Introduction to Neural Networks

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Lecture outline

- Neural units
- The XOR problem
- Feed-Forward Neural Networks
- Training Neural Nets

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Neural Network unit

- The building block of a neural network
  - Weight vector $w = w_1 \dots w_n$
  - Bias term b
  - Activation function f

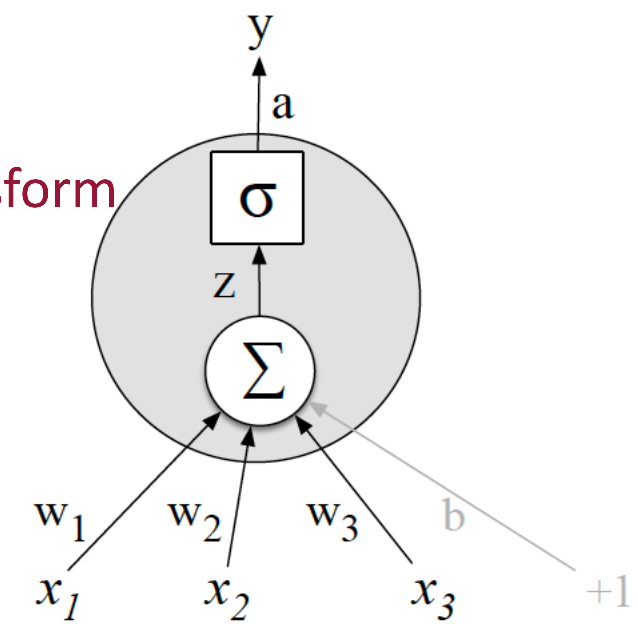
Output value

Non-linear transform

Weighted sum

Weights

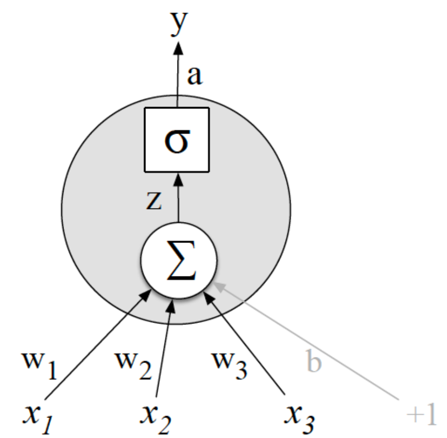
Input layer



Neural unit

- The building block of a neural network
  - Weight vector $w = w_1 \dots w_n$
  - Bias term b
  - Activation function f (non-linear)
- Output of a neural unit

$$y = a = f(z)$$



Here:

- z is the weighted sum

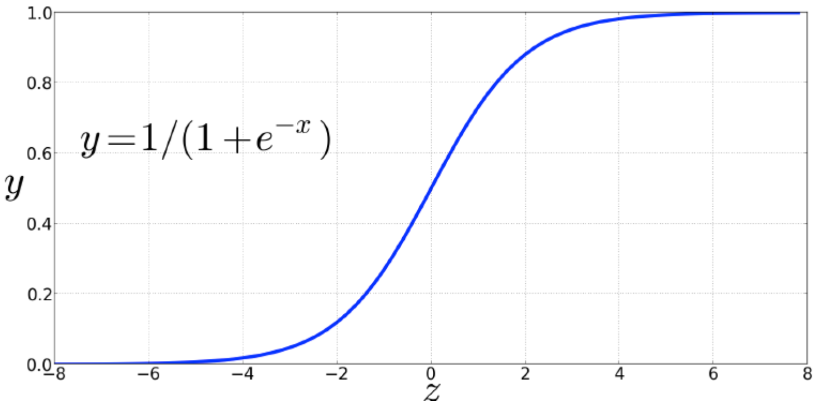
$$z = \sum_i w_i x_i + b$$

$$z = w \cdot x + b$$

Non-Linear Activation functions

- There are many non-linear activation functions
  - Sigmoid

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



  - Tanh

$$y = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

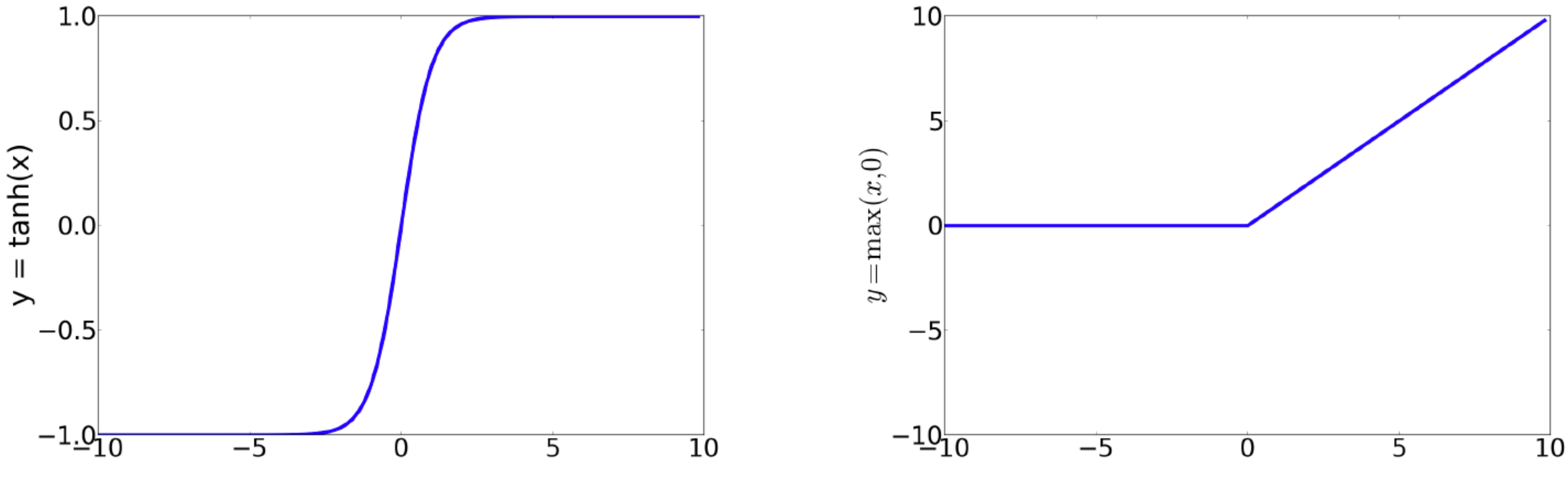
  - Rectified Linear (ReLU)

$$y = \max(x, 0)$$

  - PReLU
  - …

Activation functions

- Tanh and ReLU functions



(a) (b)

An example

Suppose a unit has:

- $w = [0.2, 0.3, 0.9]$
- $b = 0.5$

What happens with input x:

- $x = [0.5, 0.6, 0.1]$

$$y = \sigma(w \cdot x + b) =$$

An example

Suppose a unit has:

- w = [0.2,0.3,0.9]
- b = 0.5

What happens with the following input x?

- x = [0.5,0.6,0.1]

$$y = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-(w \cdot x + b)}} =$$

An example

Suppose a unit has:

- $w = [0.2, 0.3, 0.9]$
- $b = 0.5$

What happens with input x:

- $x = [0.5, 0.6, 0.1]$

$$y = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-(w \cdot x + b)}} =$$

$$\frac{1}{1 + e^{-(.5*.2+.6*.3+.1*.9+.5)}} =$$

An example

Suppose a unit has:

- $w = [0.2, 0.3, 0.9]$
- $b = 0.5$

What happens with input x:

- $x = [0.5, 0.6, 0.1]$

In Python:

```
import numpy as np
y = 1/(1+np.exp(-
(np.dot(w,x) + b)))
```

$$y = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-(w \cdot x + b)}} =$$

$$\frac{1}{1 + e^{-(.5*.2+.6*.3+.1*.9+.5)}} = \frac{1}{1 + e^{-0.87}} = .70$$

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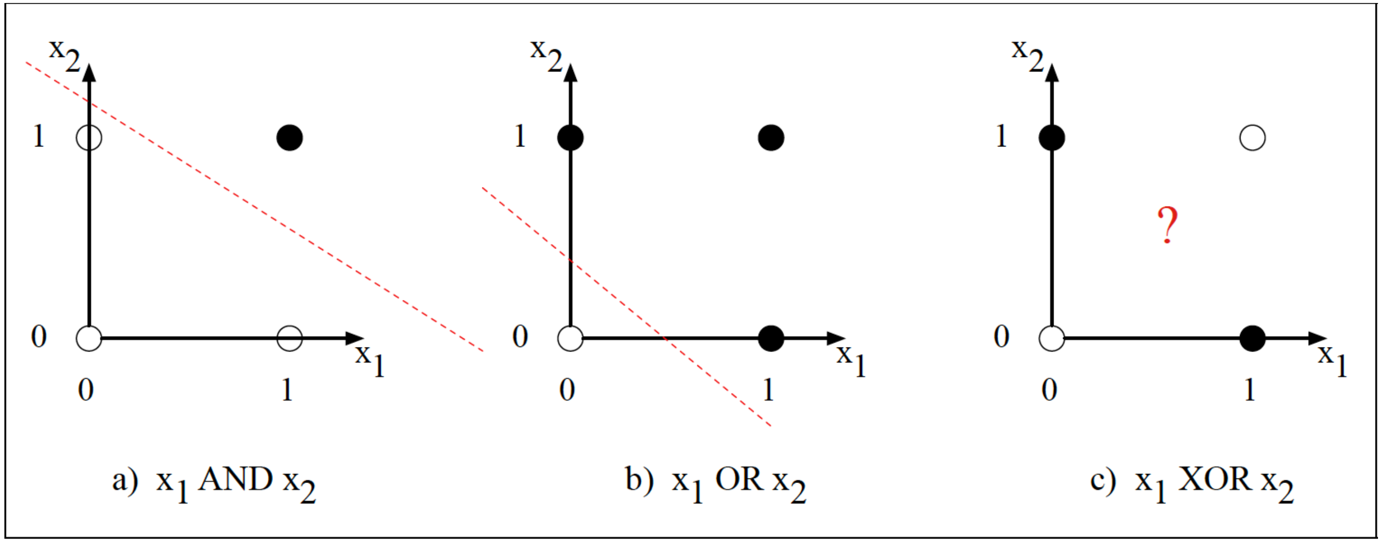
Boolean functions

- AND, OR, XOR functions

AND			OR			XOR		
x1	x2	y	x1	x2	y	x1	x2	y
0	0	0	0	0	0	0	0	0
0	1	0	0	1	1	0	1	1
1	0	0	1	0	1	1	0	1
1	1	1	1	1	1	1	1	0

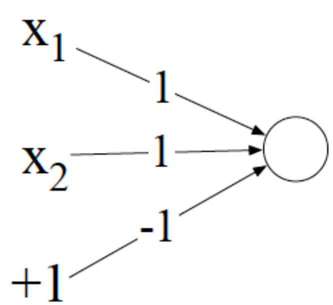


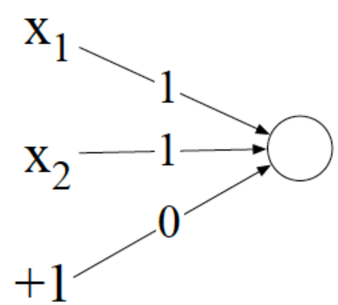
Boolean functions using Perceptron

- Using Perceptron to compute above functions

$$y = \begin{cases} 0, & \text{if } w \cdot x + b \leq 0 \\ 1, & \text{if } w \cdot x + b > 0 \end{cases}$$

- We can use Perceptron (a) for AND and (b) for OR

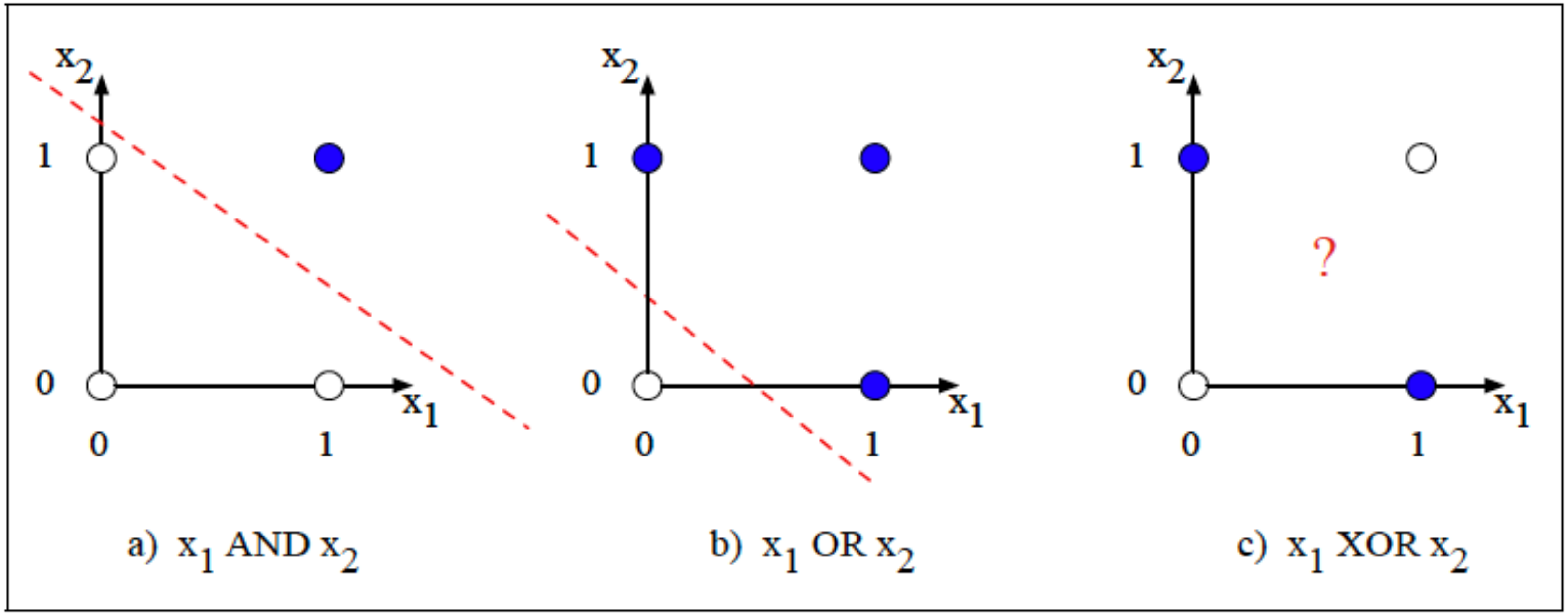




AND			OR			XOR		
x1	x2	y	x1	x2	y	x1	x2	y
0	0	0	0	0	0	0	0	0
0	1	0	0	1	1	0	1	1
1	0	0	1	0	1	1	0	1
1	1	1	1	1	1	1	1	0

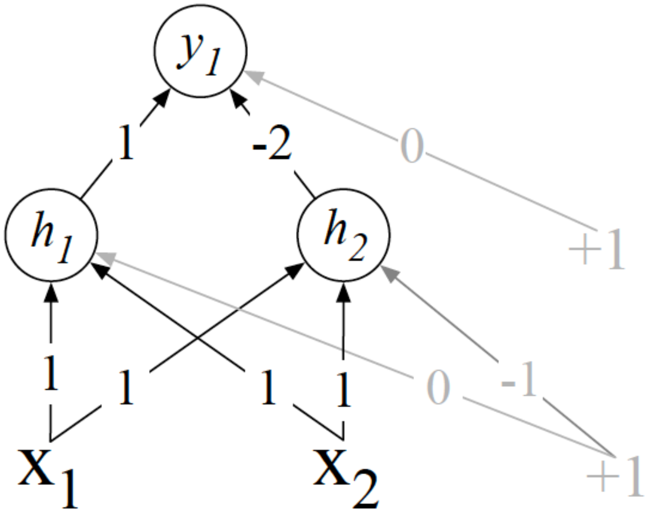
The XOR problem

- It's not possible to build a perceptron to compute logical XOR!
- The solution: neural networks!



The solution: neural networks

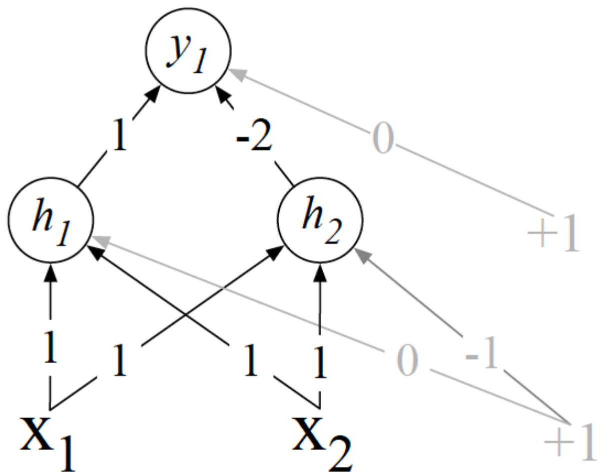
- XOR solution with two-layer neural network and ReLU activation functions



XOR

x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

The solution: neural networks



XOR

x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

x1	x2	h1	h2	y1
0	0	0	0	0
0	1	1	0	1
1	0	1	0	1
1	1	2	1	0

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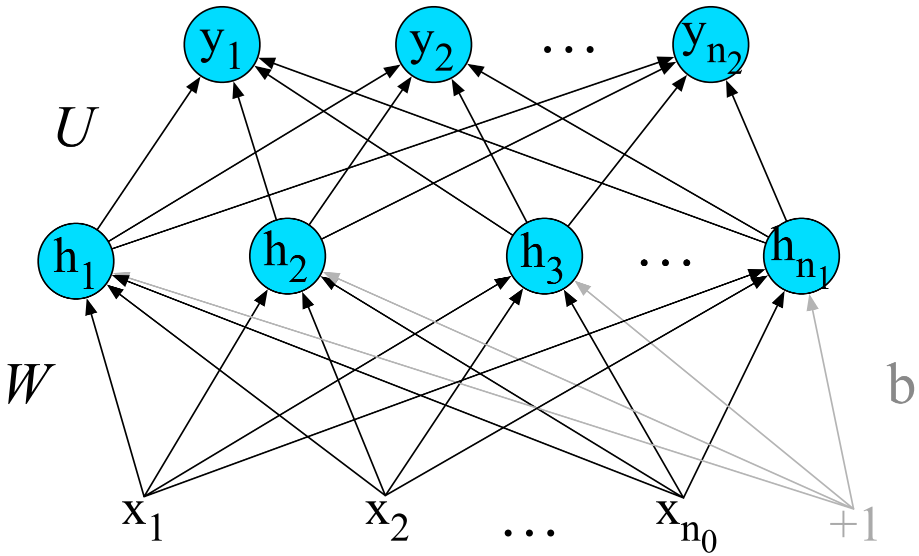
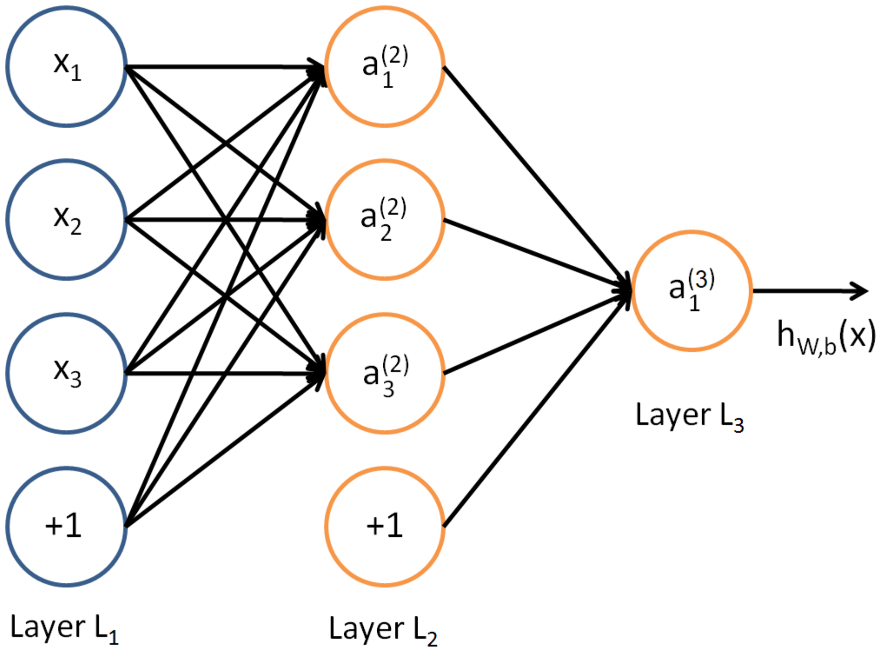
Feedforward Neural Networks

- Can also be called **multi-layer perceptrons** (or **MLPs**) for historical reasons



Feed-forward neural networks

- Simple feed-forward neural networks inclue:
  - Input units
  - Hidden units
  - Output units



Feed-forward neural networks

- A single hidden unit has:
  - parameters w (the weight vector) and
  - Bias term b (scalar)
- Combine weight vectors and bias terms of units into matrix W and vector $\mathbf{b}$

Feed-forward neural networks

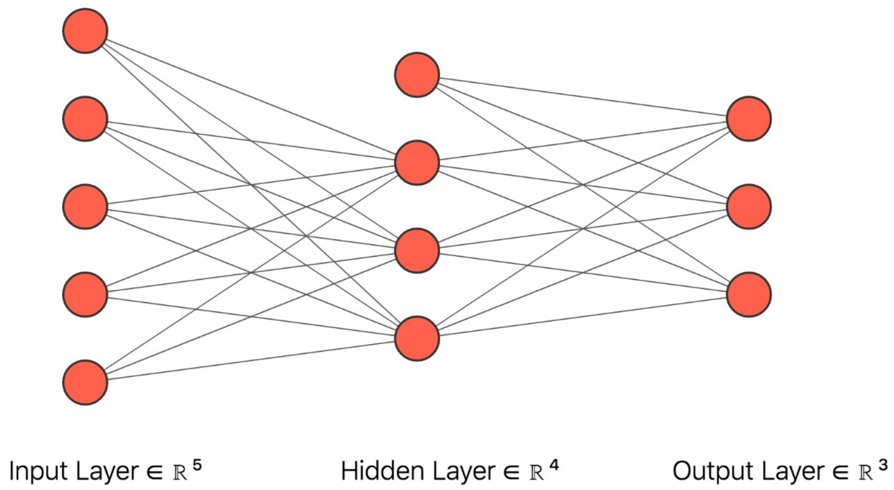
- A single hidden unit has:
  - parameters w (the weight vector) and
  - Bias term b (scalar)
- Combine weight vectors and bias terms of units into matrix W and vector $\mathbf{b}$
- Output of the hidden layer, the vector h with sigmoid as the activation function

$$h = \sigma(Wx + \mathbf{b})$$

  - The activation function is applied to vector element-wise
    - $g([z_1, z_2, z_3]) = [g(z_1), g(z_2), g(z_3)]$

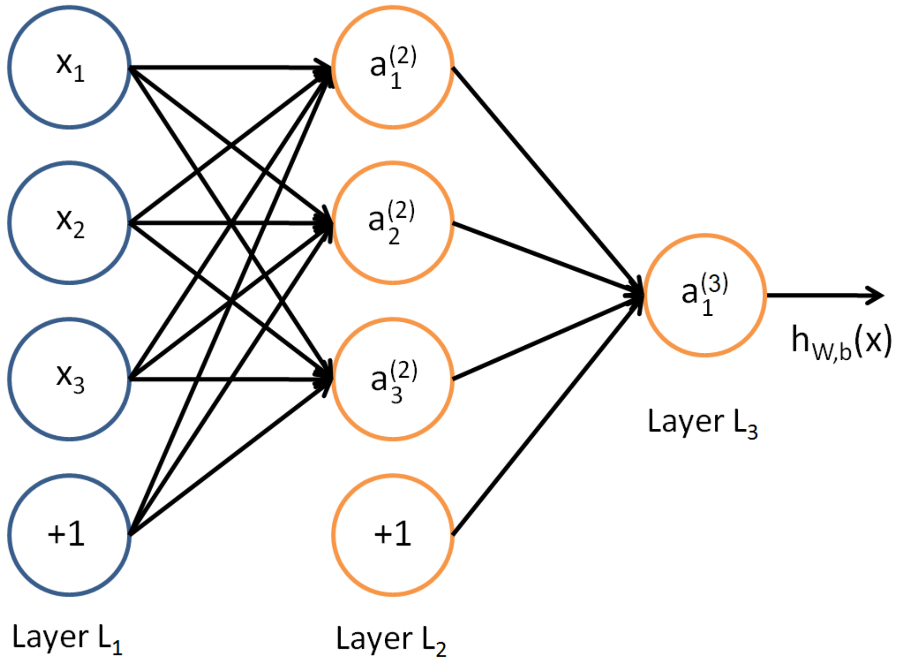
Dimensions of vectors and matrices

- Input layer (layer 0): $x \in \mathbb{R}^{n_0}$
- Hidden layer (layer 1): $h \in \mathbb{R}^{n_1}$, $b \in \mathbb{R}^{n_1}$
- Weight matrix: $W \in \mathbb{R}^{n_1 \times n_0}$



Output layer

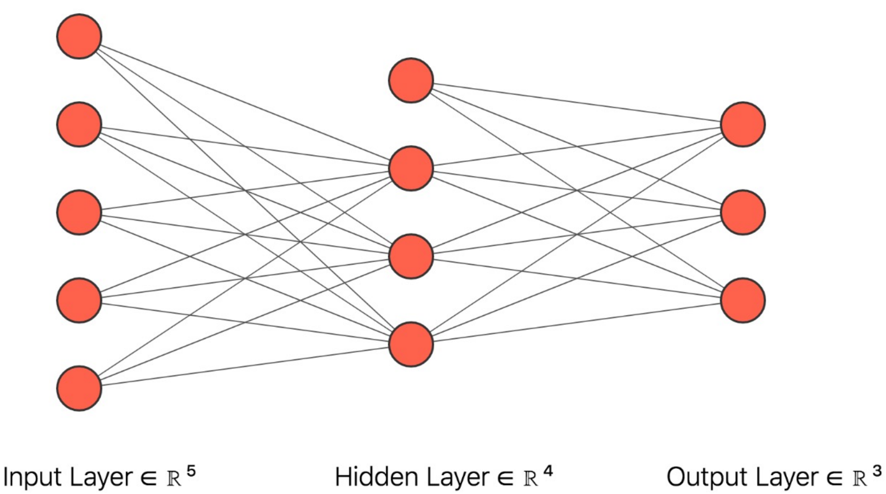
- If we do binary classification and use sigmoid function at the output layer, we use a single output unit



Output layer

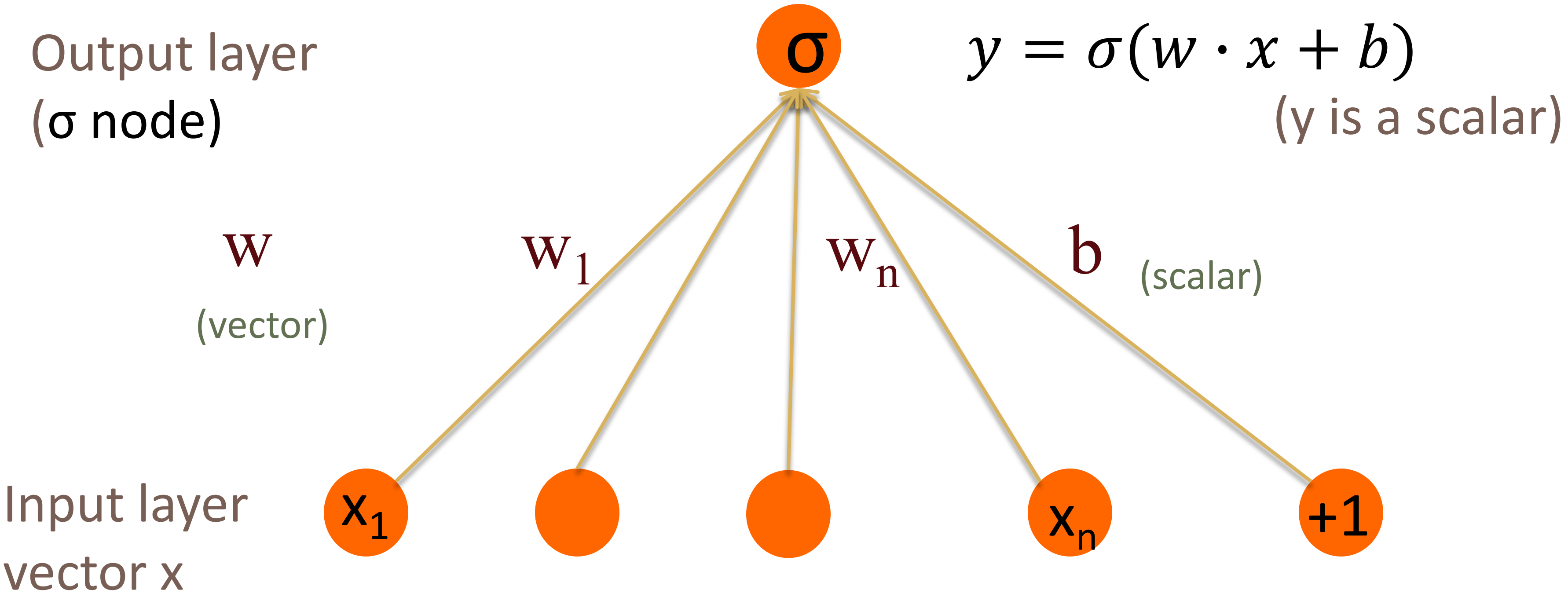
- For multi-class classification, we use *K* units in output layer and softmax function
  - *K* is the number of classes

$$p(y=c|x) = \frac{e^{w_c \cdot x + b_c}}{\sum_{j=1}^{k} e^{w_j \cdot x + b_j}}$$



Binary Logistic Regression as a 1-layer Network

(we don't count the input layer in counting layers!)



Multinomial Logistic Regression as a 1-layer Network

Fully connected single layer network

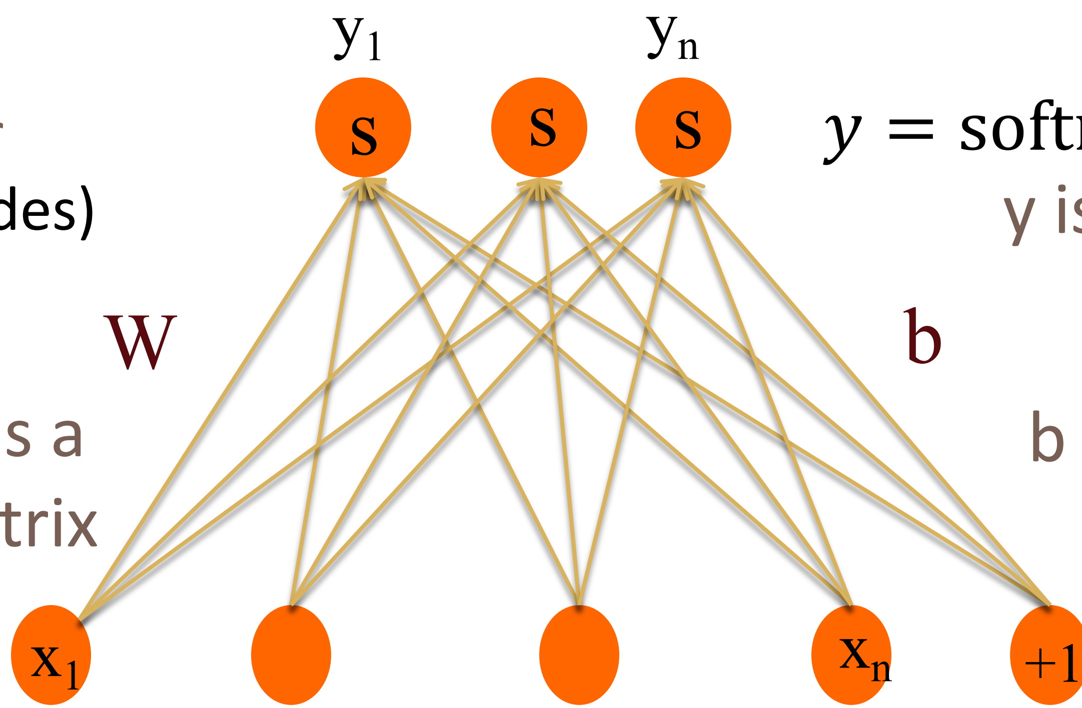
Output layer
(softmax nodes)

$$y = \mathrm{softmax}(Wx + b)$$

y is a vector

W

W is a matrix



b

b is a vector

Input layer
scalars

Reminder: softmax: a generalization of sigmoid

- For a vector *z* of dimensionality *k*, the softmax is:

$$\text{softmax}(z) = \left[\frac{\exp(z_1)}{\sum_{i=1}^{k}\exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^{k}\exp(z_i)}, \ldots, \frac{\exp(z_k)}{\sum_{i=1}^{k}\exp(z_i)}\right]$$

- Example:

$$\text{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{k}\exp(z_j)} \quad 1 \le i \le k$$

$$z = [0.6, 1.1, -1.5, 1.2, 3.2, -1.1]$$

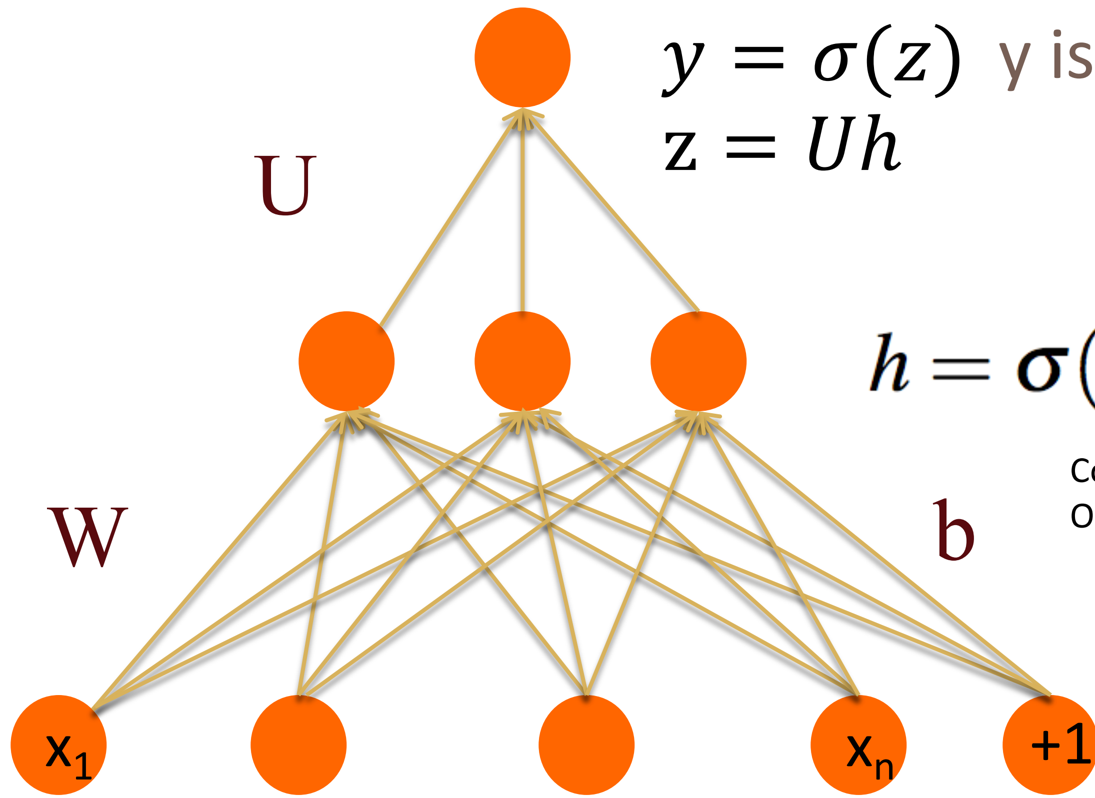
$$\text{softmax}(z) = [0.055, 0.090, 0.006, 0.099, 0.74, 0.010]$$

Two-Layer Network with scalar output

Output layer
(σ node)

hidden units
(σ node)

Input layer
(vector)



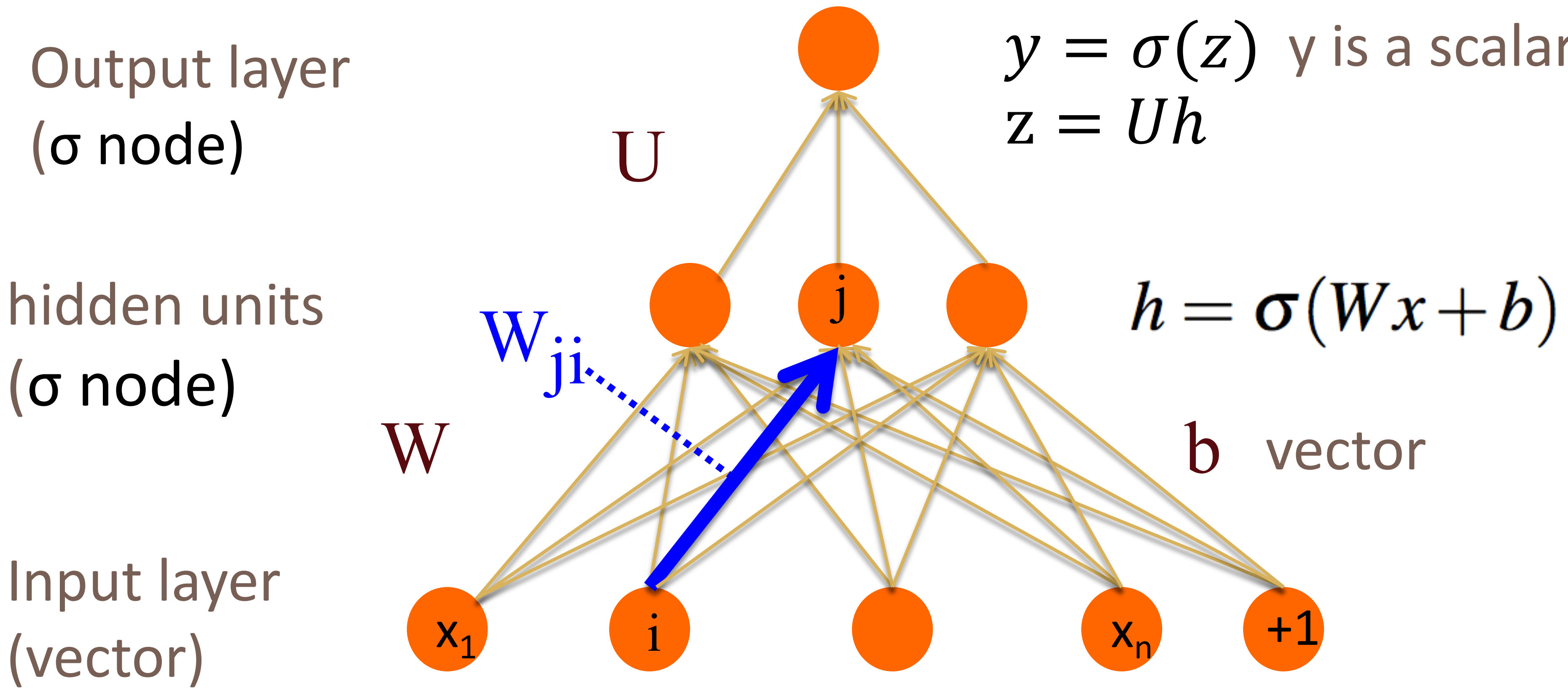
$y = \sigma(z)$ y is a scalar

$z = Uh$

$$h = \boldsymbol{\sigma}(Wx + b)$$

Could be ReLU
Or tanh

Two-Layer Network with scalar output

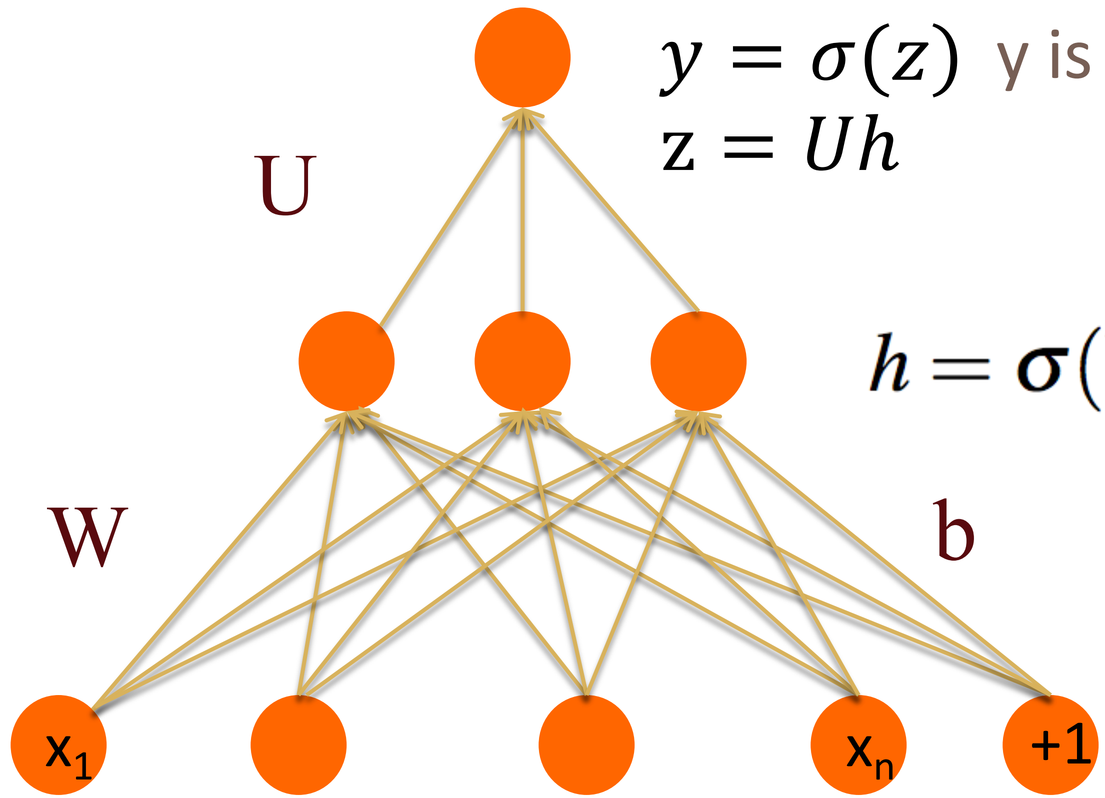


Two-Layer Network with scalar output

Output layer
(σ node)

hidden units
(σ node)

Input layer
(vector)



$y = \sigma(z)$ y is a scalar

$z = Uh$

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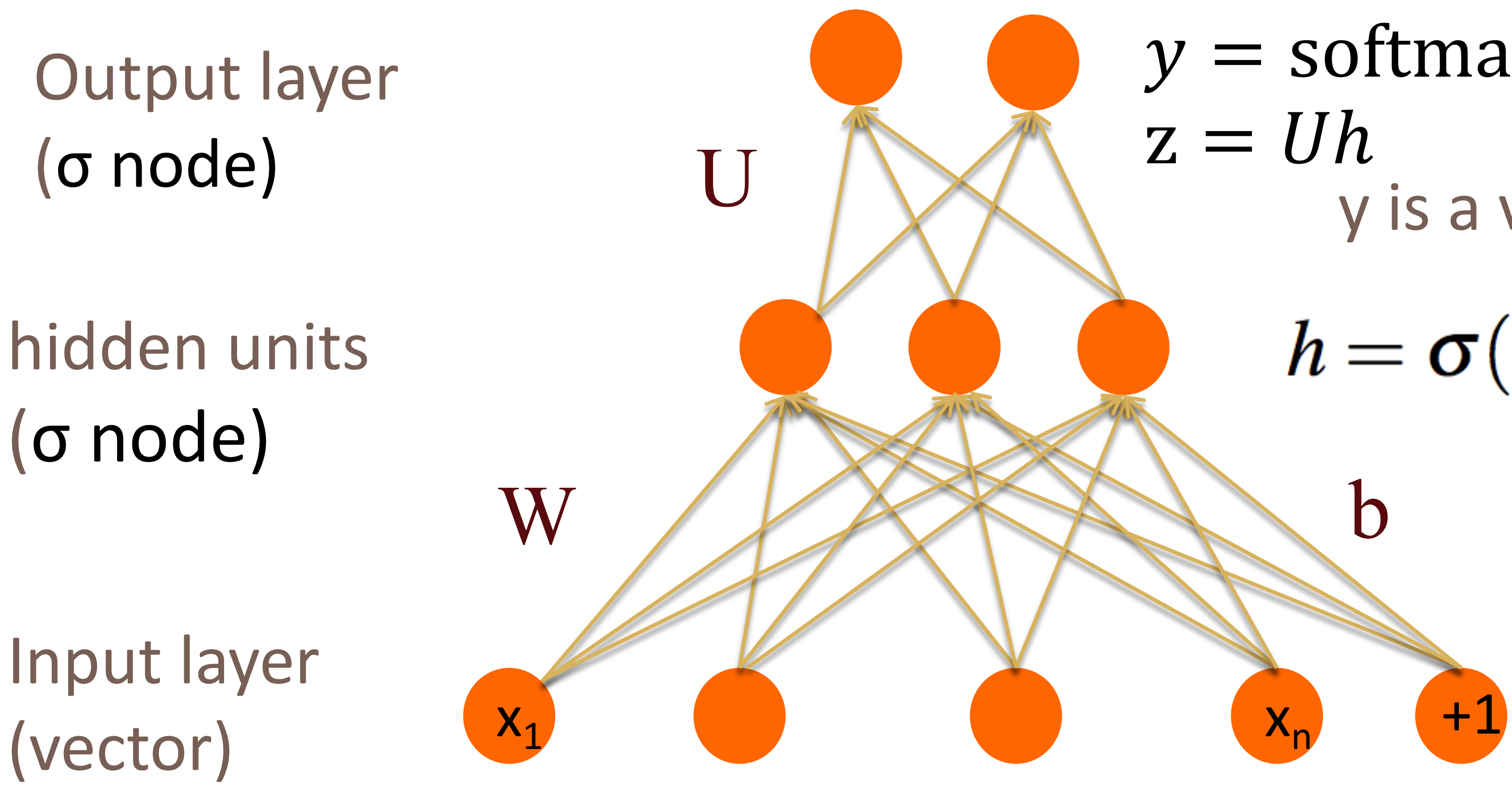
Could be ReLU
Or tanh

Two-Layer Network with softmax output



$y = \mathrm{softmax}(z)$

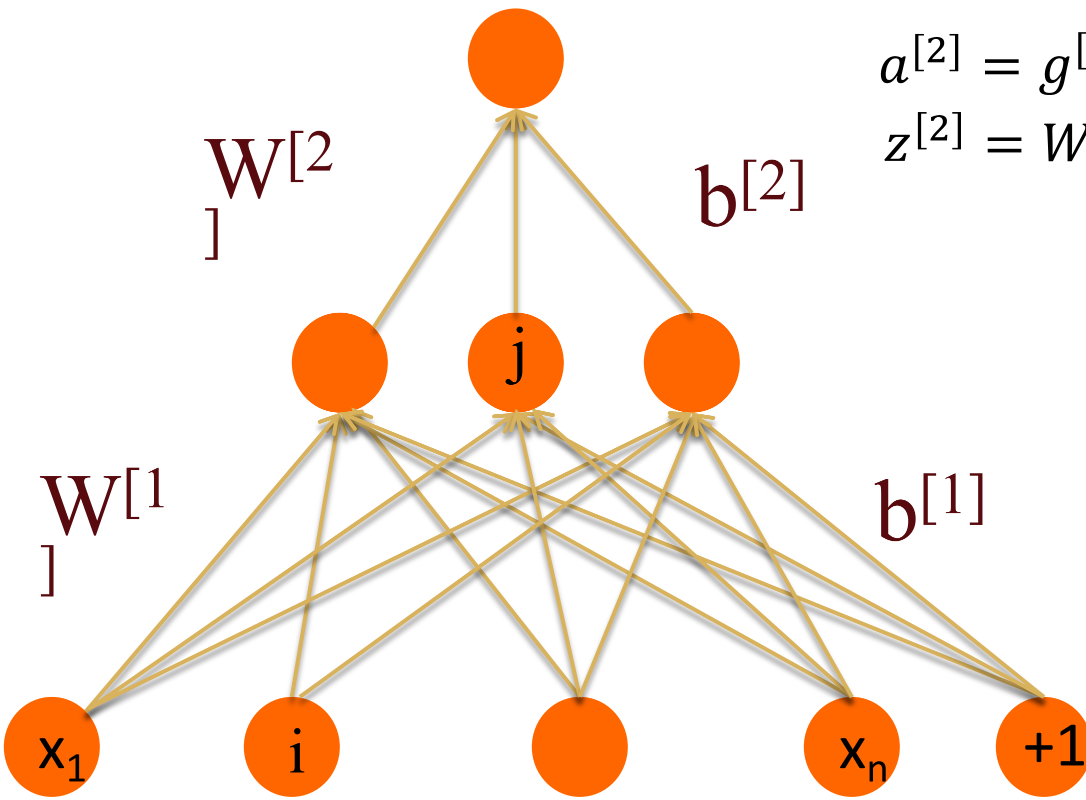
$z = Uh$

y is a vector

$h = \sigma(Wx + b)$

Could be ReLU
Or tanh

Multi-layer Notation



$$y = a^{[2]}$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$ sigmoid or softmax

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$

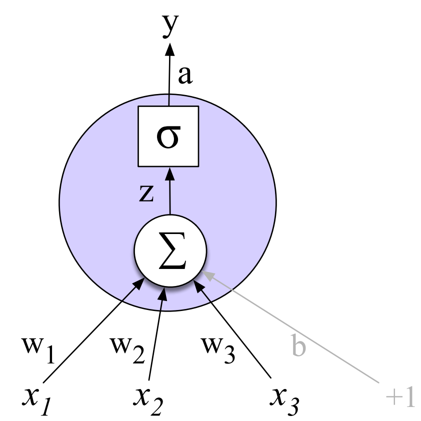
$$a^{[1]} = g^{[1]}(z^{[1]})$$ ReLU

$$z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$$

$$a^{[0]}$$

Multi Layer Notation

$$
\begin{aligned}
z^{[1]} &= W^{[1]}a^{[0]} + b^{[1]} \\
a^{[1]} &= g^{[1]}(z^{[1]}) \\
z^{[2]} &= W^{[2]}a^{[1]} + b^{[2]} \\
a^{[2]} &= g^{[2]}(z^{[2]}) \\
\hat{y} &= a^{[2]}
\end{aligned}
$$



for i **in** 1..n

$$
\begin{aligned}
z^{[i]} &= W^{[i]}\, a^{[i-1]} + b^{[i]} \\
a^{[i]} &= g^{[i]}(z^{[i]})
\end{aligned}
$$

$$\hat{y} = a^{[n]}$$

Replacing the bias unit

- Let's switch to a notation without the bias unit
- Just a notational change

1. Add a dummy node $a_0=1$ to each layer
2. Its weight w_0 will be the bias
3. So input layer $a^{[0]}_0=1$,
    - And $a^{[1]}_0=1$, $a^{[2]}_0=1$,…

Replacing the bias unit

- Instead of: We'll do this:

$x = x_1, x_2, \ldots, x_{n0}$

$$h = \sigma(Wx + b)$$

$$h_j = \sigma\left(\sum_{i=1}^{n_0} W_{ji}x_i + b_j\right)$$

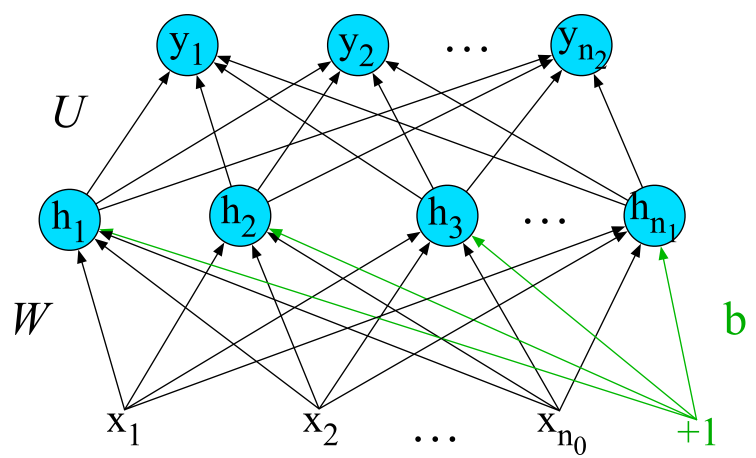
$x = x_0, x_1, x_2, \ldots, x_{n0}$

$$h = \sigma(Wx)$$

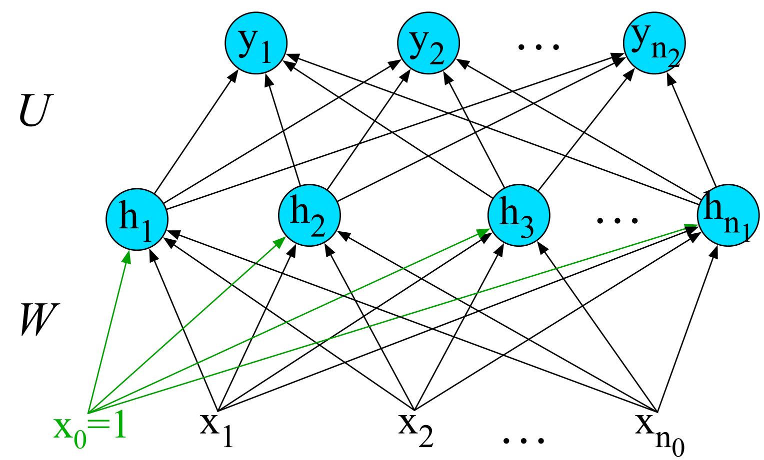
$$\sigma\left(\sum_{i=0}^{n_0} W_{ji}x_i\right)$$

Replacing the bias unit

Instead of:



We'll do this:



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Loss function

- Binary classiffication with sigmoid function at the output layer
  - Cross entropy loss (same as logistic regression)

$$L_{CE}(\hat{y}, y) = -\log p(y|x) \; = \; -[y \log \hat{y} + (1-y)\log(1-\hat{y})]$$

Loss function

- Multinomial classification with softmax function

$$L_{CE}(\hat{y}, y) = -\sum_{i=1}^{C} y_i \log \hat{y}_i$$

- Representing y as **one-hot vector**, where true class is i

$$y_i = 1 \text{ and } y_j = 0 \; \forall \; j \neq i$$

- Loss function becomes

$$L_{CE}(\hat{y}, y) = -\log \hat{y}_i = -\log \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

Computing the Gradient

- Calculate partial derivative of the loss function with respect to each parameter
- In neural networks, computing gradients for weights in layers is complicated!

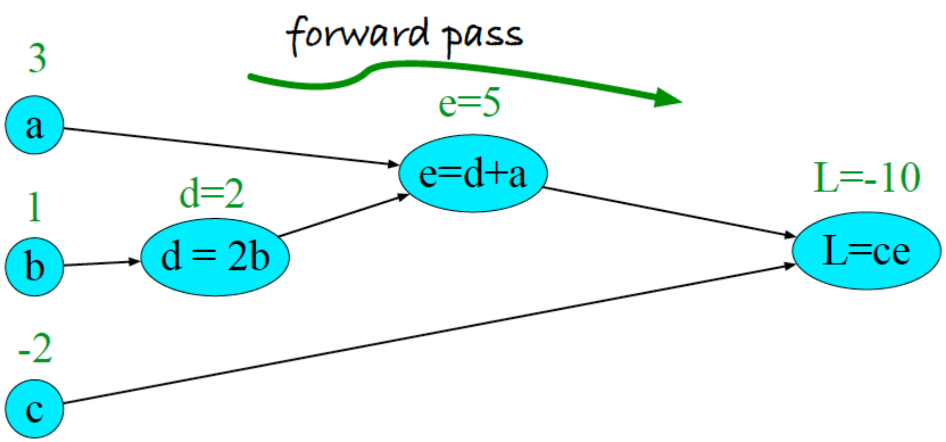
- Solution: **error backpropagation**, or **backprop** (Rumelhart et al., 1986) .

Computation graphs

- **Backpropagation** is the same as **backward differentiation**
- Backward differentiation depends on **computation graphs**

Computation graphs

- The computation is broken down into separate operations, each of which is modeled as a node in a graph
- Consider: $L(a, b, c) = c(a + 2b)$
  - series of computation
    - $d = 2 * b$
    - $e = a + d$
    - $L = c * e$



Backward differentiation on compution graphs

- We would like to compute $\frac{\partial L}{\partial a}\ \frac{\partial L}{\partial b}\ \frac{\partial L}{\partial c}$
- **Chain rule**

$$\frac{du}{dx} = \frac{du}{dv} \cdot \frac{dv}{dx}$$

  - We can apply the chain rule to more than two functions

On compution graph

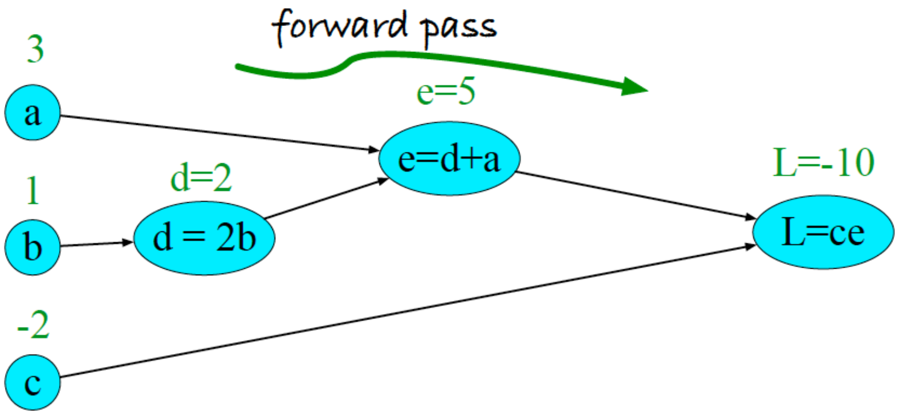
$$L = ce$$

So:

$$\frac{\partial L}{\partial c} = e$$

$$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial e}\frac{\partial e}{\partial a}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial b}$$

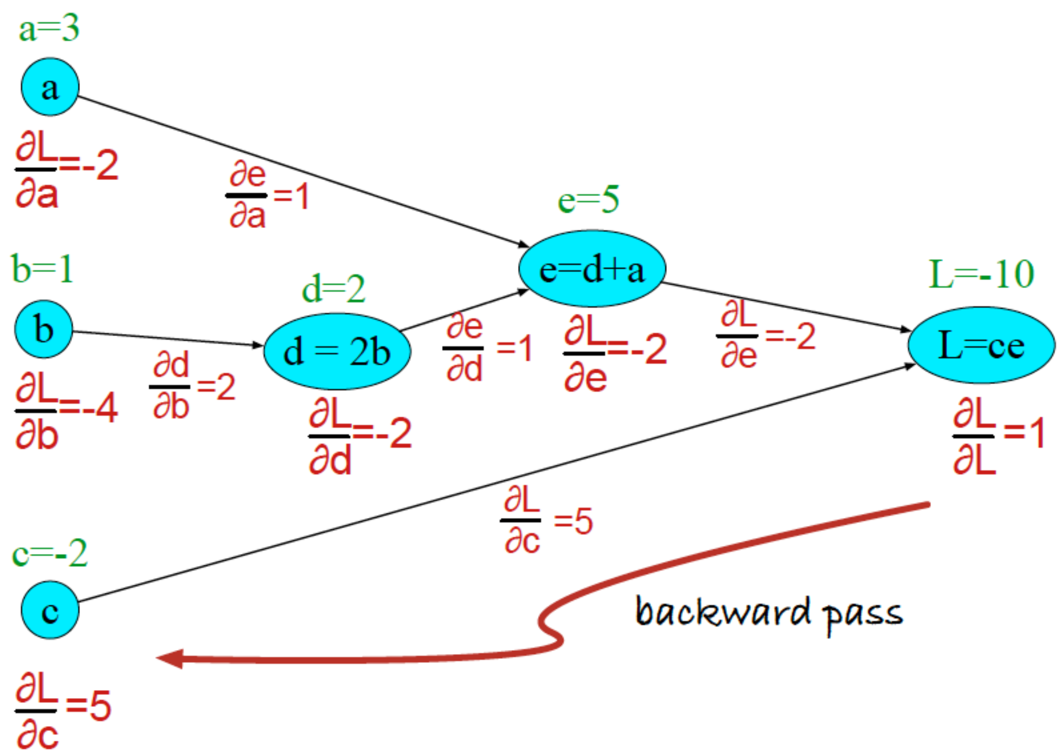


Backward differentiation on compution graphs

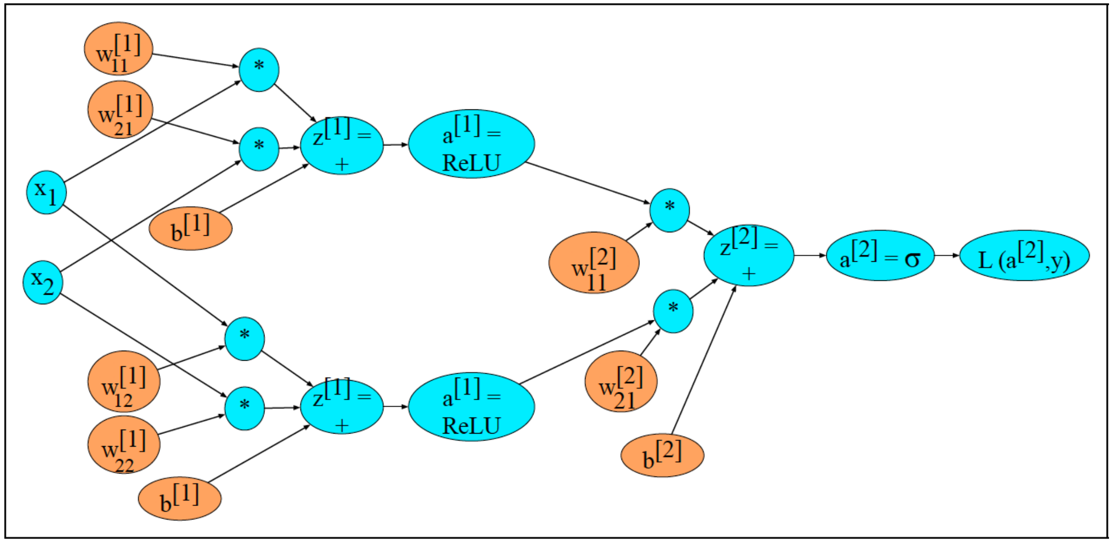
$$L = ce \; : \quad \frac{\partial L}{\partial e} = c, \frac{\partial L}{\partial c} = e$$

$$e = a + d \; : \quad \frac{\partial e}{\partial a} = 1, \frac{\partial e}{\partial d} = 1$$

$$d = 2b \; : \quad \frac{\partial d}{\partial b} = 2$$



Backward differentiation for a neural network



- Derivatives of activation functions
  - Sigmoid: $\frac{d\sigma}{dz} = \sigma(z)(1 - \sigma(z))$
  - Tanh: $\frac{d\tanh(z)}{d(z)} = 1 - \tanh^2(z)$
  - ReLU: $\frac{d\mathrm{ReLU}(z)}{d(z)} = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$

Training neural networks

- We apply gradient-based optimization algorithms
  - SGD
  - Adam
  - …
- Aspects we need to care when training
  - Weight initialization
  - Regularization: dropout,…
  - Hyperparameter tuning
    - Learning rate
    - Mini-batch size
    - Model architecture
- Some libraries that support differentiation on compution graphs: Pytorch, Tensorflow, Jax