机器学习导论

第3章 神经网络
3.2 神经网络的反向传递算法

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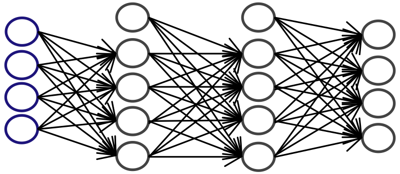
本节内容主要来自于吴恩达Coursera网课

神经网络的代价函数

Logistic regression (Cross Entropy):



$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)}\log h_\theta(x^{(i)}) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right) + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Neural network (Cross Entropy & Regularization):

$$h_\Theta(x) \in \mathbb{R}^K \qquad h_\Theta(x))_i = i^{th} \text{ output}$$

$$J(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}\left(y_k^{(i)}\log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)})\log((1-h_\Theta(x^{(i)}))_k\right)$$

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

与基于平方误差的损失函数的对比

基于交叉熵的损失函数：

$$J(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}\left(y_k^{(i)}\log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)})\log((1-h_\Theta(x^{(i)}))_k\right)$$

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

基于平方误差的损失函数：（基于教材P102公式 (5.4) ）

$$E_k = \frac{1}{2}\sum_{k=1}^{m}\sum_{j=1}^{l}(\hat{y}_j^k - y_j^k)^2$$

神经网络损失函数的优化

BP算法 (BackPropagation Algorithm)

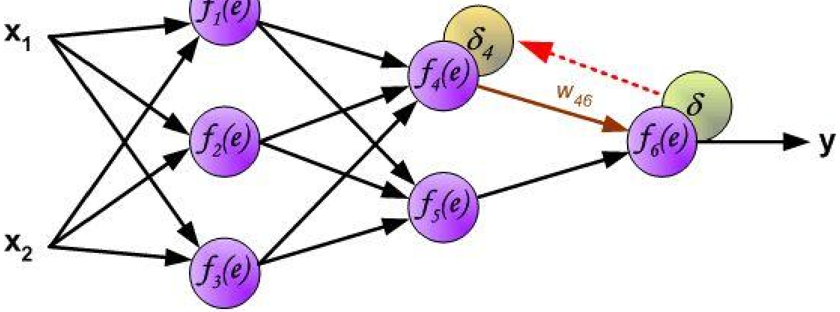
- 误差反向传播算法：用于多层前馈网络的训练
- [Werbos, 1974]， [Rumelhart, Hinton et al., 1986]

算法价值在于：最终层的误差如何分解到每个节点的输出上，尤其是隐含层的节点输出上。

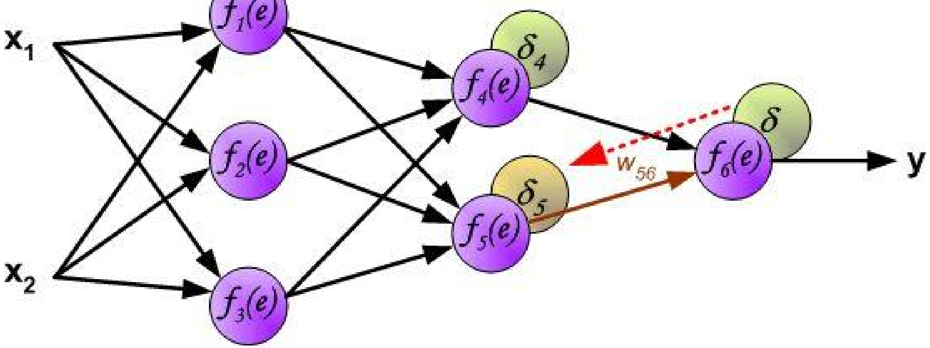
- 将误差分解到各节点的输出上，才能够通过梯度调整各节点的输入权重。

误差的反向传递示意

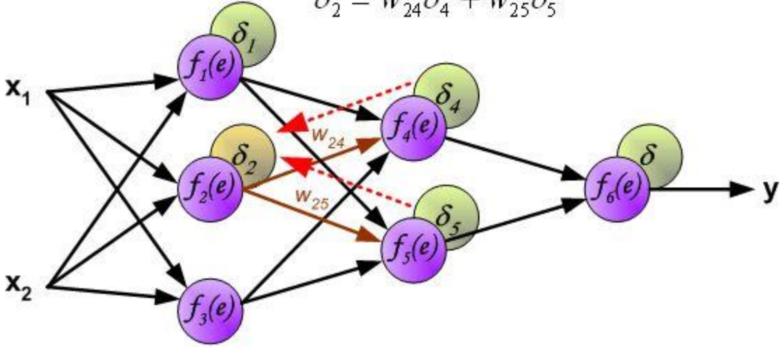
$$\delta_4 = w_{46}\delta$$



$$\delta_5 = w_{56}\delta$$



$$\delta_2 = w_{24}\delta_4 + w_{25}\delta_5$$



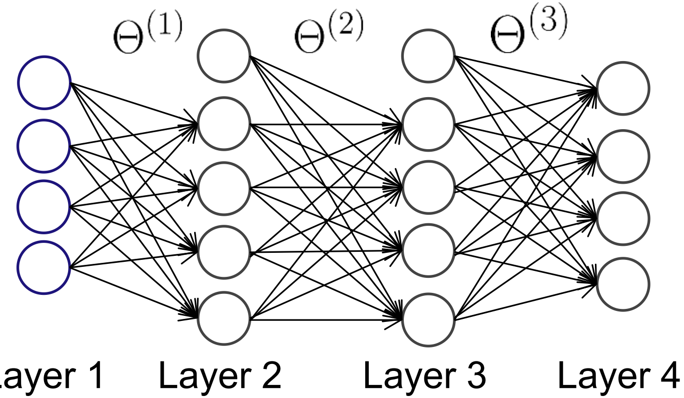
梯度的计算(基于交叉熵)

$$J(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}\left(y_k^{(i)}\log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)})\log((1-h_\Theta(x^{(i)}))_k\right)$$
$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_j^{(l)})^2$$

$$\min_\Theta J(\Theta)$$

Need code to compute:

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



$z^{(2)} = \Theta^{(1)}a^{(1)}$ $z^{(3)} = \Theta^{(2)}a^{(2)}$ $z^{(4)} = \Theta^{(3)}a^{(3)}$

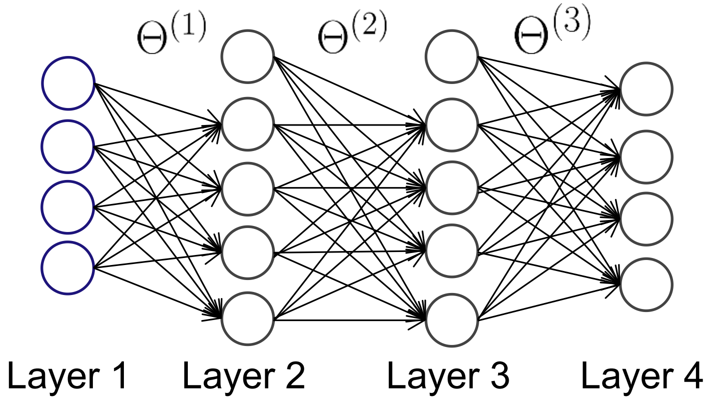
$a^{(1)} = x$ $a^{(2)} = g(z^{(2)})$ $a^{(3)} = g(z^{(3)})$ $a^{(4)} = g(z^{(4)}) = h_\Theta(\boldsymbol{x})$

$(\text{add } a_0^{(1)})$ $(\text{add } a_0^{(2)})$ $(\text{add } a_0^{(3)})$

梯度计算: 误差(可复用)、误差的反向传递

Intuition: $\delta_j^{(l)} =$ "error" of node j in layer l .

损失函数相对于模型参数(网络连接权重)的梯度使用链式求导法计算



$z^{(2)} = \Theta^{(1)} a^{(1)}$ $z^{(3)} = \Theta^{(2)} a^{(2)}$ $z^{(4)} = \Theta^{(3)} a^{(3)}$

$a^{(1)} = x$ $a^{(2)} = g(z^{(2)})$ $a^{(3)} = g(z^{(3)})$ $a^{(4)} = g(z^{(4)}) = h_\Theta(\boldsymbol{x})$

$(\text{add } a_0^{(1)})$ $(\text{add } a_0^{(2)})$ $(\text{add } a_0^{(3)})$

$$\delta^{(4)} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}}$$

$$\delta^{(3)} = \underbrace{\frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}}}_{\delta^{(4)}} \frac{\partial z^{(4)}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}}$$

$$\delta^{(2)} = \underbrace{\frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \cdot \frac{\partial z^{(4)}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}}}_{\delta^{(3)}} \cdot \frac{\partial z^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial z^{(2)}}$$

梯度计算：基于误差的梯度计算

对于一个样本和一个输出层节点的误差相对于模型参数的梯度：

$$\frac{\partial J}{\partial \Theta^{(2)}} = \underbrace{\frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} \cdot \frac{\partial z^{(4)}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}}}_{\delta^{(3)}} \cdot \frac{\partial z^{(3)}}{\partial \Theta^{(2)}}$$

$$\Theta_{ij}^{(2)}(t+1) = \Theta_{ij}^{(2)}(t) - \alpha \times \frac{\partial J}{\partial \Theta_{ij}^{(2)}}$$

BackPropagation算法的关键计算：

$$\delta^{(4)} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} = a^{(4)} - y$$

$$\frac{\partial J}{\partial a^{(4)}} = \frac{a^{(4)} - y^{(i)}}{a^{(4)}(1 - a^{(4)})}$$

求导见下一页

$$\frac{\partial a^{(4)}}{\partial z^{(4)}} = a^{(4)}(1 - a^{(4)})$$

求导见下下页

GOAL: $\delta^{(4)} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} = a^{(4)} - y$

$$
\begin{aligned}
\frac{\partial J}{\partial a^{(4)}} &= \frac{\partial}{\partial a^{(4)}} \left[- \left(y^{(i)} \mathbf{log} a^{(4)} + (1 - y^{(i)}) \mathbf{log} (1 - a^{(4)}) \right) \right] \\
&= -y^{(i)} \frac{1}{a^{(4)}} - (1 - y^{(i)}) \cdot \frac{1}{1 - a^{(4)}} \cdot (-1) \\
&= -\frac{y^{(i)}}{a^{(4)}} + \frac{1 - y^{(i)}}{1 - a^{(4)}} \\
&= \frac{-y^{(i)} + y^{(i)} a^{(4)} + a^{(4)} - a^{(4)} y^{(i)}}{a^{(4)}(1 - a^{(4)})} \\
&= \frac{a^{(4)} - y^{(i)}}{a^{(4)}(1 - a^{(4)})}
\end{aligned}
$$

GOAL: $\delta^{(4)} = \frac{\partial J}{\partial a^{(4)}} \frac{\partial a^{(4)}}{\partial z^{(4)}} = a^{(4)} - y$

$$\begin{aligned}
\frac{\partial a^{(4)}}{\partial z^{(4)}} &= \frac{\partial}{\partial z^{(4)}} \left(\frac{1}{1 + e^{-z^{(4)}}} \right) \\
&= \frac{-1}{(1 + e^{-z^{(4)}})^2} \cdot \frac{\partial}{\partial z^{(4)}} (e^{-z^{(4)}}) \\
&= \frac{-1}{(1 + e^{-z^{(4)}})^2} \cdot e^{-z^{(4)}} \cdot (-1) \\
&= \frac{1}{1 + e^{-z^{(4)}}} \cdot \frac{e^{-z^{(4)}}}{1 + e^{-z^{(4)}}} \\
&= a^{(4)}(1 - a^{(4)})
\end{aligned}$$

对于sigmoid函数

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

其导数为：

$$g'(z) = g(z)(1 - g(z))$$

汇总整理

$$\frac{\partial J}{\partial \Theta^{(2)}} = \underline{\frac{\partial J}{\partial a^{(4)}}\frac{\partial a^{(4)}}{\partial z^{(4)}} \cdot \frac{\partial z^{(4)}}{\partial a^{(3)}}\frac{\partial a^{(3)}}{\partial z^{(3)}}} \cdot \frac{\partial z^{(3)}}{\partial \Theta^{(2)}}$$

$$\delta^{(4)} = \frac{\partial J}{\partial a^{(4)}}\frac{\partial a^{(4)}}{\partial z^{(4)}} = a^{(4)} - y$$

$$\frac{\partial J}{\partial \Theta^{(3)}} = \delta^{(4)} \bullet \frac{\partial z^{(4)}}{\partial \Theta^{(3)}} = \delta^{(4)} \bullet a^{(3)}$$

$$\delta^{(3)} = \frac{\partial J}{\partial a^{(4)}}\frac{\partial a^{(4)}}{\partial z^{(4)}}\frac{\partial z^{(4)}}{\partial a^{(3)}}\frac{\partial a^{(3)}}{\partial z^{(3)}}$$

$$= (\Theta^{(3)})^T \times \delta^{(4)} \cdot * g'(z^{(3)})$$

$$\frac{\partial J}{\partial \Theta^{(2)}} = \delta^{(3)} \bullet \frac{\partial z^{(3)}}{\partial \Theta^{(2)}} = \delta^{(3)} \bullet a^{(2)}$$

$$\frac{\partial J}{\partial \Theta^{(1)}} = \delta^{(2)} \cdot \frac{\partial z^{(2)}}{\partial \Theta^{(1)}} = \delta^{(2)} \cdot a^{(1)}$$

$$\delta^{(2)} = \frac{\partial J}{\partial a^{(4)}}\frac{\partial a^{(4)}}{\partial z^{(4)}} \cdot \frac{\partial z^{(4)}}{\partial a^{(3)}}\frac{\partial a^{(3)}}{\partial z^{(3)}} \cdot \frac{\partial z^{(3)}}{\partial a^{(2)}}\frac{\partial a^{(2)}}{\partial z^{(2)}}$$

$$= (\Theta^{(2)})^T \times \delta^{(3)} \cdot * g'(z^{(2)})$$

Backpropagation算法中的梯度计算

Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$

1. Set $\triangle_{ij}^{(l)} = 0$ (for all l, i, j).
2. For $i = 1$ to m

   Set $a^{(1)} = x^{(i)}$

   Perform forward propagation to compute $a^{(l)}$ for $l = 2, 3, \ldots, L$

   Using $y^{(i)}$, compute $\delta^{(L)} = a^{(L)} - y^{(i)}$

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

   $\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ 为每个样本累计误差delta

3. $$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)} = \begin{cases} \frac{1}{m}\Delta_{ij}^{(l)} + \frac{\lambda}{m}\theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{m}\Delta_{ij}^{(l)} & \text{if } j = 0 \end{cases}$$

Backpropagation Algorithm (by Gradient Descent)

Input: Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$

Learning Rate: η

Initialize the weights of links (`randInitializeWeights.m`)

repeat

for all $(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})$ in training set

Compute all gradients $\dfrac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}}$

Update all link weights $\Theta_{ij}^{(l)}(t+1) := \Theta_{ij}^{(l)}(t) - \eta \dfrac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}}$

end

until converge or reach maximal iterations

Backpropagation算法（文字版）

- 输入与前向传播：

1. Set the input layer's values ($a^{(1)}$) to the t-th training example $x^{(t)}$. Perform a feedforward pass (Figure 2), computing the activations ($z^{(2)}$, $a^{(2)}, z^{(3)}, a^{(3)}$) for layers 2 and 3.

- 输出层误差计算：

2. For each output unit k in layer 3 (the output layer), set

$$\delta_k^{(3)} = (a_k^{(3)} - y_k),$$

- 面向隐含层的误差反向传播：

3. For the hidden layer $l = 2$, set

$$\delta^{(2)} = \left(\Theta^{(2)}\right)^T \delta^{(3)} .* g'(z^{(2)})$$

Backpropagation算法（文字版）

- 使用误差梯度计算模型参数梯度

4. Accumulate the gradient from this example using the following formula.

$$\Delta^{(l)} = \Delta^{(l)} + \delta^{(l+1)}(a^{(l)})^T$$

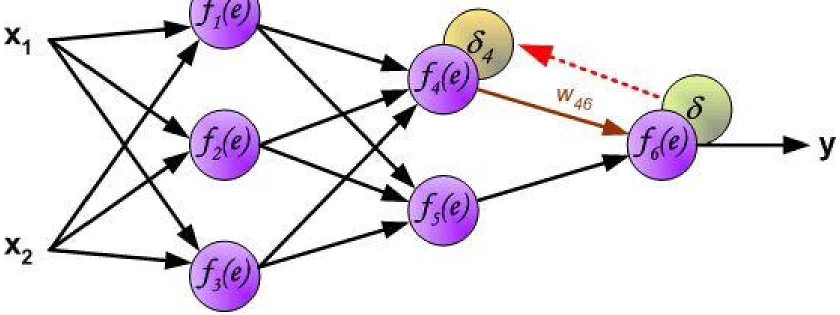
5. Obtain the (unregularized) gradient for the neural network cost function by dividing the accumulated gradients by $\frac{1}{m}$:

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)} = \frac{1}{m} \Delta_{ij}^{(l)}$$

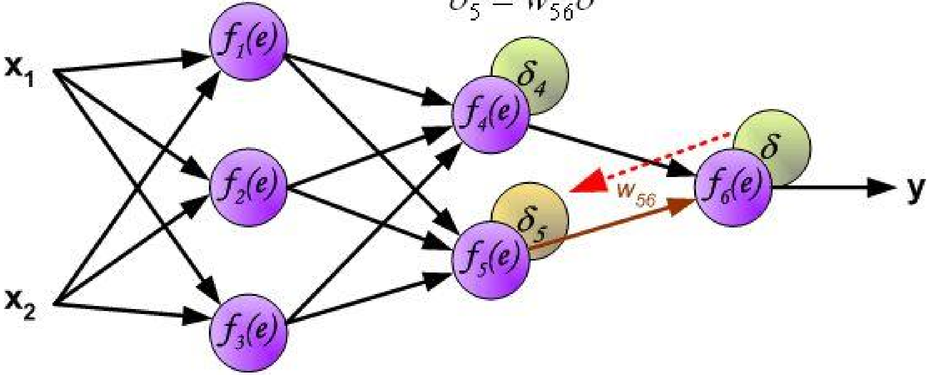
- 使用梯度下降法或梯度共轭法优化模型参数

误差的反向传递示意

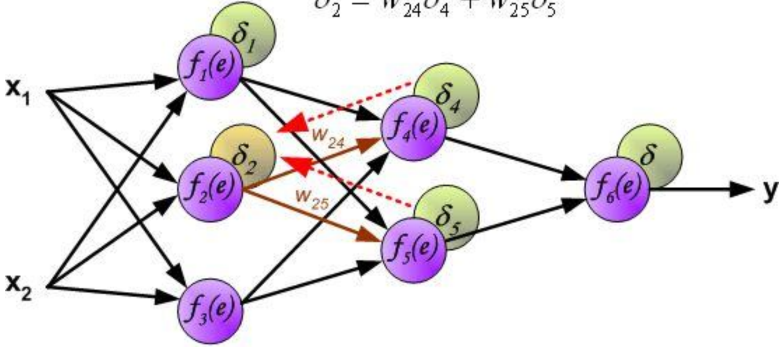
$$\delta_4 = w_{46}\delta$$



$$\delta_5 = w_{56}\delta$$



$$\delta_2 = w_{24}\delta_4 + w_{25}\delta_5$$



问题：如果将损失函数更换为误差平方和

$$E = \frac{1}{2}\sum_{i=1}^{m}\left(a^{(4)} - y^{(i)}\right)^2$$

请求解反向传递误差和对应的梯度

$$\delta = \frac{\partial E}{\partial z^{(4)}} = \frac{\partial E}{\partial a^{(4)}}\frac{\partial a^{(4)}}{\partial z^{(4)}} \qquad \frac{\partial E}{\partial \Theta_{ij}^{(3)}} = \delta^{(4)}\frac{\partial z^{(4)}}{\partial \Theta_{ij}^{(3)}}$$

请参见周志华《机器学习》第5章

总结

- 代价函数（也可看成误差）+ 梯度下降
- BP算法（梯度下降）
  - 如何将分类器的误差（即输出层节点的误差）分解到隐含层节点的输出上
  - 用隐含层节点的误差求解各输入（连接）的权重
- 代价函数
  - 基于交叉熵 或 误差平方和 的代价函数