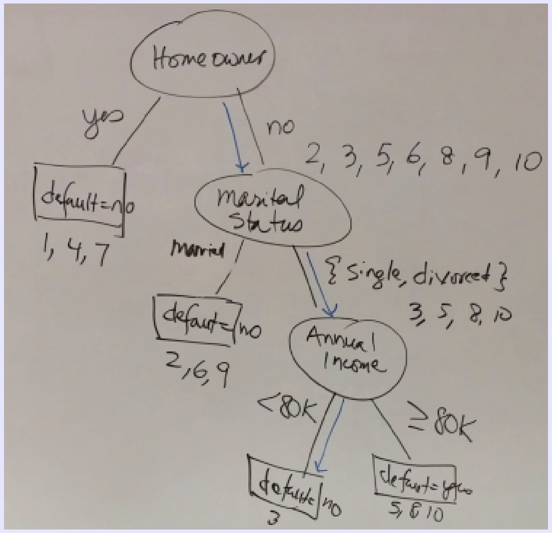
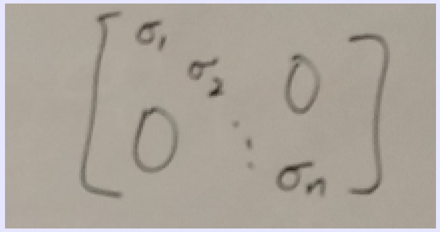
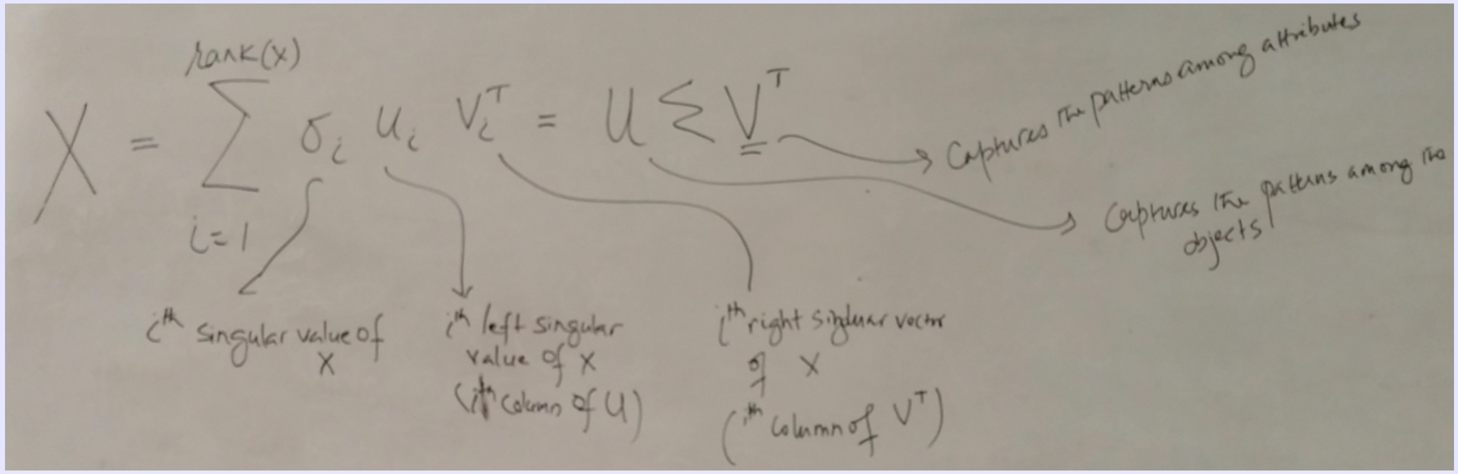
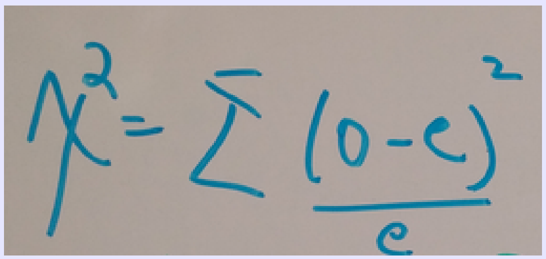
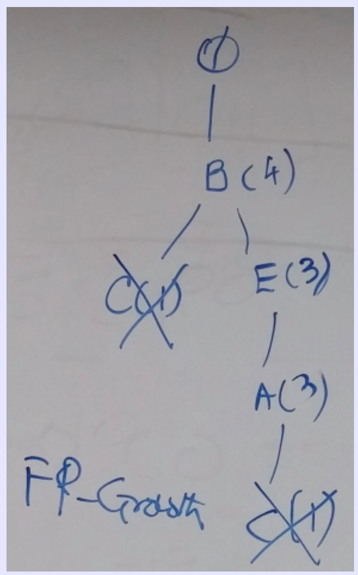
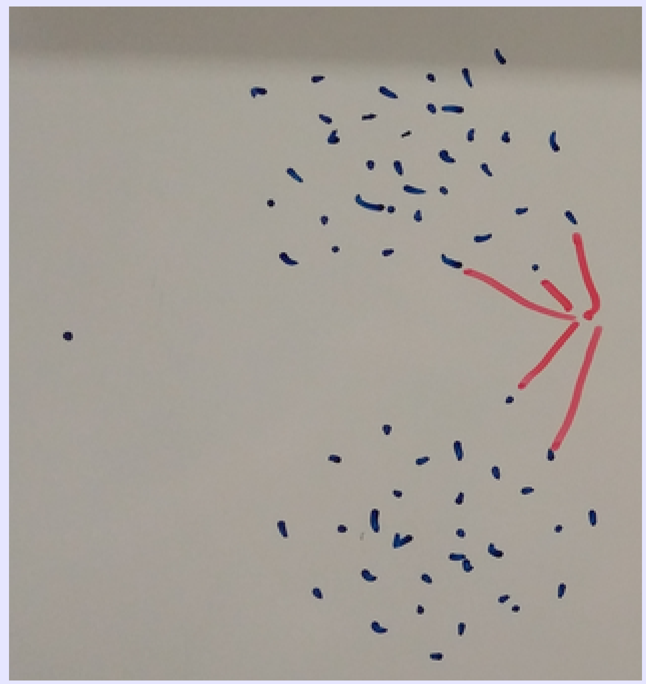












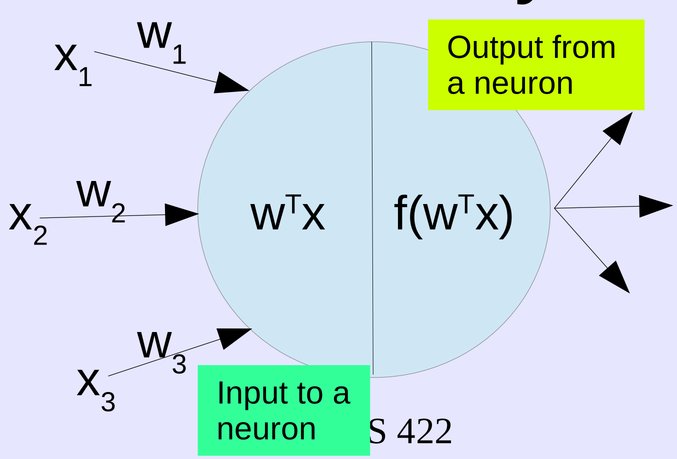
CS 422: Data Mining

Vijay K. Gurbani, Ph.D.,
Illinois Institute of Technology

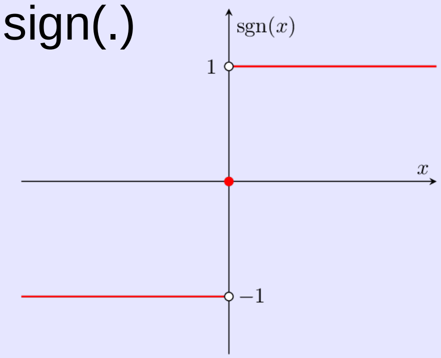
Lecture: **Introduction to Artificial Neural Networks**

Introduction

- Hidden nodes learn *latent* representation (features useful for class boundaries).
- First hidden layer captures simpler features (since it receives the predictors as input).
- Subsequent hidden layers hone into specific patterns of the data to extract features.
- So, what does a hidden layer neuron do?



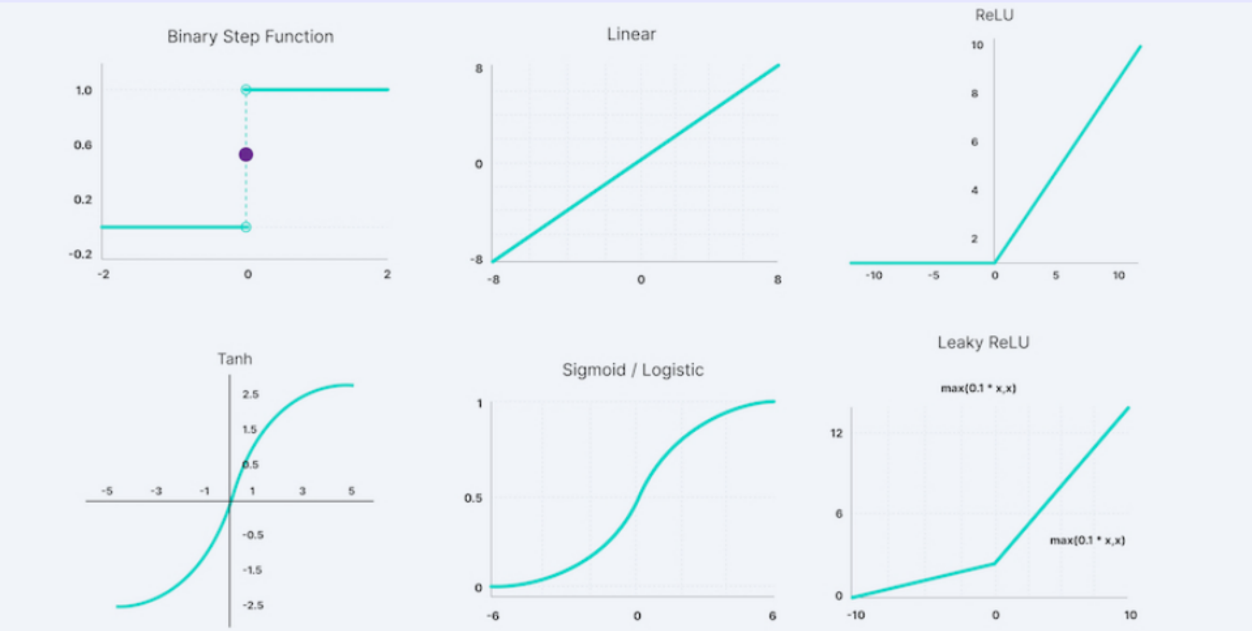
f(.) is an activation function.
You have seen this before …
… sign(.)

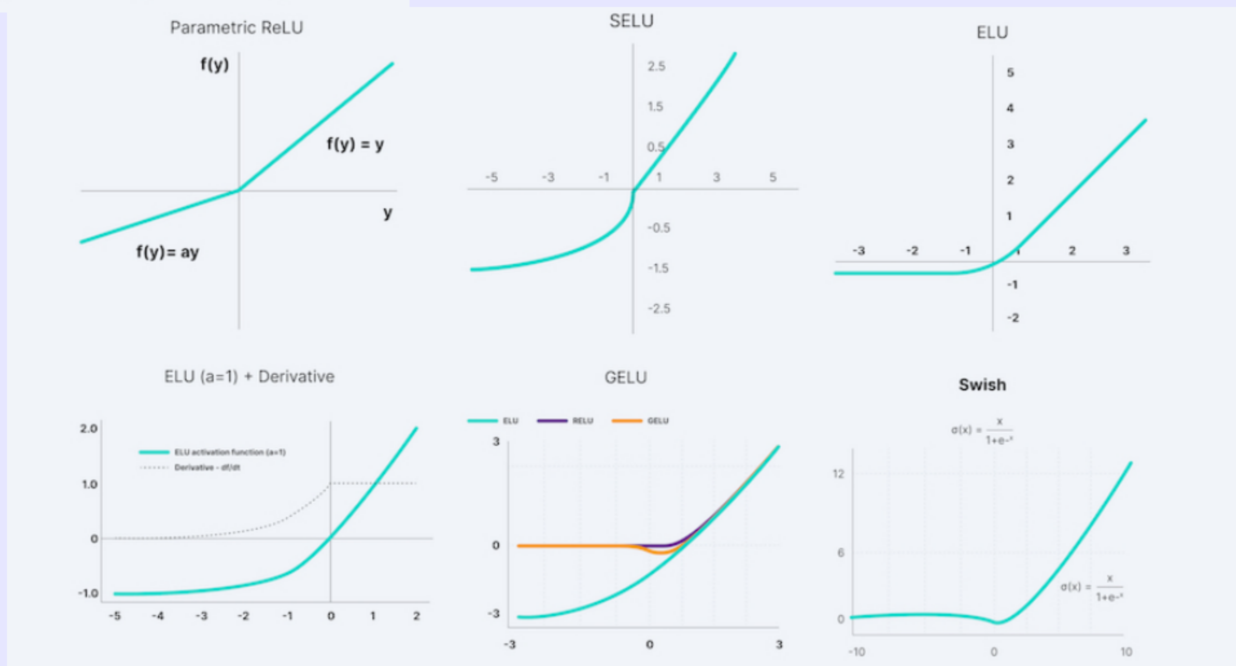


Activation functions

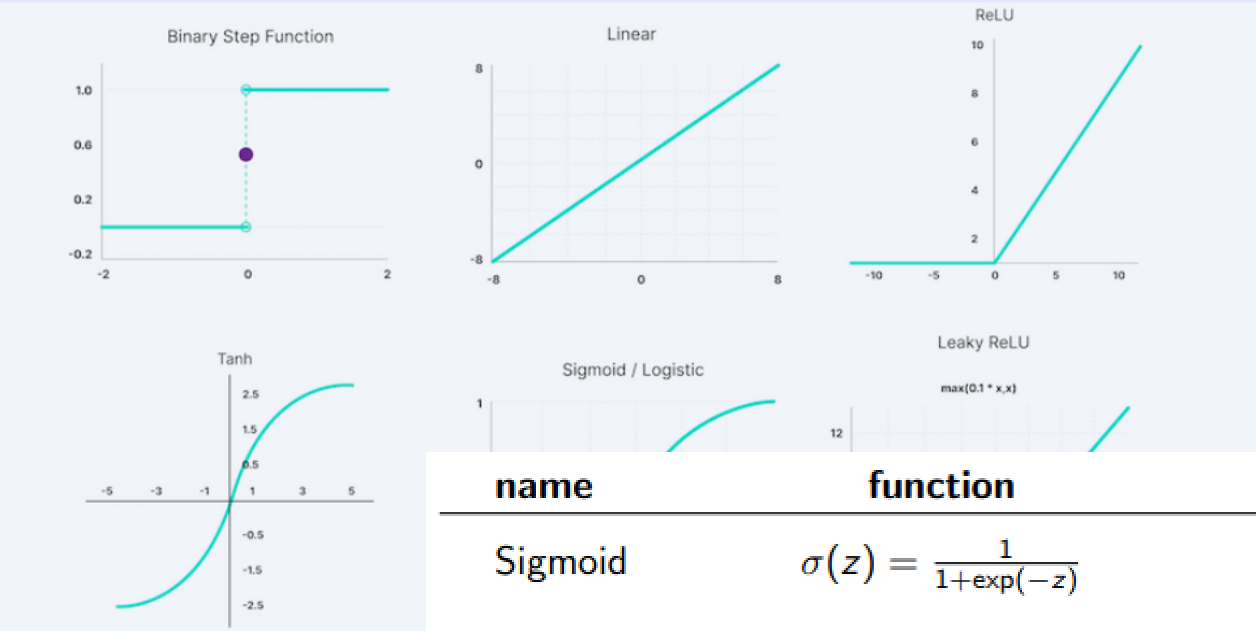
- This activation function is important, as it provides non-linearity to an ANN and allows it to create non-linear class boundaries.
- Different type of activation functions:

Activation functions





Activation functions



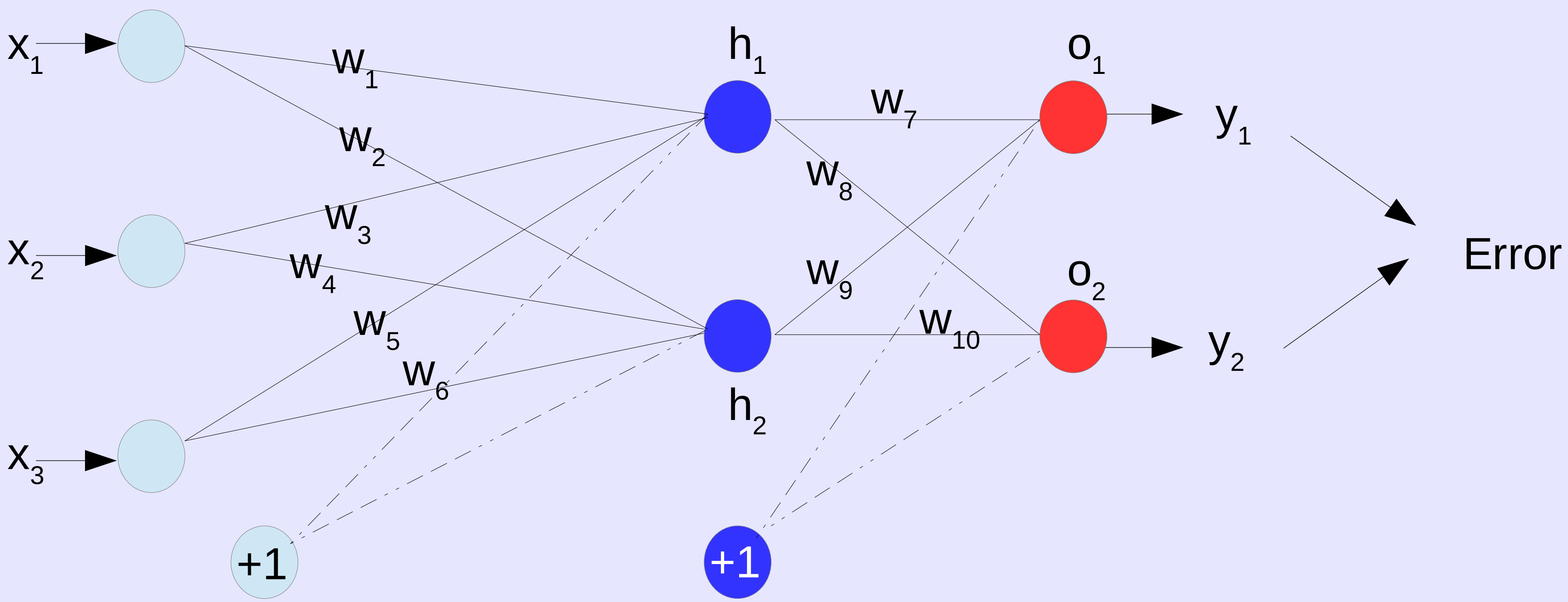
name	function	derivative
Sigmoid	$\sigma(z) = \frac{1}{1+\exp(-z)}$	$\sigma(z) \cdot (1 - \sigma(z))$
ReLU	$\mathrm{ReLU}(z) = \max(0, z)$	$\begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{if } z \leq 0 \end{cases}$

Introduction

- How do you choose an activation function?
  - Match the activation function at the output layer based on the type of prediction problem:
    - Regression: Linear activation function.
    - Binary classification: Sigmoid / Logistic activation function.
    - Multiclass classification: Softmax activation function.
  - For the hidden layers:
    - Start with relu activation function and move to others if results are sub-optimal.

Feed-Forward Neural Network

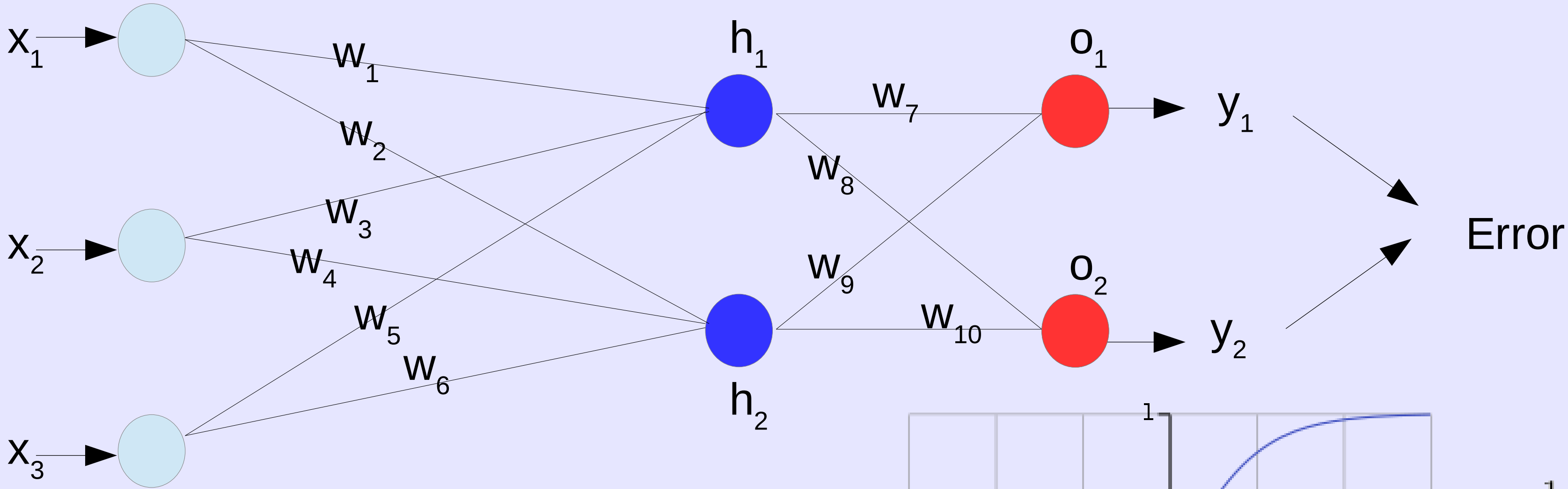
- Let’s consider the simple one hidden layer neural network to understand how it learns.



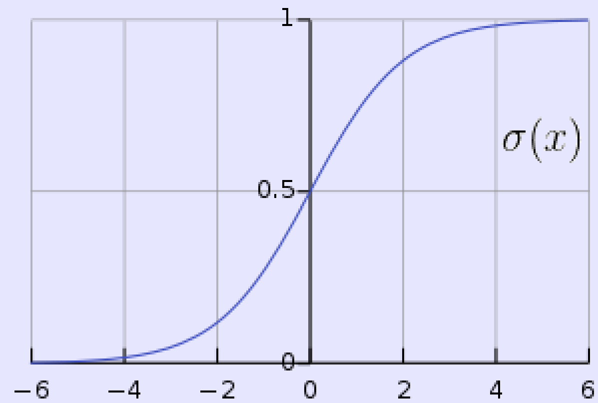
- Three inputs, plus bias, one hidden layer with two neurons, plus bias, and two output neurons.

Feed-Forward Neural Network

- Let's assume bias = 0, for simplification.



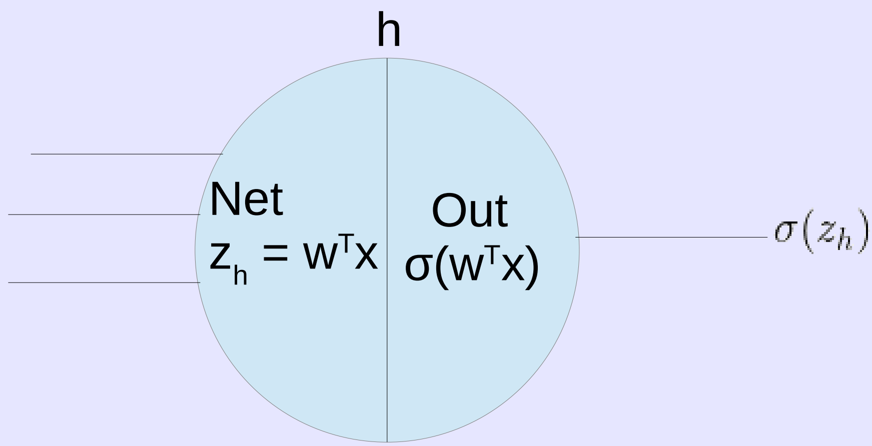
- The activation function at the hidden layers and at the output layer is the sigmoid:



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

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

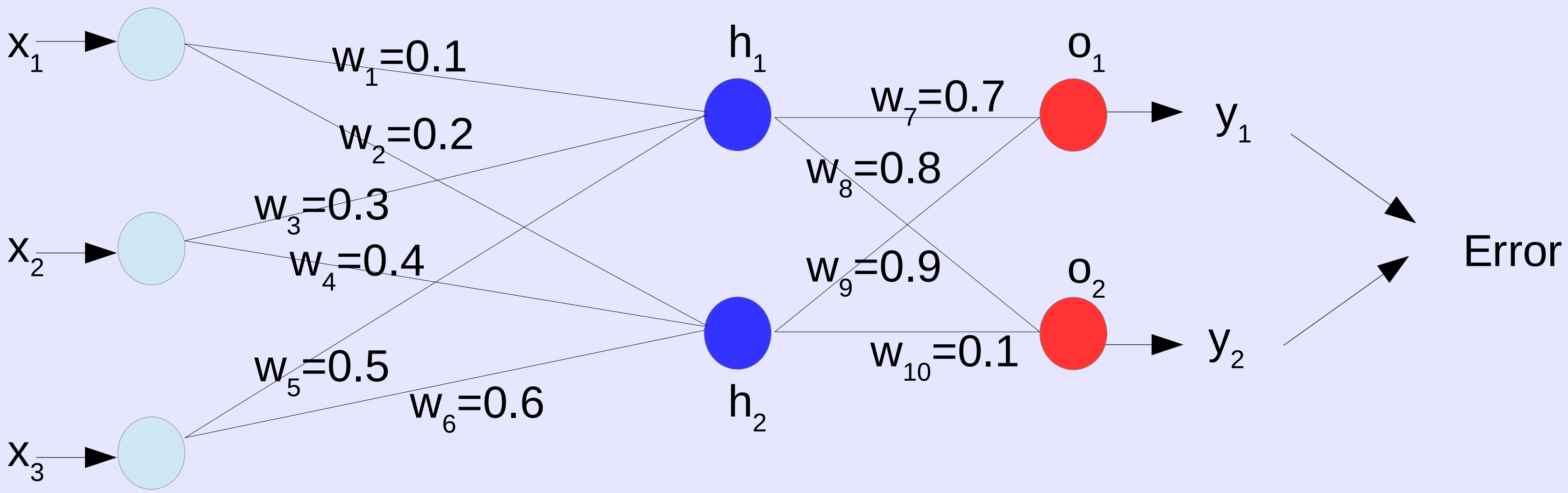
Feed-Forward Neural Network



For a neuron h, the network input to the neuron is: $z_h = w^T x = \sum_{i=1}^{n} w_i x_i = w_1 x_1 + ... + w_n x_n$

For a neuron h, the output from the neuron is: $\sigma(w^T x) = \sigma(z_h)$, where σ is the activation function.

Feed-Forward Neural Network

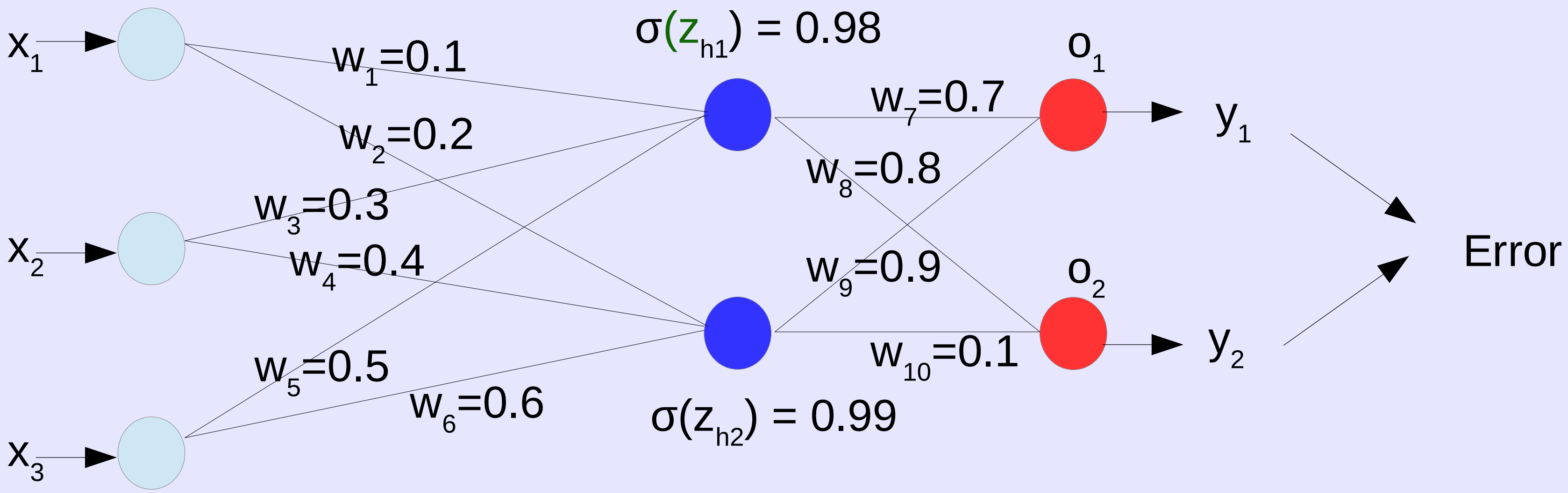


Training example: X = [1,4,5], y = [0.1, 0.05]; weights initialized as shown.

$z_{h1} = (x_1 * w_1 + x_2 * w_3 + x_3 * w_5) = (1*0.1)+(4*0.3)+(5*0.5) = 3.8$
$\sigma(z_{h1}) = \sigma(3.8) = 0.98$

$z_{h2} = (x_1 * w_2 + x_2 * w_4 + x_3 * w_6) = (1*0.2)+(4*0.4)+(5*0.6) = 4.8$
$\sigma(z_{h2}) = \sigma(4.8) = 0.99$

Feed-Forward Neural Network

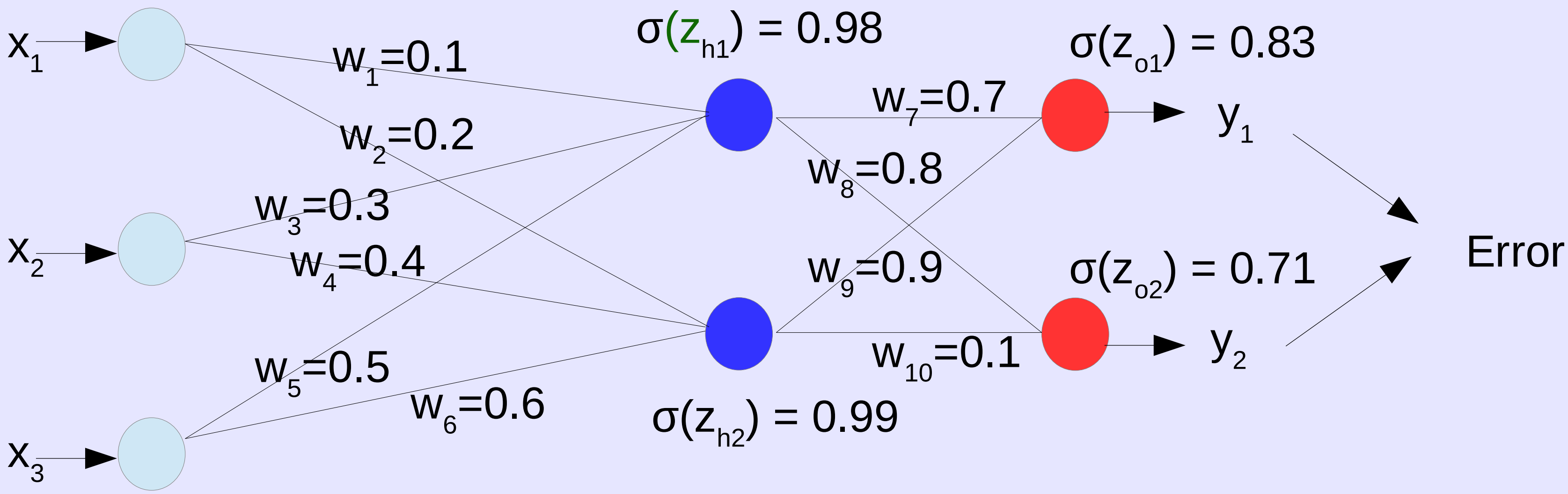


Training example: X = [1,4,5], y = [0.1, 0.05]; weights initialized as shown.

$z_{o1} = (\sigma(Z_{h1}) * w_7 + \sigma(Z_{h2}) * w_9) = (0.98*0.7) + (0.99*0.9) = 1.58$
$\sigma(z_{o1}) = \sigma(1.58) = 0.83$

$z_{o2} = (\sigma(Z_{h1}) * w_8 + \sigma(Z_{h2}) * w_{10}) = (0.98*0.8) + (0.99*0.1) = 0.88$
$\sigma(z_{o2}) = \sigma(0.88) = 0.71$

Feed-Forward Neural Network

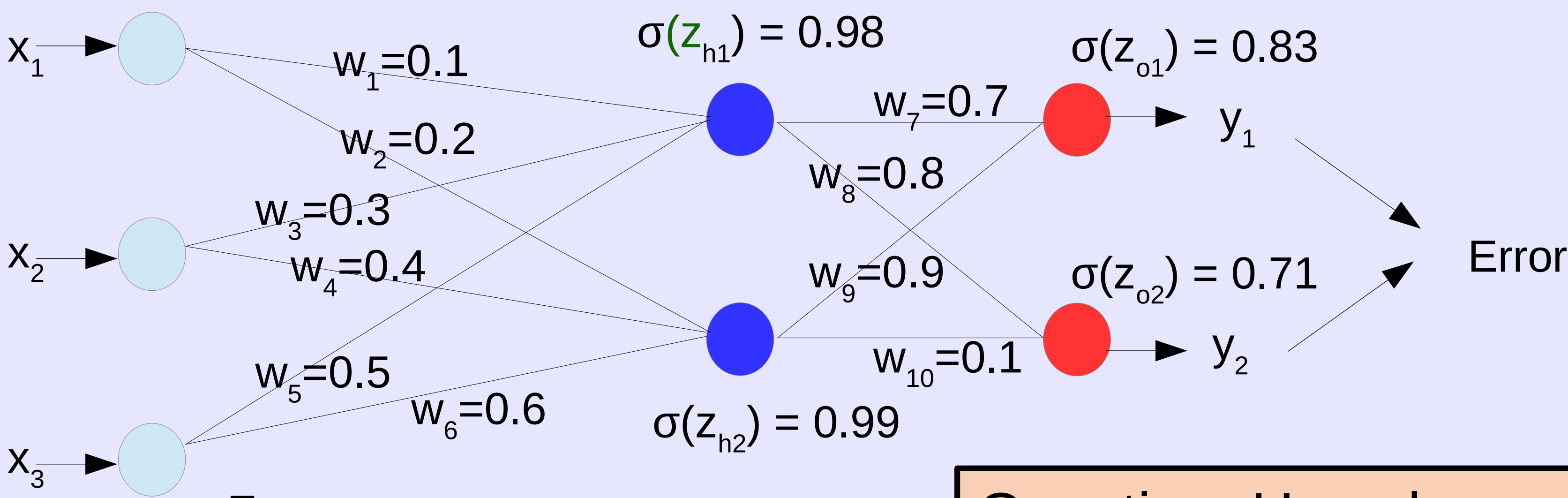


Training example: X = [1,4,5], y = [0.10, 0.05]; weights initialized as shown.

$z_{o1} = (\sigma(Z_{h1}) * w_7 + \sigma(Z_{h2}) * w_9) = (0.98*0.7) + (0.99*0.9) = 1.58$
$\sigma(z_{o1}) = \sigma(1.58) = 0.83$

$z_{o2} = (\sigma(Z_{h1}) * w_8 + \sigma(Z_{h2}) * w_{10}) = (0.98*0.8) + (0.99*0.1) = 0.88$
$\sigma(z_{o2}) = \sigma(0.88) = 0.71$

Feed-Forward Neural Network

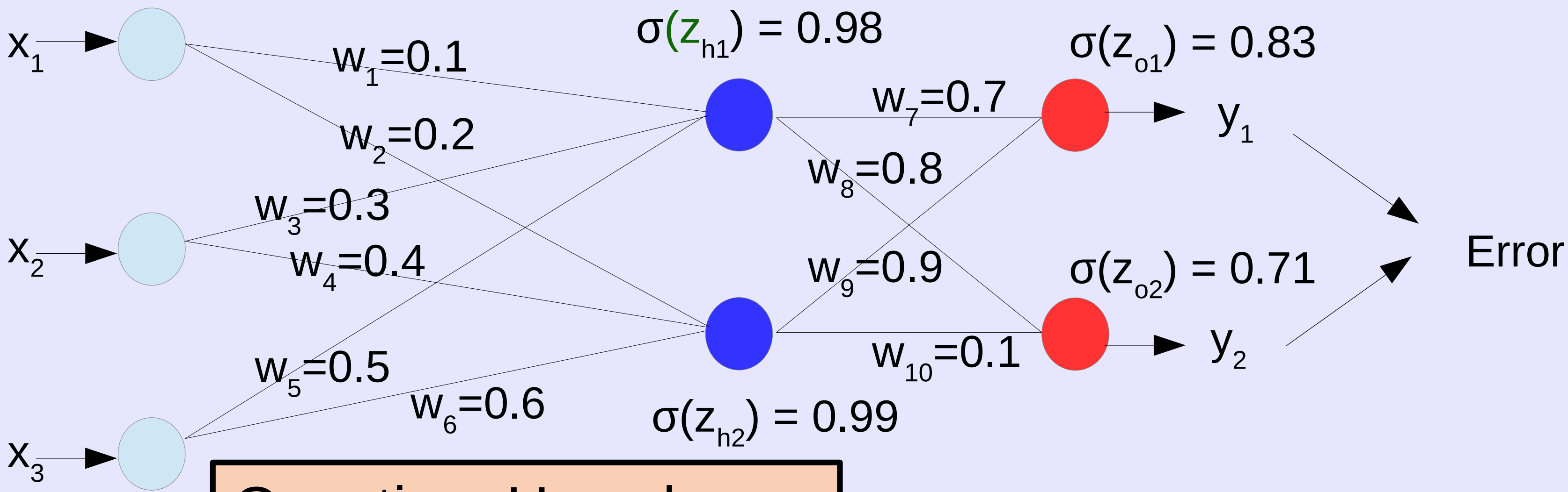


Error:

$$\frac{1}{2}[(\sigma(z_{o_1}) - y_1)^2 + (\sigma(z_{o_2}) - y_2)^2] =$$
$$\frac{1}{2}[(0.83 - 0.1)^2 + (0.71 - 0.05)^2] = 0.48$$

Question: How do we reduce the error?

Feed-Forward Neural Network



Question: How do we reduce the error?

By nudging the weights towards the direction of the error.

But how?

- Using the chain rule from calculus to derive a **gradient** vector. Recall:

$$\nabla f(x) = \left[\partial \frac{f(x_1,\ldots,x_n)}{\partial(x_1)},\ \partial \frac{f(x_1,\ldots,x_n)}{\partial(x_2)}, \ldots,\ \partial \frac{f(x_1,\ldots,x_n)}{\partial(x_n)}\right]$$

- Here, the gradient will be of the error function with respect to each weight (and bias):

$$E(\mathrm{w,b}) = \frac{1}{2}\sum_{i=1}^{n} \mathrm{Loss}(y_i, \hat{y}_i)^2$$

- Typical choice of a loss function is the squared loss function discussed previously.

- Use the gradients to explore the minima of the error function: Gradient Descent algorithm.

Backpropagation

- Chain Rule:

  y = f(g(x)),

  What is $\frac{dy}{dx}$?

Backpropagation

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y = f(g(x)),

What is $\frac{dy}{dx}$?

Let u = g(x), then
y = f(u), and

$$\frac{dy}{dx} = \frac{dy}{du} . \frac{du}{dx}$$

Backpropagation

- Chain Rule:

y = f(g(x)),

What is $\frac{dy}{dx}$?

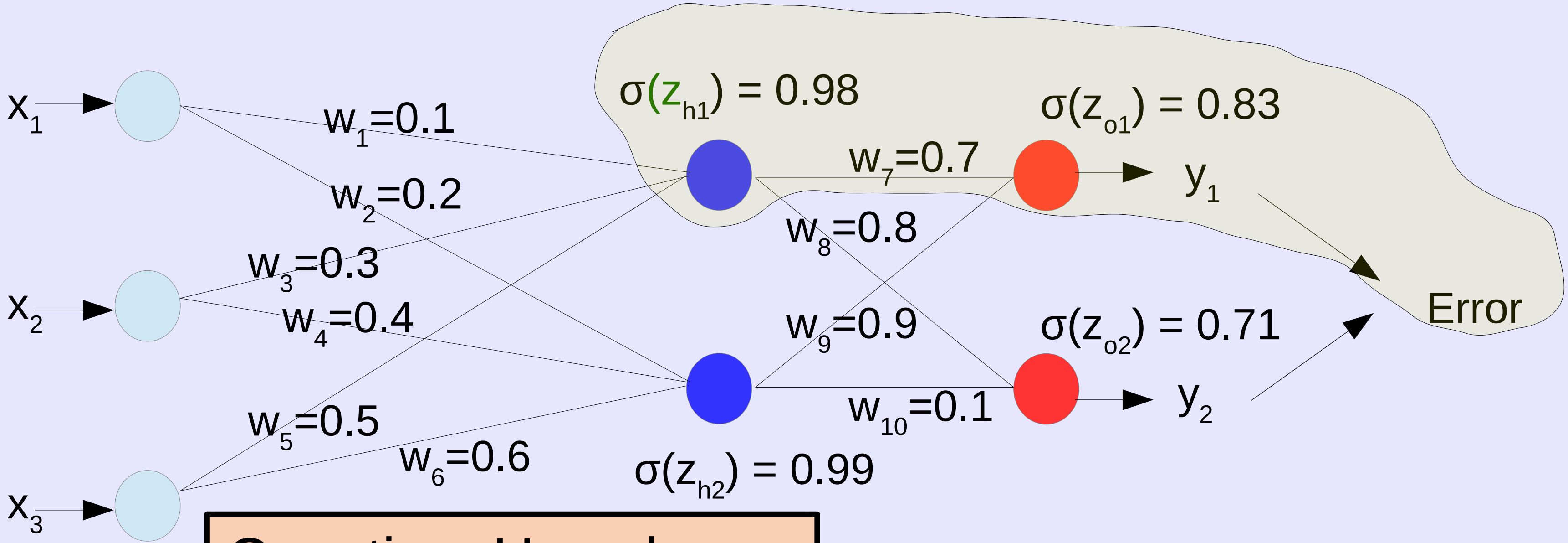
Let u = g(x), then
y = f(u), and

$$\frac{dy}{dx} = \frac{dy}{du} . \frac{du}{dx}$$

y = f(g(h(x)))
Let u = h(x)
v = g(u)
y = f(v)

$$\frac{dy}{dx} = \frac{dy}{dv} . \frac{dv}{du} . \frac{du}{dx}$$

Backpropagation



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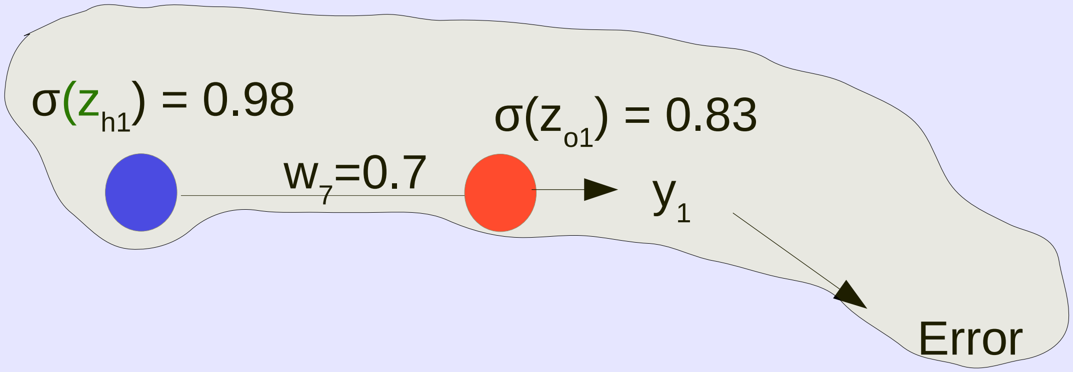


$$y = [0.10, 0.05]$$

Activation function is Sigmoid, $\sigma(x) = \dfrac{1}{1+e^{-x}}$

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \sigma(x)(1-\sigma(x))$$

$$\sigma(Z_{o1}) = 0.83, y = 0.10, \sigma(Z_{h1}) = 0.98$$

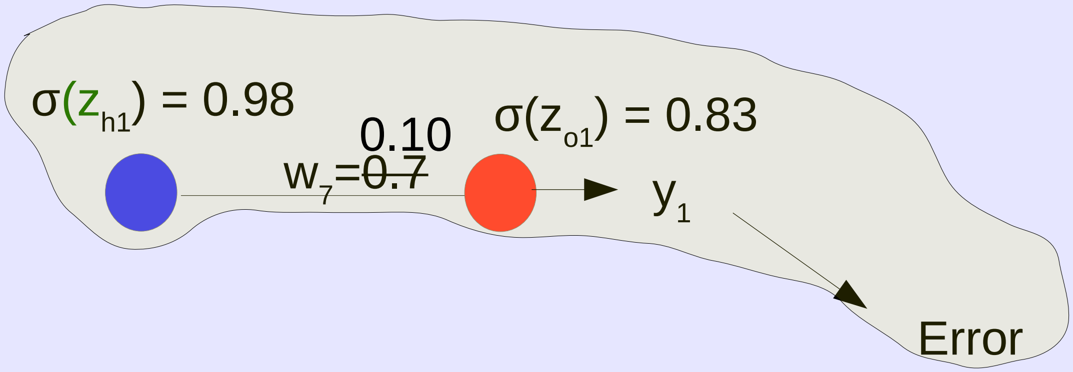
Our error is 0.48 See slide 20 We need to nudge the error to 0.00

$$E(\text{w,b}) = \frac{1}{2}\sum_{i=1}^{n} \text{Loss}(y_i, \hat{y}_i)^2$$

$$= \frac{1}{2}\left[(\sigma(Z_{o1}) - y_1)^2 + (\sigma(Z_{o2}) - y_2)^2\right]$$

$$\frac{\partial E}{\partial \sigma(Z_{o1})} = \sigma(Z_{o1}) - y_1$$

Backpropagation



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$$= \frac{1}{2}\left[(\sigma(Z_{o1}) - y_1)^2 + (\sigma(Z_{o2}) - y_2)^2\right]$$

$$\frac{\partial E}{\partial \sigma(Z_{o1})} = \sigma(Z_{o1}) - y_1$$

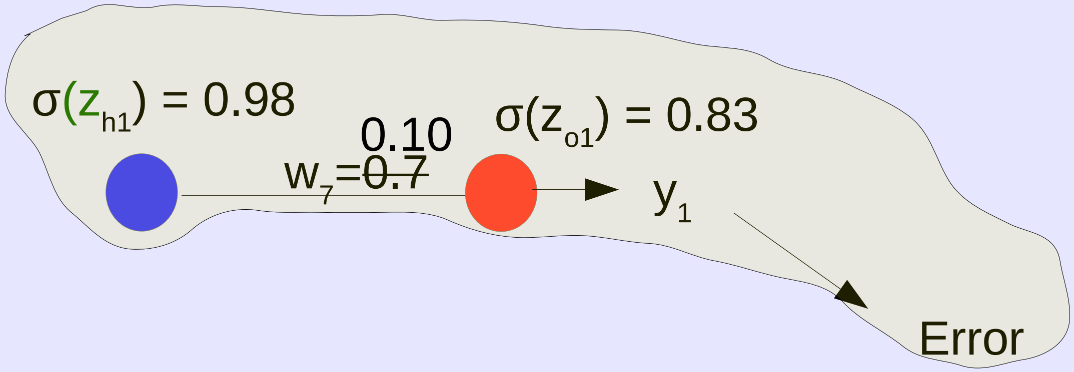
$$\frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \sigma(Z_{o1})} \cdot \frac{\partial \sigma(Z_{o1})}{\partial Z_{o1}} \cdot \frac{\partial Z_{o1}}{\partial w_7}$$

$$= [(\sigma(Z_{o1}) - y_1)] \cdot [\sigma(Z_{o1})(1-\sigma(Z_{o1}))] \cdot [\sigma(Z_{h1})]$$

$$= [(0.83 - 0.1)] \cdot [(0.83 - (1 - 0.83))] \cdot [0.98]$$

$$= 0.10$$

Backpropagation



$y = [0.10, 0.05]$

Activation function is Sigmoid, $\sigma(x) = \frac{1}{1+e^{-x}}$

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \sigma(x)(1-\sigma(x))$$

$\sigma(Z_{o1}) = 0.83, y = 0.10, \sigma(Z_{h1}) = 0.98$

Our error is 0.48 See slide 20 We need to nudge the error to 0.00

$$E(\text{w,b}) = \frac{1}{2}\sum_{i=1}^{n} \text{Loss}(y_i, \hat{y}_i)^2$$

$$= \frac{1}{2}\left[(\sigma(Z_{o1}) - y_1)^2 + (\sigma(Z_{o2}) - y_2)^2\right]$$

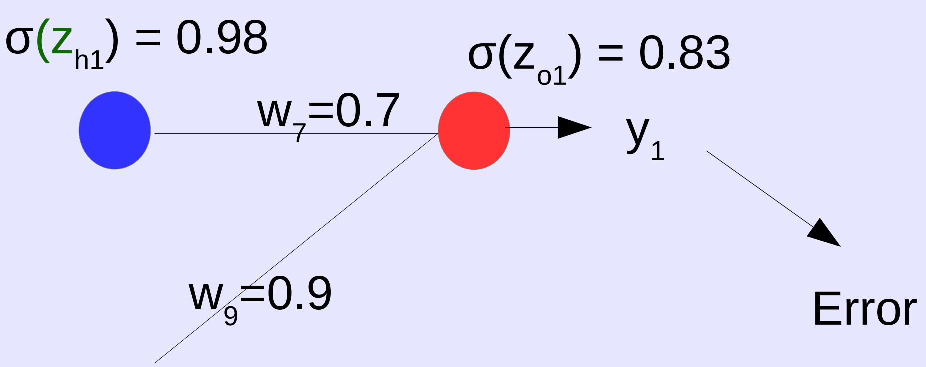
$$\frac{\partial E}{\partial \sigma(Z_{o1})} = \sigma(Z_{o1}) - y_1$$

$$\frac{\partial E}{\partial w_7} = \frac{\partial E}{\partial \sigma(Z_{o1})} \cdot \frac{\partial \sigma(Z_{o1})}{\partial Z_{o1}} \cdot \frac{\partial Z_{o1}}{\partial w_7}$$

$$= [(\sigma(Z_{o1}) - y_1)] \cdot [\sigma(Z_{o1})(1 - \sigma(Z_{o1}))] \cdot [\sigma(Z_{h1})]$$

$$= [(0.83 - 0.1)] \cdot [(0.83 - (1 - 0.83))] \cdot [0.98]$$

$$= 0.10$$

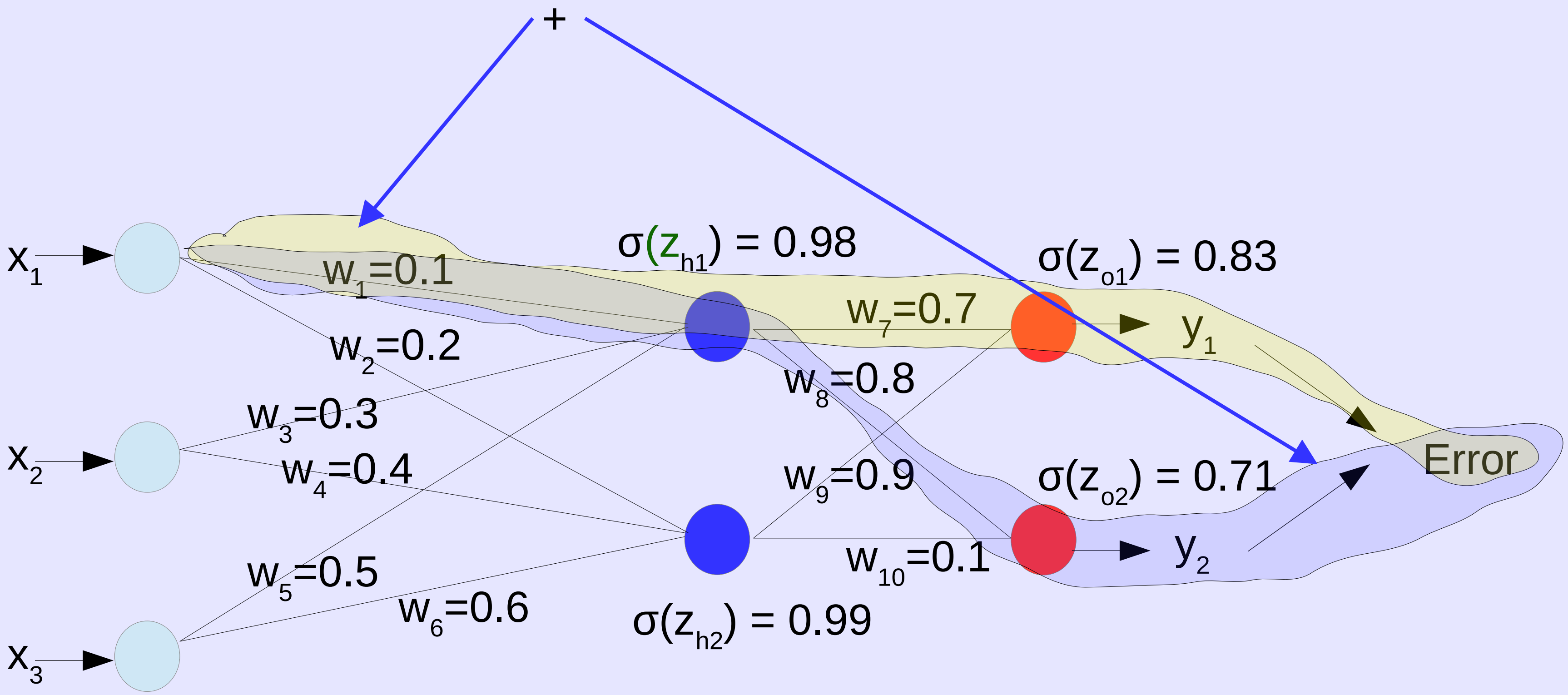


$$\frac{\partial E}{\partial w_9} = \frac{\partial E}{\partial \sigma(Z_{o1})} \cdot \frac{\partial \sigma(Z_{o1})}{\partial Z_{o1}} \cdot \frac{\partial Z_{o1}}{\partial w_9} = 0.10 \quad \text{(Work it out!)}$$

Backpropagation

Propagating errors through the hidden layers.

$$\frac{\partial E}{\partial w_1} = \frac{\partial E}{\partial \sigma(Z_{h1})} \cdot \frac{\partial \sigma(Z_{h1})}{\partial Z_{h1}} \cdot \frac{\partial Z_{h1}}{\partial w_1}$$



Backpropagation

- Result of backpropagation:
  - A gradient vector of weights used for updating the weights to get to the minimum gradient (Jacobian matrix).

$$\nabla E = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \frac{\partial E}{\partial w_3}, ..., \frac{\partial E}{\partial w_n}\right]^T = [0.61, 0.87, 0.21, ..., 0.99]^T$$

- Summary of backpropagation:
  - Feed forward computation
  - Backpropagation to the output layer
  - Backpropagation to the hidden layer(s)
  - Weight updates.

$$w_{new} = w_{old} - \eta \nabla E$$

Gradient descent

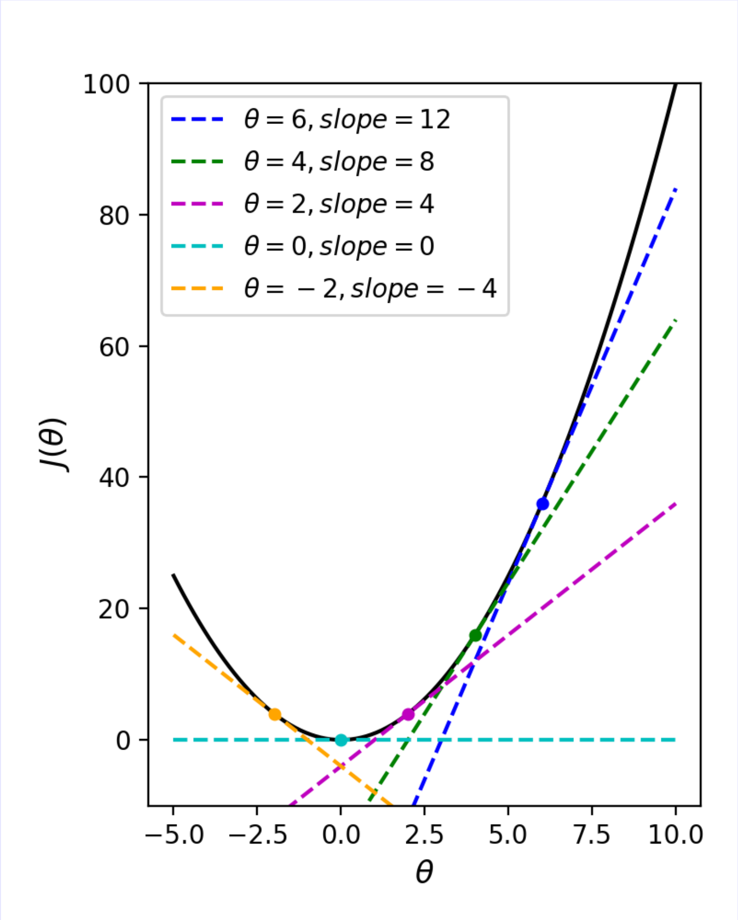
Gradient descent

- Relates two concepts:
  - Error (or cost) function minimization.
  - Minimizes the error function with respect to the weights. (Recall: $\nabla E = \frac{\partial E}{\partial w_i} \text{ for all } i \in \{1, 2, ..., n\}$)
- A gradient descent algorithm iteratively goes through the training dataset, modifying weights during each pass (epoch) to minimize the cost.

$$w_{new} = w_{old} - \eta \nabla E$$

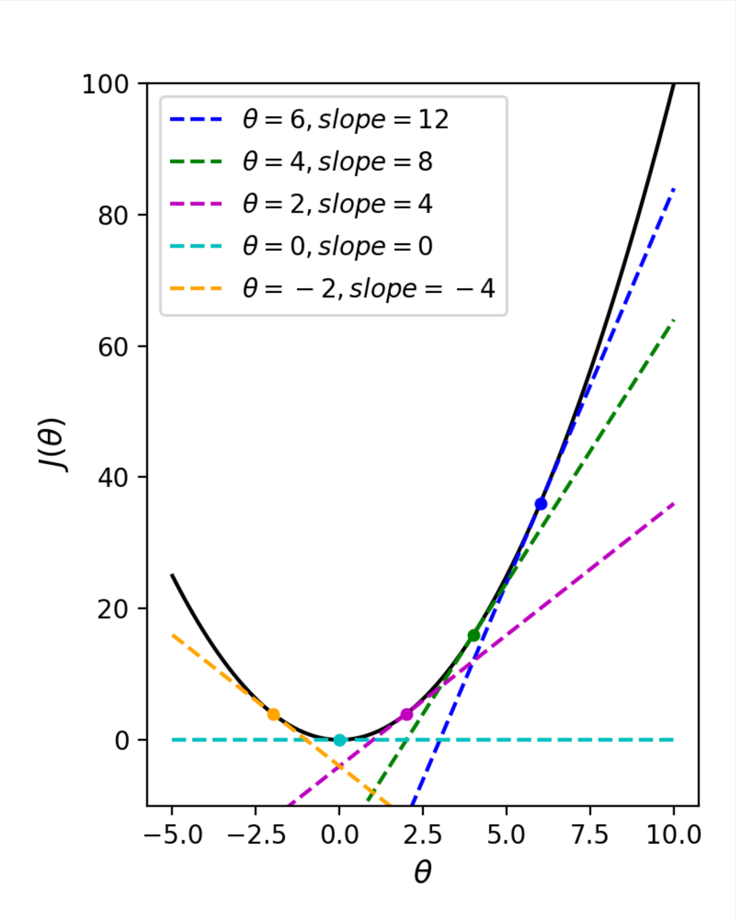
Gradient descent

Intuitive feel of the gradient.

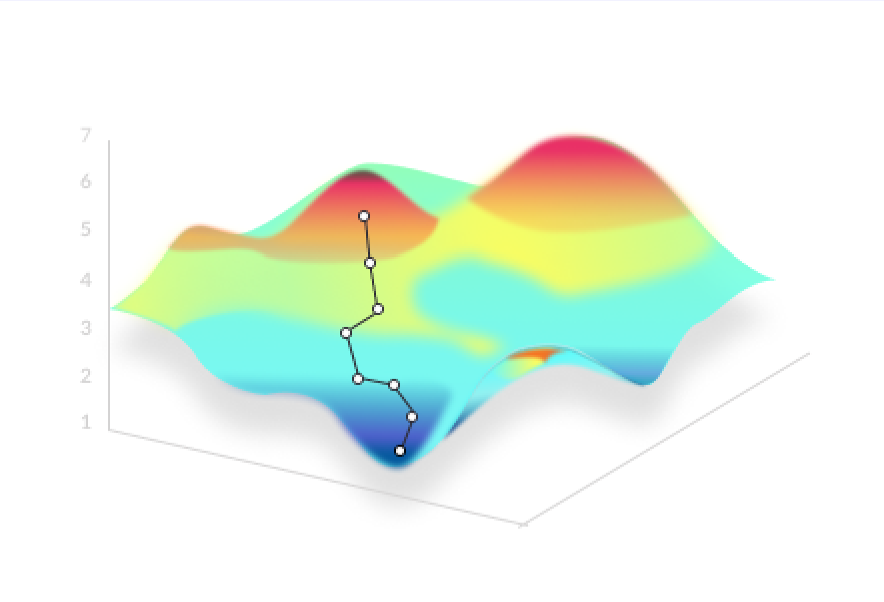


Gradient descent

Intuitive feel of the gradient.



Gradient descent in neural networks



Gradient descent

- Types of gradient descent algorithms:
  - Batch gradient descent
    - Calculate error for each observation, and at end of the training data calculate average error and update *w*.
  - Stochastic gradient descent
    - Calculate error for each observation, and update *w*.
  - Mini-batch gradient descent
    - Split data into small batches, calculate error for each observation in a batch, and at end of the batch calculate average error and update *w*.
    - Preferred method.

Gradient descent

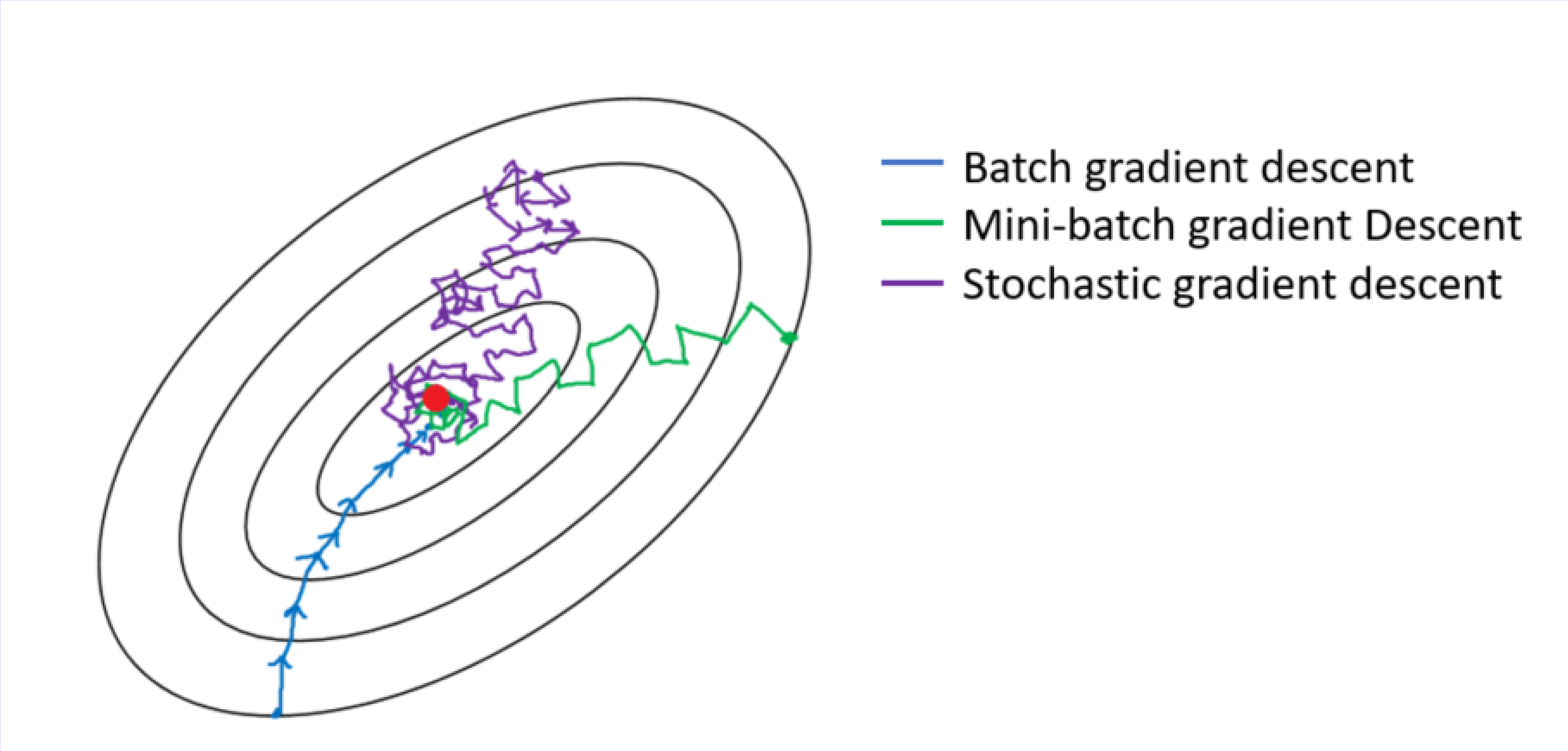
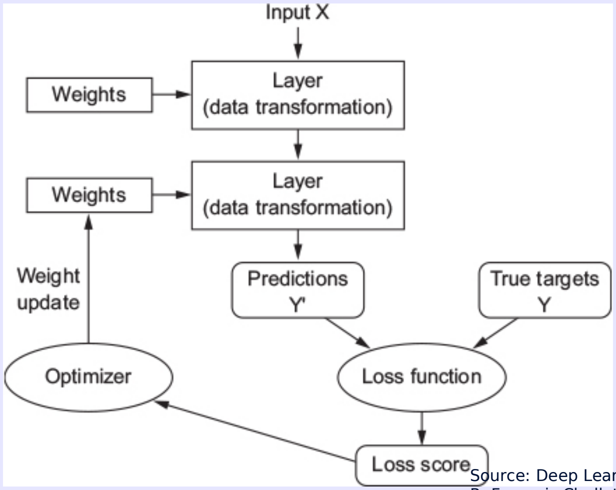


Image source: https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3

Summary

- The learning process in neural networks



Source: Deep Learning with R, Francois Chollet and J.J. Allaire, Manning Press, 2018.

Code

- iris-nn.r
- The Fashion MNIST dataset (neural-main.r)