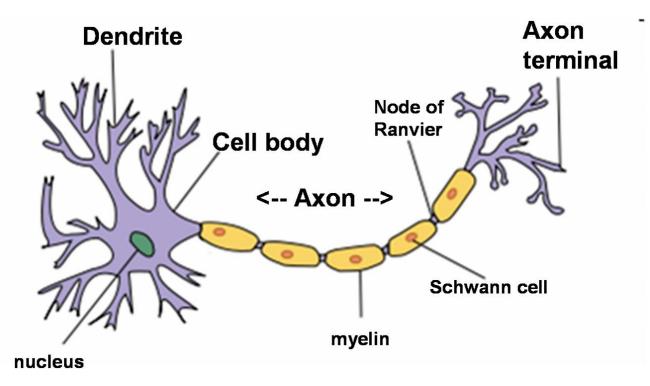
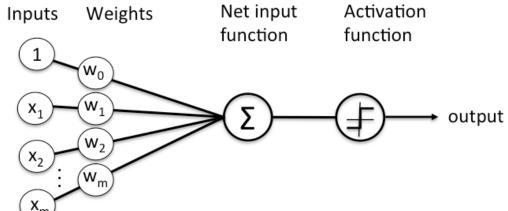
Unit 2 Neural Networks

TFIP-Al Artificial Neural Networks and Deep Learning

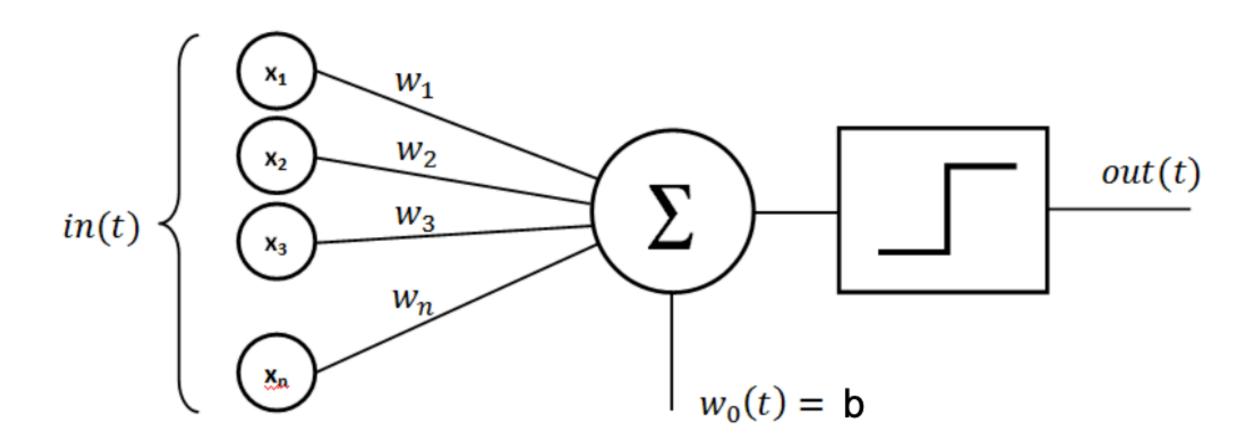
Feed-forward Neural Network

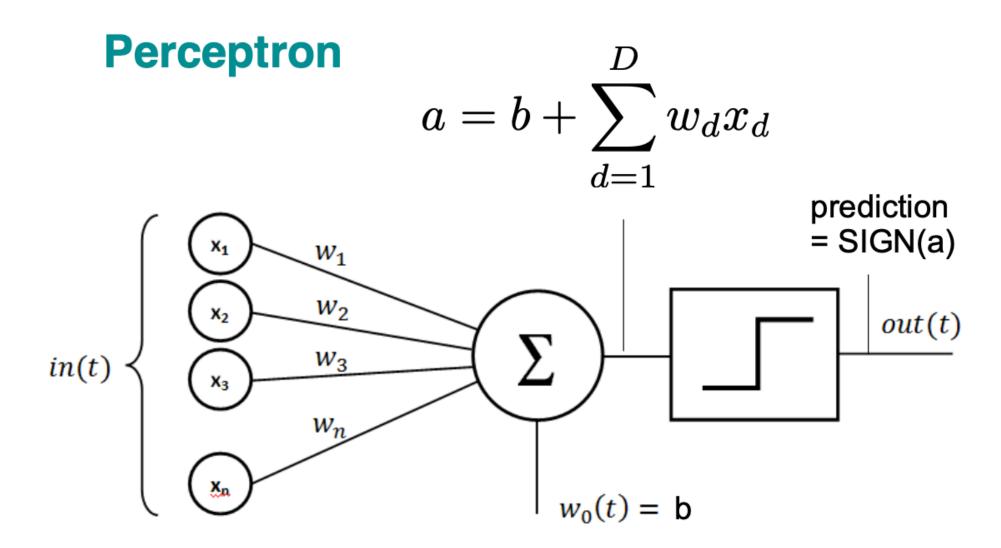
Neuron - perceptron





Perceptrons





Error driven learning $a = b + \sum_{d=1}^{D} w_d x_d$

- At each step, return SIGN(a)
- if SIGN(a)≠ y update parameter
- otherwise don't change

Algorithm 5 PerceptronTrain(D, MaxIter)

```
w_d \leftarrow o, for all d = 1 \dots D
                                                                           // initialize weights
b \leftarrow 0
                                                                                // initialize bias
_{3:} for iter = 1 \dots MaxIter do
     for all (x,y) \in D do
     a \leftarrow \sum_{d=1}^{D} w_d x_d + b
                                                      // compute activation for this example
    if ya \leq o then
           w_d \leftarrow w_d + yx_d, for all d = 1 \dots D
                                                                             // update weights
           b \leftarrow b + y
                                                                                  // update bias
8:
         end if
      end for
11: end for
return w_0, w_1, ..., w_D, b
```

Does this move a in the right direction?

- update w' = w + yx = w + x
- b' = b + y = b+1

$$a' = \sum_{d=1}^{D} w'_d x_d + b'$$

$$= \sum_{d=1}^{D} (w_d + x_d) x_d + (b+1)$$

$$= \sum_{d=1}^{D} w_d x_d + b + \sum_{d=1}^{D} x_d x_d + 1$$

$$= a + \sum_{d=1}^{D} x_d^2 + 1 > a$$

Does this move a in the right direction?

- update w' = w +yx = w + x
- b' = b + y = b+1

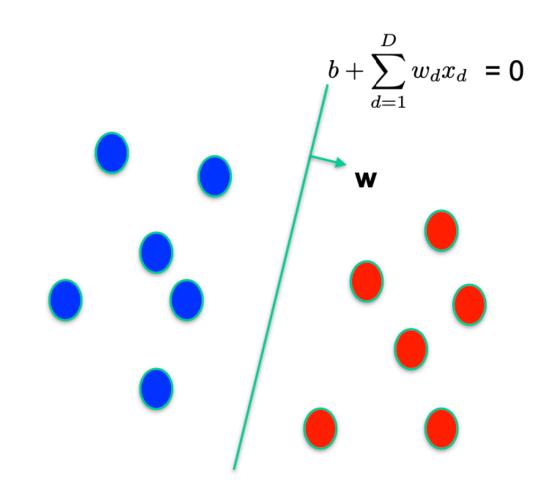
$$a' = \sum_{d=1}^{D} w'_d x_d + b'$$

$$= \sum_{d=1}^{D} (w_d + x_d) x_d + (b+1)$$

$$= \sum_{d=1}^{D} w_d x_d + b + \sum_{d=1}^{D} x_d x_d + 1$$

$$= a + \sum_{d=1}^{D} x_d^2 + 1 \qquad \text{a becomes more positive (not guaranteed that a>0)}$$

What is the decision boundary?



How good is this algorithm?

 Convergence: an entire pass without changing the weights.

 If the data is linearly separable, the algorithm will converge. But not necessarily to the "best" boundary

Notion of margin

$$margin(\mathbf{D}, w, b) = \begin{cases} \min_{(x,y) \in \mathbf{D}} y(w \cdot x + b) & \text{if } w \text{ separates } \mathbf{D} \\ -\infty & \text{otherwise} \end{cases}$$

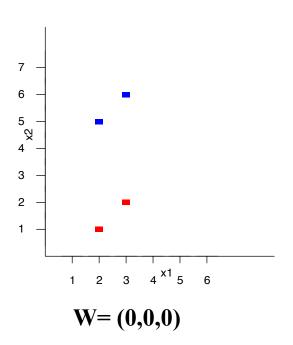
$$margin(\mathbf{D}) = \sup_{w,b} margin(\mathbf{D}, w, b)$$

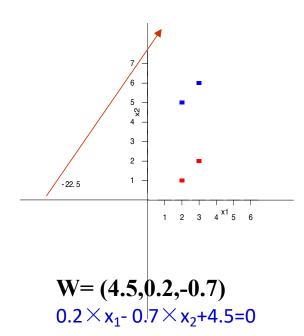
If data is linearly separable with margin γ and $||\mathbf{x}|| \le 1$, then algorithm will converge in $\frac{1}{\sqrt{2}}$ updates

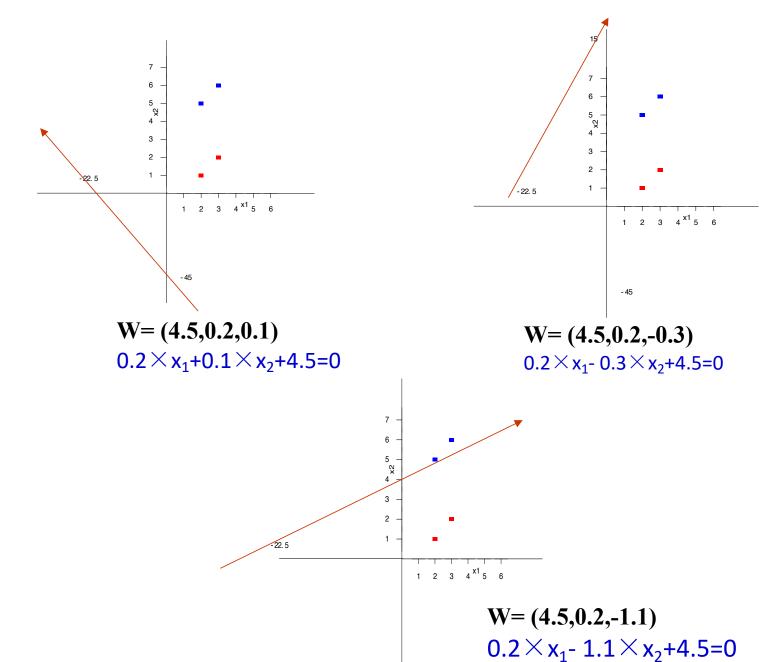
- The first generation of neural networks
- They were popularised by Frank Rosenblatt in the early 1960's.
 - They appeared to have a very powerful learning algorithm.
 - Lots of grand claims were made for what they could learn to do.
- In 1969, Minsky and Papert published a book called "Perceptrons" that analysed what they could do and showed their limitations.
 - Many people thought these limitations applied to all neural network models.
- The perceptron learning procedure is still widely used today for tasks with enormous feature vectors that contain many millions of features.

Perceptrons: training

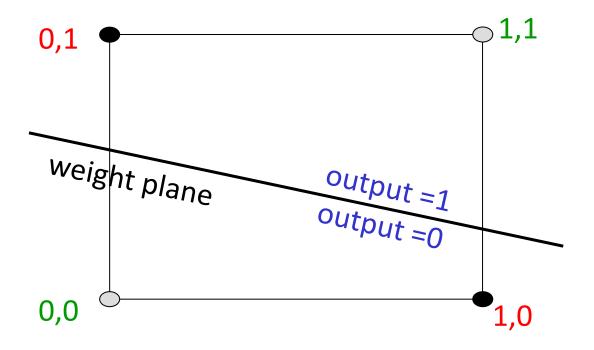
- Same as the learning method of logistic regression (with hard threshold or sigmoid function)
- Pick training cases using any policy that ensures that every training case will keep getting picked.
 - If the output unit is correct, leave its weights alone.
 - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
 - If the output unit incorrectly outputs a 1, subtract the input vector from the weight vector.
- This is guaranteed to find a set of weights that gets the right answer for all the training cases if any such set exists.







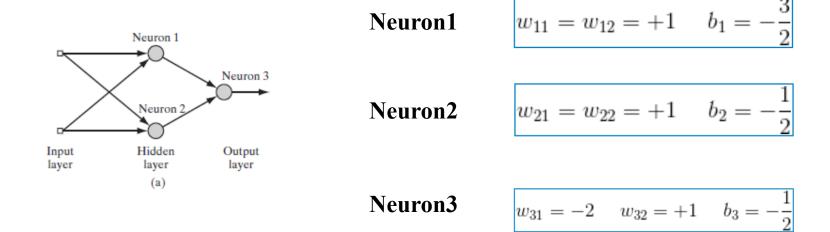
What perceptrons can't do



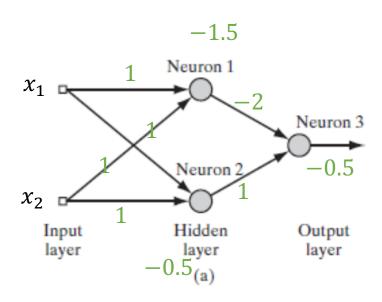
The positive and negative cases cannot be separated by a plane

Hidden units

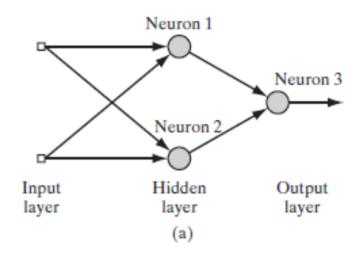
- Without hidden units, perceptrons are very limited
 - More layers of linear units do not help. It's still linear.
- We need multiple layers of adaptive, non-linear hidden units.



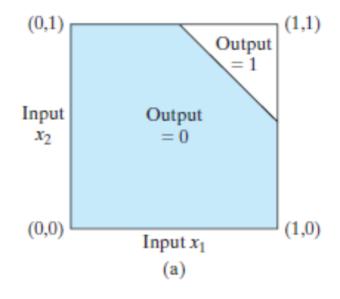
N.N. Inference

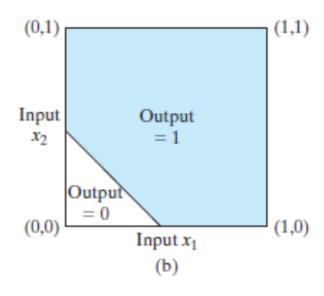


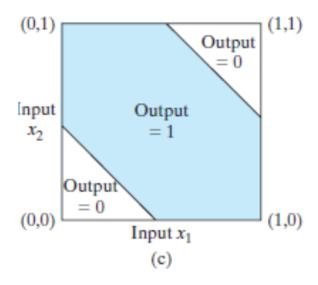
N.N. Inference



XOR Problem







Neuron1

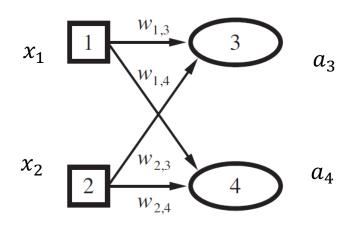
Neuron2

Neuron3

Loss function

- how can we train such nets?
 - We need an efficient way of adapting all the weights, not just the last layer. This is hard.
 - Learning the weights going into hidden units is equivalent to learning features.
 - This is difficult because nobody is telling us directly what the hidden units should do.

Learning - single layered



For a single sample (x1,x2)

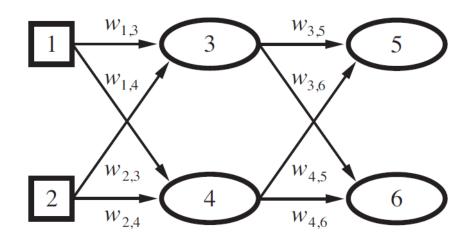
$$a3 = g(w_{1,3} * x_1 + w_{2,3} * x_2 + w_{0,3})$$

$$a4 = g(w_{1,4} * x_1 + w_{2,4} * x_2 + w_{0,4})$$

$$E(\mathbf{w}) = \frac{1}{2} [(y_1 - a_3)^2 + (y_2 - a_4)^2]$$

$$\frac{\partial}{\partial \mathbf{w}} E(\mathbf{w}) = \frac{\partial}{\partial \mathbf{w} \mathbf{1}} \frac{1}{2} (y_1 - a_3)^2 + \frac{\partial}{\partial \mathbf{w} \mathbf{2}} \frac{1}{2} (y_2 - a_4)^2$$

Difficulty in learning with multilayer



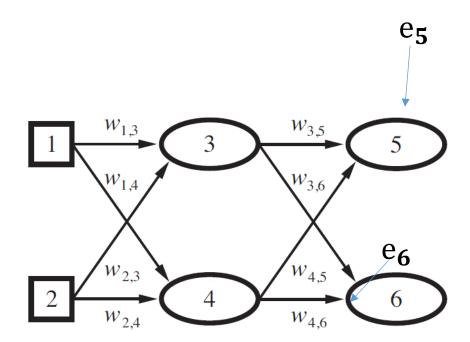
Error at the output layer is clear,

Error at the hidden layers seems mysterious

- the training data do not say what value the hidden nodes should have.

Error Back-propagate

Now Error at the hidden layers can be estimated



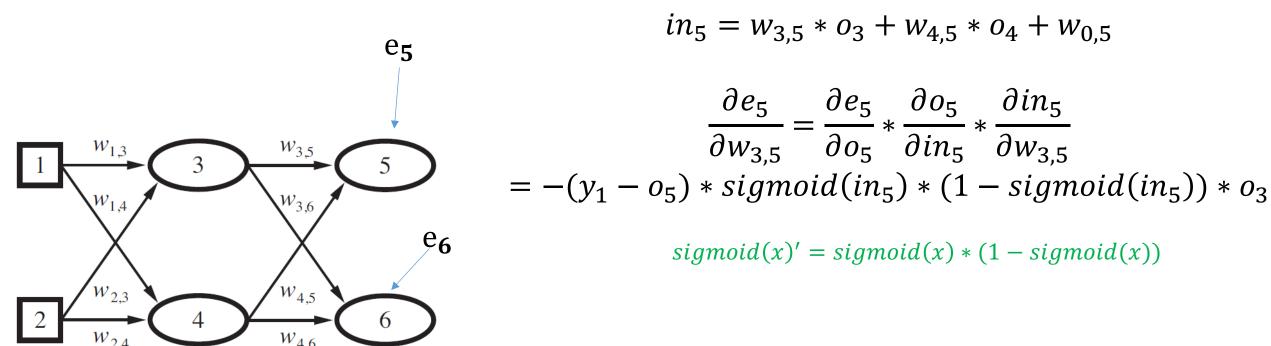
Error of Node3 is back propagated from e5 and e6

Output layer weight learning – chain rule

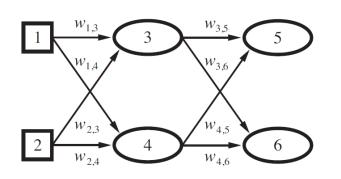
$$e_5 = \frac{1}{2}(y_1 - o_5)^2$$

$$o_5 = sigmoid(in_5)$$

Now Error at the hidden layers can be estimated



Output layer weight learning – delta rule



Gradient e5

$$\frac{\partial e_5}{\partial w_{3,5}} = -(y_1 - o_5) * sigmoid(in_5) * (1 - sigmoid(in_5)) * o_3$$
$$= -(y_1 - o_5) * o_5 * (1 - o_5) * o_3$$

Gradient Descent

$$w_{3,5} = w_{3,5} - \alpha * \delta_5 * o_3$$

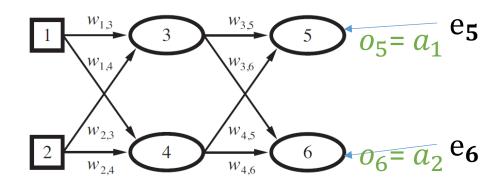
$$w_{4,5} = w_{4,5} - \alpha * \delta_5 * o_4$$

$$w_{0,5} = w_{0,5} - \alpha * \delta_5$$

$$\frac{\partial e_5}{\partial w_{4,5}} = \delta_5 * o_4$$

$$\frac{\partial e_5}{\partial w_{0,5}} = \delta_5$$

Hidden layer weight learning



$$\frac{\partial e_5}{\partial w_{1,3}} = \delta_5^* w_{3,5}^* o_3^* (1 - o_3) * x_1$$

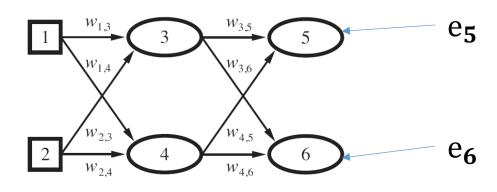
$$\frac{\partial e_5}{\partial w_{2,3}} = \delta_5 * w_{3,5} * o_3 * (1 - o_3) * x_2$$

$$e_3 = e_5 + e_6$$

$$\frac{\partial e_3}{\partial w_{1,3}} = \frac{\partial e_5}{\partial w_{1,3}} + \frac{\partial e_6}{\partial w_{1,3}}$$

• • •

Hidden layer weight learning



$$\frac{\partial e_5}{\partial w_{1,3}} = \delta_5 * w_{3,5} * o_3 * (1 - o_3) * x_1$$

$$\frac{\partial e_5}{\partial w_{2,3}} = \delta_5 * w_{3,5} * o_3 * (1 - o_3) * x_2$$

$$e_3 = e_5 + e_6$$

$$\frac{\partial e_3}{\partial w_{1,3}} = \frac{\partial e_5}{\partial w_{1,3}} + \frac{\partial e_6}{\partial w_{1,3}}$$

$$\frac{\partial e_3}{\partial w_{1,3}} = \delta_5^* w_{3,5}^* o_3^* (1 - o_3) * x_1^+$$
$$\delta_6^* w_{3,6}^* o_3^* (1 - o_3) * x_1$$

$$= \frac{(\delta_5 * w_{3,5} + \delta_6 * w_{3,6}) * o_3 * (1 - o_3)}{\uparrow} * x_1$$

$$\delta_3 \qquad sigmoid(x)'$$

...

BP algorithm (stochastic + sigmoid)

- Step0 define # of layers, # of nodes
- Step1 initialize parameters: weights and bias
- Step2 feed forward
 - Calculate output for each non-input layer node
- Step3 back propagate
 - Compute sensitivity for each non-input layer node i
 - Update parameters
- Step4 Convergence
 - Compute cost function
 - Repeat step2 until convergence

sensitivity

$$\delta_i = error_i \cdot o_i \cdot (1 - o_i)$$

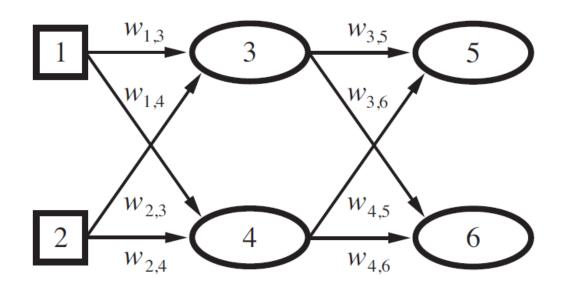
$$error_i = -(y - o_i) \quad \text{output-layer}$$

$$error_i = \sum_j (\delta_j * w_{i,j}) \quad \text{hidden-layer}$$

$$w_{k,i} = w_{k,i} - \alpha \cdot \delta_i \cdot o_k$$

Back-propagate - Example

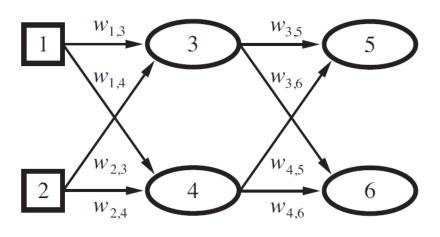
B.P. Example – the Network



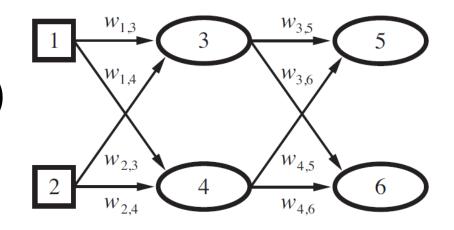
$$in_3 = x_1 \cdot w_{1,3} + x_2 \cdot w_{2,3} + w_{0,3}$$

$$o_3 = sigmoid(in_3)$$

B.P. Example – Feed Forward



B.P. Example – Learning (stochastic)



$$\delta_3 = o_3 \cdot (1 - o_3) \cdot (\delta_5 \cdot w_{3,5} + \delta_6 \cdot w_{3,6})$$

$$\delta_4 = o_4 \cdot (1 - o_4) \cdot (\delta_5 \cdot w_{4,5} + \delta_6 \cdot w_{4,6})$$

$$w_{1,3} = w_{1,3} - \alpha \cdot \delta_3 \cdot x_1 \qquad w_{1,4} = w_{1,4} - \alpha \cdot \delta_4 \cdot x_1$$

$$w_{2,3} = w_{2,3} - \alpha \cdot \delta_3 \cdot x_2 \qquad w_{2,4} = w_{2,4} - \alpha \cdot \delta_4 \cdot x_2$$

$$w_{0,3} = w_{0,3} - \alpha \cdot \delta_3 \cdot 1 \qquad w_{0,4} = w_{0,4} - \alpha \cdot \delta_4 \cdot 1$$

$$w_{3,5} = w_{3,5} - \alpha \cdot \delta_5 \cdot o_3$$

$$w_{4,5} = w_{4,5} - \alpha \cdot \delta_5 \cdot o_4$$

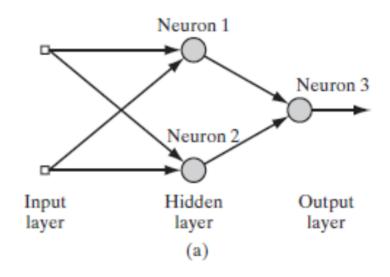
$$w_{0,5} = w_{0,5} - \alpha \cdot \delta_5 \cdot 1$$

$$w_{3,6} = w_{3,6} - \alpha \cdot \delta_6 \cdot o_3$$

$$w_{4,6} = w_{4,6} - \alpha \cdot \delta_6 \cdot o_4$$

$$w_{0,6} = w_{0,6} - \alpha \cdot \delta_6 \cdot 1$$

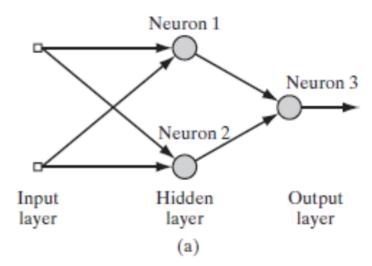
XOR with 2 nodes hidden layer



X1	X2	Y
0	0	0
0	1	1
1	0	1
1	1	0

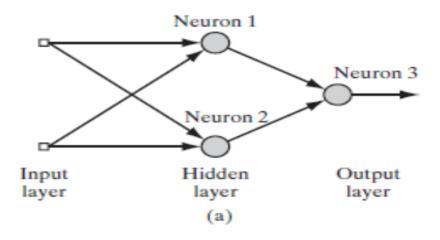
Parameter initialization

- To avoid symmetry problem, the initial value for the weights would not be zeros any longer,
- Instead, they would be a small randomized value
 - $w_{i1.1} = 0.02$ (randomly generated)
 - $w_{i2.1} = 0.03$
 - $w_{0.1} = 0$
 - $w_{i1.2} = 0.01$
 - $w_{i2.2} = 0.02$
 - $w_{0.2} = 0$
 - $w_{1.3} = 0.01$
 - $w_{2.3} = 0.03$
 - $w_{0,3} = 0$



Feed forward – input(0,0)

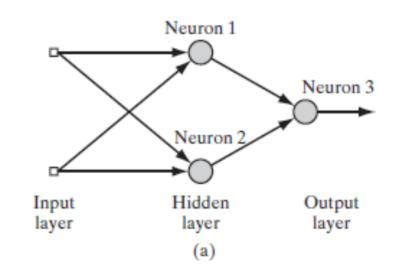
- $o_1 = sigmoid(0) = 0.5$
- $o_2 = sigmoid(0) = 0.5$
- $o_3 = sigmoid(0.5 \cdot 0.01 + 0.5 \cdot 0.03 + 0) = 0.505$



Back propagate - input(0,0)

We have

- o[3]={0.5, 0.5, 0.505}
- $o_3 = 0.505$, and y = 0



Sensitivities for all nodes

•
$$\delta_3 = -(y - o_3) \cdot o_3 \cdot (1 - o_3) = -(0 - 0.505)0.505(1 - 0.505) = 0.126$$

•
$$\delta_1 = (\delta_3 w_{1.3}) o_1 (1 - o_1) = (0.126) \cdot 0.01 \cdot 0.5 \cdot (1 - 0.5) = 0.000315$$

•
$$\delta_2 = (\delta_3 w_{2.3}) o_2 (1 - o_2) = (0.126) \cdot 0.03 \cdot 0.5 \cdot (1 - 0.5) = 0.000945$$

• Hidden-Output Weight

•
$$w_{1,3} = w_{1,3} - \alpha \cdot \delta_3 \cdot o_1 = 0.01 - 0.1 \cdot 0.126 \cdot 0.5 = -0.0037$$

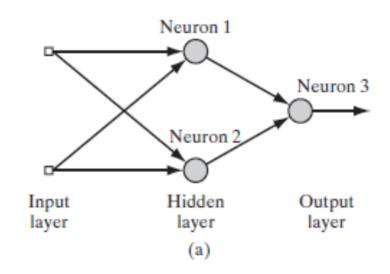
•
$$w_{2,3} = w_{2,3} - \alpha \cdot \delta_3 \cdot o_2 = 0.03 - 0.1 \cdot 0.126 \cdot 0.5 = -0.0237$$

•
$$w_{0.3} = w_{0.3} - \alpha \cdot \delta_3 = 0 - 0.1 \cdot 0.126 = -0.0126$$

Back propagate — input(0,0)

We have

- o[3]={0.5, 0.5, 0.505}
- $\delta[3]=\{0.000315, 0.000945, 0.126\}$



Input-Hidden

•
$$w_{i_{1,1}} = w_{i_{1,1}} - \alpha \cdot \delta_1 \cdot x_1 = 0.02 - 0.1 \cdot 0.000315 \cdot 0 = 0.02$$

•
$$w_{i2,1} = w_{i2,1} - \alpha \cdot \delta_1 \cdot x_2 = 0.03 - 0.1 \cdot 0.000315 \cdot 0 = 0.03$$

•
$$w_{0.1} = w_{0.1} - \alpha \cdot \delta_1 = 0 - 0.1 \cdot 0.000315 = -0.0000315$$

•
$$w_{i_{1,2}} = w_{i_{1,2}} - \alpha \cdot \delta_2 \cdot x_1 = 0.01 - 0.1 \cdot 0.000945 \cdot 0 = 0.01$$

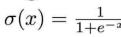
•
$$w_{i2,2} = w_{i2,2} - \alpha \cdot \delta_2 \cdot x_2 = 0.02 - 0.1 \cdot 0.000945 \cdot 0 = 0.02$$

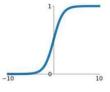
•
$$w_{0,2} = w_{0,2} - \alpha \cdot \delta_2 = 0 - 0.1 \cdot 0.000945 = -0.0000945$$

Activation Functions

- sigmoid
 - Gradient vanishing
 - Output is not zero-centered slow down the learning
 - Power operation time cost
- tanh (Hyperbolic Tangent)
 - Gradient vanishing
 - Output is not zero-centered
 - Power operation
- Relu
 - Gradient vanishing
 - Output is not zero-centered
 - Power operation
 - Dead Relu Problem

Sigmoid

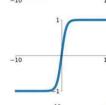




$$\sigma(x) = rac{1}{1 + e^{-x}}$$

$$\sigma(x)\cdot(1-\sigma(x))$$

tanh(x)



$$anh x = rac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$1 - \tanh(x)^2$$

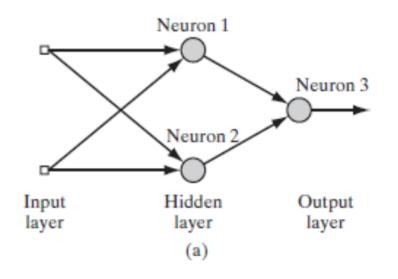
 $\max(0, x)$



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

$$= \begin{cases} 0, x < 0 \\ 1, x \ge 0 \end{cases}$$

XOR with 2 nodes hidden layer - vectorization



- Hidden layer
 - tanh
- Output layer
 - sigmoid

X0	X1	X2	Y
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	0

- X is a 4×3 matrix
- Y is a 4×1 vector

Parameter initialization

Hidden layer

• Weight_hidden =
$$\begin{bmatrix} 0.02 & 0.01 \\ 0.03 & 0.02 \end{bmatrix}$$

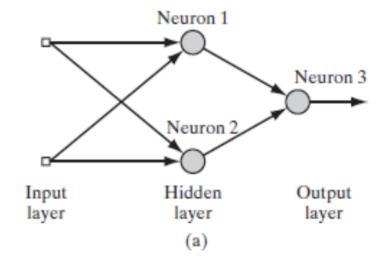
- Bias_hidden=[0 0]
- Output layer

• Weight_output =
$$\begin{bmatrix} 0.01 \\ 0.03 \end{bmatrix}$$

• Bias_output=[0]

$$w_{i1,1} = 0.02$$

 $w_{i2,1} = 0.03$
 $w_{0,1} = 0$
 $w_{i1,2} = 0.01$
 $w_{i2,2} = 0.02$
 $w_{0,2} = 0$
 $w_{1,3} = 0.01$
 $w_{2,3} = 0.03$
 $w_{0,3} = 0$



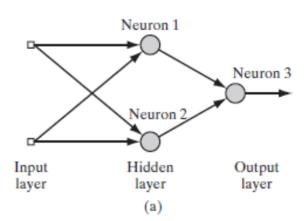
Feed forward – Hidden layer output

•
$$X = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} Y = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

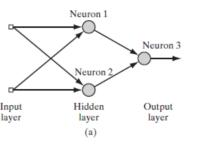
• Weight_hidden = $\begin{bmatrix} 0.02 & 0.01 \\ 0.03 & 0.02 \end{bmatrix}$
• Bias hidden= $\begin{bmatrix} 0 & 0 \end{bmatrix}$

hidden_output = tanh(np.dot(X,weight_hidden)+ bias_hidden))

hidden_output =
$$\begin{bmatrix} o_1^{(1)} & o_2^{(1)} \\ o_1^{(2)} & o_2^{(2)} \\ o_1^{(3)} & o_2^{(3)} \\ o_1^{(4)} & o_2^{(4)} \end{bmatrix}$$



Feed forward – output layer output

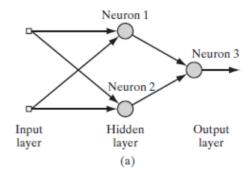


yhat = expit(np.dot(hidden_output,weight_output) + bias_output)

• hidden_output =
$$\begin{bmatrix} o_1^{(1)} & o_2^{(1)} \\ o_1^{(2)} & o_2^{(2)} \\ o_1^{(3)} & o_2^{(3)} \\ o_1^{(4)} & o_2^{(4)} \end{bmatrix}, \text{ yhat } = \begin{bmatrix} o_1^{(1)} \\ o_3^{(2)} \\ o_3^{(3)} \\ o_3^{(4)} \end{bmatrix}$$

- Weight_output = $\begin{bmatrix} 0.01 \\ 0.03 \end{bmatrix}$
- Bias_output=[0]

Sensitivity computing



- $delta_output = -(Y-yhat)*(yhat)*(1-yhat)$
- delta_hidden = np.dot(delta_output,weight_output.T)*(1-np.square(hidden_output))

• delta_output =
$$\begin{bmatrix} \delta_3^{(1)} \\ \delta_3^{(2)} \\ \delta_3^{(3)} \\ \delta_3^{(4)} \end{bmatrix}$$
, delta_hidden = =
$$\begin{bmatrix} \delta_1^{(1)} & \delta_2^{(1)} \\ \delta_1^{(2)} & \delta_2^{(2)} \\ \delta_1^{(3)} & \delta_2^{(3)} \\ \delta_1^{(4)} & \delta_2^{(4)} \end{bmatrix}$$

Parameters Update

- weight_output = weight_output α*np.dot(hidden_output.T,delta_output)/4
- bias_output = bias_output - α *np.sum(delta_output)/4

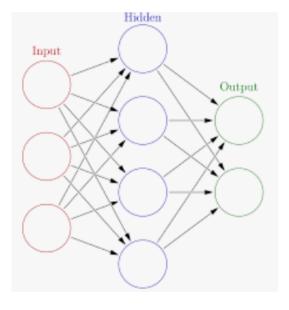
- weight_hidden = weight_hidden - α *np.dot(X.T, delta_hidden)/4
- bias_hidden = bias_hidden - α *np.sum(delta_hidden,axis=0)/4

Weight Initialization

All Zero Initialization(pitfall)

- We assume: with proper data normalization
 - Half of the weights will be positive
 - Half of them will be negative
 - 0 would be the best guess
- It is a mistake
 - Same output → same gradient → same parameter updates

- Logistic Regression
 - All 0 initialization is ok



Small random numbers

Close to zero, but not identically zero

- Symmetry breaking
- $W \sim N(0, \sigma)$
 - ${f \cdot}$ W is initialized as a random vector sampled from a multidimensional gaussian

- Smaller numbers ≠ work better
 - very small weights → small gradient → gradient diminish

Uniform distribution initialization

$$W \sim U\left[-\frac{1}{\sqrt{n_{in}}}, \frac{1}{\sqrt{n_{in}}}\right]$$

where U[-a, a] is the uniform distribution in the interval (-a, a), and n_{in} is the size of the previous layer

- Problems in weights initialization
 - If the weights in a network start too small, then the signal shrinks as it passes through each layer until it's too tiny to be useful. (Gradient Vanishing)
 - If the weights in a network start too large, then the signal grows as it passes through each layer until it's too massive to be useful. (Gradient Exploding)

Gaussian distribution with zero mean and a suitable variance

$$n_{in} = n, n_{out} = m$$

• For simplicity, let's assume m=1

$$y = W^T X = w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$

- to help keep the signal from exploding to a high value or vanishing to zero
- we want the variance to remain the same after passing the layer

$$var(y) = var(w_1x_1 + w_2x_2 + \dots + w_nx_n) = var(w_1x_1) + \dots var(w_nx_n)$$

• Assume W and X are independent, both of them have zero mean

$$var(w_i x_i) = E[x_i]^2 var(w_i) + E[w_i]^2 var(x_i) + var(w_i) var(x_i)$$

$$var(w_i x_i) = E[x_i]^2 var(w_i) + E[w_i]^2 var(x_i) + var(w_i) var(x_i)$$

• I.ID assumption on each w_i and x_i

$$var(y) = n \cdot var(w_i) var(x_i)$$

• if we want to make sure the variance of y to be the same as X, then we need $n \cdot \text{var}(w_i) = 1$. Hence,

$$var(w_i) = \frac{1}{n} = \frac{1}{n_{in}}$$

 Similarly, if you go through the same steps for the backpropagated signal, you find that you need

$$var(w_i) = \frac{1}{n_{out}}$$

- These two constraints can only be satisfied simultaneously if $n_{in}=n_{out}$
- As a compromise,

$$var(w_i) = \frac{2}{n_{in} + n_{out}}$$

 Moreover, the author also introduced a normalized initialization version follows uniform distribution

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_{in} + n_{out}}}, \frac{\sqrt{6}}{\sqrt{n_{in} + n_{out}}}\right]$$

• What's more, Xavier with uniform distribution + sigmoid activation

$$W \sim U\left[-\frac{4 \cdot \sqrt{6}}{\sqrt{n_{in} + n_{out}}}, \frac{4 \cdot \sqrt{6}}{\sqrt{n_{in} + n_{out}}}\right]$$

Xavier is aimed to deal with gradient vanishing or exploding problems

• Xavier initialization would not be use with ReLU activation, which would not lead to vanishing or exploding gradients

ReLU initialization

- Proposed to handle the issue that some very deep CNNs have difficulties to converge
- Weights in those CNN are initialized by random weights drawn from Gaussian distributions with fixed standard deviations
- n_l : size of layer l

$$W \sim N(0, \sqrt{\frac{2}{n_l}}) \qquad W \sim U[-\sqrt{\frac{6}{n_l}}, \sqrt{\frac{6}{n_l}}]$$