



Machine Learning

Neural Networks: Learning

Cost function

Neural Network (Classification)



$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})\}$$

$L =$ total no. of layers in network

$s_l =$ no. of units (not counting bias unit) in layer l

Binary classification

$y = 0$ or 1

1 output unit

Multi-class classification (K classes)

$y \in \mathbb{R}^K$ E.g. $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$
pedestrian car motorcycle truck

K output units

Cost function

Logistic regression:

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

Neural network:

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

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



Machine Learning

Neural Networks: Learning

Backpropagation algorithm

Gradient computation

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

$$\rightarrow \min_{\Theta} J(\Theta)$$

Need code to compute:

$$\rightarrow - \underline{J(\Theta)}$$

$$\rightarrow - \underline{\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)} \quad \leftarrow$$

$$\Theta_{ij}^{(l)} \in \mathbb{R}$$

Gradient computation

Given one training example (x, y) :

Forward propagation:

$$\begin{aligned} &\rightarrow \underline{a^{(1)}} = \underline{x} \\ &\rightarrow z^{(2)} = \Theta^{(1)} a^{(1)} \\ &\rightarrow a^{(2)} = g(z^{(2)}) \quad (\text{add } \underline{a_0^{(2)}}) \\ &\rightarrow z^{(3)} = \Theta^{(2)} a^{(2)} \\ &\rightarrow a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)}) \\ &\rightarrow z^{(4)} = \Theta^{(3)} a^{(3)} \\ &\rightarrow \underline{a^{(4)}} = \underline{h_{\Theta}(x)} = g(z^{(4)}) \end{aligned}$$



Gradient computation: Backpropagation algorithm

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

For each output unit (layer $L = 4$)

$$\delta_j^{(4)} = a_j^{(4)} - y_j$$

(handwritten note: $(\text{activation})_j$ $\delta_j^{(4)} = a_j^{(4)} - y_j$)



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

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

(handwritten notes for $g'(z)$):
 $a^{(3)} \cdot (1 - a^{(3)})$
 $a^{(2)} \cdot (1 - a^{(2)})$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$

(ignoring λ ; if $\lambda = 0$)

Backpropagation algorithm

THIS SHOULD BE $\Theta^{(L+1)}$

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

Set $\Delta_{ij}^{(l)} = 0$ (for all l, i, j).

(used to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$)

For $i = 1$ to $m \leftarrow (\underline{x^{(i)}}, \underline{y^{(i)}})$

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

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

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

→ Compute $\underline{\delta^{(L-1)}}, \underline{\delta^{(L-2)}}, \dots, \underline{\delta^{(2)}}$ ~~set~~

→ $\underline{\Delta_{ij}^{(l)}} := \underline{\Delta_{ij}^{(l)}} + \underline{a_j^{(l)}} \underline{\delta_i^{(l+1)}}$ ← Δ

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

→ $\underline{D_{ij}^{(l)}} := \frac{1}{m} \underline{\Delta_{ij}^{(l)}} + \underline{\lambda \Theta_{ij}^{(l)}}$ if $\underline{j \neq 0}$

→ $\underline{D_{ij}^{(l)}} := \frac{1}{m} \underline{\Delta_{ij}^{(l)}}$ if $\underline{j = 0}$

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



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Backpropagation intuition

Forward Propagation



Forward Propagation



What is backpropagation doing?

$$J(\Theta) = -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log(h_{\Theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - (h_{\Theta}(x^{(i)}))) \right] + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{ji}^{(l)})^2$$

(x⁽ⁱ⁾, y⁽ⁱ⁾)

Focusing on a single example x⁽ⁱ⁾, y⁽ⁱ⁾, the case of 1 output unit, and ignoring regularization (λ = 0),

Note: Mistake on lecture, it is supposed to be 1-h(x).

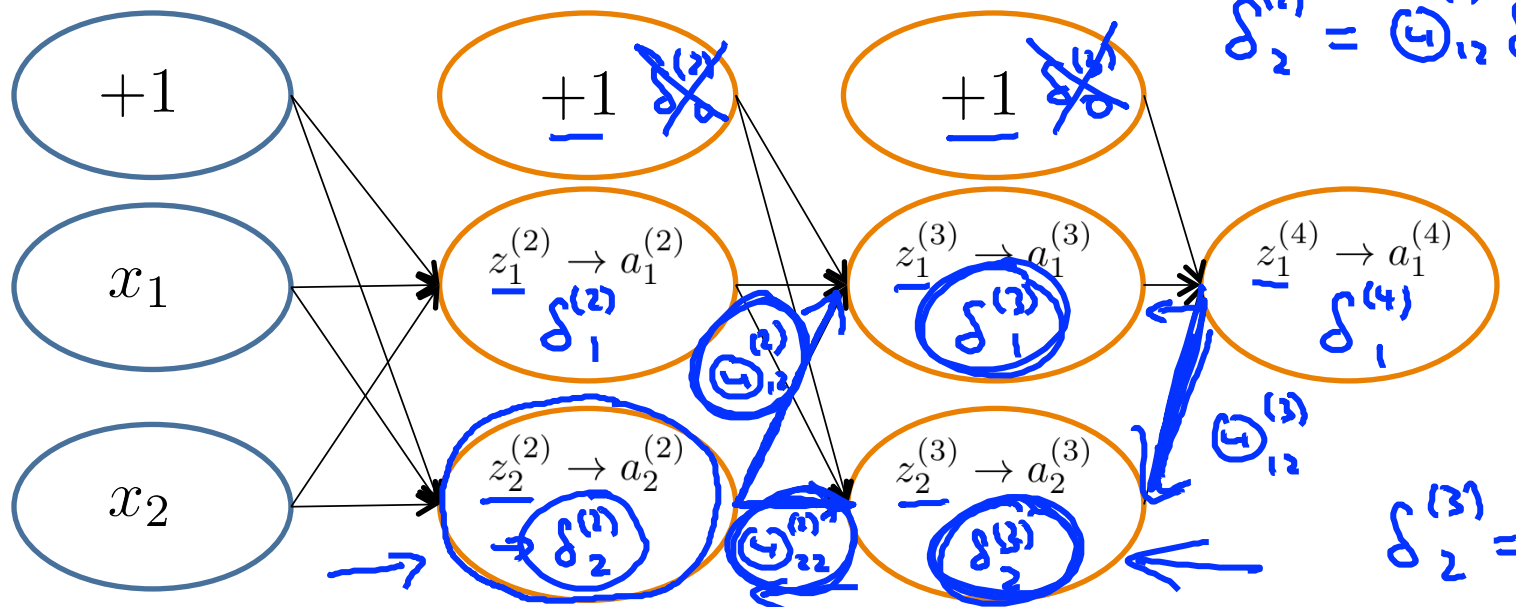
$$\text{cost}(i) = y^{(i)} \log h_{\Theta}(x^{(i)}) + (1 - y^{(i)}) \log h_{\Theta}(x^{(i)})$$

(Think of cost(i) ≈ (h_Θ(x⁽ⁱ⁾) - y⁽ⁱ⁾)²)

I.e. how well is the network doing on example i?

NOTE THAT THIS WEIGHTED SUM IS TO GIVE SOME INTUITION BEHIND WHAT IS GOING ON WITH DELTAS. IN REALITY YOU MUST CALCULATE THE PARTIAL DERIVATIVE OF COST WITH RESPECT TO z_j .

Forward Propagation



$$\delta_1^{(4)} = y^{(i)} - a_1^{(4)}$$

$$\delta_2^{(4)} = w_{12}^{(4)} \delta_1^{(3)} + w_{22}^{(4)} \delta_2^{(3)}$$

$\rightarrow \delta_j^{(l)} = \text{"error" of cost for } a_j^{(l)} \text{ (unit } j \text{ in layer } l).$

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(i)$ (for $j \geq 0$), where

$$\text{cost}(i) = y^{(i)} \log h_{\Theta}(x^{(i)}) + (1 - y^{(i)}) \log h_{\Theta}(x^{(i)})$$



Machine Learning

Neural Networks: Learning

Implementation
note: Unrolling
parameters

Advanced optimization

```
function [jVal, gradient] = costFunction(theta)  
...  
optTheta = fminunc(@costFunction, initialTheta, options)
```

Handwritten annotations: \mathbb{R}^{n+1} (under gradient), \mathbb{R}^{n+1} (vectors) (under theta), and an arrow pointing to initialTheta.

Neural Network (L=4):

→ $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ - matrices (Theta1, Theta2, Theta3)

→ $D^{(1)}$, $D^{(2)}$, $D^{(3)}$ - matrices (D1, D2, D3)

“Unroll” into vectors

Example

$$s_1 = 10, s_2 = 10, s_3 = 1$$

$$\rightarrow \Theta^{(1)} \in \mathbb{R}^{10 \times 11}, \Theta^{(2)} \in \mathbb{R}^{10 \times 11}, \Theta^{(3)} \in \mathbb{R}^{1 \times 11}$$

$$\rightarrow D^{(1)} \in \mathbb{R}^{10 \times 11}, D^{(2)} \in \mathbb{R}^{10 \times 11}, D^{(3)} \in \mathbb{R}^{1 \times 11}$$



$$\rightarrow \text{thetaVec} = [\text{Theta1}(:); \text{Theta2}(:); \text{Theta3}(:)] ;$$

$$\rightarrow \text{DVec} = [\text{D1}(:); \text{D2}(:); \text{D3}(:)] ;$$

$$\text{Theta1} = \text{reshape}(\text{thetaVec}(1:110), 10, 11) ;$$

$$\rightarrow \text{Theta2} = \text{reshape}(\text{thetaVec}(111:220), 10, 11) ;$$

$$\rightarrow \text{Theta3} = \text{reshape}(\text{thetaVec}(221:231), 1, 11) ;$$

Learning Algorithm

- Have initial parameters $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$.
- Unroll to get `initialTheta` to pass to
- `fminunc(@costFunction, initialTheta, options)`

```
function [jval, gradientVec] = costFunction(thetaVec)
```

- From thetaVec, get $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$. *reshape*
- Use forward prop/back prop to compute $D^{(1)}, D^{(2)}, D^{(3)}$ $J(\Theta)$
and $D^{(1)}, D^{(2)}, D^{(3)}$
Unroll _____ to get gradientVec.

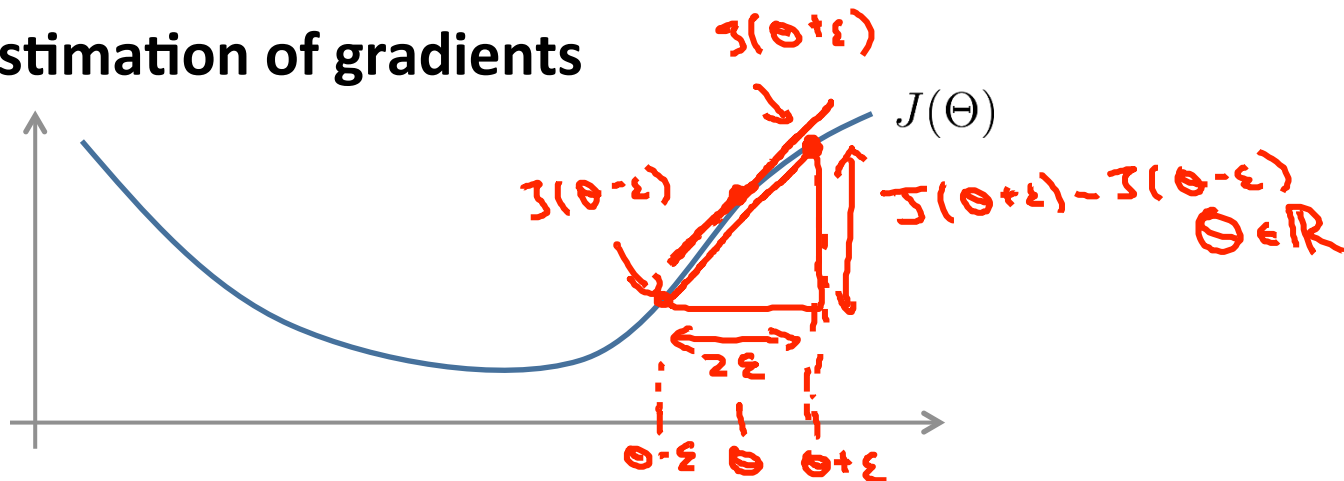


Machine Learning

Neural Networks: Learning

Gradient checking

Numerical estimation of gradients



$$\frac{d}{d\Theta} J(\Theta) \approx$$

$$\frac{J(\Theta + \epsilon) - J(\Theta - \epsilon)}{2\epsilon}$$

$\epsilon = 10^{-4}$

~~$$\frac{J(\Theta + \epsilon) - J(\Theta)}{\epsilon}$$~~

Implement: gradApprox = (J(theta + EPSILON) - J(theta - EPSILON)) / (2*EPSILON)

Parameter vector θ

→ $\theta \in \mathbb{R}^n$ (E.g. θ is “unrolled” version of $\underline{\Theta^{(1)}}$, $\underline{\Theta^{(2)}}$, $\underline{\Theta^{(3)}}$)

→ $\theta = [\theta_1, \theta_2, \theta_3, \dots, \theta_n]$

→ $\frac{\partial}{\partial \theta_1} J(\theta) \approx \frac{J(\theta_1 + \epsilon, \theta_2, \theta_3, \dots, \theta_n) - J(\theta_1 - \epsilon, \theta_2, \theta_3, \dots, \theta_n)}{2\epsilon}$

→ $\frac{\partial}{\partial \theta_2} J(\theta) \approx \frac{J(\theta_1, \theta_2 + \epsilon, \theta_3, \dots, \theta_n) - J(\theta_1, \theta_2 - \epsilon, \theta_3, \dots, \theta_n)}{2\epsilon}$

⋮

→ $\frac{\partial}{\partial \theta_n} J(\theta) \approx \frac{J(\theta_1, \theta_2, \theta_3, \dots, \theta_n + \epsilon) - J(\theta_1, \theta_2, \theta_3, \dots, \theta_n - \epsilon)}{2\epsilon}$

```

for i = 1:n, ←
    [
        thetaPlus = theta;
        thetaPlus(i) = thetaPlus(i) + EPSILON;
        thetaMinus = theta;
        thetaMinus(i) = thetaMinus(i) - EPSILON;
        gradApprox(i) = (J(thetaPlus) - J(thetaMinus))
                        / (2*EPSILON);
    ]
end;

```

$\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_i + \epsilon \\ \vdots \\ \theta_n \end{bmatrix} \rightarrow \theta_i - \epsilon$


$\frac{2}{2\theta_i} J(\theta).$

Check that gradApprox \approx DVec ←

↑
From back prop.

Implementation Note:

- - Implement backprop to compute DVec (unrolled $D^{(1)}$, $D^{(2)}$, $D^{(3)}$).

- - Implement numerical gradient check to compute gradApprox.
- - Make sure they give similar values.
- - Turn off gradient checking. Using backprop code for learning.


Important:

- - Be sure to disable your gradient checking code before training your classifier. If you run numerical gradient computation on every iteration of gradient descent (or in the inner loop of `costFunction(...)`) your code will be very slow.



Machine Learning

Neural Networks: Learning

Random initialization

Initial value of Θ

For gradient descent and advanced optimization method, need initial value for Θ .

```
optTheta = fminunc(@costFunction,  
    initialTheta, options)
```

Consider gradient descent

Set initialTheta = zeros(n,1) ?

Zero initialization



$$\rightarrow \Theta_{ij}^{(l)} = 0 \text{ for all } i, j, l.$$

$$a_1^{(2)} = a_2^{(2)} \quad \text{Also} \quad \delta_1^{(2)} = \delta_2^{(2)}$$

$$\frac{\partial}{\partial \Theta_{0,1}^{(1)}} J(\Theta) = \frac{\partial}{\partial \Theta_{0,2}^{(1)}} J(\Theta)$$

$$\underline{\Theta_{0,1}^{(1)}} = \underline{\Theta_{0,2}^{(1)}}$$

After each update, parameters corresponding to inputs going into each of two hidden units are identical.

$$\underline{a_1^{(2)} = a_2^{(2)}}$$

Random initialization: Symmetry breaking

→ Initialize each $\Theta_{ij}^{(l)}$ to a random value in $[-\epsilon, \epsilon]$
(i.e. $-\epsilon \leq \Theta_{ij}^{(l)} \leq \epsilon$)

E.g.

Random 10x11 matrix (betw. 0 and 1)

→ `Theta1 = rand(10, 11) * (2 * INIT_EPSILON) - INIT_EPSILON;` $[-\epsilon, \epsilon]$

→ `Theta2 = rand(1, 11) * (2 * INIT_EPSILON) - INIT_EPSILON;`



Machine Learning

Neural Networks: Learning

Putting it together

Training a neural network

Pick a network architecture (connectivity pattern between neurons)



→ No. of input units: Dimension of features $x^{(i)}$

→ No. of output units: Number of classes

Reasonable default: 1 hidden layer, or if >1 hidden layer, have same no. of hidden units in every layer (usually the more the better)

$y \in \{1, 2, 3, \dots, 10\}$
 ~~$y = 5$~~

$y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$

Training a neural network

- 1. Randomly initialize weights
- 2. Implement forward propagation to get $h_{\Theta}(x^{(i)})$ for any $x^{(i)}$
- 3. Implement code to compute cost function $J(\Theta)$
- 4. Implement backprop to compute partial derivatives $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$

→ for $i = 1:m$ { $(x^{(1)}, y^{(1)})$ $(x^{(2)}, y^{(2)})$, ..., $(x^{(m)}, y^{(m)})$

→ Perform forward propagation and backpropagation using example $(x^{(i)}, y^{(i)})$

(Get activations $a^{(l)}$ and delta terms $\delta^{(l)}$ for $l = 2, \dots, L$).

→ $\Delta^{(2)} := \Delta^{(2)} + \delta^{(L)} (a^{(2)})^T$

...

}

compute $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$.



Training a neural network

- 5. Use gradient checking to compare $\frac{\partial}{\partial \Theta_{ik}^{(l)}} J(\Theta)$ computed using backpropagation vs. using numerical estimate of gradient of $J(\Theta)$.
- Then disable gradient checking code.
- 6. Use gradient descent or advanced optimization method with backpropagation to try to minimize $J(\Theta)$ as a function of parameters Θ

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

$J(\Theta)$ — non-convex.





Machine Learning

Neural Networks: Learning

Backpropagation
example: Autonomous
driving (optional)

