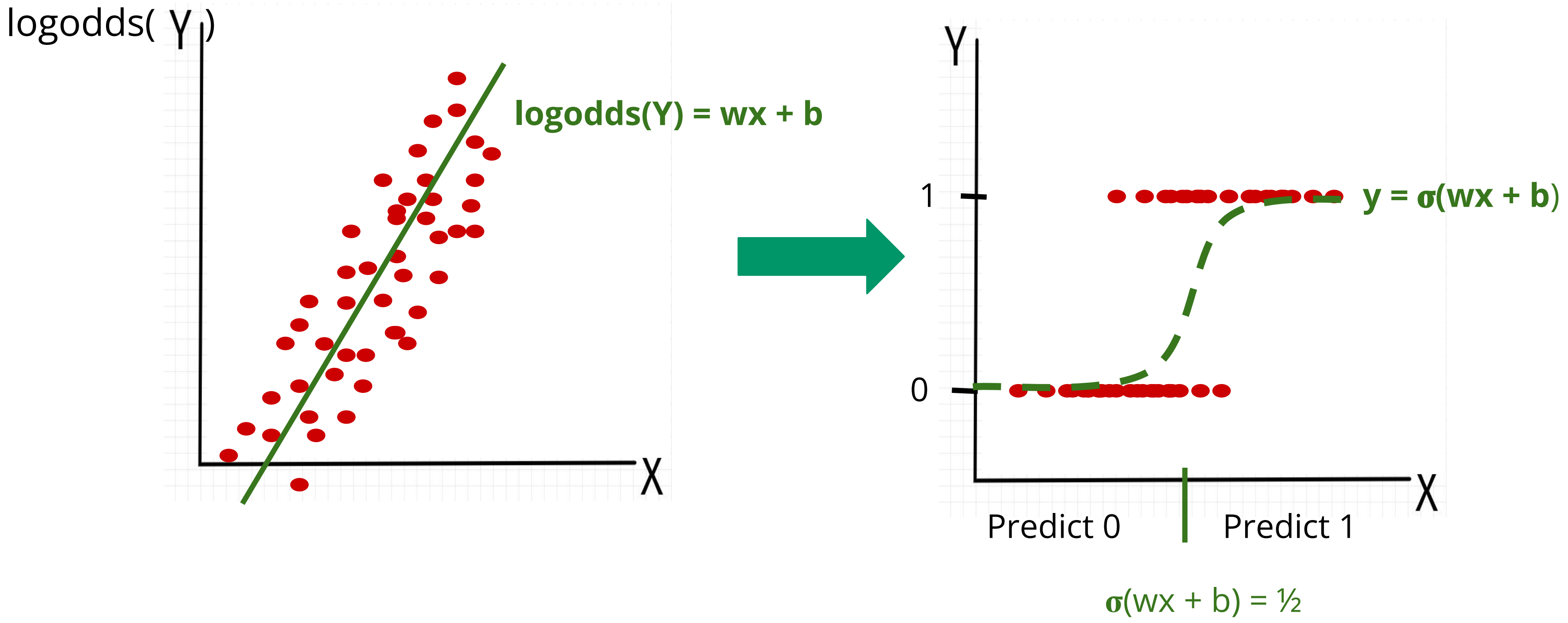
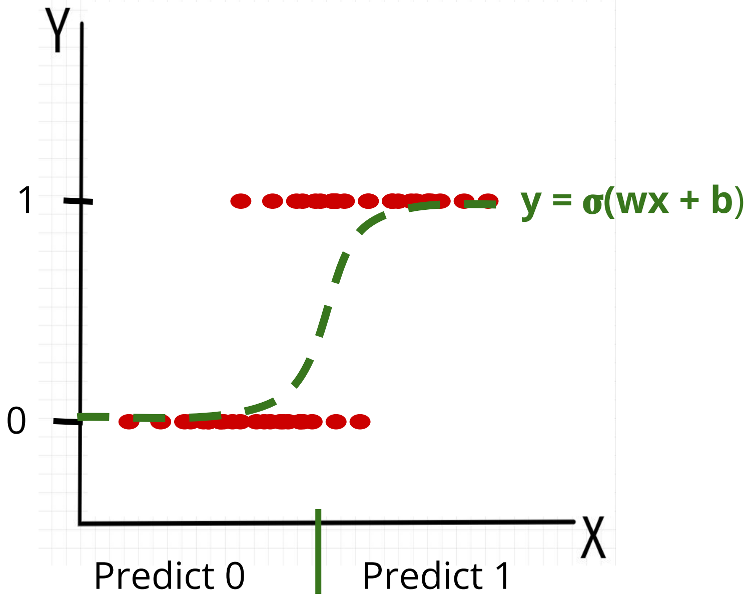
Neural Networks

Boston University CS 506 - Lance Galletti

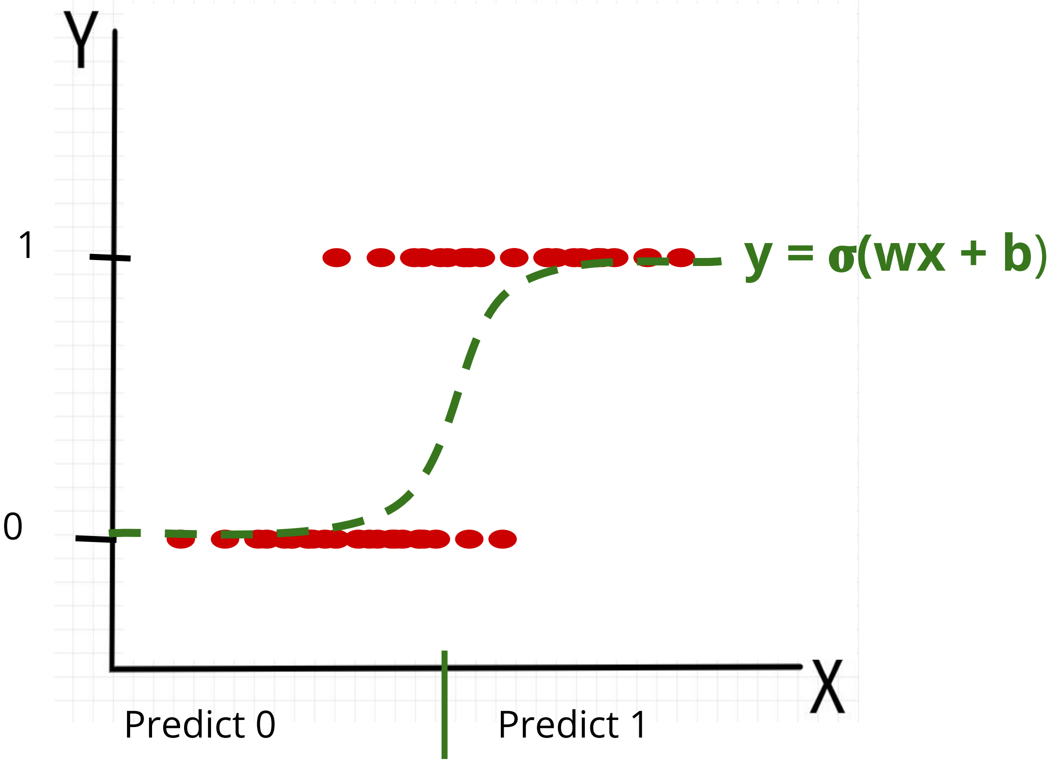
DECISION RULE:
IF P(Y=1|X) > ½ THEN 1 ELSE 0



DECISION RULE:
IF P(Y=1|X) > ½ THEN 1 ELSE 0



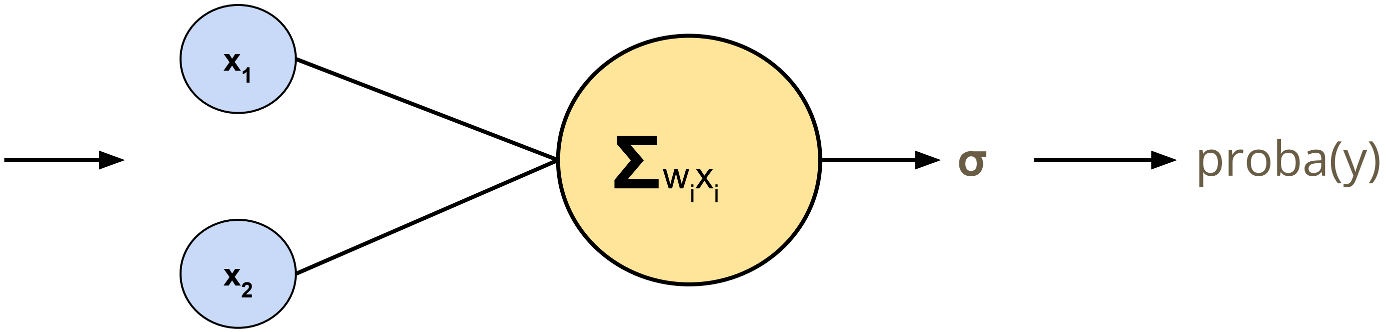
$\sigma(wx + b) = \frac{1}{2}$



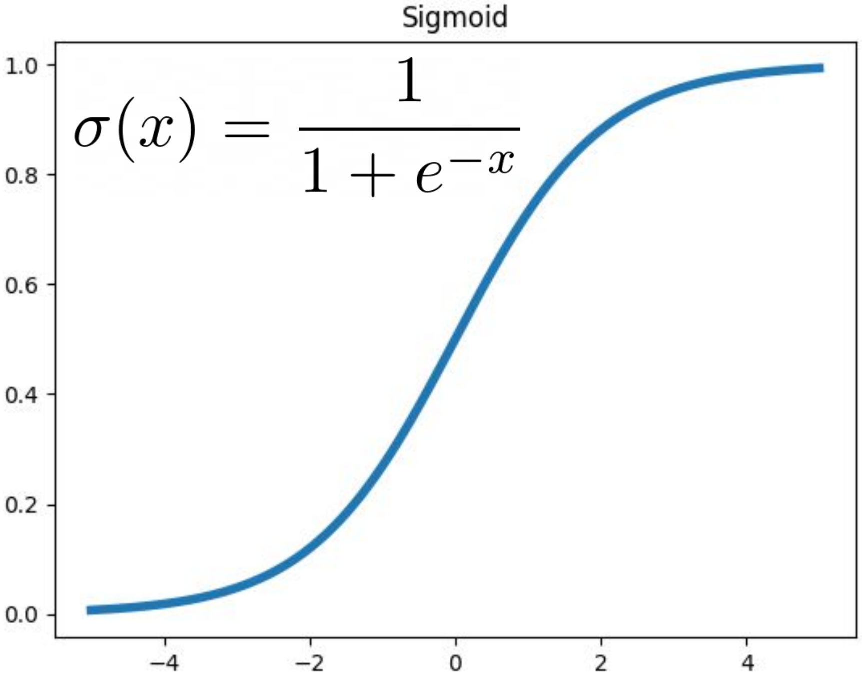
$$\sigma(wx + b) = \frac{1}{2}$$

Logistic Regression Revisited

x_1	x_2	y
...	...	0
...	...	1
...	...	1
...	...	0



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



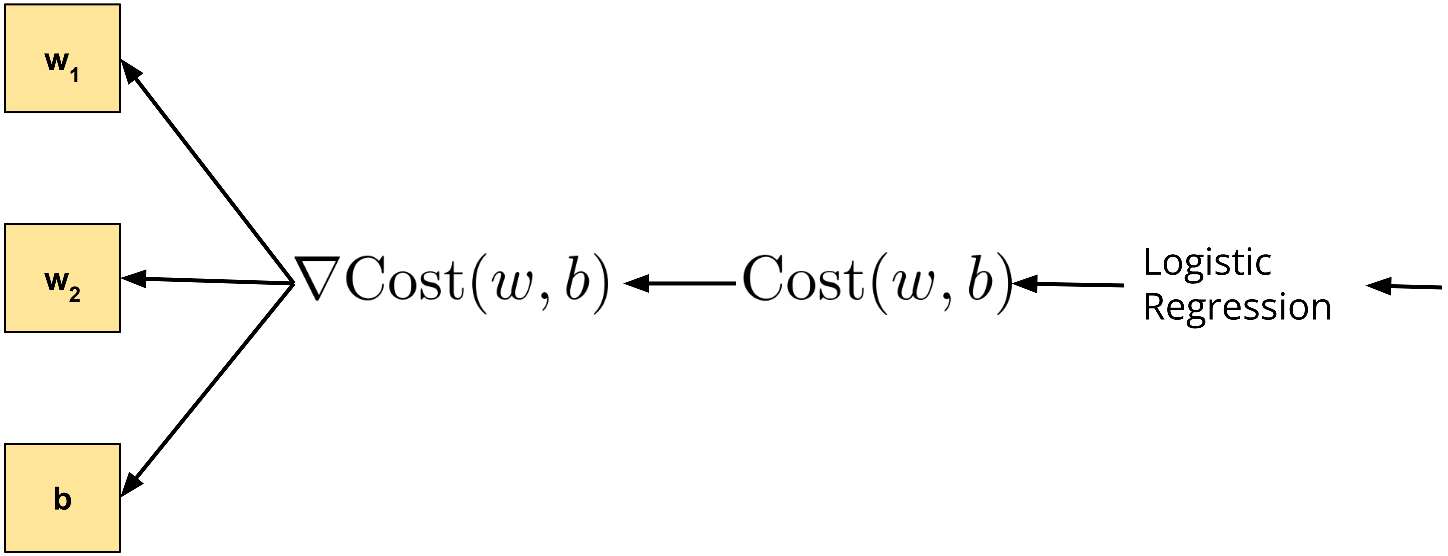
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

$$\max \prod_{i=1}^{n} P(y_i|x_i) = \prod_{i} (logit^{-1}(w^T x_i + b))^{y_i} (1 - logit^{-1}(w^T x_i + b))^{1-y_i}$$

$$= \min -\frac{1}{n} \sum_{i=1}^{n} \left[yi \log(\sigma(-w^T x_i + b)) + (1 - y_i) \log(1 - \sigma(-w^T x_i + b)) \right]$$

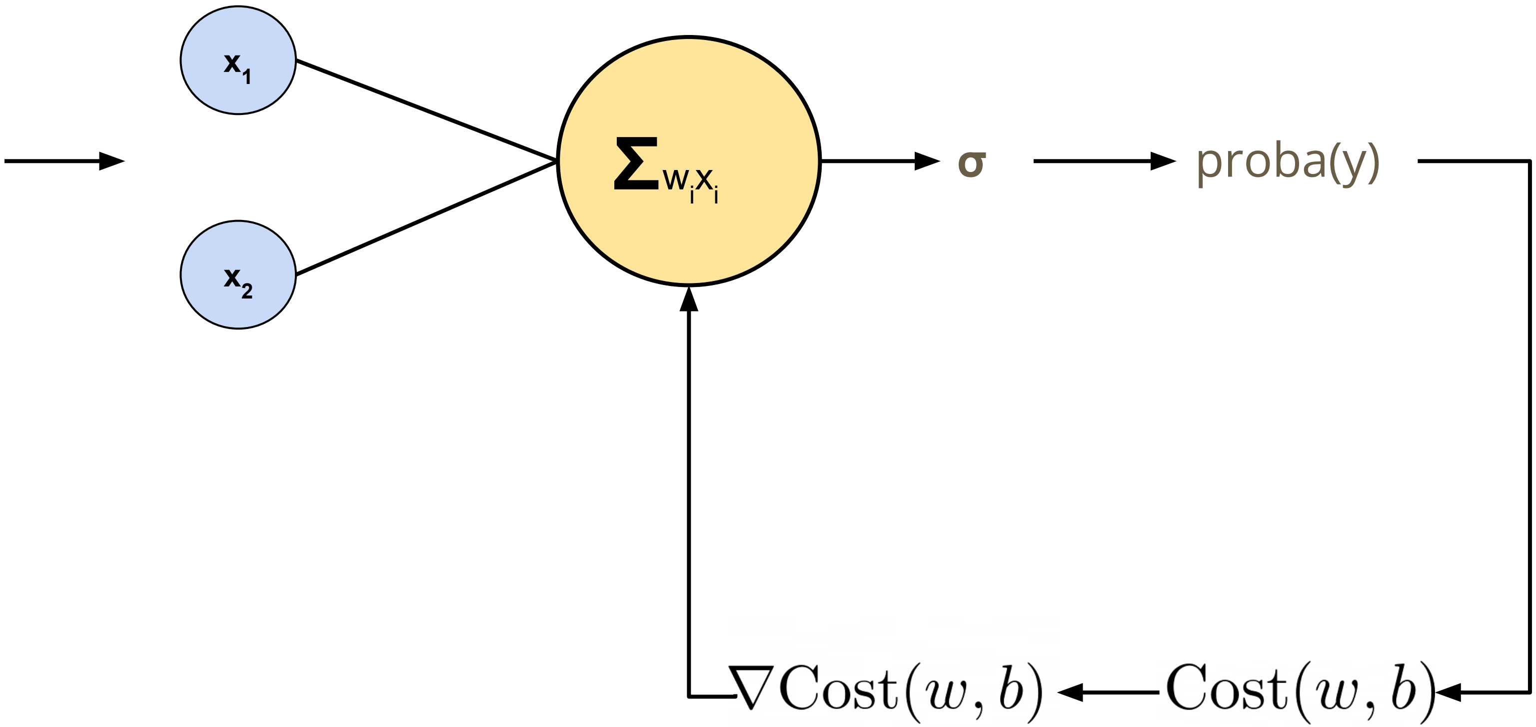
$$= \min \mathrm{Cost}(w, b)$$

Gradient Descent



x_1	x_2	y
...	...	0
...	...	1
...	...	1
...	...	0

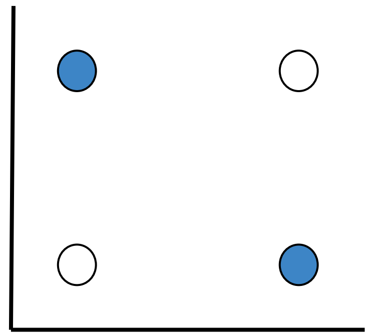
x_1	x_2	y
...	...	0
...	...	1
...	...	1
...	...	0



Logistic Regression Revisited

XOR function

x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	0



Logistic Regression Revisited

XOR function

x_1	x_2	y
0	0	0
1	0	1
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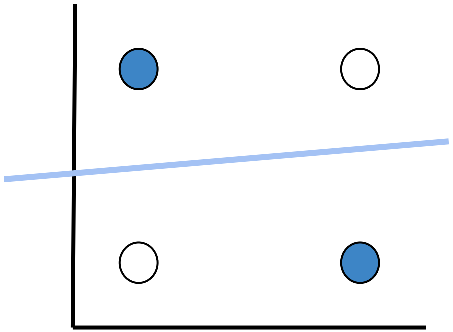
1	1	0



Logistic Regression Revisited

XOR function

x_1	x_2	y
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1	0	1
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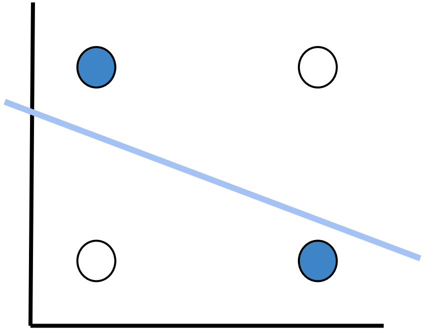

Logistic Regression Revisited

XOR function

x_1	x_2	y
0	0	0
1	0	1
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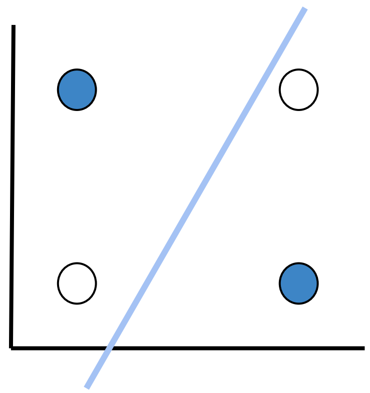
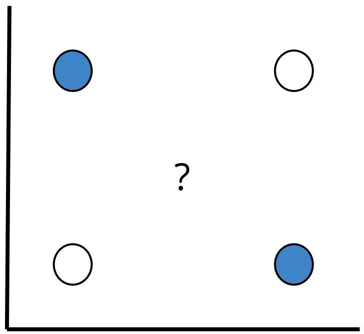


Logistic Regression Revisited

XOR function

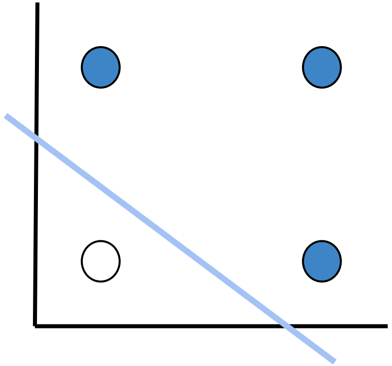
x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	0



Logistic Regression Revisited

Recall, the **OR** function is linearly separable:

x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	1



Logistic Regression Revisited

XOR(x_1, x_2) = **OR**(**AND**$(x_1 = 0 , x_2 = 1)$, **AND**$(x_1 = 1 , x_2 = 0)$)

$$= (x_1 = 0 \wedge x_2 = 1) \vee (x_1 = 1 \wedge x_2 = 0)$$

x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	0

Logistic Regression Revisited

$$\textbf{XOR}(x_1, x_2) = \textbf{OR}(\ \textbf{AND}(x_1 = 0\ , x_2 = 1), \textbf{AND}(x_1 = 1\ , x_2 = 0))$$

$$= (x_1 = 0 \wedge x_2 = 1) \vee (x_1 = 1 \wedge x_2 = 0)$$

$$= h_1 \vee\ h_2$$

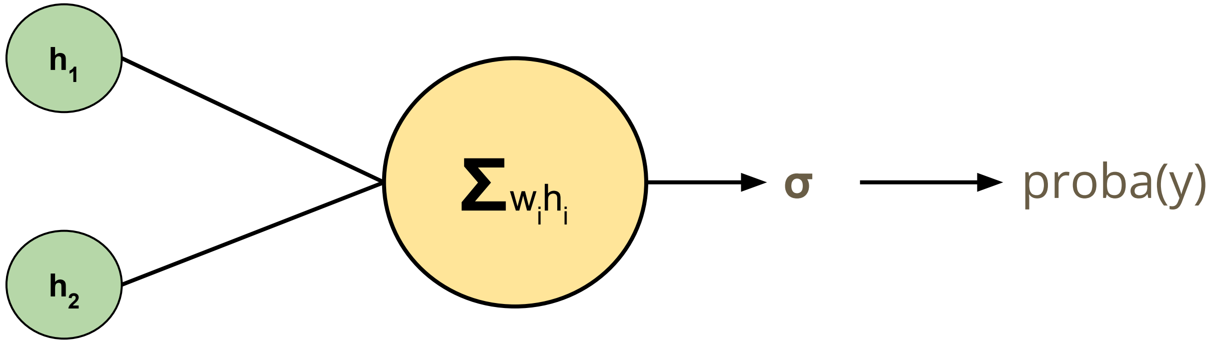
$h_1 = \textbf{AND}(x_1 = 0\ , x_2 = 1)$

$h_2 = \textbf{AND}(x_1 = 1\ , x_2 = 0)$

x_1	x_2	$\mathbf{h_1}$	$\mathbf{h_2}$	y
0	0	0	0	0
1	0	0	1	1
0	1	1	0	1
1	1	0	0	0

Logistic Regression Revisited

h_1	h_2	y
0	0	0
0	1	1
1	0	1
0	0	0

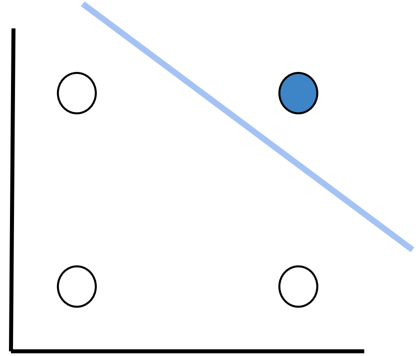


where $$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Logistic Regression Revisited

But, the **AND** function is also linearly separable:

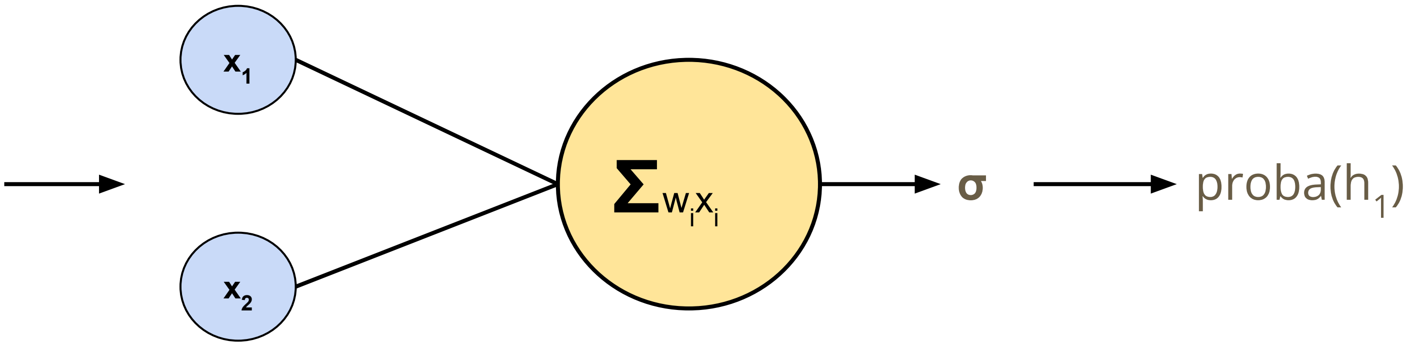
x_1	x_2	y
0	0	0
1	0	0
0	1	0
1	1	1



Logistic Regression Revisited

Since we can learn h_1 and h_2 automatically through logistic regression

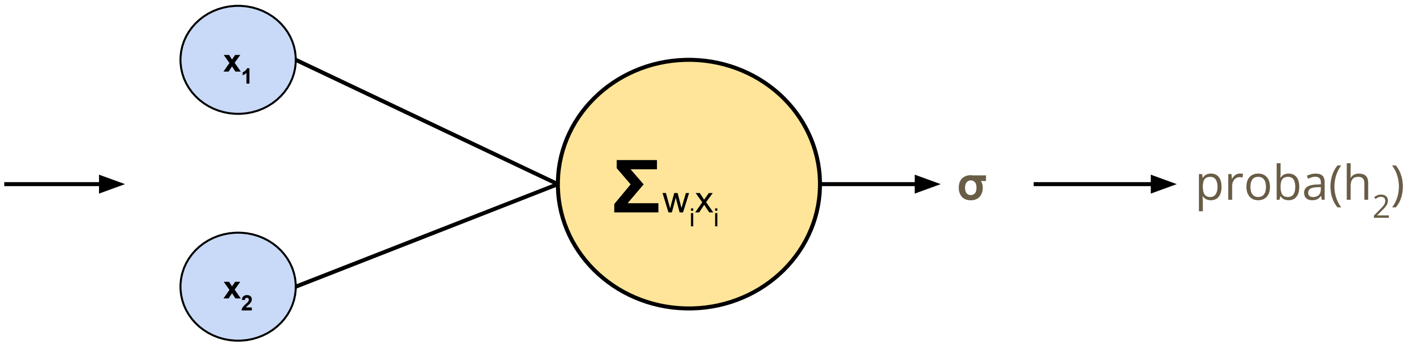
x_1	x_2	h_1
0	0	0
0	1	0
1	0	1
1	1	0



Logistic Regression Revisited

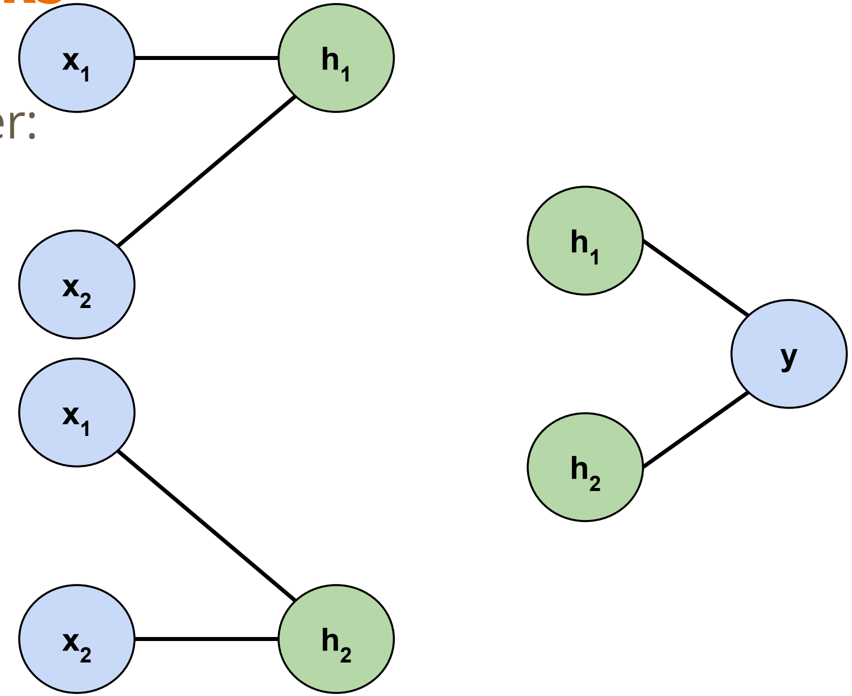
Since we can learn h_1 and h_2 automatically through logistic regression

x_1	x_2	h_2
0	0	0
0	1	1
1	0	0
1	1	0



Neural Networks

Putting it all together:



Neural Networks

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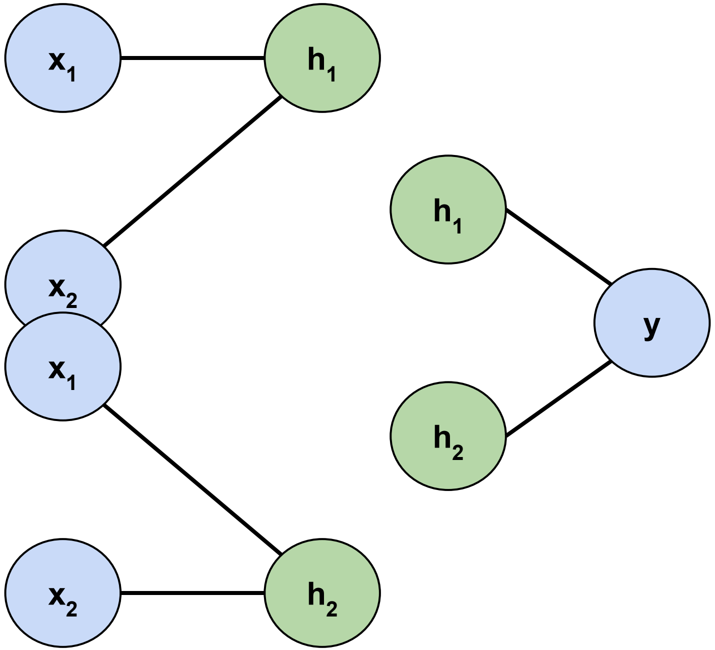

Neural Networks

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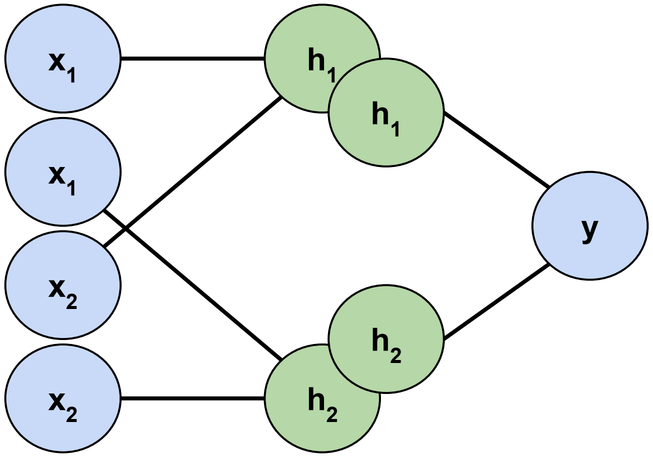

Neural Networks

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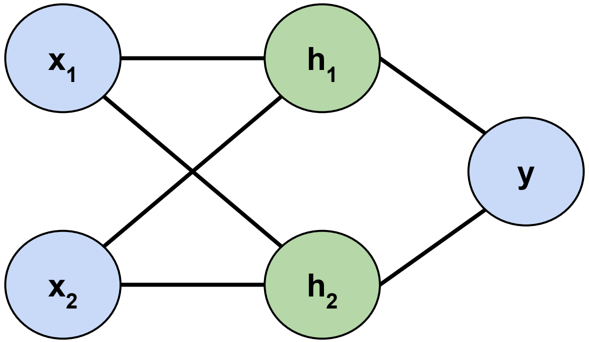
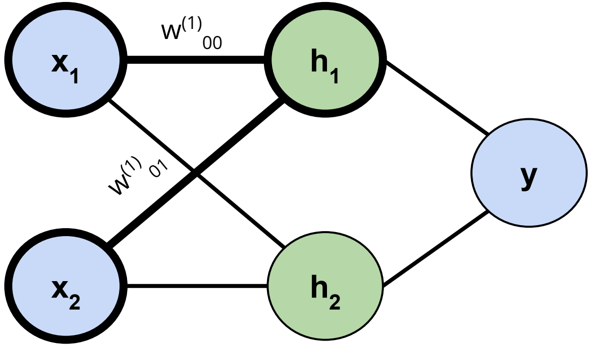
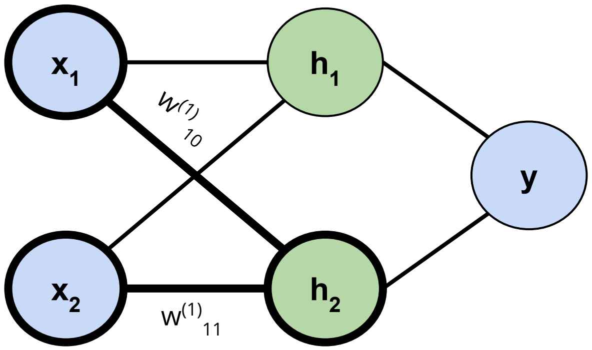


Neural Networks



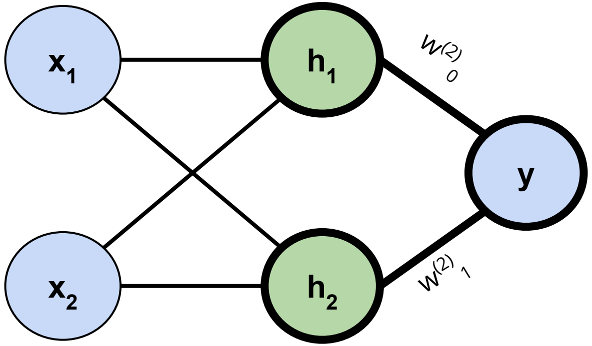
$$h_1 = \boldsymbol{\sigma}(w^{(1)}_{00}\, x_1 + w^{(1)}_{01}\, x_2 + b^{(1)}_{1})$$

Neural Networks



$$h_2 = \boldsymbol{\sigma}(w^{(1)}_{10}\, x_1 + w^{(1)}_{11}\, x_2 + b^{(1)}_{2})$$

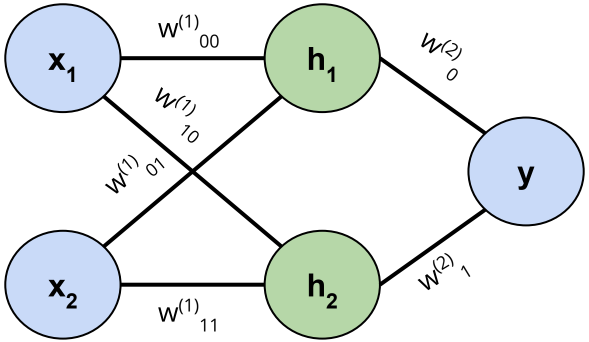
Neural Networks



$y = \boldsymbol{\sigma}(\ w^{(2)}_0\ h_1 + w^{(2)}_1\ h_2 + b^{(2)}_1)$

Neural Networks

Putting it all together:



Neural Networks

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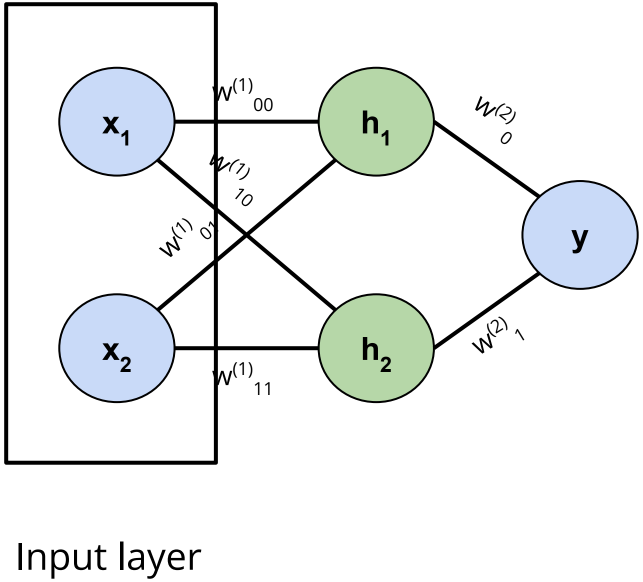
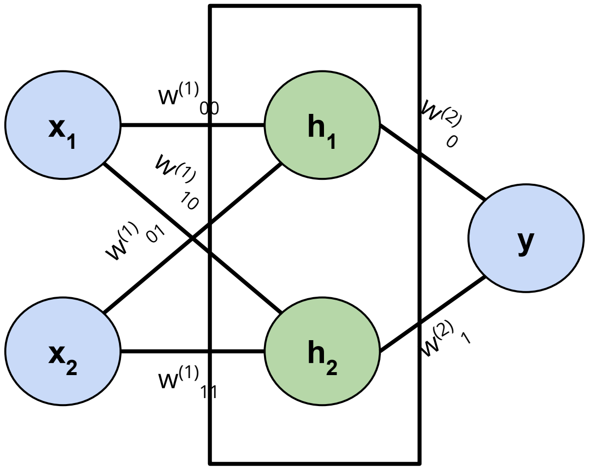


Neural Networks

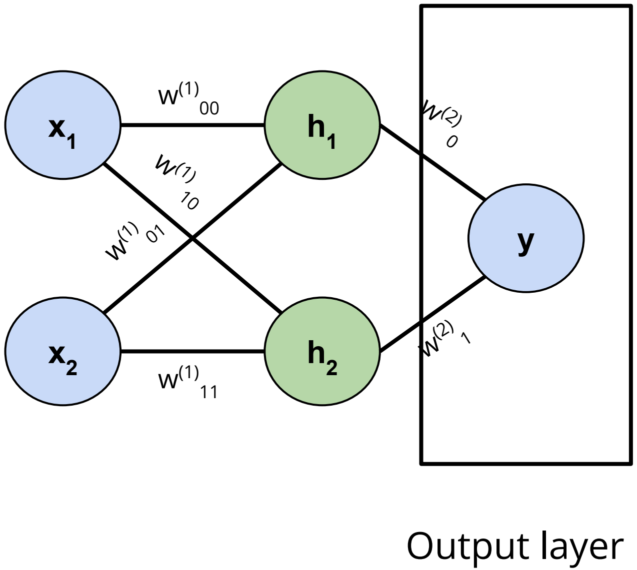
Putting it all together:



Hidden layer

Neural Networks

Putting it all together:



Neural Networks

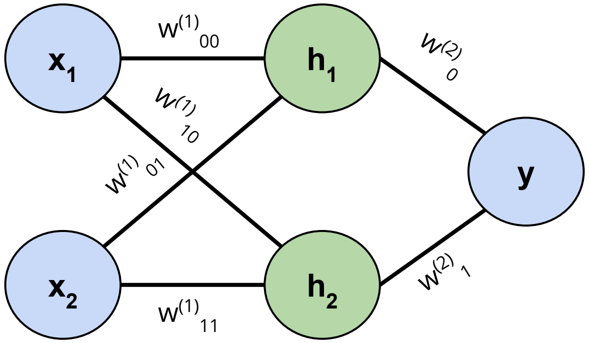
It’s all about learning features (created in the hidden layer(s)) automatically

Neural Networks

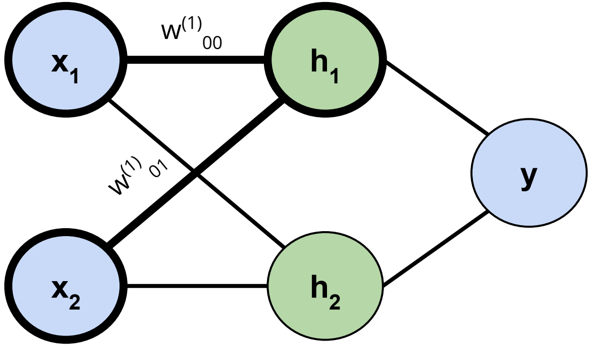
We need to define:

1. How the input flows through the network to get the output (forward propagation)
2. How weights and biases get updated (backward propagation)

Neural Networks - Forward Propagation

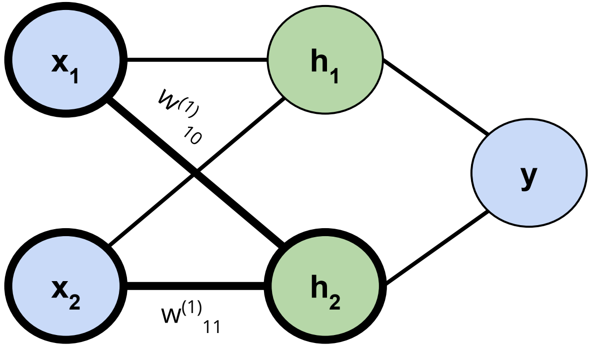


Neural Networks - Forward Propagation



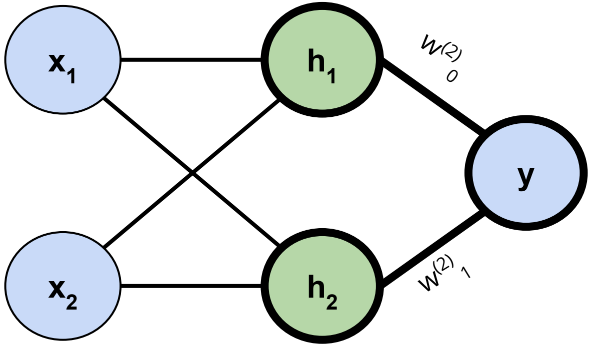
$h_1 = \boldsymbol{\sigma}(w^{(1)}_{00}\, x_1 + w^{(1)}_{01}\, x_2 + b^{(1)}_1)$

Neural Networks - Forward Propagation



$$h_2 = \boldsymbol{\sigma}(w^{(1)}_{10}\, x_1 + w^{(1)}_{11}\, x_2 + b^{(1)}_{2})$$

Neural Networks - Forward Propagation



$$y = \boldsymbol{\sigma}(w^{(2)}_0\, h_1 + w^{(2)}_1\, h_2 + b^{(2)}_1)$$

Neural Networks - Forward Propagation

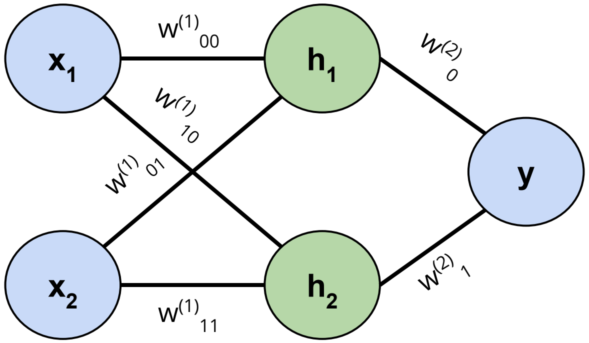
Using matrix notation:

$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \sigma \left(\begin{bmatrix} w_{00}^{(1)} & w_{01}^{(1)} \\ w_{10}^{(1)} & w_{11}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} \right)$$

$$y = \sigma(\begin{bmatrix} w_{00}^{(2)} \\ w_{01}^{(2)} \end{bmatrix}^T \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + b^{(2)})$$

Neural Networks - Forward Propagation

Q: if all the weights and biases are initialized to 0, what will be the output of the network?



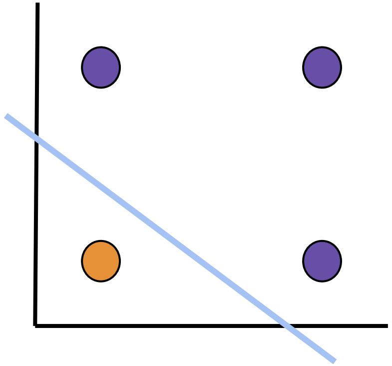
Recall in Logistic Regression

Decision Boundary is where

$\sigma(wx+b) = ½$

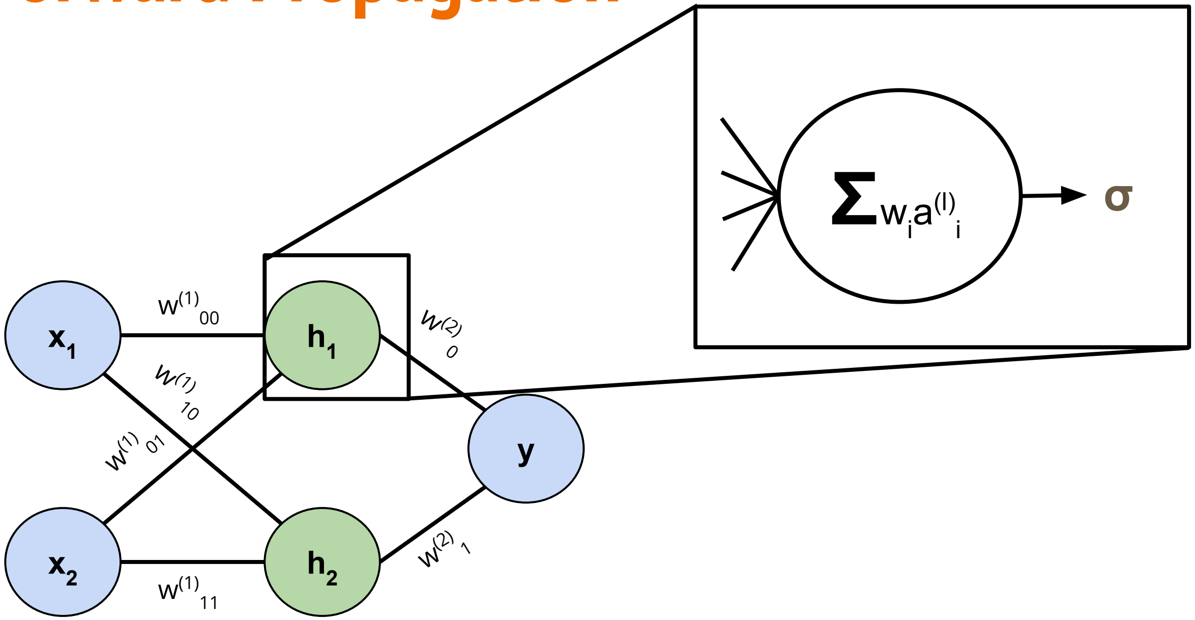
which is exactly where

$wx+b = 0$



Neural Networks - Forward Propagation

Q: what happens if we don't have **σ** in the hidden layer here? What will the decision boundary look like? What will our features be?



Neural Networks - Forward Propagation

If we don't, we just end up with normal logistic regression on x_1 and x_2.

$h_1 = w^{(1)}_{00}\, x_1 + w^{(1)}_{01}\, x_2 + b^{(1)}_1$

$h_2 = w^{(1)}_{10}\, x_1 + w^{(1)}_{11}\, x_2 + b^{(1)}_2$

Then

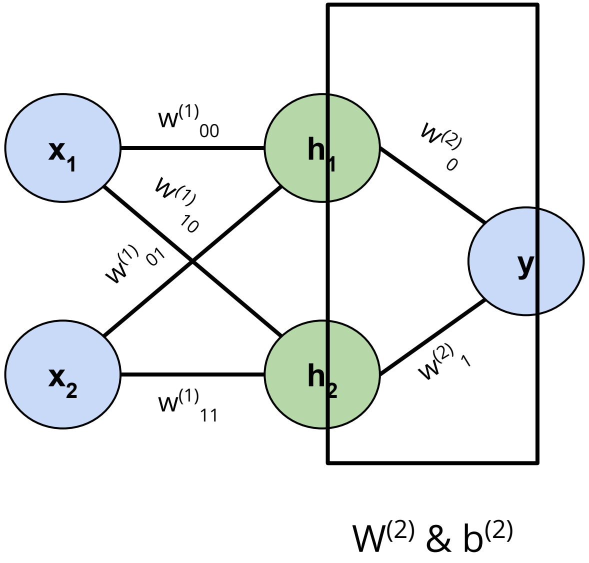
$y = \boldsymbol{\sigma}(\, w^{(2)}_0\, h_1 + w^{(2)}_1\, h_2 + b^{(2)}_1)$

$= \boldsymbol{\sigma}(\, w^{(2)}_0(w^{(1)}_{00}\, x_1 + w^{(1)}_{01}\, x_2 + b^{(1)}_1) + w^{(2)}_1(w^{(1)}_{10}\, x_1 + w^{(1)}_{11}\, x_2 + b^{(1)}_2) + b^{(2)}_1)$

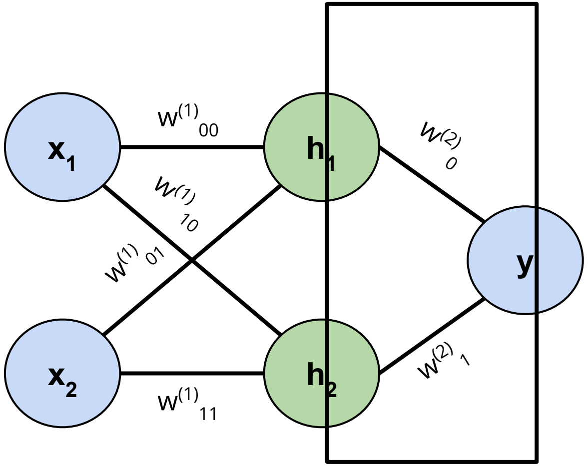
$= \boldsymbol{\sigma}(\, w_1\, x_1 + w_2\, x_2 + b_2)$

Neural Networks - BackPropagation

How do weights and biases get updated?



Neural Networks - BackPropagation



This is the same update from logistic regression except relative to the learned features **h**

$$\mathrm{Cost}(w, b)$$

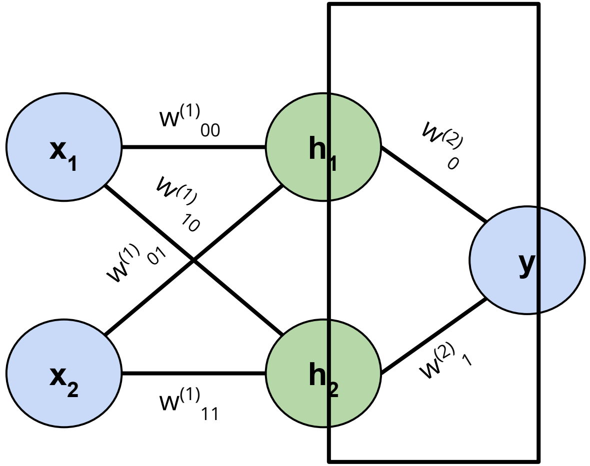
$$= \quad -\frac{1}{n}\sum_{i=1}^{n}\left[yi\log(\sigma(-w^T h_i + b)) + (1 - y_i)\log(1 - \sigma(-w^T h_i + b))\right]$$

Neural Networks - BackPropagation

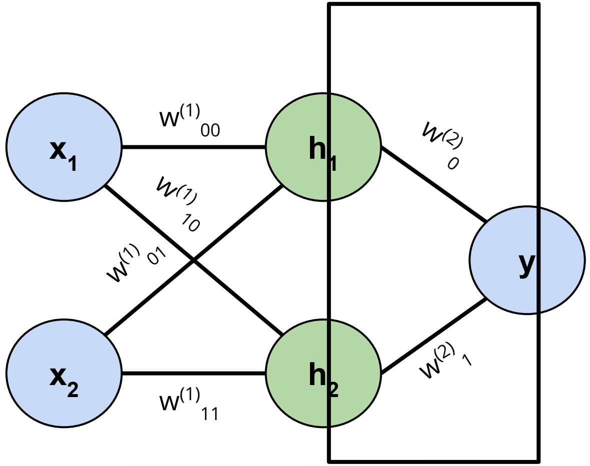
$$\nabla \mathrm{Cost}(w,b) = \left[\frac{\partial}{\partial w}\mathrm{Cost}, \frac{\partial}{\partial b}\mathrm{Cost}\right]$$

$$\frac{\partial}{\partial w}\mathrm{Cost} = \frac{1}{n}\sum_{i=1}^{n} h_i(y_i - \sigma(-w^T h_i + b))$$

$$\frac{\partial}{\partial b}\mathrm{Cost} = \frac{1}{n}\sum_{i=1}^{n} \sigma(-w^T h_i + b) - y_i$$



Neural Networks - BackPropagation



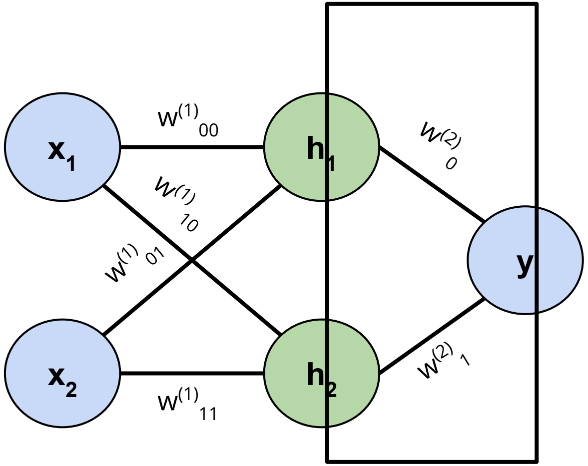
Using the chain rule:

$$\frac{\partial C}{\partial W^{(2)}} = \frac{\partial C}{\partial u^{(2)}} \frac{\partial u^{(2)}}{\partial W^{(2)}} \quad \text{where} \quad u^{(2)} = W^{(2)} h + b^{(2)}$$

$$= \frac{\partial C}{\partial u^{(2)}} \cdot h = \frac{1}{n} \sum_{i=1}^{n} h(y_i - \sigma(u^{(2)}))$$

$h = \boldsymbol{\sigma}(W^{(1)} X + b^{(1)})$

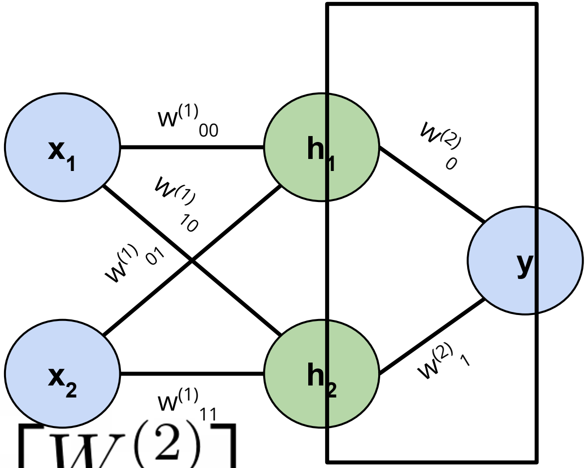
Neural Networks - BackPropagation



Similarly:

$$\frac{\partial C}{\partial b^{(2)}} = \frac{\partial C}{\partial u^{(2)}} \frac{\partial u^{(2)}}{\partial b^{(2)}} = \frac{1}{n} \sum_{i=1}^{n} y_i - \sigma(u^{(2)})$$

Neural Networks - BackPropagation



So we can update $W^{(2)}$ and $b^{(2)}$ as follows:

$$\begin{bmatrix} W^{(2)}_{new} \\ \\ b^{(2)}_{new} \end{bmatrix} = -\alpha \begin{bmatrix} \frac{\partial C}{\partial W^{(2)}} \\ \\ \frac{\partial C}{\partial b^{(2)}} \end{bmatrix} + \begin{bmatrix} W^{(2)} \\ \\ b^{(2)} \end{bmatrix}$$

So far this is identical to logistic regression. But how do we update $W^{(1)}$ and $b^{(1)}$

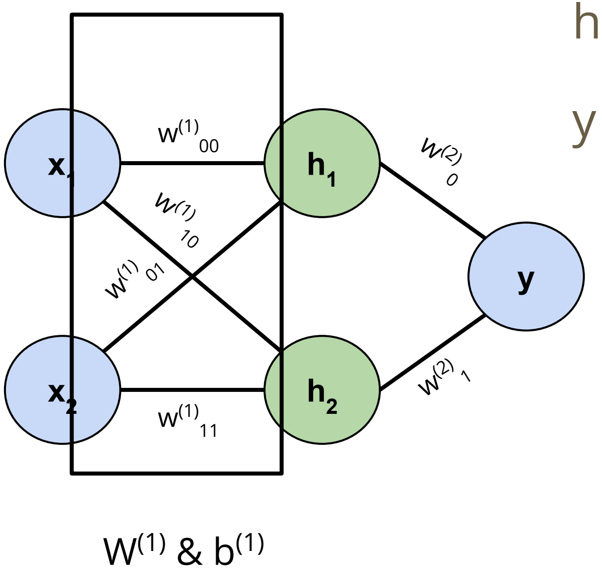
Neural Networks - BackPropagation

How do weights and biases get updated?

$$h_1 = \boldsymbol{\sigma}(w^{(1)}_{00}\, x_1 + w^{(1)}_{01}\, x_2 + b^{(1)}_{1})$$

$$h_2 = \boldsymbol{\sigma}(w^{(1)}_{10}\, x_1 + w^{(1)}_{11}\, x_2 + b^{(1)}_{2})$$

$$y = \boldsymbol{\sigma}(w^{(2)}_{0}\, h_1 + w^{(2)}_{1}\, h_2 + b^{(2)}_{1})$$



Neural Networks - BackPropagation

$$\text{Cost}(w, b)$$

$$= \quad -\frac{1}{n}\sum_{i=1}^{n}\left[yi \log(\sigma(-w^T h_i + b)) + (1 - y_i) \log(1 - \sigma(-w^T h_i + b))\right]$$

Neural Networks - BackPropagation

$$\mathrm{Cost}(w, b)$$

$$= -\frac{1}{n}\sum_{i=1}^{n}\left[yi\log(\sigma(-w^T h_i + b)) + (1 - y_i)\log(1 - \sigma(-w^T h_i + b))\right]$$

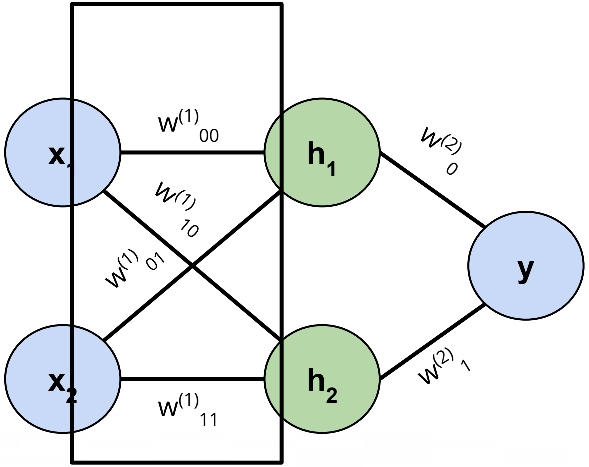
Neural Networks - BackPropagation

$$\text{Cost}(w, b)$$

$$= -\frac{1}{n}\sum_{i=1}^{n}\left[yi\log(\sigma(-w^T h_i + b)) + (1 - y_i)\log(1 - \sigma(-w^T h_i + b))\right]$$

$$h_i = \boldsymbol{\sigma}(\, w^{(1)}_{i0}\, x_1 + w^{(1)}_{i1}\, x_2 + b^{(1)}_i)$$

Neural Networks - BackPropagation



Using the chain rule:

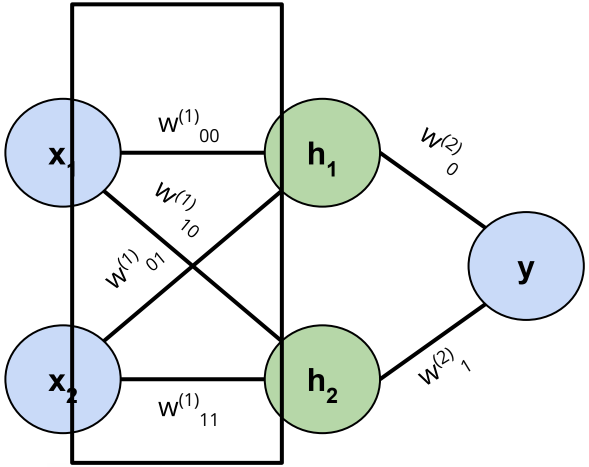
$$\frac{\partial C}{\partial W^{(1)}} = \frac{\partial C}{\partial h} \cdot \frac{\partial h}{\partial W^{(1)}} = \frac{\partial C}{\partial h} \cdot \frac{\partial h}{\partial u^{(1)}} \cdot \frac{\partial u^{(1)}}{\partial W^{(1)}} \quad \text{where} \quad u^{(1)} = w^{(1)}x + b^{(1)}$$

$W^{(1)}$ & $b^{(1)}$

$$= \frac{\partial C}{\partial u^{(2)}} \cdot \frac{\partial u^{(2)}}{\partial h} \cdot \frac{\partial h}{\partial u^{(1)}} \cdot \frac{\partial u^{(1)}}{\partial W^{(1)}} = \frac{\partial C}{\partial u^{(2)}} \cdot W^{(2)} \cdot \sigma'(u^{(1)}) \cdot x$$

Already computed

Neural Networks - BackPropagation



Similarly:

$$\frac{\partial C}{\partial b^{(1)}} = \frac{\partial C}{\partial u^{(2)}} \cdot W^{(2)} \cdot \sigma'(u^{(1)})$$

Already computed

Neural Networks - BackPropagation

Backpropagation: update $W^{(1)}$ and $b^{(1)}$ without recomputing values that are computed when getting the gradients of the previously updated layer.

http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf

Neural Networks - BackPropagation

Important Note:

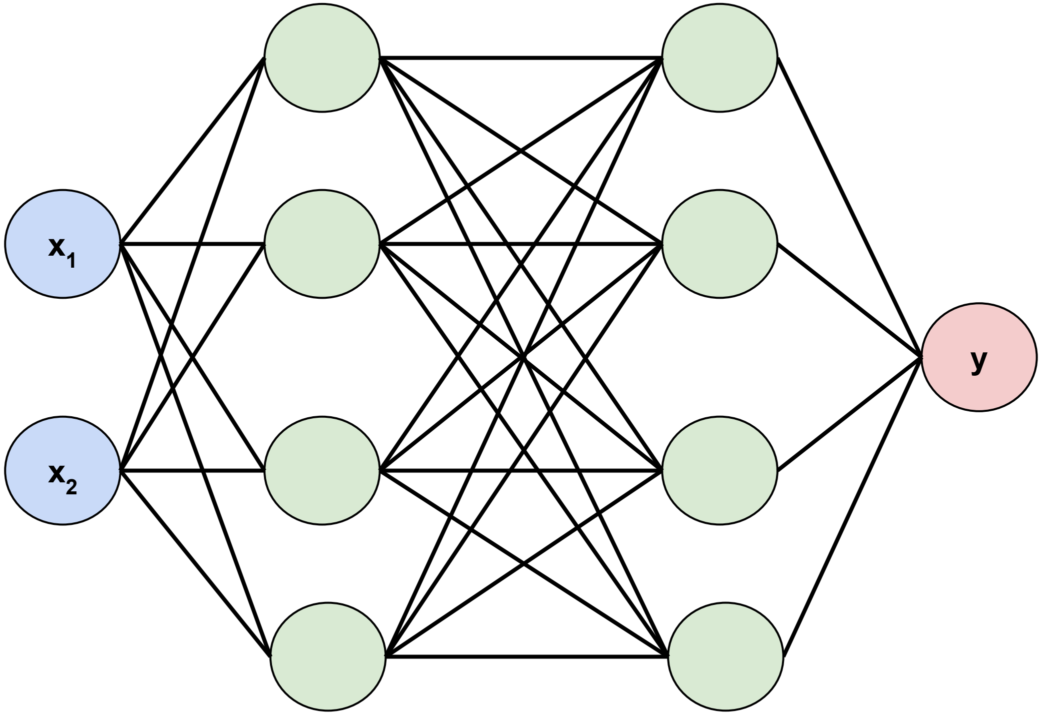
$$\frac{\partial C}{\partial W^{(1)}} = \frac{\partial C}{\partial h} \cdot \frac{\partial h}{\partial W^{(1)}} = \frac{\partial C}{\partial h} \cdot \frac{\partial h}{\partial u^{(1)}} \cdot \frac{\partial u^{(1)}}{\partial W^{(1)}} \quad \text{where} \quad u^{(1)} = w^{(1)}x + b^{(1)}$$

$$= \frac{\partial C}{\partial u^{(2)}} \cdot \frac{\partial u^{(2)}}{\partial h} \cdot \frac{\partial h}{\partial u^{(1)}} \cdot \frac{\partial u^{(1)}}{\partial W^{(1)}} = \frac{\partial C}{\partial u^{(2)}} \cdot W^{(2)} \cdot \sigma'(u^{(1)}) \cdot x$$

Depends on both data and weights
Initializing all weights to zero then is not a good idea

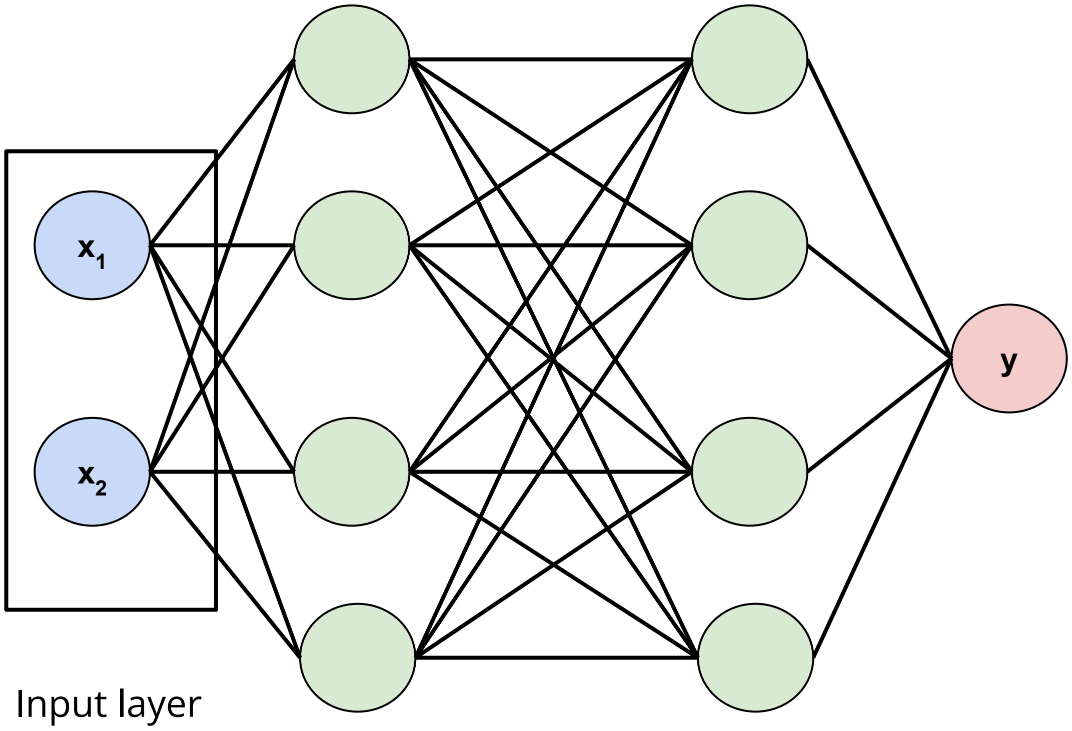
Feedforward Neural Networks

In general:



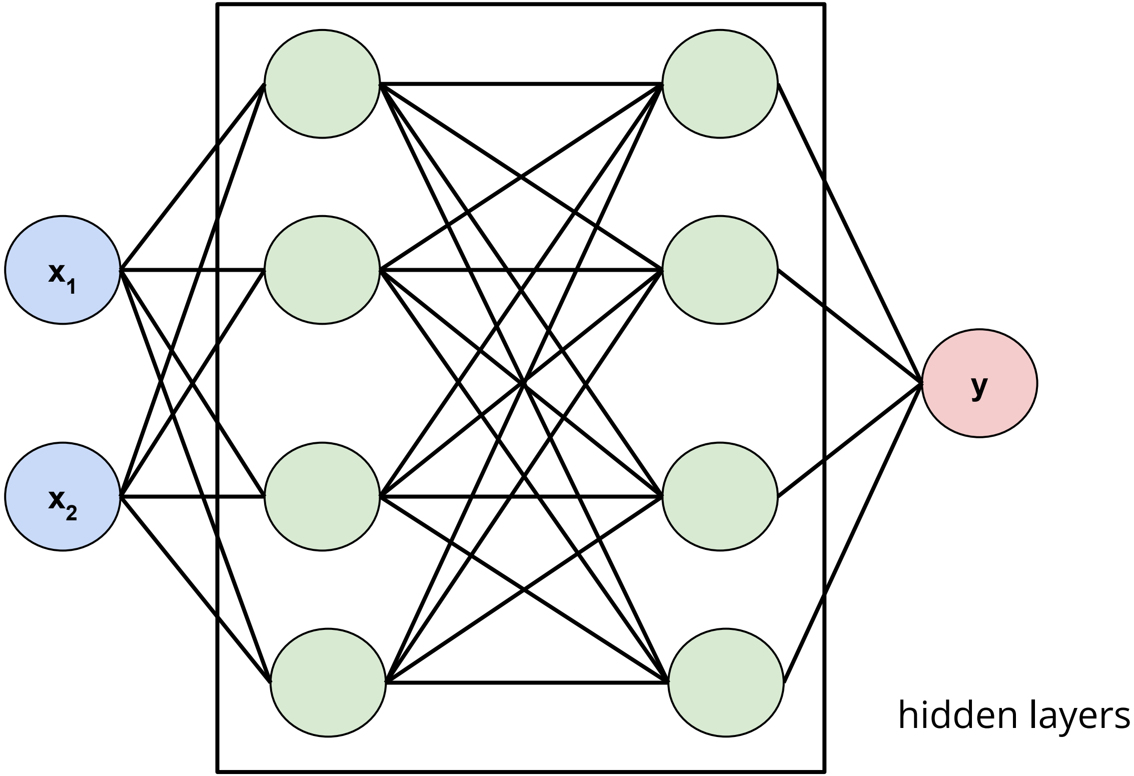
Feedforward Neural Networks

In general:



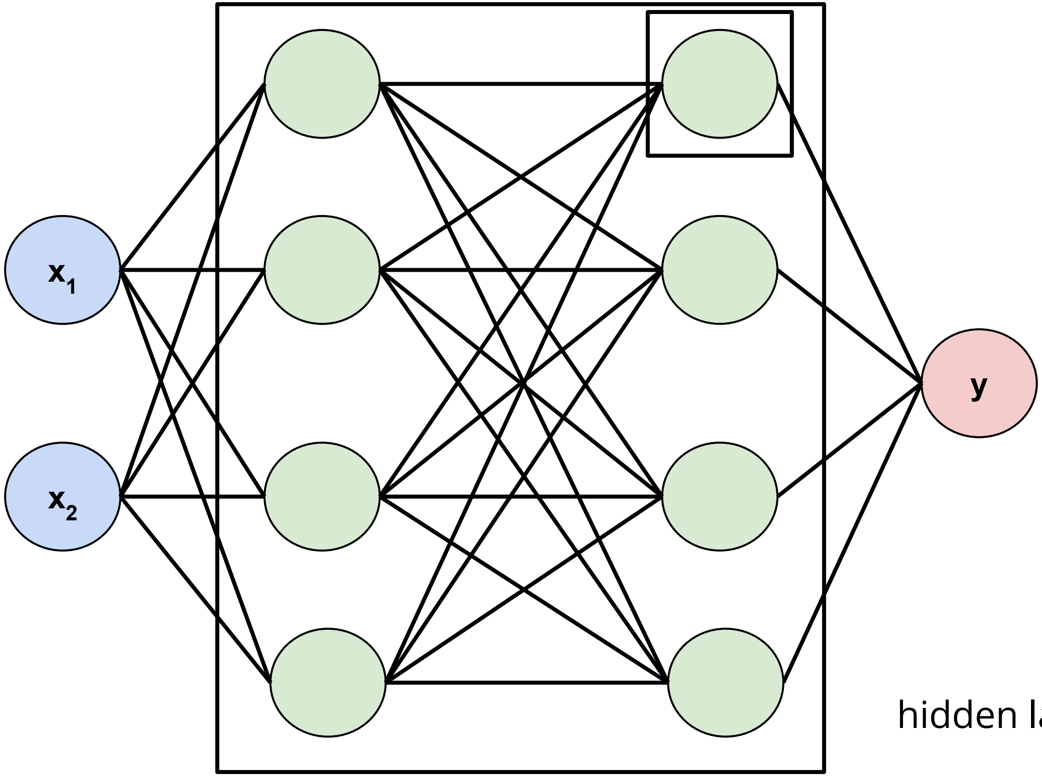
Feedforward Neural Networks

In general:



Feedforward Neural Networks

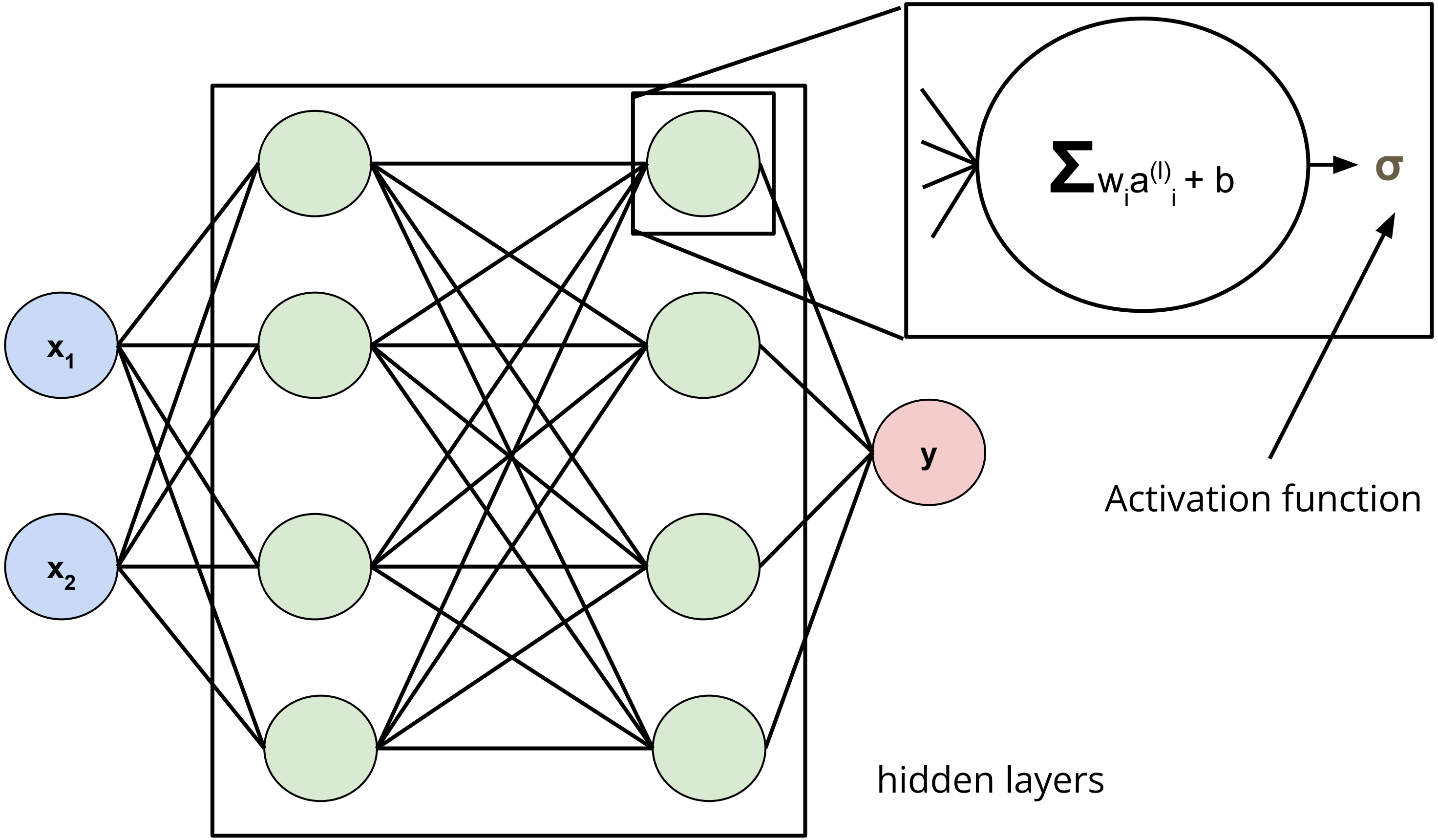
In general:



hidden layers

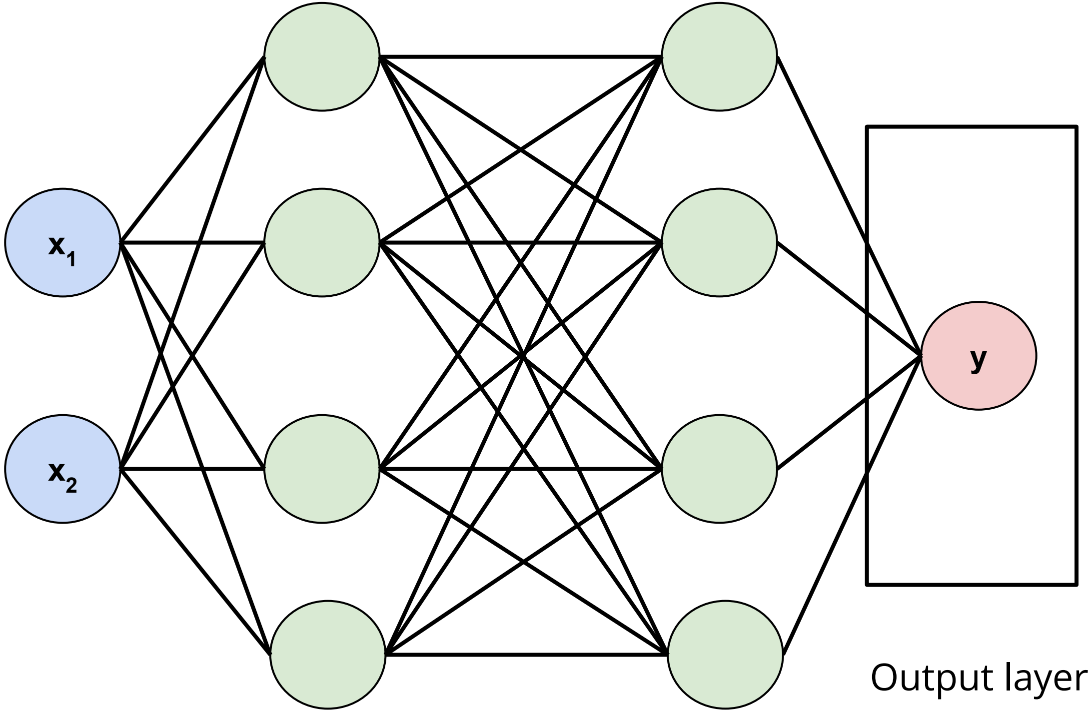
Feedforward Neural Networks

In general:



Feedforward Neural Networks

In general:



Feedforward Neural Networks

The hope:

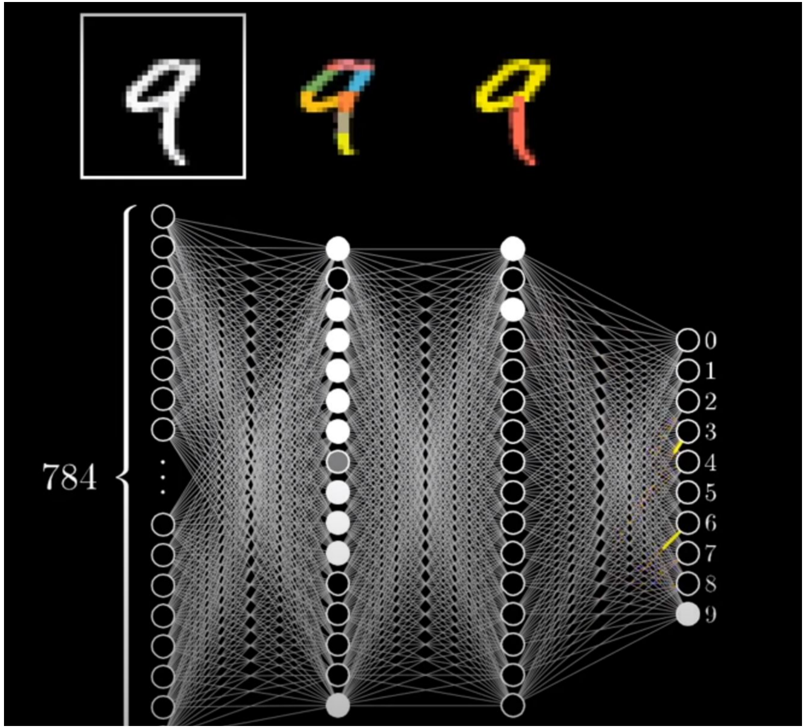


Image from 3b1b

Feedforward Neural Networks

The reality:

(a) Husky classified as wolf (b) Explanation

Figure 11: Raw data and explanation of a bad model's prediction in the "Husky vs Wolf" task.

	Before	After
Trusted the bad model	10 out of 27	3 out of 27
Snow as a potential feature	12 out of 27	25 out of 27

Table 2: "Husky vs Wolf" experiment results.

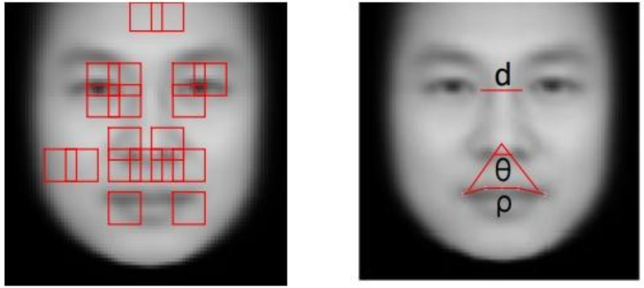
Image from "Why Should I Trust You?": Explaining the Predictions of Any Classifier (2016) Marco Tulio Ribeiro, Sameer Singh, Carlos Guestrin

Feedforward Neural Networks

The scary reality:

(a) Three samples in criminal ID photo set S_c.

(b) Three samples in non-criminal ID photo set S_n



(a) (b)

Figure 8. (a) FGM results; (b) Three discriminative features ρ, d and θ.

from "Automated Inference on Criminality using Face Images", Xiaolin Wu, Xi Zhang

According to this model, if you don't smile, you're a criminal

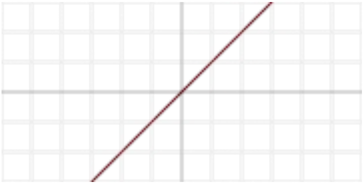
Neural Networks

Can do both **Classification** and **Regression**

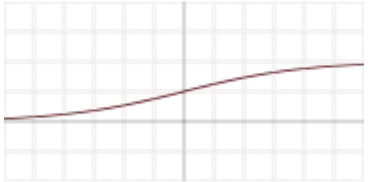
Neural Networks - Tuning Parameters

1. Step size α
2. Number of BackPropagation iterations
3. Batch Size
4. Number of hidden layers
5. Size of each hidden layer
6. Activation function used in each layer
7. Cost function
8. Regularization (to avoid overfitting)

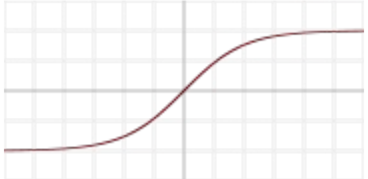
Activation Functions



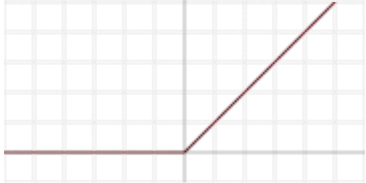
Identity -> x



Sigmoid -> **σ**(x)



Tanh -> tanh(x)



ReLU -> max(0, x)

Note: can use any function you want in order to introduce non-linearity. These are just the popular ones that have been shown to work in practice.

Tuning the activation function is equivalent to feature engineering.

Demo

Universal Approximation Theorem

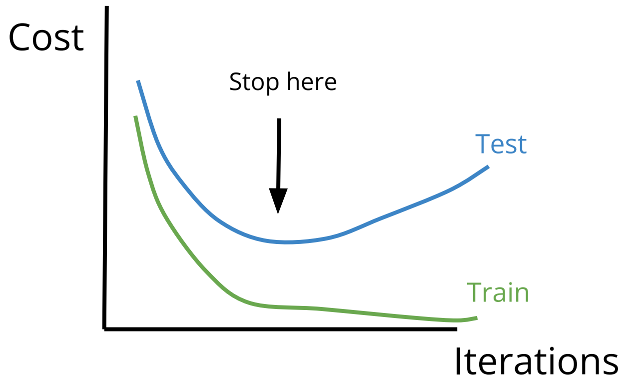
Neural Networks - Challenges

1. High risk of overfitting as you’re optimizing on the training set.
2. As the dimensionality of the input increases:
   a. So does the number of weights
   b. The gradients typically get smaller: Vanishing gradient problem
3. Doesn’t do well for computer vision where the object of detection can be anywhere in the image
4. Doesn’t handle sequences of inputs (i.e. when provided with context for data)

Neural Networks - Regularization

Two main ways:

1. Early termination of weight / bias updates



2. Dropout - kill neurons (by setting them to 0) randomly

Neural Networks

First: Normalize your data

https://medium.com/mlearning-ai/tuning-neural-networks-part-i-normalize-your-data-6821a28b2cd8

Neural Networks - Initialization Gotchas

Divide and conquer

https://medium.com/mlearning-ai/tuning-neural-networks-part-ii-considerations-for-initialization-4f82e525da69

Zero initialization:

If act(0) != 0 then weights all move together (same as constant init)

If act(0) == 0 then no updates can be made

Neural Networks - Activation Functions

https://medium.com/@gallettilance/tuning-neural-networks-part-iii-43dfd0c8600f