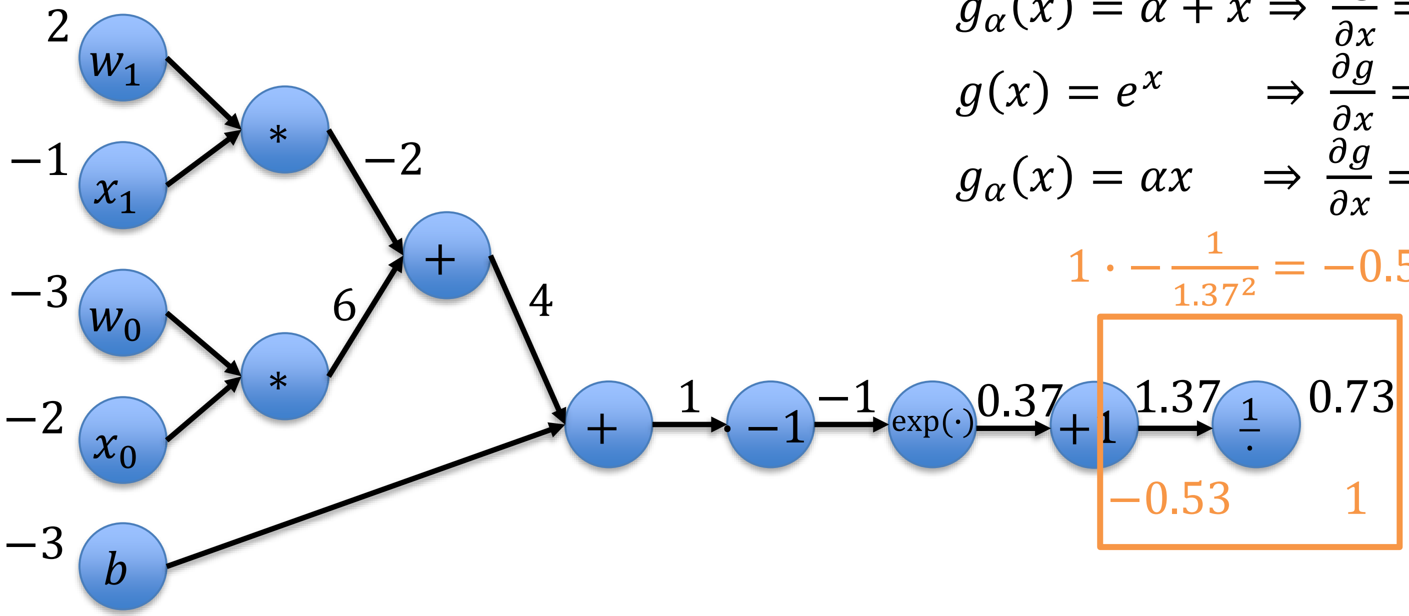
$$\boxed{g(x) = \frac{1}{x} \quad \Rightarrow \frac{\partial g}{\partial x} = -\frac{1}{x^2}}$$

$$g_\alpha(x) = \alpha + x \Rightarrow \frac{\partial g}{\partial x} = 1$$

$$g(x) = e^x \quad \Rightarrow \frac{\partial g}{\partial x} = e^x$$

$$g_\alpha(x) = \alpha x \quad \Rightarrow \frac{\partial g}{\partial x} = \alpha$$

$$1 \cdot -\frac{1}{1.37^2} = -0.53$$



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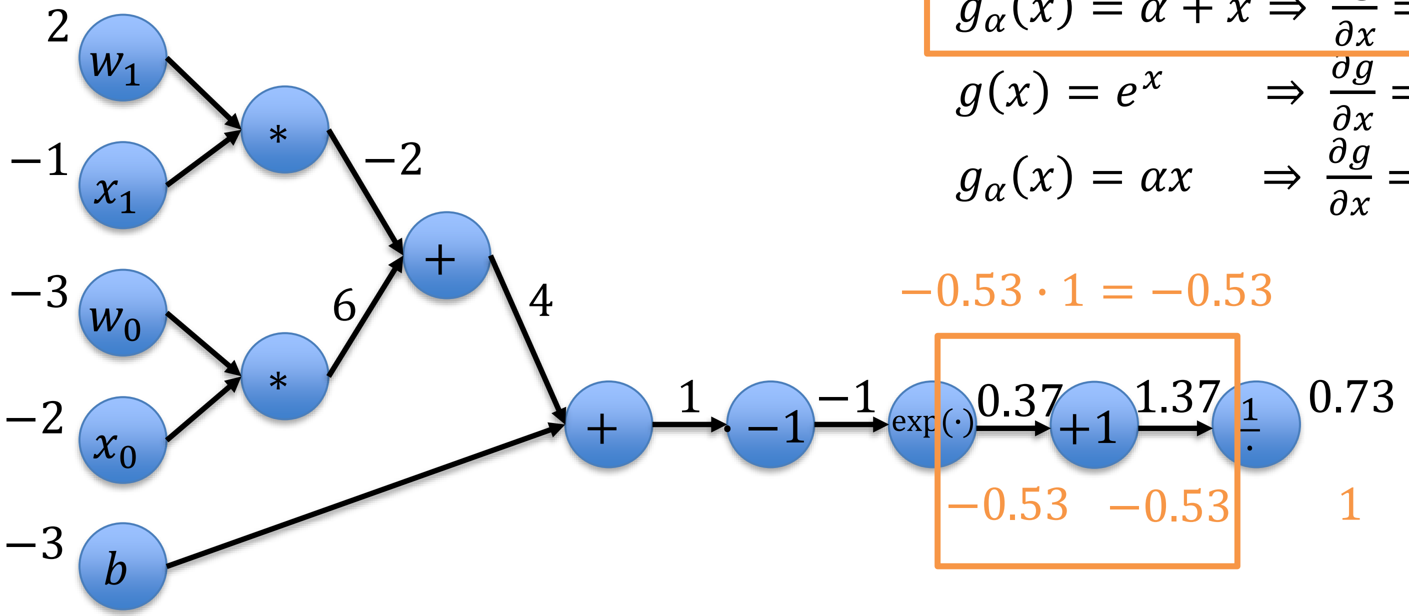

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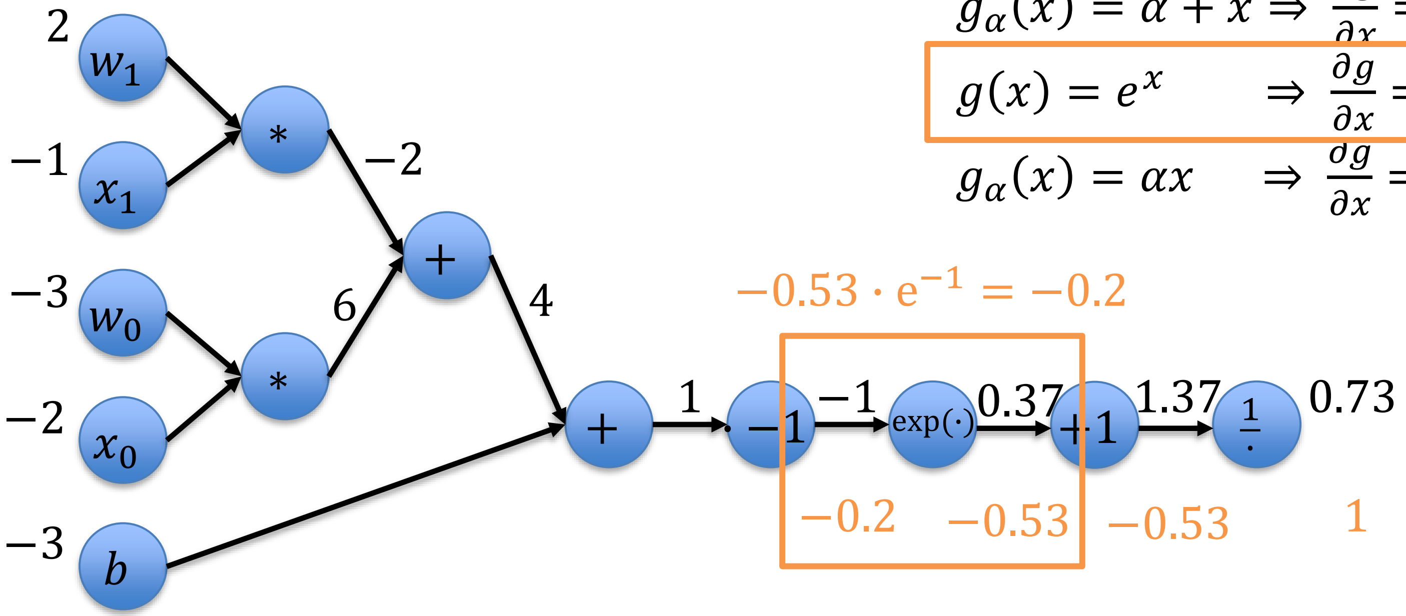

NNs as Computational Graphs

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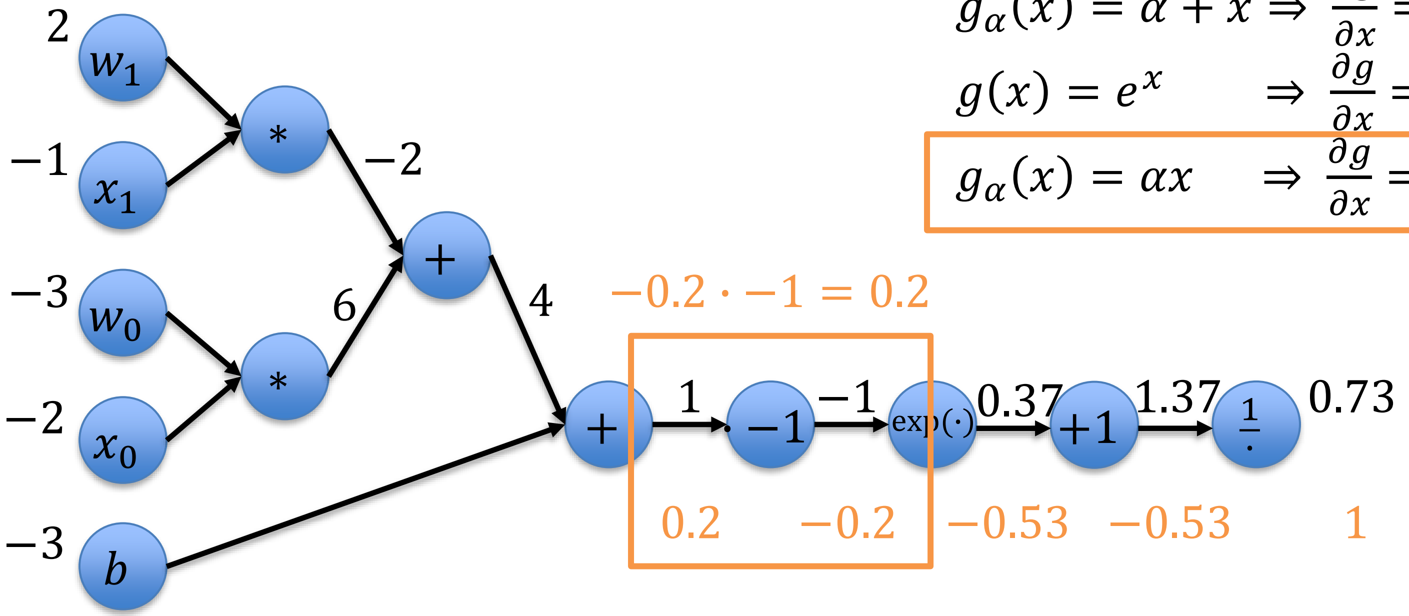

NNs as Computational Graphs

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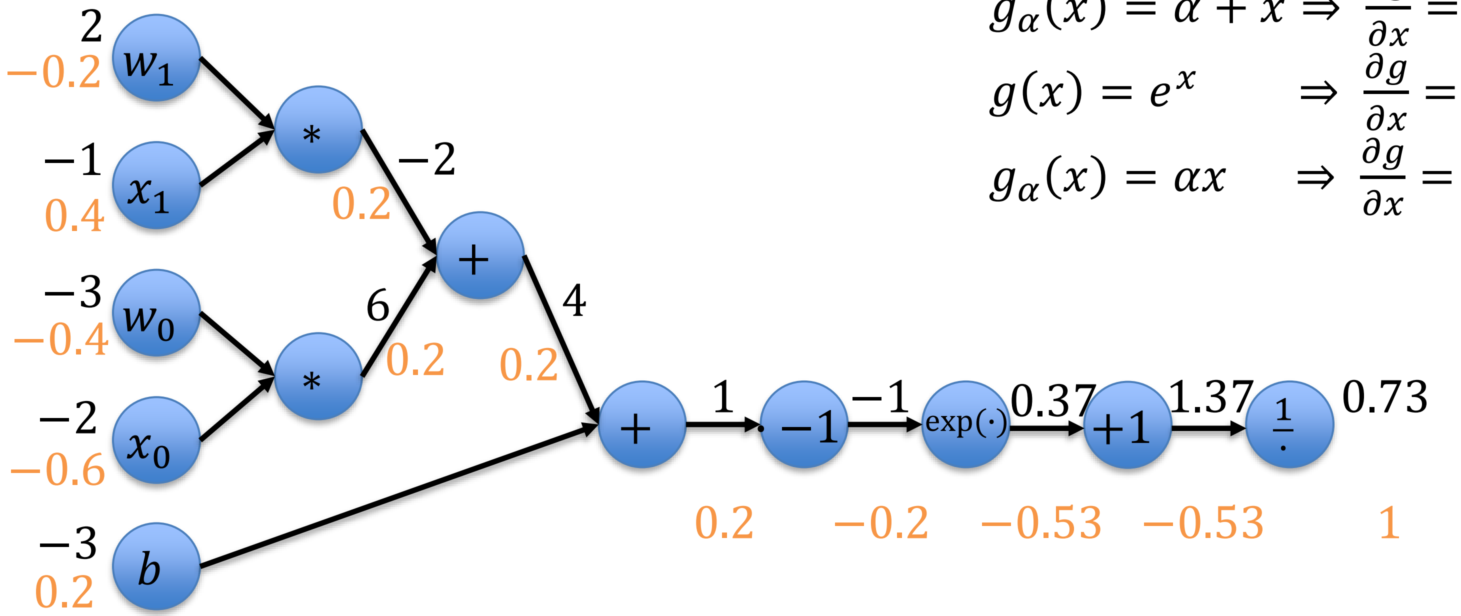
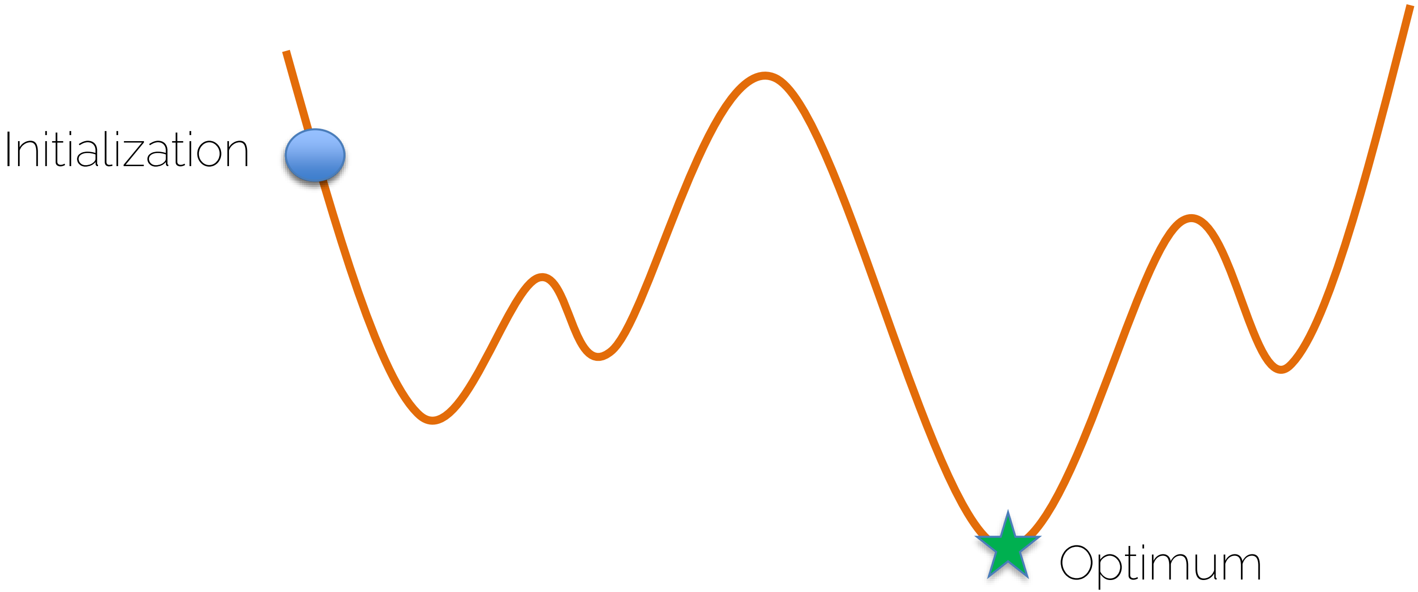


Gradient Descent

Gradient Descent

$$\boldsymbol{x}^* = \arg\min f(\boldsymbol{x})$$



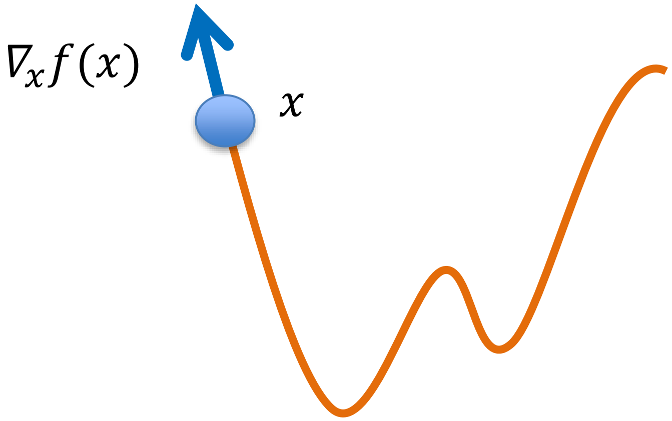
Gradient Descent

- From derivative to gradient

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \longrightarrow \nabla_x f(x)$$

Direction of greatest increase of the function

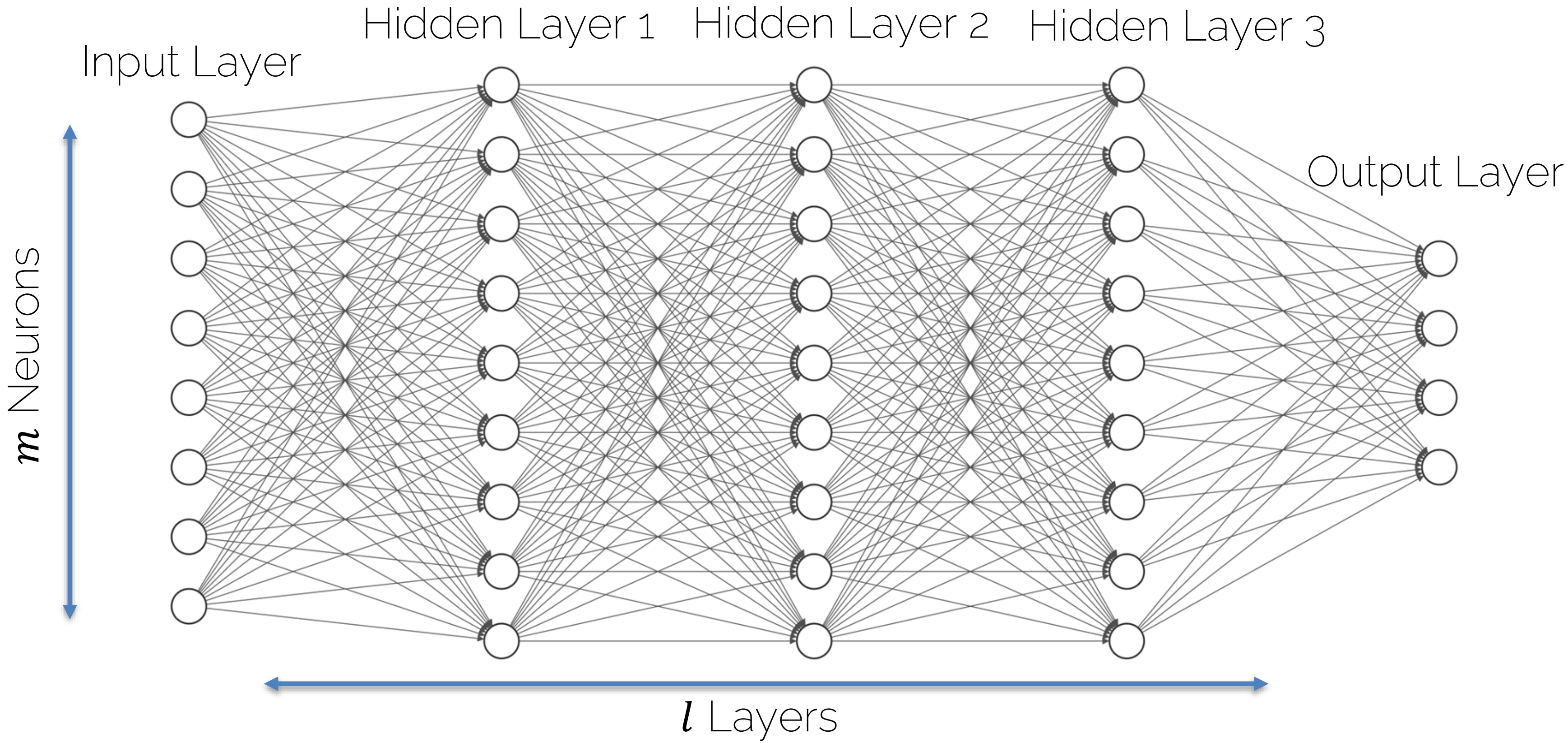
- Gradient steps in direction of negative gradient



$$x' = x - \alpha \nabla_x f(x)$$

Learning rate

Gradient Descent for Neural Networks



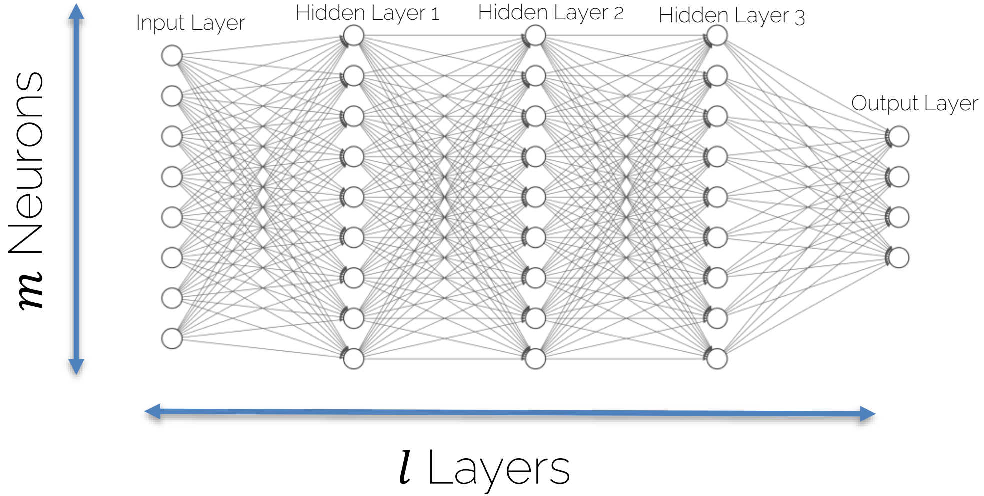
Gradient Descent for Neural Networks

For a given training pair $\{\boldsymbol{x}, \boldsymbol{y}\}$, we want to update all weights, i.e., we need to compute the derivatives w.r.t. to all weights:

$$\nabla_{\boldsymbol{W}} f_{\{\boldsymbol{x},\boldsymbol{y}\}}(\boldsymbol{W}) = \begin{bmatrix} \frac{\partial f}{\partial w_{0,0,0}} \\ \cdots \\ \cdots \\ \frac{\partial f}{\partial w_{l,m,n}} \end{bmatrix}$$

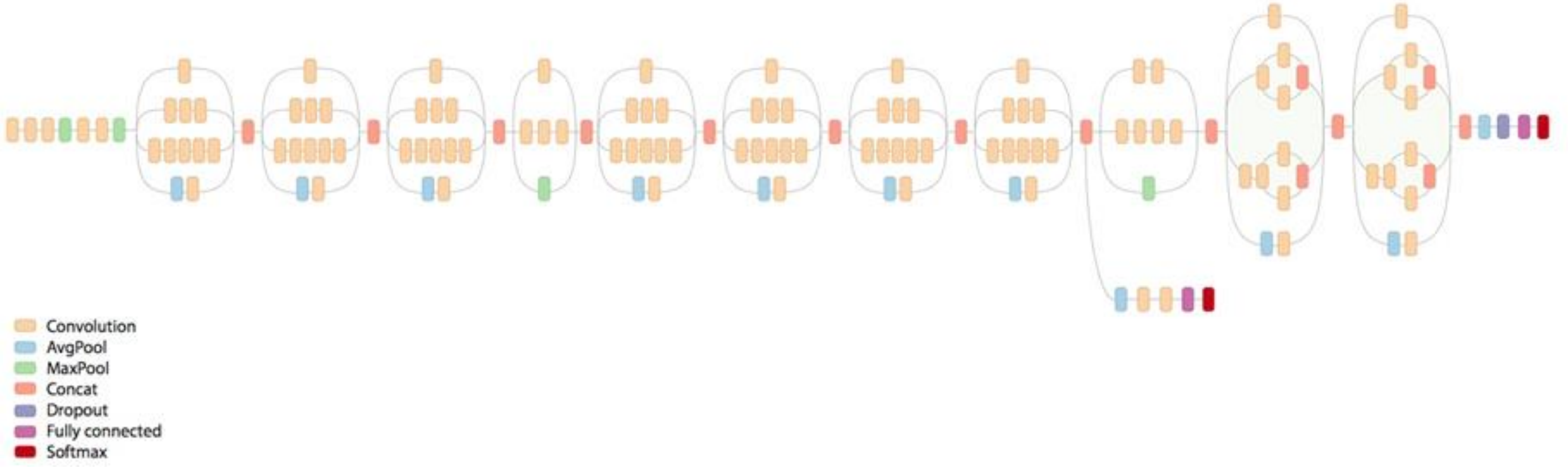
Gradient step:

$$\boldsymbol{W}' = \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} f_{\{\boldsymbol{x},\boldsymbol{y}\}}(\boldsymbol{W})$$



NNs can Become Quite Complex…

- These graphs can be huge!



[Szegedy et al.,CVPR'15] Going Deeper with Convolutions

The Flow of the Gradients

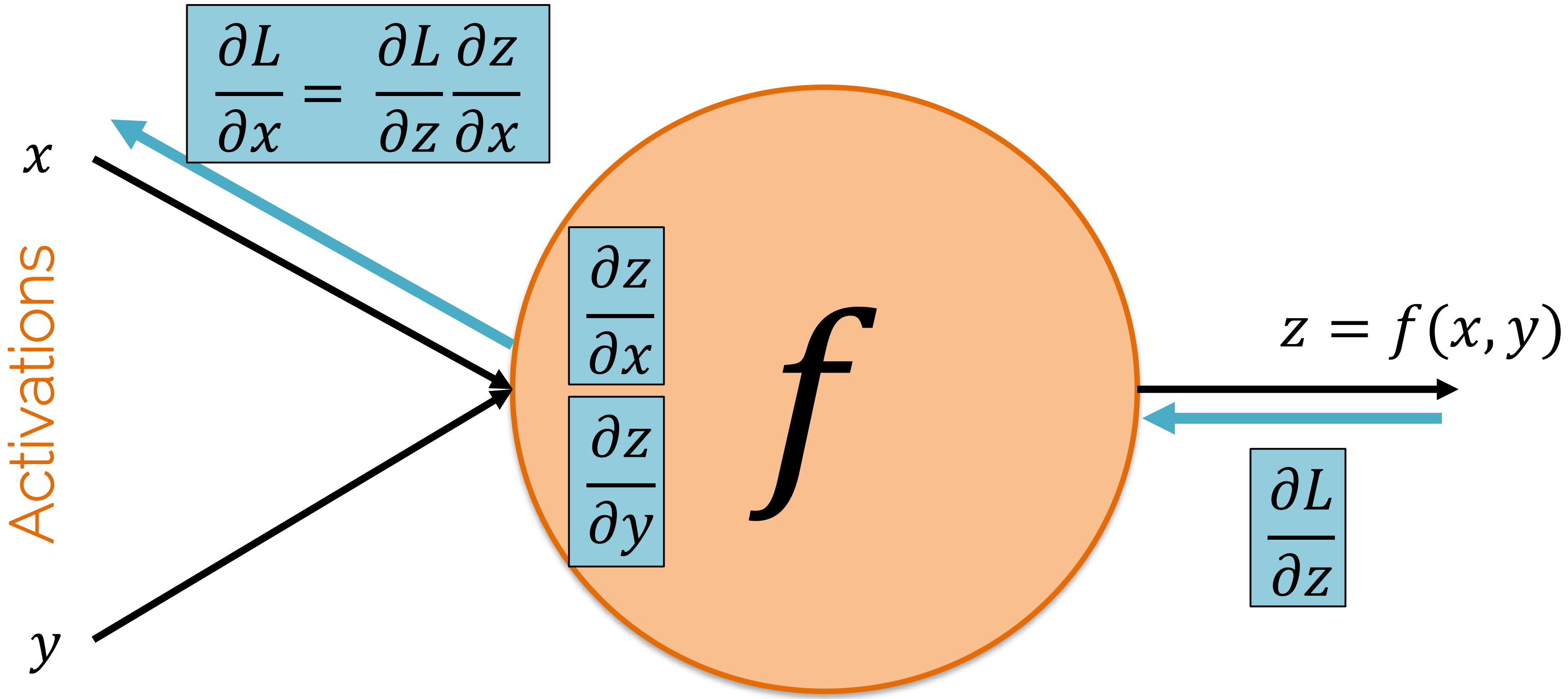
- Many many many many of these nodes form a neural network

NEURONS

- Each one has its own work to do

FORWARD AND BACKWARD PASS

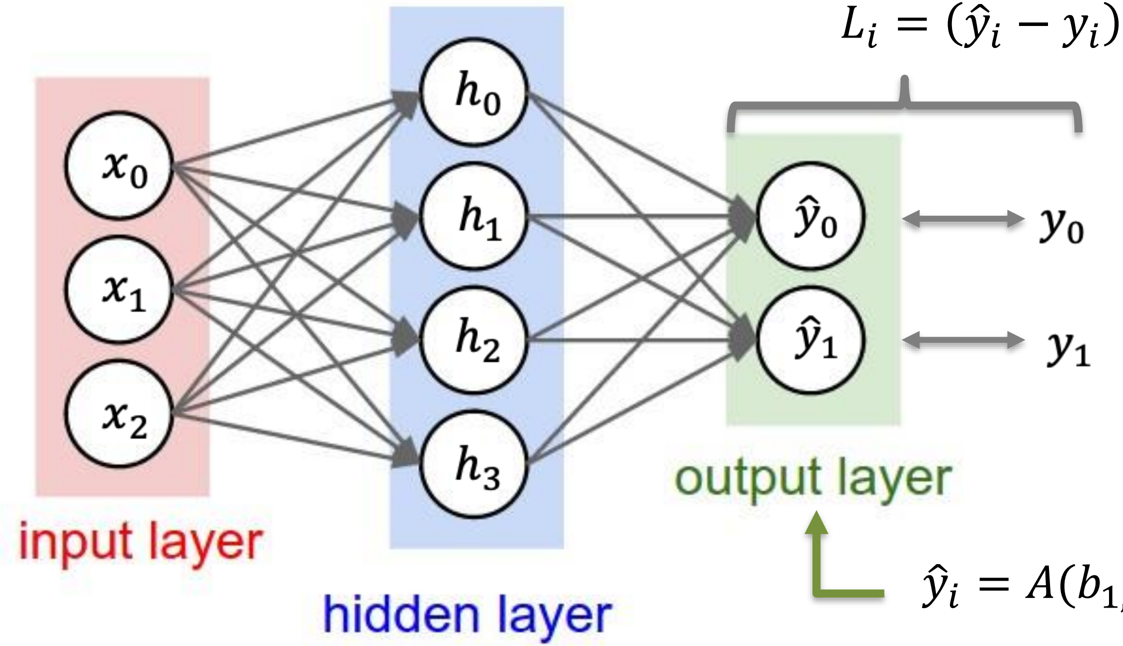
The Flow of the Gradients



Activation function

Gradient Descent for Neural Networks

Loss function
$L_i = (\hat{y}_i - y_i)^2$

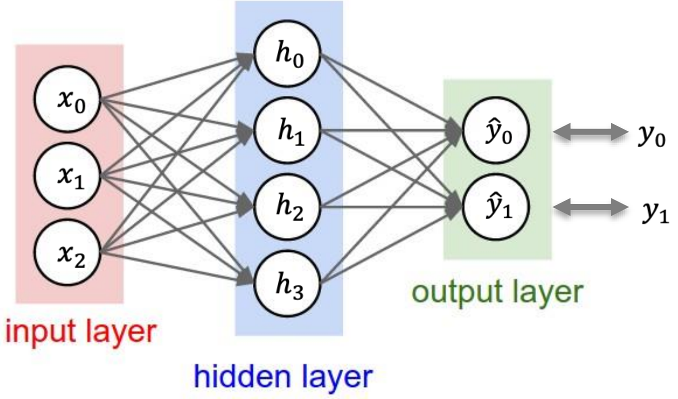


$$\hat{y}_i = A(b_{1,i} + \sum_j h_j w_{1,i,j})$$

$$h_j = A(b_{0,j} + \sum_k x_k w_{0,j,k})$$

Just simple:
$A(x) = \max(0, x)$

Gradient Descent for Neural Networks



$$h_j = A(b_{0,j} + \sum_k x_k w_{0,j,k})$$

$$\hat{y}_i = A(b_{1,i} + \sum_j h_j w_{1,i,j})$$

$$L_i = (\hat{y}_i - y_i)^2$$

Just go through layer by layer

Backpropagation

$$\frac{\partial L}{\partial w_{1,i,j}} = \frac{\partial L}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial w_{1,i,j}}$$

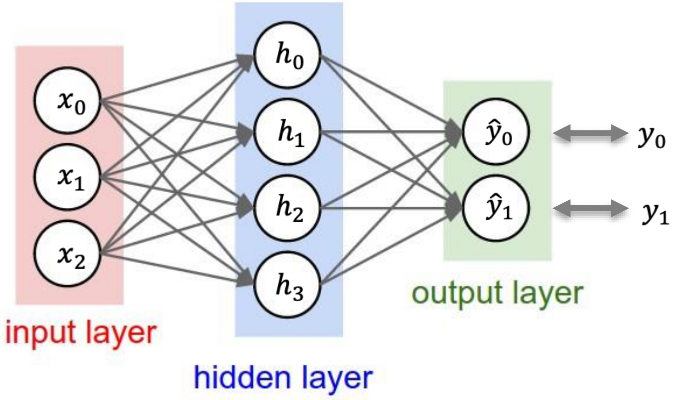
$$\frac{\partial L_i}{\partial \hat{y}_i} = 2(\hat{y}_i - y_i)$$

$$\frac{\partial \hat{y}_i}{\partial w_{1,i,j}} = h_j \quad \text{if} > 0, \text{ else } 0$$

$$\frac{\partial L}{\partial w_{0,j,k}} = \frac{\partial L}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial h_j} \cdot \frac{\partial h_j}{\partial w_{0,j,k}}$$

…

Gradient Descent for Neural Networks



$$h_j = A(b_{0,j} + \sum_k x_k w_{0,j,k})$$

$$\hat{y}_i = A(b_{1,i} + \sum_j h_j w_{1,i,j})$$

$$L_i = (\hat{y}_i - y_i)^2$$

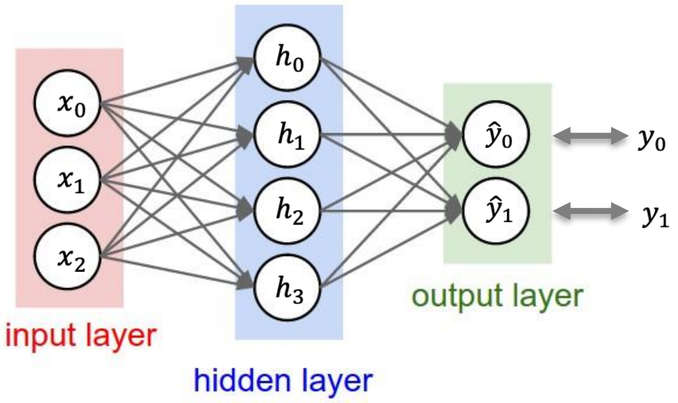
How many unknown weights?

- Output layer: $2 \cdot 4 + 2$
- Hidden Layer: $4 \cdot 3 + 4$

#neurons · #input channels + #biases

Note that some activations have also weights

Derivatives of Cross Entropy Loss



Binary Cross Entropy loss

$$L = -\sum_{i=1}^{n_{out}} (y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i))$$

$$\hat{y}_i = \frac{1}{1 + e^{-s_i}} \qquad s_i = \sum_{j} h_j w_{ji}$$

output scores

Gradients of weights of last layer:

$$\frac{\partial L}{\partial w_{ji}} = \boxed{\frac{\partial L}{\partial \hat{y}_i}} \cdot \boxed{\frac{\partial \hat{y}_i}{\partial s_i}} \cdot \boxed{\frac{\partial s_i}{\partial w_{ji}}}$$

$$\boxed{\frac{\partial L}{\partial \hat{y}_i}} = \frac{-y_i}{\hat{y}_i} + \frac{1 - y_i}{1 - \hat{y}_i} = \frac{\hat{y}_i - y_i}{\hat{y}_i(1 - \hat{y}_i)},$$

$$\boxed{\frac{\partial \hat{y}_i}{\partial s_i}} = \hat{y}_i\,(1 - \hat{y}_i),$$

$$\boxed{\frac{\partial s_i}{\partial w_{ji}}} = h_j$$

$$\Rightarrow \frac{\partial L}{\partial w_{ji}} = (\hat{y}_i - y_i)h_j, \quad \frac{\partial L}{\partial s_i} = \hat{y}_i - y_i$$

Derivatives of Cross Entropy Loss

Gradients of weights of first layer:

$$\boxed{\frac{\partial L}{\partial h_j}} = \sum_{i=1}^{n_{out}} \frac{\partial L}{\partial \hat{y}_i} \frac{\partial \hat{y}_i}{\partial s_i} \frac{\partial s_i}{\partial h_j} = \sum_{i=1}^{n_{out}} \frac{\partial L}{\partial \hat{y}_i} \hat{y}_i (1 - \hat{y}_i) w_{ji} = \sum_{i=1}^{n_{out}} (\hat{y}_i - y_i) w_{ji}$$

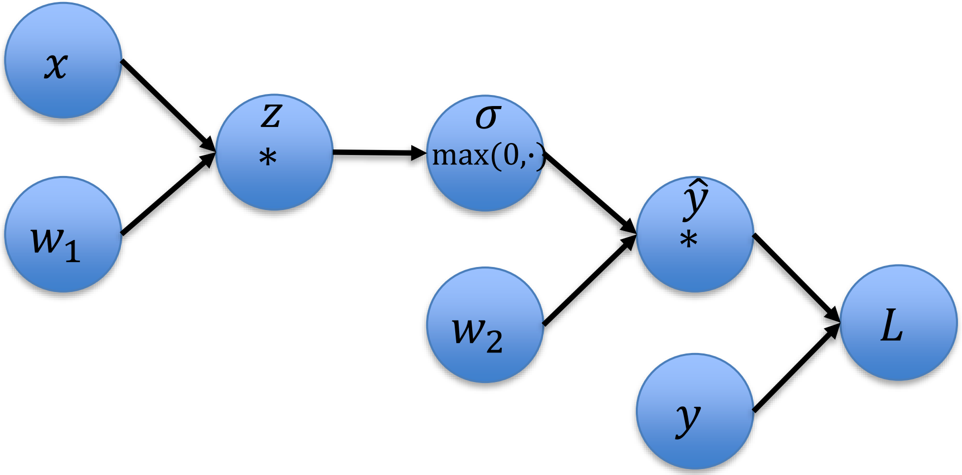
$$\boxed{\frac{\partial L}{\partial s_j^1}} = \boxed{\sum_{i=1}^{n_{out}} \frac{\partial L}{\partial s_i} \frac{\partial s_i}{\partial h_j}} \frac{\partial h_j}{\partial s_j^1} = \boxed{\sum_{i=1}^{n_{out}} (\hat{y}_i - y_i) w_{ji}} \left(h_j (1 - h_j)\right)$$

$$\frac{\partial L}{\partial w_{kj}^1} = \boxed{\sum_{i=1}^{n_{out}} \frac{\partial L}{\partial s_j^1}} \frac{\partial s_j^1}{\partial w_{kj}^1} = \boxed{\sum_{i=1}^{n_{out}} (\hat{y}_i - y_i) w_{ji} \left(h_j (1 - h_j)\right)} x_k$$

Back to Compute Graphs & NNs

- Inputs $\boldsymbol{x}$ and targets $\boldsymbol{y}$
- Two-layer NN for regression with ReLU activation
- Function we want to optimize:

$$\sum_{i=1}^{n} \|w_2 \max(0, w_1 x_i) - y_i\|_2^2$$



Gradient Descent for Neural Networks

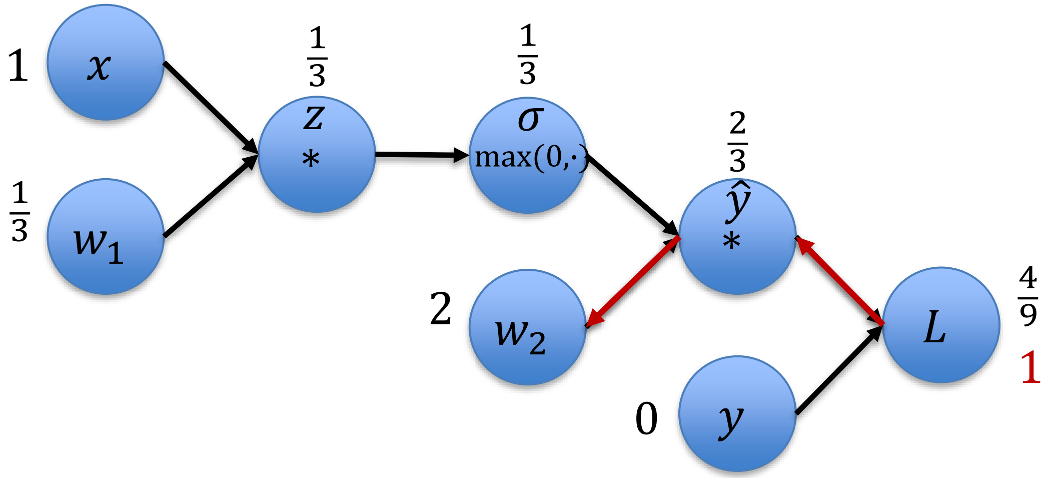
Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

$L(\boldsymbol{y}, \widehat{\boldsymbol{y}}; \boldsymbol{\theta}) = \frac{1}{n}\sum_i^n ||\hat{y}_i - y_i||_2^2$

In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$

$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \frac{\partial \hat{y}}{\partial w_2} = \sigma$



Backpropagation

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_2}$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

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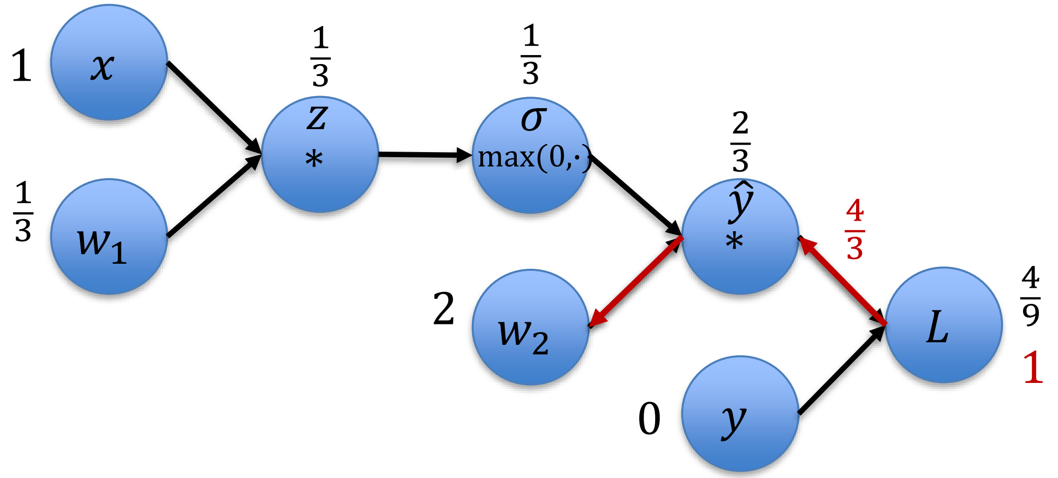

Backpropagation

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_2}$$

$$2 \cdot \frac{2}{3}$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

$L(\boldsymbol{y}, \hat{\boldsymbol{y}}; \boldsymbol{\theta}) = \frac{1}{n}\sum_i^n ||\hat{y}_i - y_i||_2^2$

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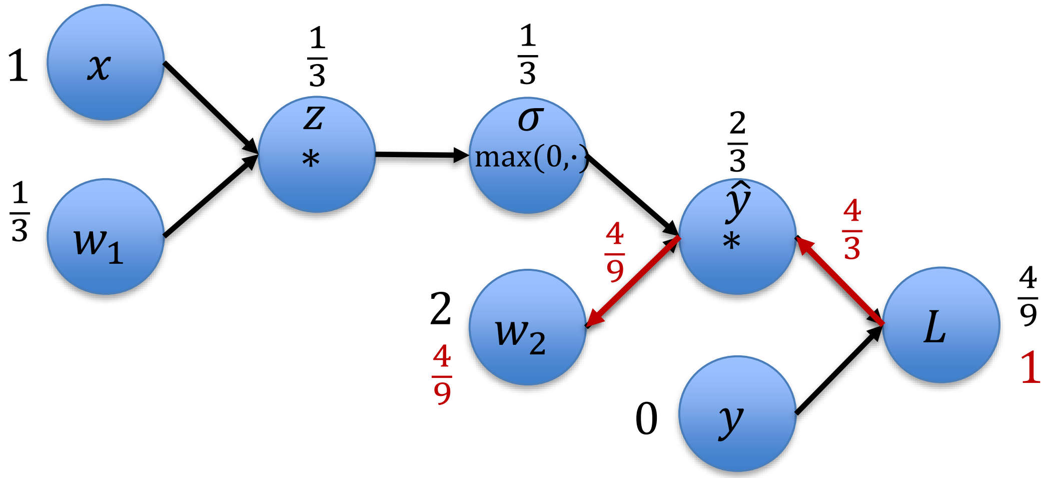
$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \boxed{\frac{\partial \hat{y}}{\partial w_2} = \sigma}$



Backpropagation

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_2}$$

$$2 \cdot \frac{2}{3} \quad \cdot \frac{1}{3}$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

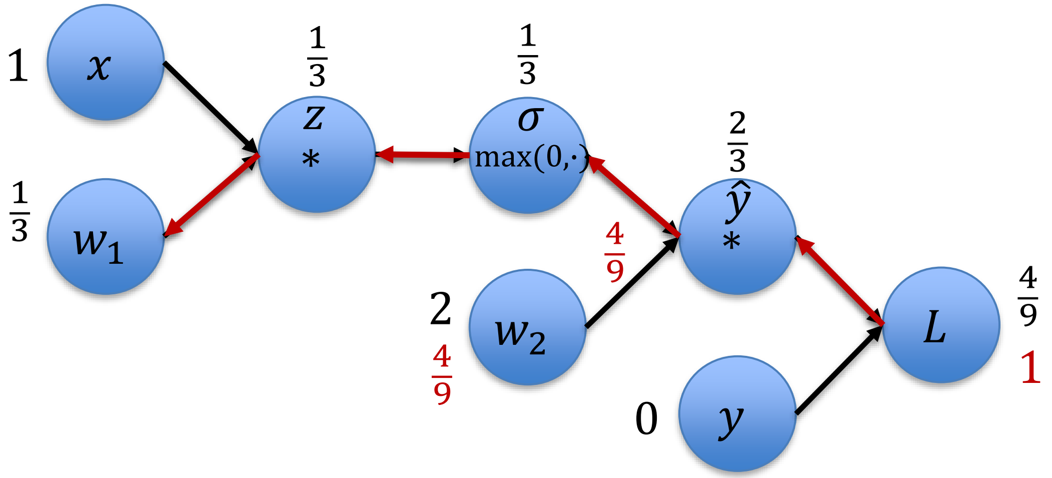
In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$

$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \frac{\partial \hat{y}}{\partial \sigma} = w_2$

$\sigma = \max(0, z) \Rightarrow \frac{\partial \sigma}{\partial z} = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ else} \end{cases}$

$z = x \cdot w_1 \quad \Rightarrow \frac{\partial z}{\partial w_1} = x$



Backpropagation

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \boxed{\frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)}$

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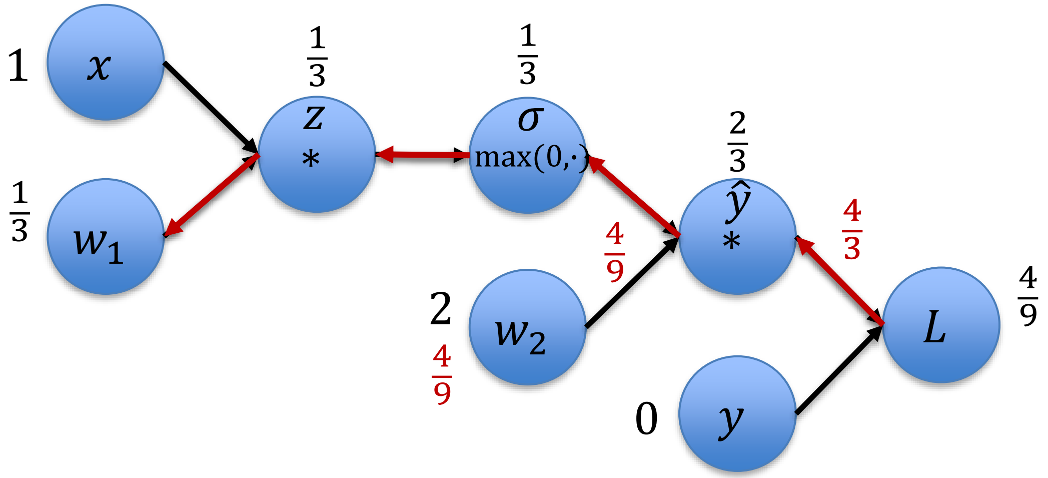

Backpropagation

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

$2 \cdot \frac{2}{3}$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$

$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \boxed{\frac{\partial \hat{y}}{\partial \sigma} = w_2}$

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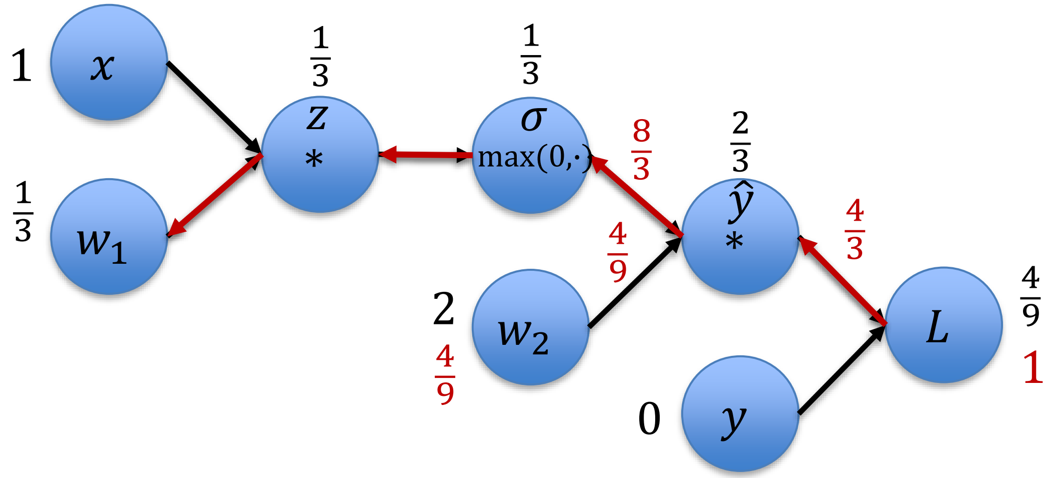


Backpropagation

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

$$2 \cdot \frac{2}{3} \quad \cdot 2$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

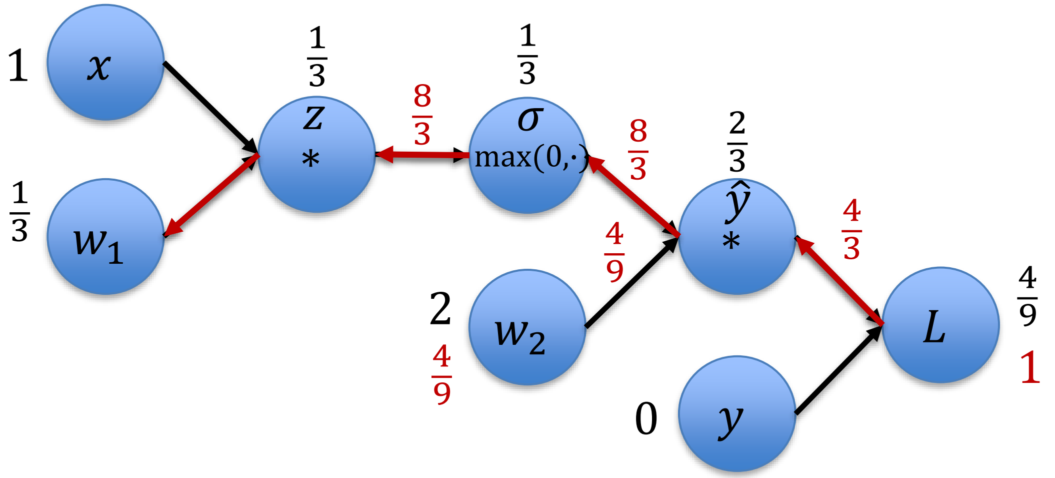
In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$

$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \frac{\partial \hat{y}}{\partial \sigma} = w_2$

$\sigma = \max(0, z) \Rightarrow \boxed{\frac{\partial \sigma}{\partial z} = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ else} \end{cases}}$

$z = x \cdot w_1 \quad \Rightarrow \frac{\partial z}{\partial w_1} = x$



Backpropagation

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

$$2 \cdot \frac{2}{3} \cdot 2 \cdot 1$$

Gradient Descent for Neural Networks

Initialize $x = 1,\ y = 0,$
$w_1 = \frac{1}{3}, w_2 = 2$

In our case $n, d = 1$:

$L = (\hat{y} - y)^2 \quad \Rightarrow \frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$

$\hat{y} = w_2 \cdot \sigma \quad \Rightarrow \frac{\partial \hat{y}}{\partial \sigma} = w_2$

$\sigma = \max(0, z) \Rightarrow \frac{\partial \sigma}{\partial z} = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ else} \end{cases}$

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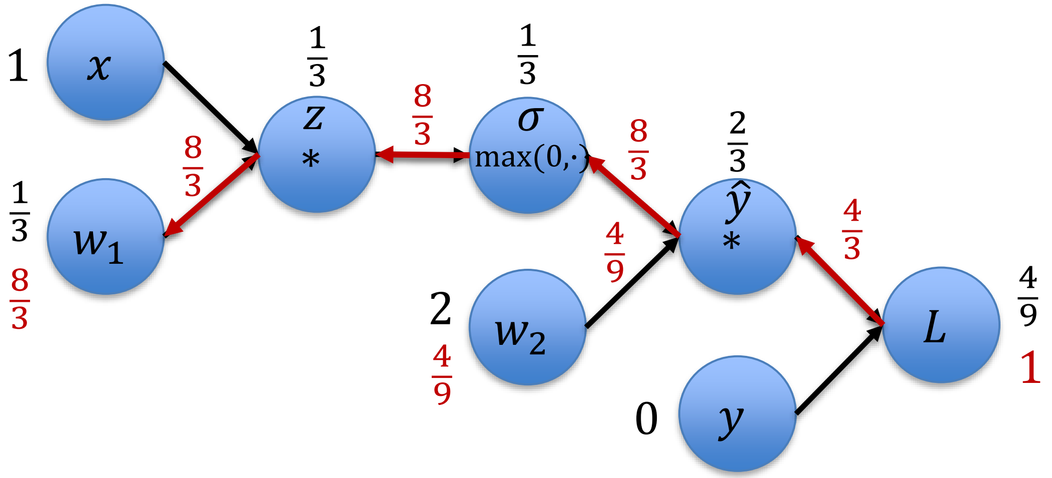


Backpropagation

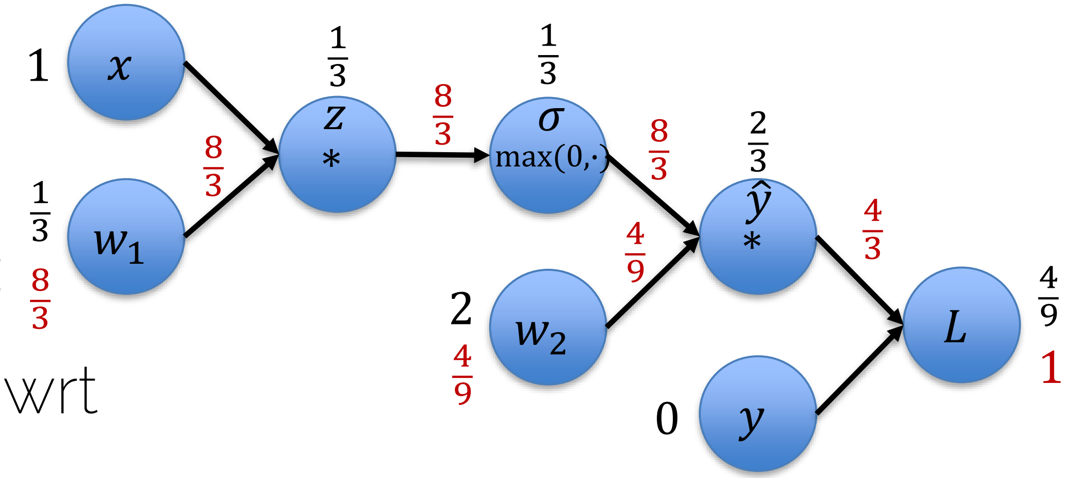
$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

$$2 \cdot \frac{2}{3} \quad \cdot 2 \quad \cdot 1 \quad \cdot 1$$

Gradient Descent for Neural Networks

- Function we want to optimize:

$$f(x, \boldsymbol{w}) = \sum_{i=1}^{n} \| w_2 \max(0, w_1 x_i) - y_i \|_2^2$$



- Computed gradients wrt to weights $\boldsymbol{w_1}$ and $\boldsymbol{w_2}$
- Now: update the weights

$$\boldsymbol{w}' = \boldsymbol{w} - \alpha \cdot \nabla_{\boldsymbol{w}} f = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} - \alpha \cdot \begin{pmatrix} \nabla_{w_1} f \\ \nabla_{w_2} f \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{3} \\ 2 \end{pmatrix} - \alpha \cdot \begin{pmatrix} \frac{8}{3} \\ \frac{4}{9} \end{pmatrix}$$

But: how to choose a good learning rate $\boldsymbol{\alpha}$?

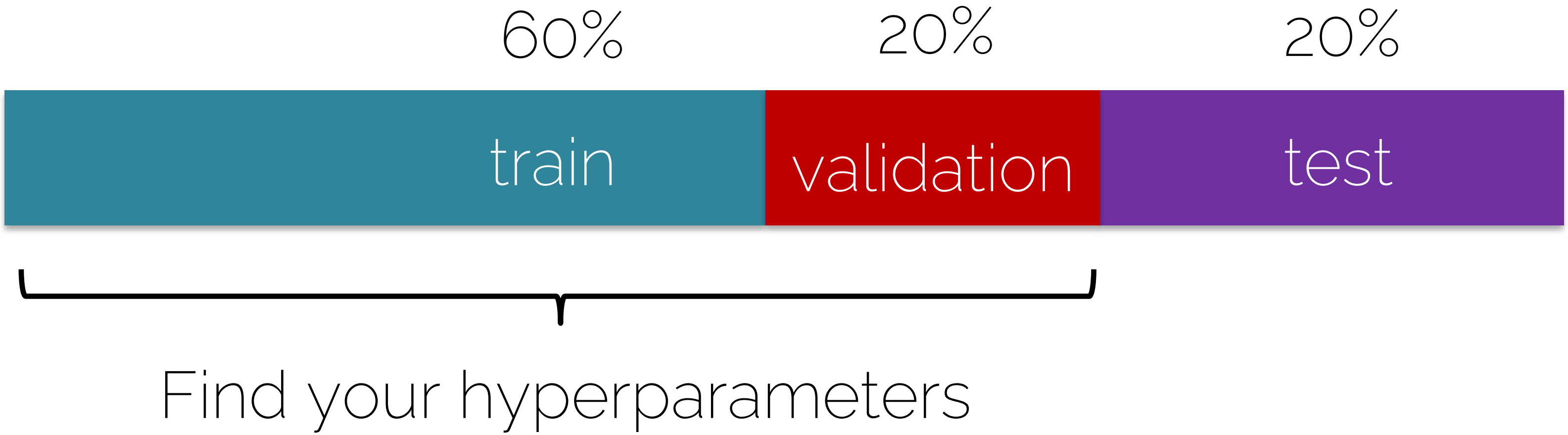
Gradient Descent

- How to pick good learning rate?
- How to compute gradient for single training pair?
- How to compute gradient for large training set?
- How to speed things up? More to see in next lectures…

Regularization

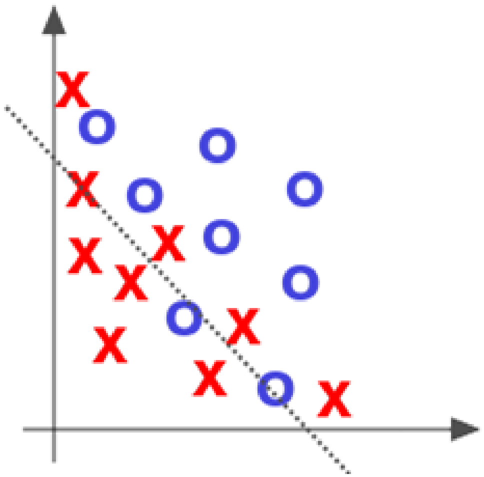
Recap: Basic Recipe for ML

- Split your data

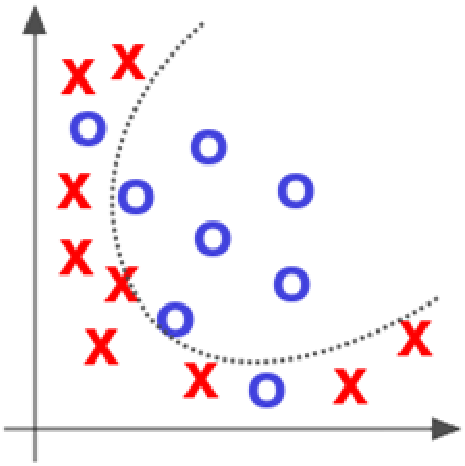


Other splits are also possible (e.g., 80%/10%/10%)

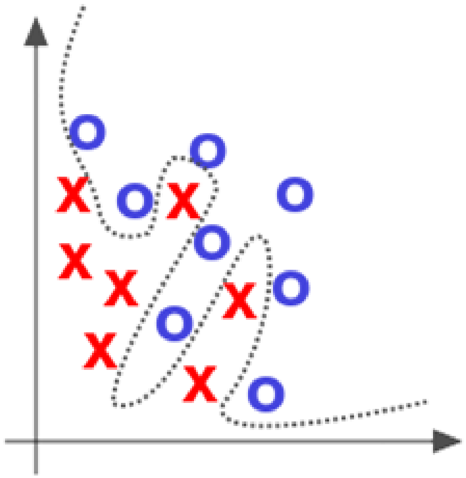
Over- and Underfitting



Underfitted



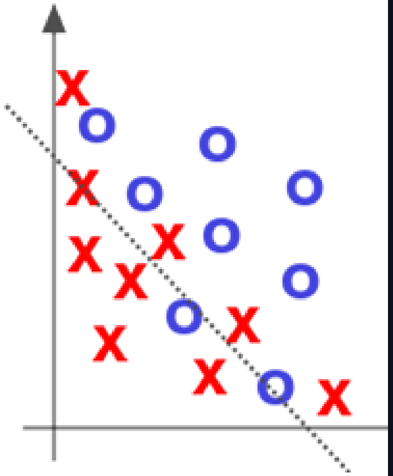
Appropriate



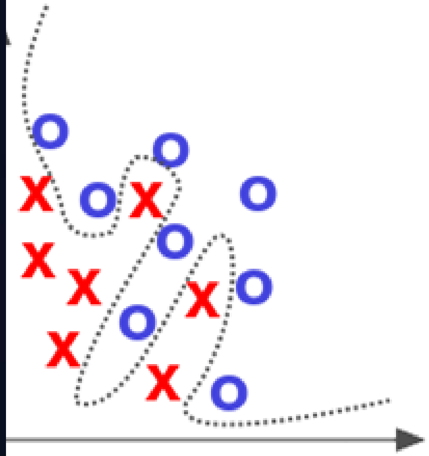
Overfitted

Source: Deep Learning by Adam Gibson, Josh Patterson, O'Reily Media Inc., 2017

Over- and Underfitting



Underfitted

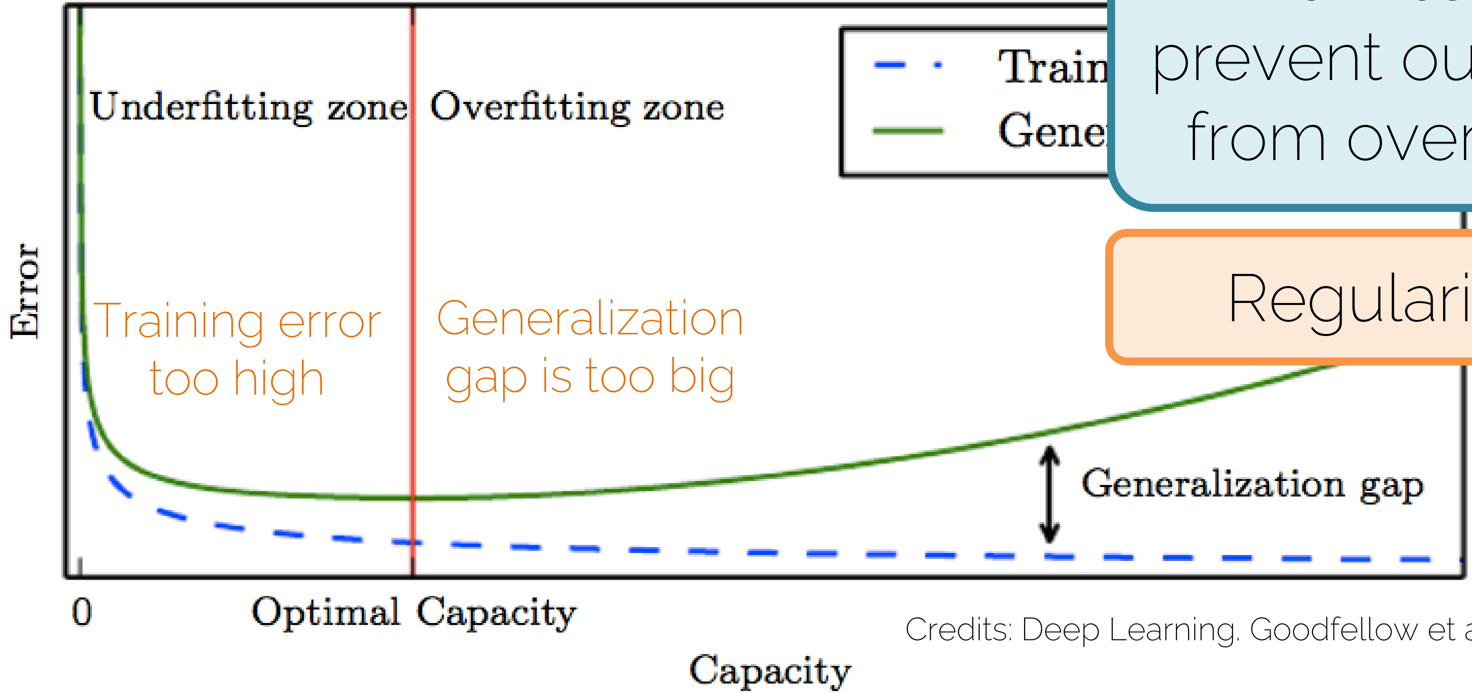


Overfitted

eily Media Inc., 2017

Training a Neural Network

- Training/ Validation curve



How can we prevent our model from overfitting?

Regularization

Credits: Deep Learning. Goodfellow et al.

Regularization

- Loss function $\boldsymbol{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}, \boldsymbol{\theta}) = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$

- Regularization techniques
  - L2 regularization
  - L1 regularization
  - Max norm regularization
  - Dropout
  - Early stopping
  - ...

Add **regularization term** to loss function

Regularization

- Loss function $L(\boldsymbol{y}, \hat{\boldsymbol{y}}, \boldsymbol{\theta}) = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \boxed{+ \lambda R(\boldsymbol{\theta})}$

- Regularization techniques
  - L2 regularization
  - L1 regularization
  - Max norm regularization
  - Dropout
  - Early stopping
  - …

Add **regularization term** to loss function

More details later

Regularization: Example

- Input: 3 features $\boldsymbol{x} = [1, 2, 1]$

- Two linear classifiers that give the same result:

- $\theta_1 = [0, 0.75, 0]$ $\longrightarrow$ Ignores 2 features

- $\theta_2 = [0.25, 0.5, 0.25]$ $\longrightarrow$ Takes information from all features

Regularization: Example

- Loss $L(\boldsymbol{y}, \hat{\boldsymbol{y}}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \left(x_i \theta_{ji} - y_i\right)^2 \boxed{+ \lambda R(\boldsymbol{\theta})}$

- L2 regularization $R(\boldsymbol{\theta}) = \sum_{i=1}^{n} \theta_i^2$

$$\theta_1 \longrightarrow 0 + 0.75^2 + 0 = 0.5625$$

$$\theta_2 \longrightarrow 0.25^2 + 0.5^2 + 0.25^2 = \boxed{0.375}$$ Minimization

$$x = [1, 2, 1], \theta_1 = [0, 0.75, 0], \theta_2 = [0.25, 0.5, 0.25]$$

Regularization: Example

- Loss $L(\boldsymbol{y}, \hat{\boldsymbol{y}}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \left(x_i \theta_{ji} - y_i\right)^2 \boxed{+ \lambda R(\boldsymbol{\theta})}$

- L1 regularization $R(\boldsymbol{\theta}) = \sum_{i=1}^{n} |\theta_i|$

$$\theta_1 \longrightarrow 0 + 0.75 + 0 = \boxed{0.75}$$ Minimization

$$\theta_2 \longrightarrow 0.25 + 0.5 + 0.25 = 1$$

$$x = [1, 2, 1], \theta_1 = [0, 0.75, 0], \theta_2 = [0.25, 0.5, 0.25]$$

Regularization: Example

- Input: 3 features $\boldsymbol{x} = [1, 2, 1]$

- Two linear classifiers that give the same result:

- $\theta_1 = [0, 0.75, 0]$ → Ignores 2 features

- $\theta_2 = [0.25, 0.5, 0.25]$ → Takes information from all features

Regularization: Example

- Input: 3 features $\boldsymbol{x} = [1, 2, 1]$

- Two linear classifiers that give the same result:

- $\theta_1 = [0, 0.75, 0]$ → L1 regularization enforces **sparsity**

- $\theta_2 = [0.25, 0.5, 0.25]$ → L2 regularization enforces that the weights have **similar values**

Regularization: Effect

- Dog classifier takes different inputs

Furry

Has two eyes

Has a tail

Has paws

Has two ears

L1 regularization will focus all the attention to a few key features

Regularization: Effect

- Dog classifier takes different inputs

Furry

Has two eyes

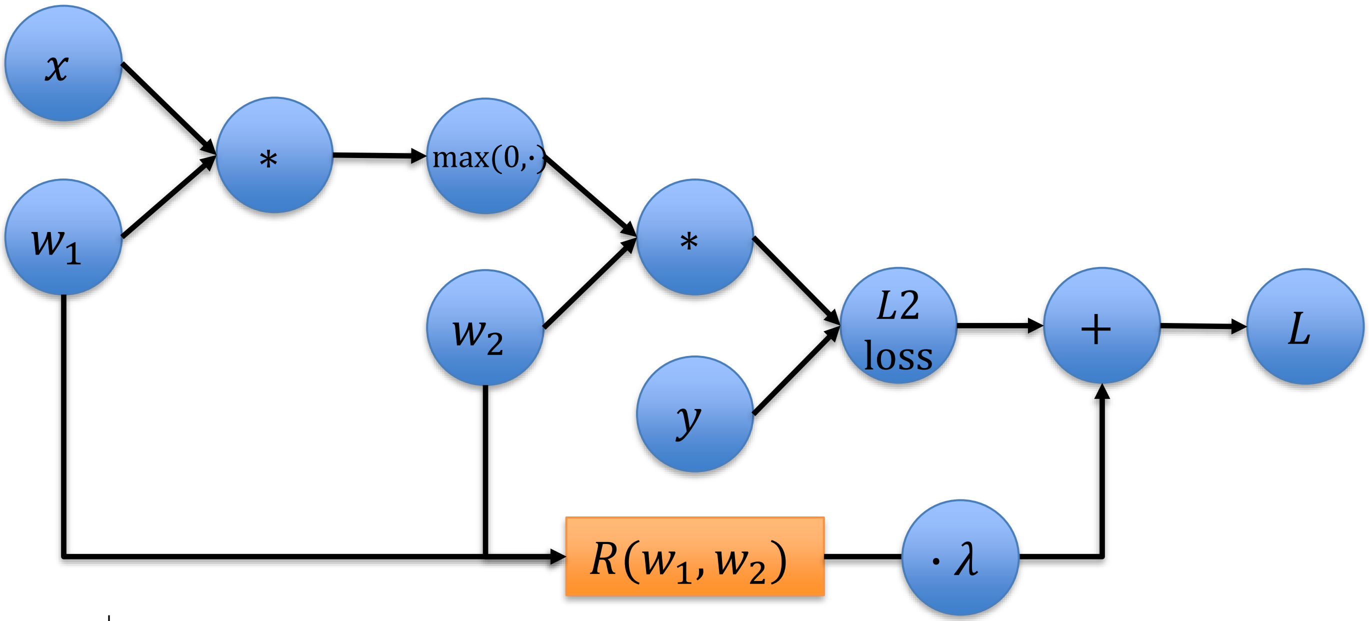
Has a tail

Has paws

Has two ears

L2 regularization will take all information into account to make decisions

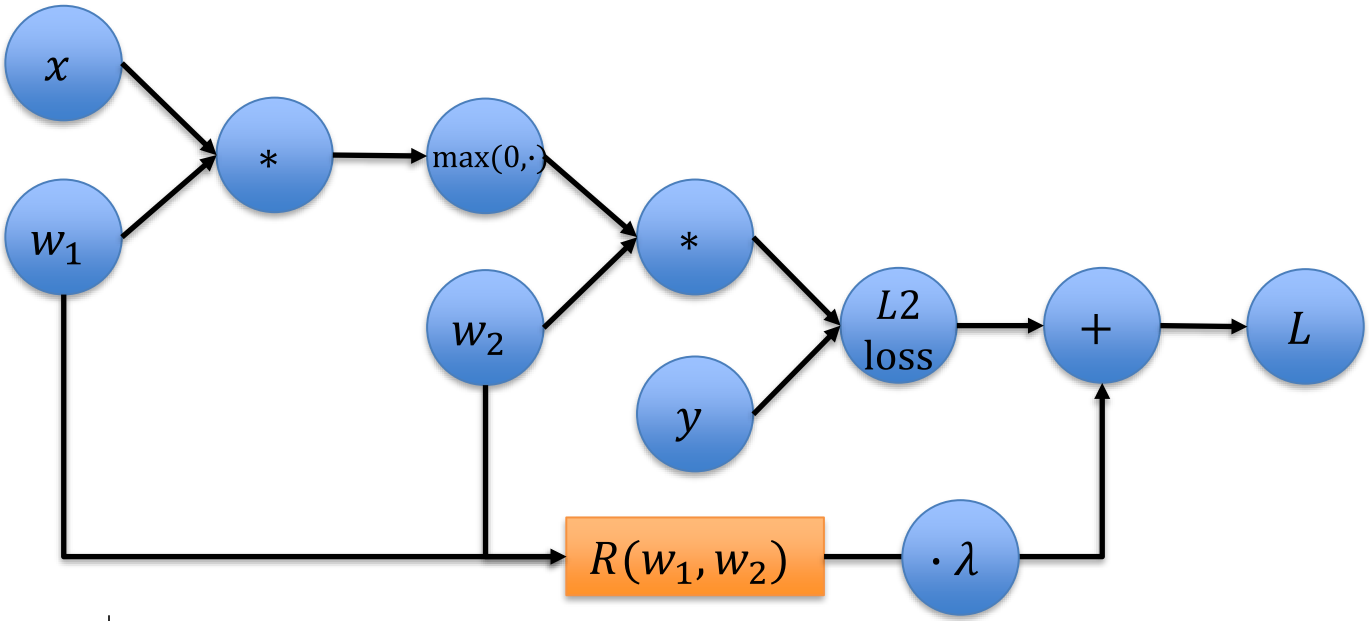
Regularization for Neural Networks



Combining nodes:
Network output + L2-loss + regularization

$$\sum_{i=1}^{n} \|w_2 \max(0, w_1 x_i) - y_i\|_2^2 + \lambda R(w_1, w_2)$$

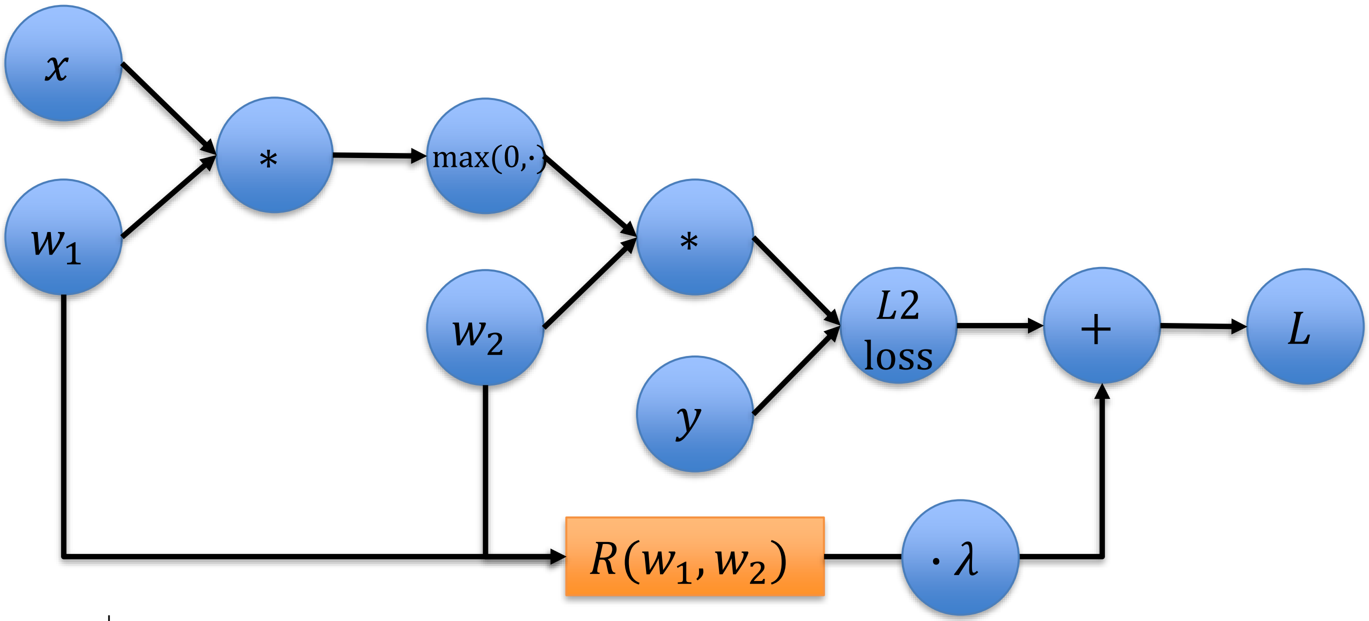
Regularization for Neural Networks



Combining nodes:
Network output + L2-loss + regularization

$$\sum_{i=1}^{n} \|w_2 \max(0, w_1 x_i) - y_i\|_2^2 + \lambda \left\| \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \right\|_2^2$$

Regularization for Neural Networks



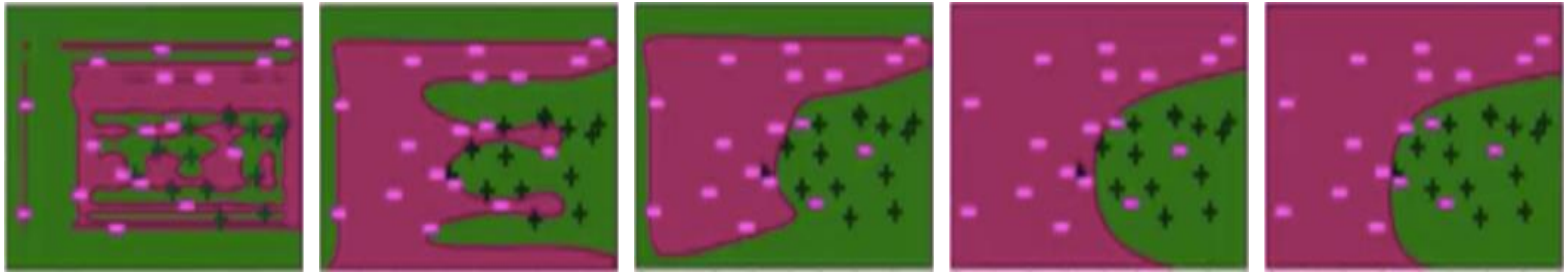
Combining nodes:
Network output + L2-loss + regularization

$$\sum_{i=1}^{n} \| w_2 \max(0, w_1 x_i) - y_i \|_2^2 + \lambda(w_1^2 + w_2^2)$$

Regularization

Regularization $\lambda = 0$ $\lambda = 0.00001$ $\lambda = 0.001$ $\lambda = 1$ $\lambda = 10$

Decision Boundary



Credit: University of Washington

What happens to the training error?

What is the goal of regularization?

Regularization

- Any strategy that aims to

Lower validation error

Increasing training error

Next Lecture

- This week:
  - Check exercises!
  - Check piazza / post questions ☺
- Next lecture
  - Optimization of Neural Networks
  - In particular, introduction to SGD (our main method!)

See you next week ☺

Further Reading

- Backpropagation
  - Chapter 6.5 (6.5.1 - 6.5.3) in http://www.deeplearningbook.org/contents/mlp.html
  - Chapter 5.3 in Bishop, Pattern Recognition and Machine Learning
  - http://cs231n.github.io/optimization-2/
- Regularization
  - Chapter 7.1 (esp. 7.1.1 & 7.1.2) http://www.deeplearningbook.org/contents/regularization.html
  - Chapter 5.5 in Bishop, Pattern Recognition and Machine Learning