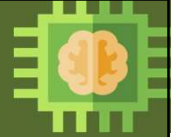


Elective Course

Course Code: CS4103

Autumn 2025-26



Lecture #40

Artificial Intelligence for Data Science

Week-11:

MACHINE LEARNING (Part VIII)

Neural Network Learning

Course Instructor:

Dr. Monidipa Das

Assistant Professor

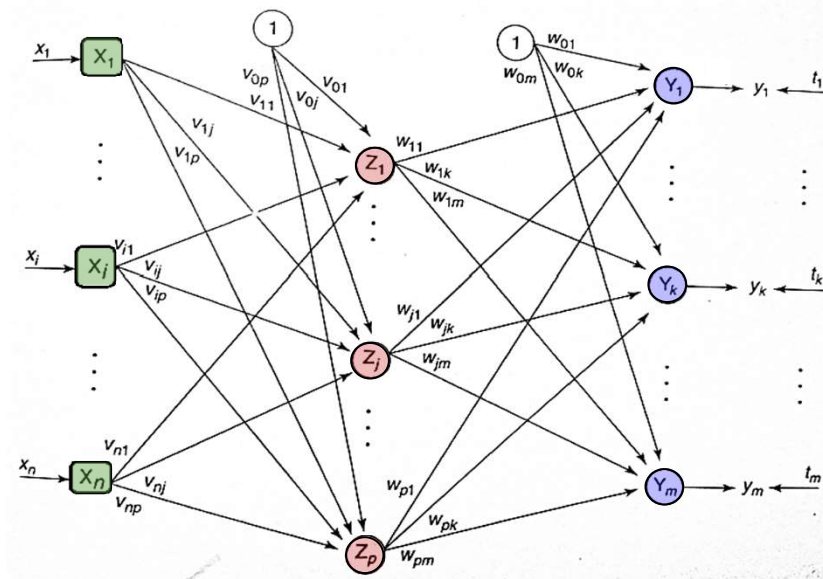
Department of Computational and Data Sciences

Indian Institute of Science Education and Research Kolkata, India 741246

Back Propagation Network (BPN)

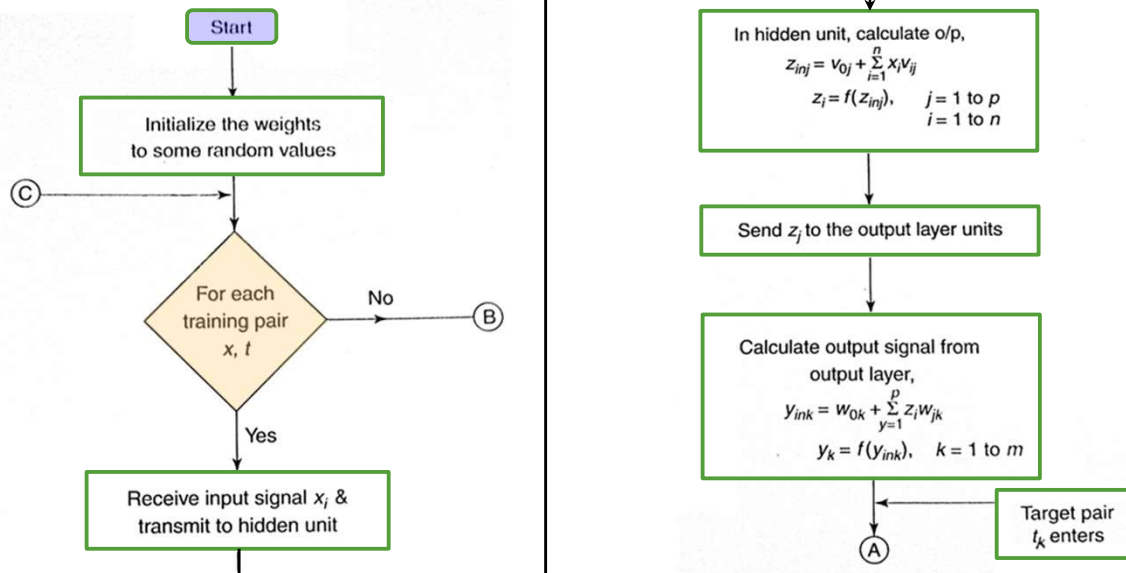


- Architecture



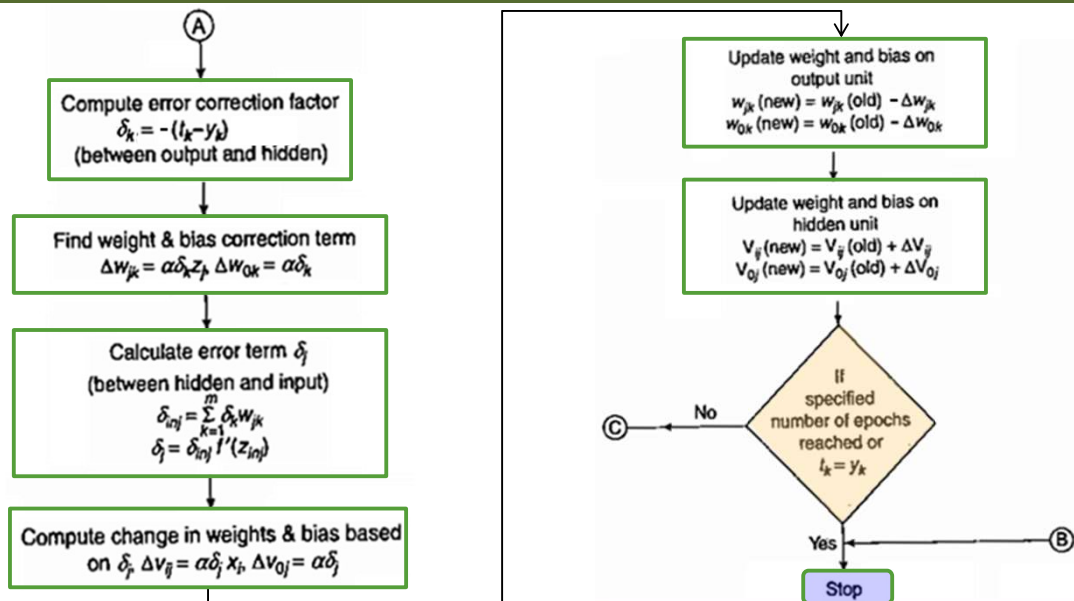
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BPN Training



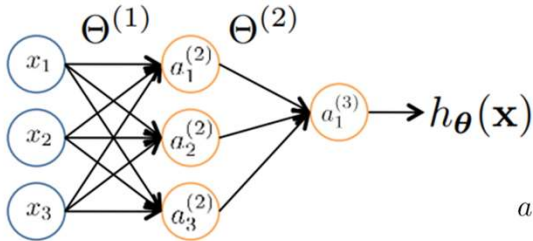
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BPN Training



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Neural Network



$a_i^{(j)}$ = "activation" of unit i in layer j

$\Theta^{(j)}$ = weight matrix controlling function mapping from layer j to layer $j+1$

$$\begin{aligned} a_1^{(2)} &= g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3) \\ a_2^{(2)} &= g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3) \\ a_3^{(2)} &= g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3) \\ h_{\Theta}(x) &= a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)}) \end{aligned}$$

If network has s_j units in layer j and s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$.

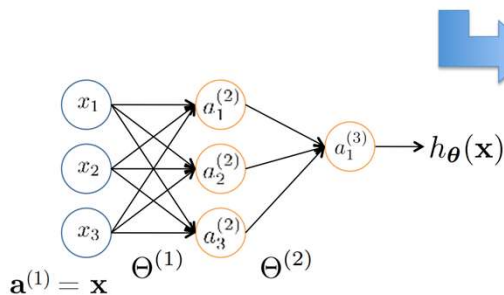
$$\Theta^{(1)} \in \mathbb{R}^{3 \times 4} \quad \Theta^{(2)} \in \mathbb{R}^{1 \times 4}$$

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Vectorization



$$\begin{aligned} a_1^{(2)} &= g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3) = g(z_1^{(2)}) \\ a_2^{(2)} &= g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3) = g(z_2^{(2)}) \\ a_3^{(2)} &= g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3) = g(z_3^{(2)}) \\ h_{\Theta}(\mathbf{x}) &= g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)}) = g(z_1^{(3)}) \end{aligned}$$



Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)} \mathbf{x}$$

$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

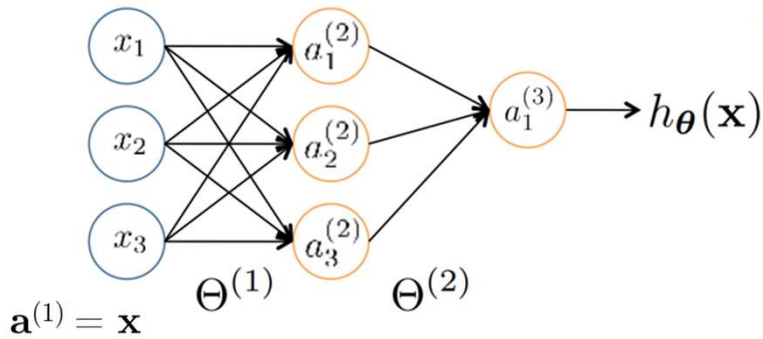
$$\text{Add } a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)} \mathbf{a}^{(2)}$$

$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

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Forward Propagation



Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)} \mathbf{x} = \Theta^{(1)} \mathbf{a}^{(1)}$$

$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

$$\text{Add } a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)} \mathbf{a}^{(2)}$$

$$h_{\theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

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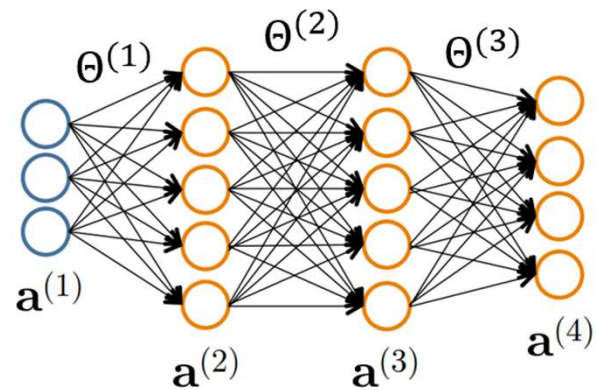
Forward Propagation



- Given one labeled training instance (\mathbf{x}, y) :

Forward Propagation

- $\mathbf{a}^{(1)} = \mathbf{x}$
- $\mathbf{z}^{(2)} = \Theta^{(1)} \mathbf{a}^{(1)}$
- $\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$ [add $a_0^{(2)}$]
- $\mathbf{z}^{(3)} = \Theta^{(2)} \mathbf{a}^{(2)}$
- $\mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$ [add $a_0^{(3)}$]
- $\mathbf{z}^{(4)} = \Theta^{(3)} \mathbf{a}^{(3)}$
- $\mathbf{a}^{(4)} = h_{\theta}(\mathbf{x}) = g(\mathbf{z}^{(4)})$



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Cost Function



Neural Network:

$$h_{\Theta} \in \mathbb{R}^K \quad (h_{\Theta}(\mathbf{x}_i))_k = k^{\text{th}} \text{ output of the } i\text{-th sample}$$

$$J(\Theta) = -\frac{1}{n} \left[\sum_{i=1}^n \sum_{k=1}^K y_{ik} \log (h_{\Theta}(\mathbf{x}_i))_k + (1 - y_{ik}) \log (1 - (h_{\Theta}(\mathbf{x}_i))_k) \right]$$

k^{th} class: true, predicted
not k^{th} class: true, predicted

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Optimizing the Neural Network



$$J(\Theta) = -\frac{1}{n} \left[\sum_{i=1}^n \sum_{k=1}^K y_{ik} \log (h_{\Theta}(\mathbf{x}_i))_k + (1 - y_{ik}) \log (1 - (h_{\Theta}(\mathbf{x}_i))_k) \right]$$

$$+ \frac{\lambda}{2n} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{ji}^{(l)})^2$$

Solve via: $\min_{\Theta} J(\Theta)$

We can use Gradient Descent (GD)

Need code to compute:

- $J(\Theta)$
- $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

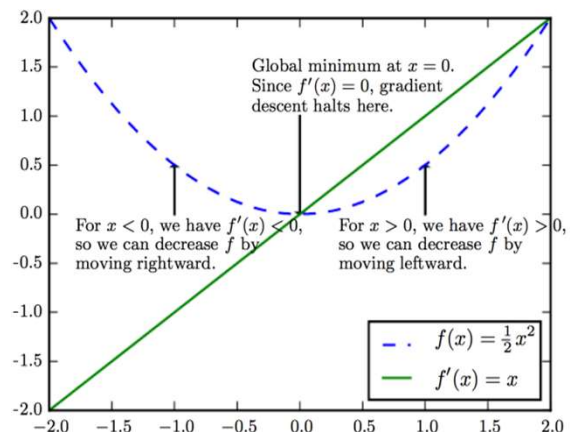
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How Gradient Descent (GD) works using derivatives



- Criterion $f(x)$ minimized by moving from current solution in direction of the negative of gradient

- For $x > 0$, $f(x)$ increases with x and $f'(x) > 0$
- For $x < 0$, $f(x)$ decreases with x and $f'(x) < 0$
- Use $f'(x)$ to follow function downhill
- Reduce $f(x)$ by going in direction opposite sign of derivative $f'(x)$



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Method of Gradient Descent



- Decrease f by moving in the direction of the negative gradient
 - This is known as the method of **gradient descent**
- The method proposes a new point
$$\mathbf{x}' = \mathbf{x} - \alpha \nabla_{\mathbf{x}} f(\mathbf{x})$$
 - where α is the **learning rate**, a positive scalar. Set to a small constant.
- This converges when every element of the gradient is zero
 - In practice, very close to zero
- We may be able to avoid iterative algorithm and jump to the critical point by solving the equation $\nabla_{\mathbf{x}} f(\mathbf{x}) = 0$ for \mathbf{x}

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Gradient Descent Algorithm



Gradient Descent: Algorithmic representation

repeat until convergence {
 $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ (simultaneously update $j = 0$ and $j = 1$)
 }
 Parameters Cost function, which is to be minimized

Correct updating of parameters

temp0 := $\theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
 temp1 := $\theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$
 $\theta_0 :=$ temp0
 $\theta_1 :=$ temp1

Incorrect updating of parameters

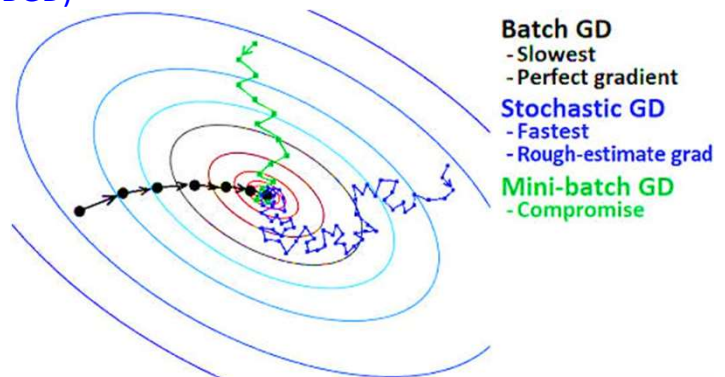
temp0 := $\theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
 $\theta_0 :=$ temp0
 temp1 := $\theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$
 $\theta_1 :=$ temp1

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Types of Gradient Descent

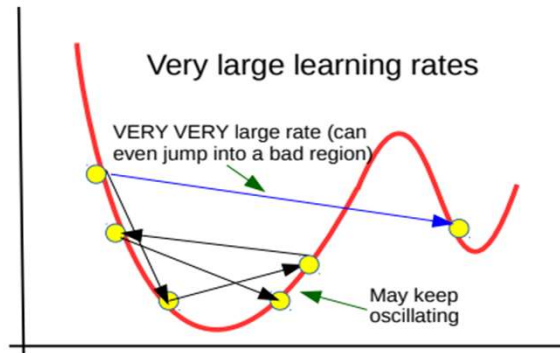


- There are **three major types** of Gradient Descent Algorithms:
 - Batch Gradient Descent (BGD)
 - Stochastic Gradient Descent (SGD)
 - Mini-Batch Gradient Descent (MBGD)

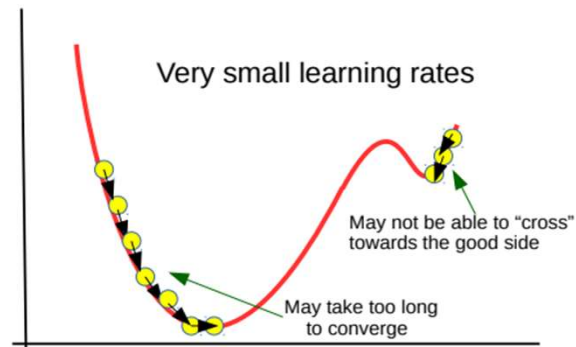


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Learning rate is very important



Too large, the next point will perpetually bounce haphazardly across the bottom of the well



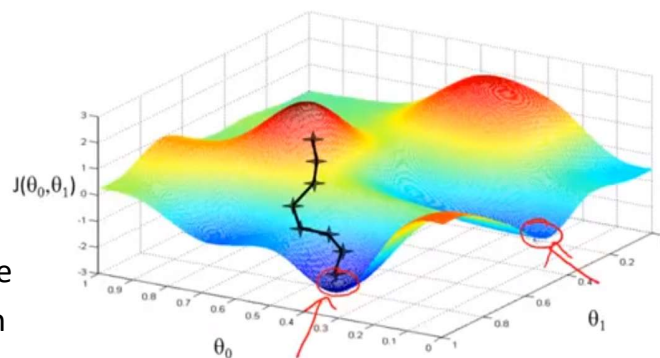
Too small learning rate will take too long

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GD: Advantages and Disadvantages



- Advantages
 - Ease of implementation
 - Convergence guarantee
 - Scalability
- Disadvantages
 - Sensitivity to learning rate
 - Sensitivity to initialization
 - Convergence speed



Courtesy: Andrew Ng

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Optimizing the Neural Network



$$J(\Theta) = -\frac{1}{n} \left[\sum_{i=1}^n \sum_{k=1}^K y_{ik} \log(h_{\Theta}(\mathbf{x}_i))_k + (1 - y_{ik}) \log(1 - (h_{\Theta}(\mathbf{x}_i))_k) \right] + \frac{\lambda}{2n} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l-1}} \sum_{j=1}^{s_l} (\Theta_{ji}^{(l)})^2$$

Solve via: $\min_{\Theta} J(\Theta)$

$J(\Theta)$ is not convex, so GD on a neural net yields a local optimum

- But, tends to work well in practice

Need code to compute:

- $J(\Theta)$
- $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

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Backpropagation

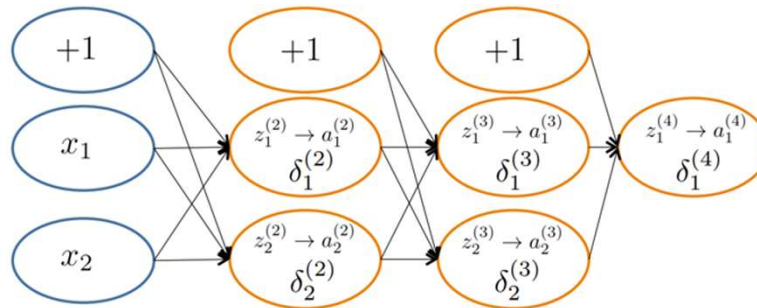


- Similar to the perceptron learning algorithm, we cycle through our examples
 - If the output of the network is correct, no changes are made
 - If there is an error, weights are adjusted to reduce the error

- The trick is to assess the blame for the error and divide it among the contributing weights

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Backpropagation Intuition



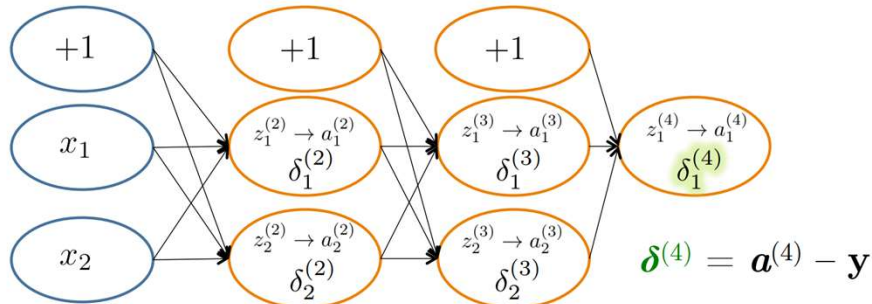
$\delta_j^{(l)}$ = “error” of node j in layer l

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

where $\text{cost}(\mathbf{x}_i) = -[y_i \log h_{\Theta}(\mathbf{x}_i) + (1 - y_i) \log(1 - h_{\Theta}(\mathbf{x}_i))]$

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Backpropagation Intuition



$\delta_j^{(l)}$ = “error” of node j in layer l

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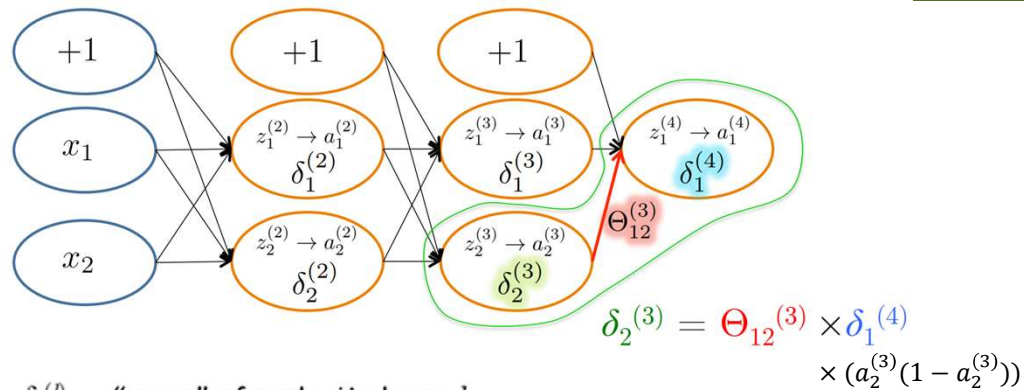
$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(4)} = g(\mathbf{z}^{(4)})$$

$$\frac{\partial \mathbf{a}}{\partial \mathbf{z}} = g'(\mathbf{z}) = g(\mathbf{z})(1 - g(\mathbf{z})) = \mathbf{a}(1 - \mathbf{a})$$

When g is logistic sigmoid

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Backpropagation Intuition



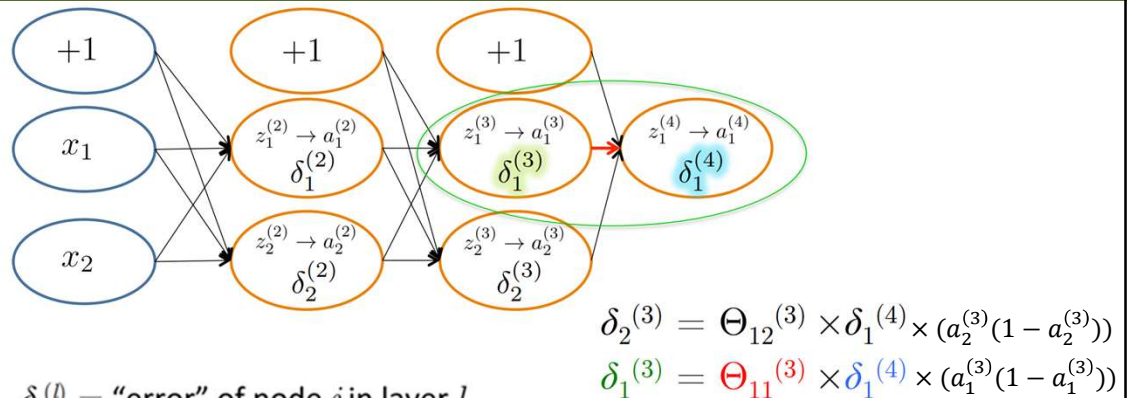
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Backpropagation Intuition



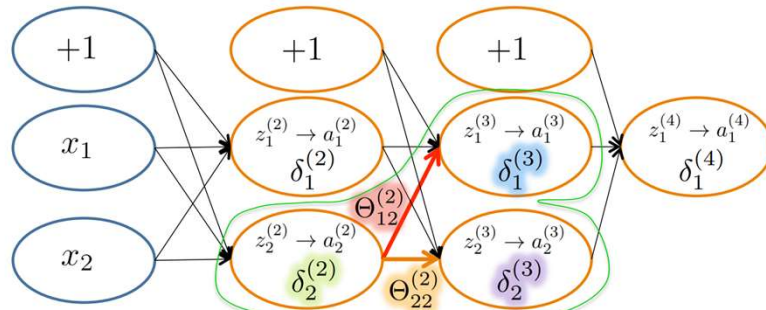
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Backpropagation Intuition



$$\delta_2^{(2)} = (\Theta_{12}^{(2)} \times \delta_1^{(3)} + \Theta_{22}^{(2)} \times \delta_2^{(3)}) \times (a_2^{(2)}(1 - a_2^{(2)}))$$

$\delta_j^{(l)}$ = “error” of node j in layer l

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

where $\text{cost}(\mathbf{x}_i) = -[y_i \log h_{\Theta}(\mathbf{x}_i) + (1 - y_i) \log(1 - h_{\Theta}(\mathbf{x}_i))]$

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Backpropagation Intuition: Gradient Computation



Let $\delta_j^{(l)}$ = “error” of node j in layer l

(#layers $L = 4$)

Backpropagation

- $\delta^{(4)} = \mathbf{a}^{(4)} - \mathbf{y}$
- $\delta^{(3)} = (\Theta^{(3)})^T \delta^{(4)} \cdot g'(\mathbf{z}^{(3)})$
- $\delta^{(2)} = (\Theta^{(2)})^T \delta^{(3)} \cdot g'(\mathbf{z}^{(2)})$
- (No $\delta^{(1)}$)

Element-wise product \cdot^*

$$g'(\mathbf{z}^{(3)}) = \mathbf{a}^{(3)} \cdot^* (1 - \mathbf{a}^{(3)})$$

$$g'(\mathbf{z}^{(2)}) = \mathbf{a}^{(2)} \cdot^* (1 - \mathbf{a}^{(2)})$$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)} \quad (\text{ignoring } \lambda; \text{ if } \lambda = 0)$$

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Training a Neural Network via Gradient Descent with Backprop



Given: training set $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

Initialize all $\Theta^{(l)}$ randomly (NOT to 0!)

Loop // each iteration is called an epoch

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)

For each training instance $(\mathbf{x}^{(s)}, y^{(s)})$:

Set $\mathbf{a}^{(1)} = \mathbf{x}^{(s)}$

Compute $\{\mathbf{a}^{(2)}, \dots, \mathbf{a}^{(L)}\}$ via forward propagation

Compute $\delta^{(L)} = \mathbf{a}^{(L)} - y^{(s)}$

Compute errors $\{\delta^{(L-1)}, \dots, \delta^{(2)}\}$

Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n} \Delta_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n} \Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$

Until weights converge or max #epochs is reached

Backpropagation

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Questions?

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