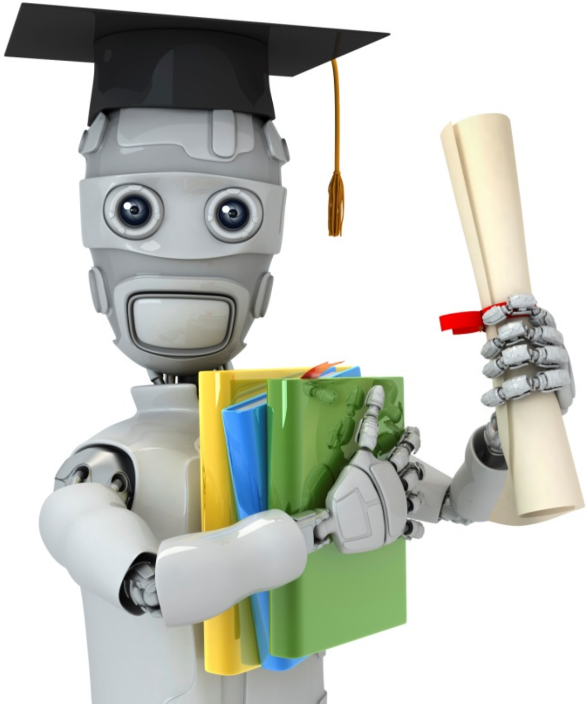
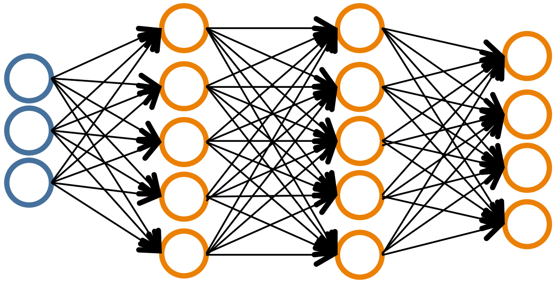


Machine Learning

Neural Networks: Learning

Cost function

Neural Network (Classification)



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

$L =$ total no. of layers in network

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

Binary classification

$y = 0 \text{ or } 1$

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:

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

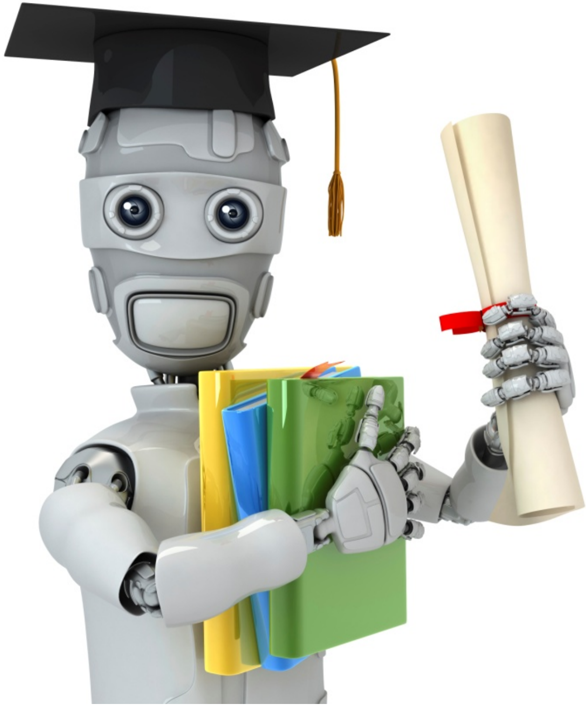
Neural network:

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

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

h(x) is a k-dimensional vector

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



Neural Networks: Learning

Backpropagation algorithm

Machine Learning

Gradient computation

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

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

l表示第l層,
i表示本層第i個node
j表示下一層第j個node

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

Need code to compute:

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

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

Gradient computation

Given one training example (x, y):

Forward propagation:

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

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

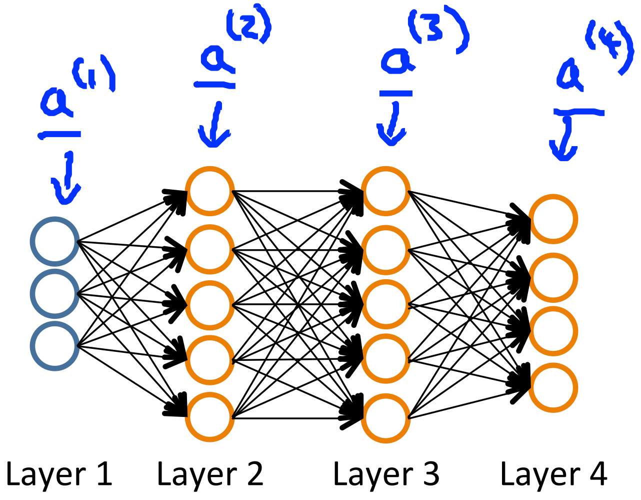
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$

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

$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$

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

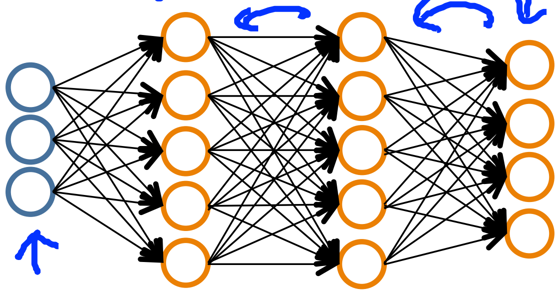
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



Gradient computation: Backpropagation algorithm

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

$\delta^{(2)}$ $a_j^{(l)}$ $\delta^{(3)}$ $\delta^{(4)}$



For each output unit (layer L = 4)

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

$(h_\Theta(x))_j$ $\quad \delta^{(4)} = a^{(4)} - y$

Theta 3 transpose delta 4, that's a vector; g prime z3 that's also a vector

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

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

$a^{(3)} .* (1 - a^{(3)})$ (這就是g')

$a^{(2)} .* (1 - a^{(2)})$

(No $\delta^{(1)}$)

we're sort of back propagating the errors from the output layer to layer 3 to their to hence the name back complication.

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

(ignoring λ; if $\lambda = 0$)

大寫的Delta可以理解為跟cost的偏導成正比

It's possible to prove that if you ignore regularization then the partial derivative terms you want are exactly given by the activations and these delta terms. We'll fix this detail later about the regularization term.

Backpropagation algorithm

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

Set $\triangle_{ij}^{(l)} = 0$ (for all l, i, j). (use to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$)

For $i = 1$ to m $(x^{(i)}, y^{(i)})$ l, i, j意思見p5

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

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

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

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

$\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

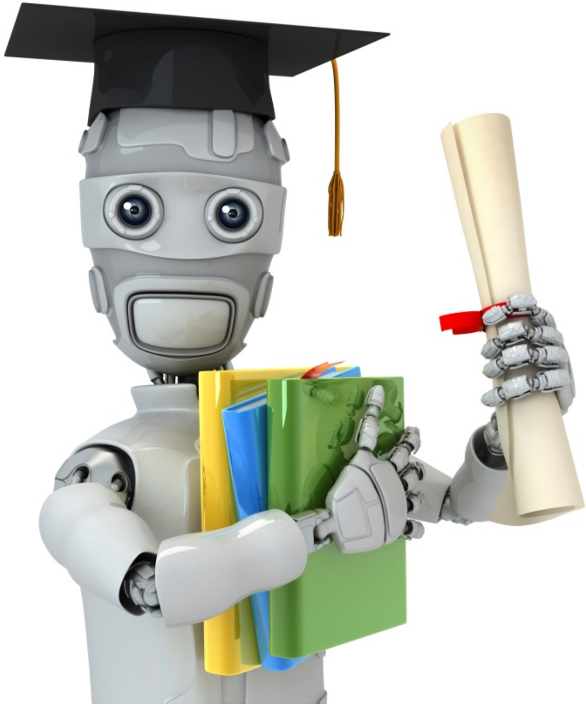
$\triangle^{(l)} := \triangle^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

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

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

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

these D terms, that is exactly the partial derivative of the cost function

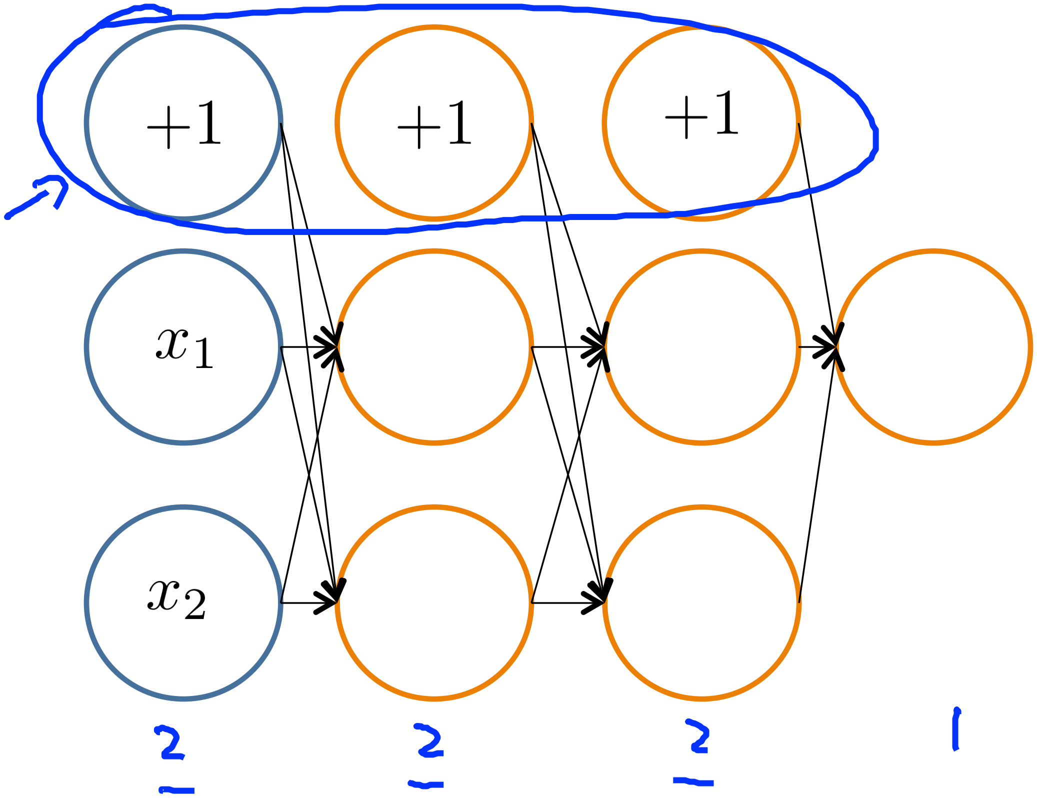


Neural Networks: Learning

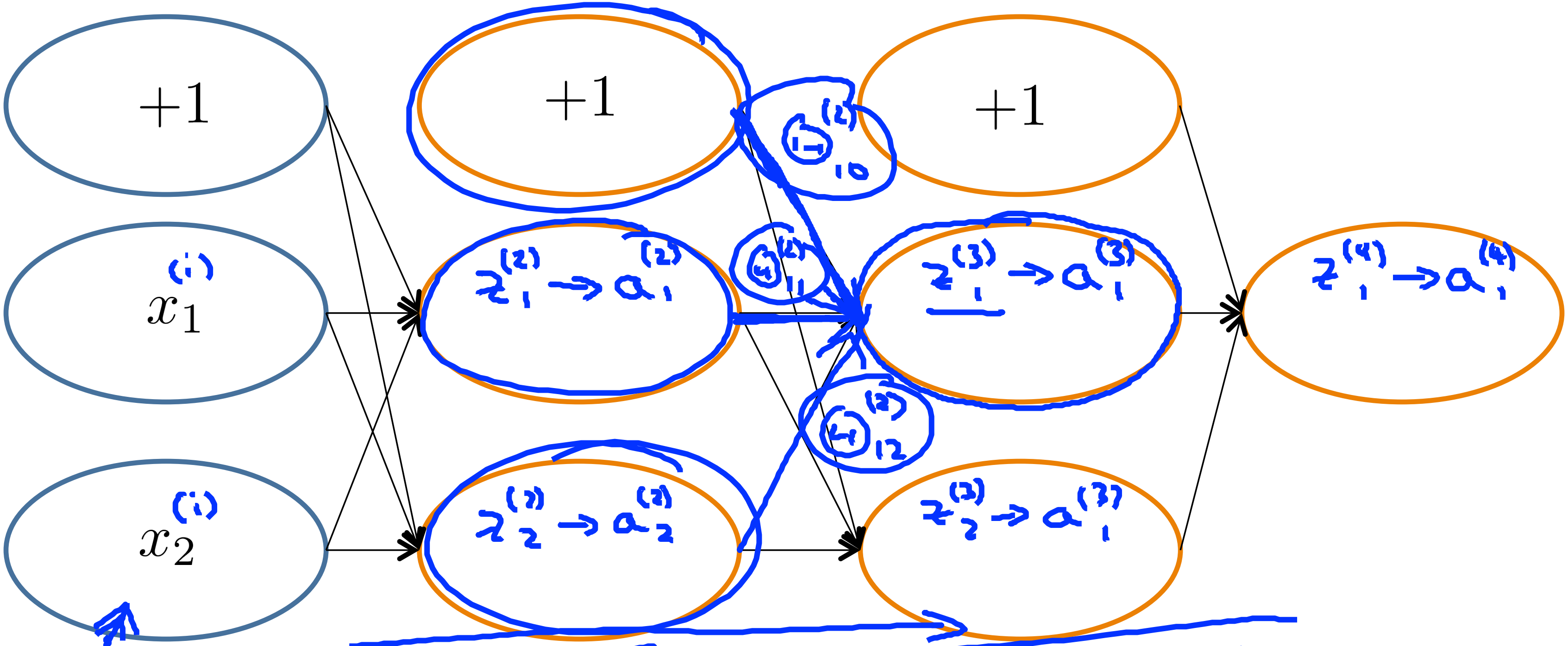
Backpropagation intuition

Machine Learning

Forward Propagation



Forward Propagation



$(x^{(i)}, y^{(i)})$

$$z_1^{(3)} = \Theta_{10}^{(2)} \times 1 + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} \cdot a_1^{(2)}$$

What is backpropagation doing?

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} \underbrace{y^{(i)} \log(h_\Theta(x^{(i)})) + (1-y^{(i)}) \log(1-(h_\Theta(x^{(i)})))}_{(x^{(i)},\, y^{(i)})}\right]$$

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

Focusing on a single example $x^{(i)}$, $y^{(i)}$, the case of 1 output unit, and ignoring regularization ($\lambda = 0$),

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

(Think of $\text{cost(i)} \approx (\boxed{h_\Theta(x^{(i)})} - \boxed{y^{(i)}})^2$)

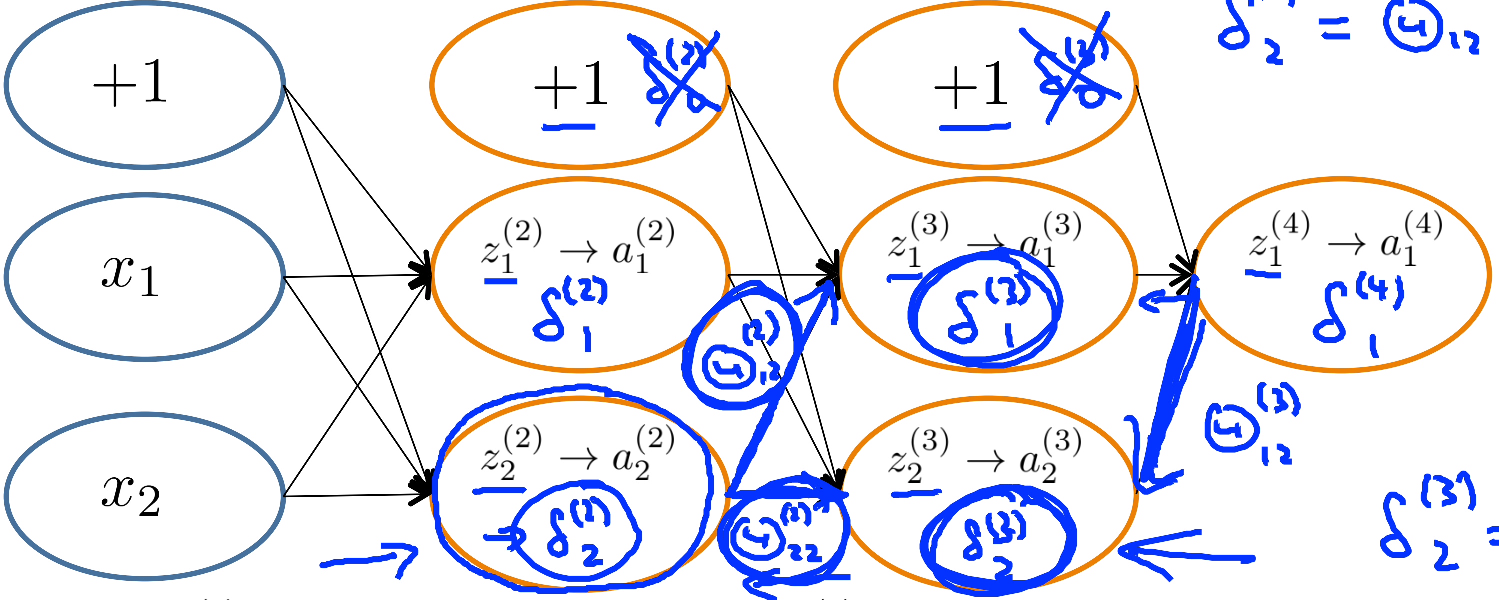
I.e. how well is the network doing on example i?

$y^{(i)}$

Forward Propagation

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

$\delta_2^{(2)} = \Theta_{12}^{(2)} \delta_1^{(3)} + \Theta_{12}^{(2)} \delta_2^{(3)}$

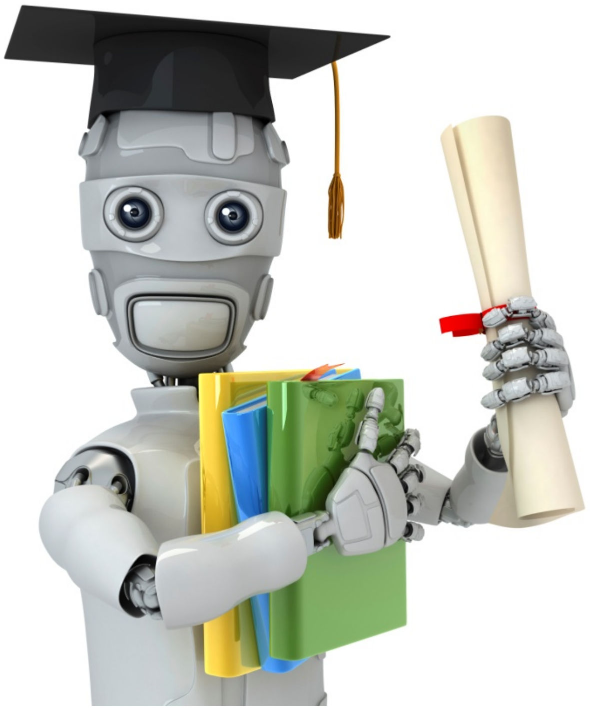


$\delta_2^{(3)} = \Theta_{12}^{(3)} \cdot \delta_1^{(4)}$.

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

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

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



Neural Networks: Learning

Implementation note: Unrolling parameters

Machine Learning

Advanced optimization

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

$\mathbb{R}^{n+1}$ $\mathbb{R}^{n+1}$ (vectors)

Neural Network (L=4):

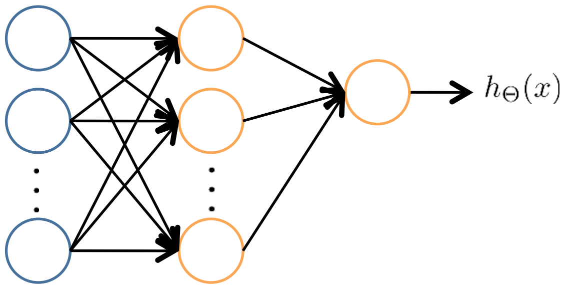
→ $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ - matrices (`Theta1`, `Theta2`, `Theta3`)

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

"Unroll" into vectors

Example

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



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

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

$\Theta^{(1)}$ $\Theta^{(2)}$ $\Theta^{(3)}$

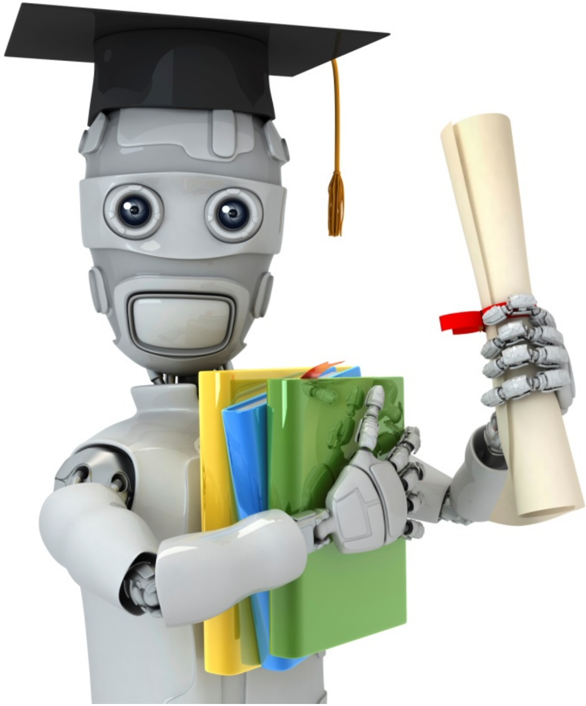
```
thetaVec = [ Theta1(:); Theta2(:); Theta3(:)];
DVec = [D1(:); D2(:); D3(:)];

Theta1 = reshape(thetaVec(1:110),10,11);
Theta2 = reshape(thetaVec(111:220),10,11);
Theta3 = reshape(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 $\boxed{\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}}$. reshape
- Use forward prop/back prop to compute $D^{(1)}, D^{(2)}, D^{(3)}$ and $J(\Theta)$
- Unroll $D^{(1)}, D^{(2)}, D^{(3)}$ to get `gradientVec`.

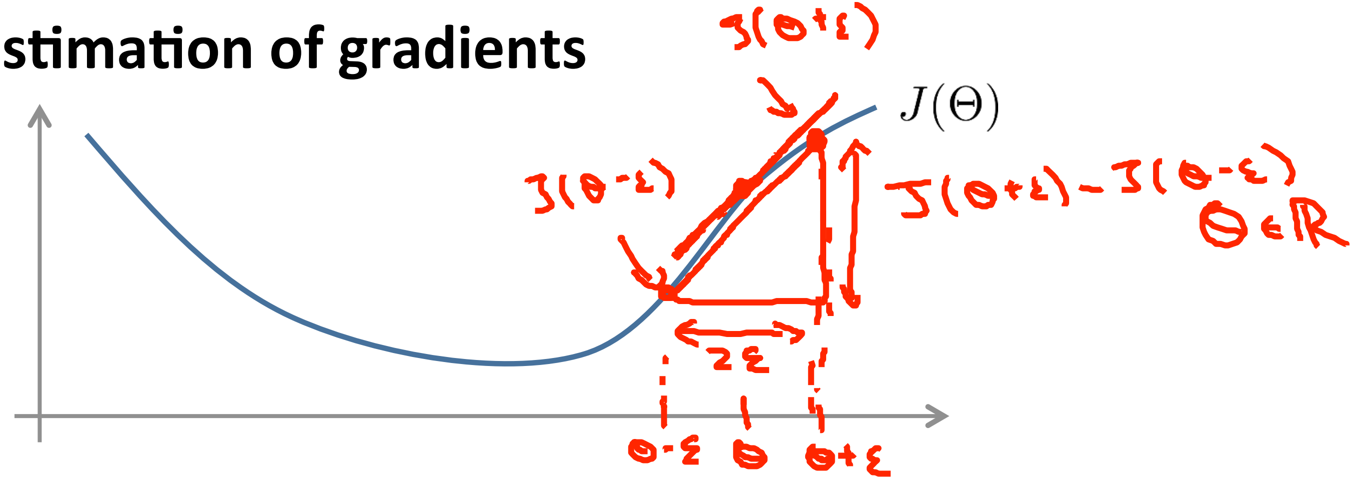


Machine Learning

Neural Networks: Learning

Gradient checking

Numerical estimation of gradients



$$\frac{d}{d\theta}J(\theta) \approx \frac{J(\theta+\epsilon)-J(\theta-\epsilon)}{2\epsilon} \qquad \cancel{\frac{J(\theta+\epsilon)-J(\theta)}{\epsilon}}$$

$\epsilon = 10^{-4}$

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 $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$)
- $\theta = [\theta_1, \theta_2, \theta_3, \dots, \theta_n]$

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

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

$$\vdots$$

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

```
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;
```

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

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

Check that $\boxed{\texttt{gradApprox}} \approx \boxed{\texttt{DVec}}$

From backprop.

Implementation Note:

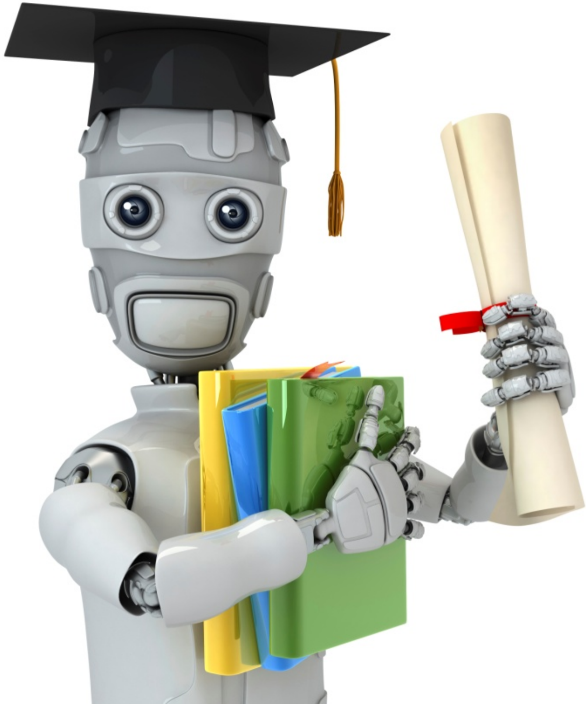
- Implement backprop to compute **DVec** (unrolled $D^{(1)}, D^{(2)}, D^{(3)}$).
- Implement numerical gradient check to compute **gradApprox**.
- Make sure they give similar values.
- Turn off gradient checking. Using backprop code for learning.

DVec

$\delta^{(4)}, \delta^{(3)}, \delta^{(2)}$

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)
```

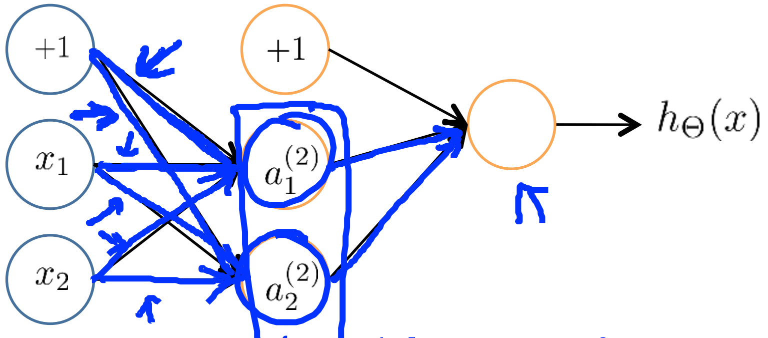
Consider gradient descent

Set `initialTheta = zeros(n,1)` ?

Zero initialization

Is it possible to set the initial value of theta to the vector of all zeros? Whereas this worked okay when we were using logistic regression, initializing all of your parameters to zero actually does not work when you are trading on your own network.

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



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

$$\frac{\partial}{\partial \Theta_{01}^{(1)}} J(\Theta) = \frac{\partial}{\partial \Theta_{02}^{(1)}} J(\Theta) \qquad \Theta_{01}^{(1)} = \Theta_{02}^{(1)}$$

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

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

Random initialization: Symmetry breaking

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

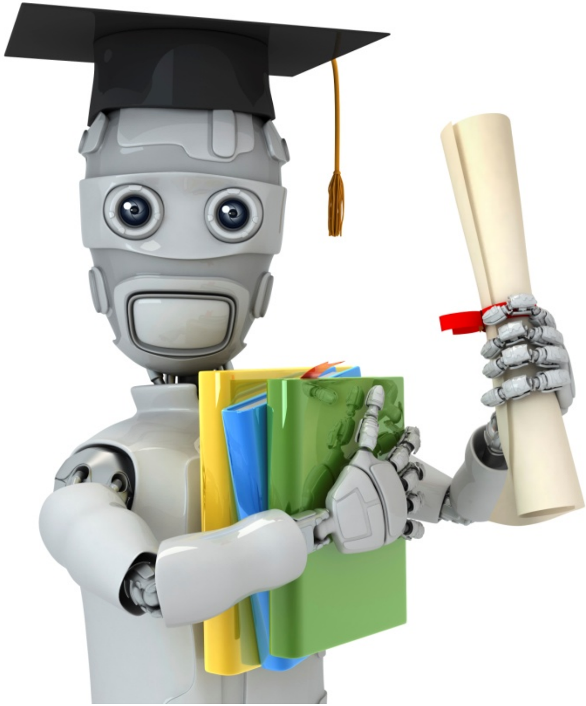
E.g.

random 10×11 matrix (betw. 0 and 1)

```
Theta1 = rand(10,11)*(2*INIT_EPSILON)
         - INIT_EPSILON;
```

[-ε, ε]

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



Machine Learning

Neural Networks: Learning

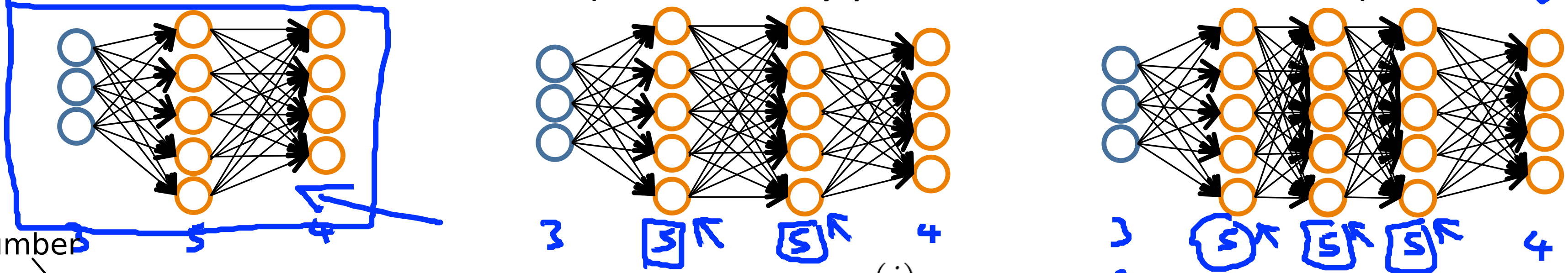
Putting it together

When training a neural network, the first thing you need to do is pick some network architecture

Training a neural network

And usually the number of hidden units in each layer will be maybe comparable to the dimension of x, comparable to the number of features, or it could be any where from same number of hidden units of input features to maybe so that three or four times of that.

Pick a network architecture (connectivity pattern between neurons)



Number

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

$y \in \{1, 2, 3, \ldots, 10\}$

$\cancel{y}$

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

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 $\boxed{\frac{\partial}{\partial\Theta^{(l)}_{jk}} J(\Theta)}$

```
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 $l = 2, \ldots, L$).

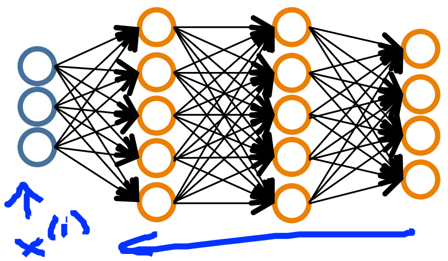
$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

....

}

...

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



Andrew Ng

Training a neural network

5. Use gradient checking to compare $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$ computed using backpropagation vs. using numerical estimate of gradient of $J(\Theta)$. Having done gradient checking just now reassures us that our implementation of back propagation is correct

   Then disable gradient checking code.

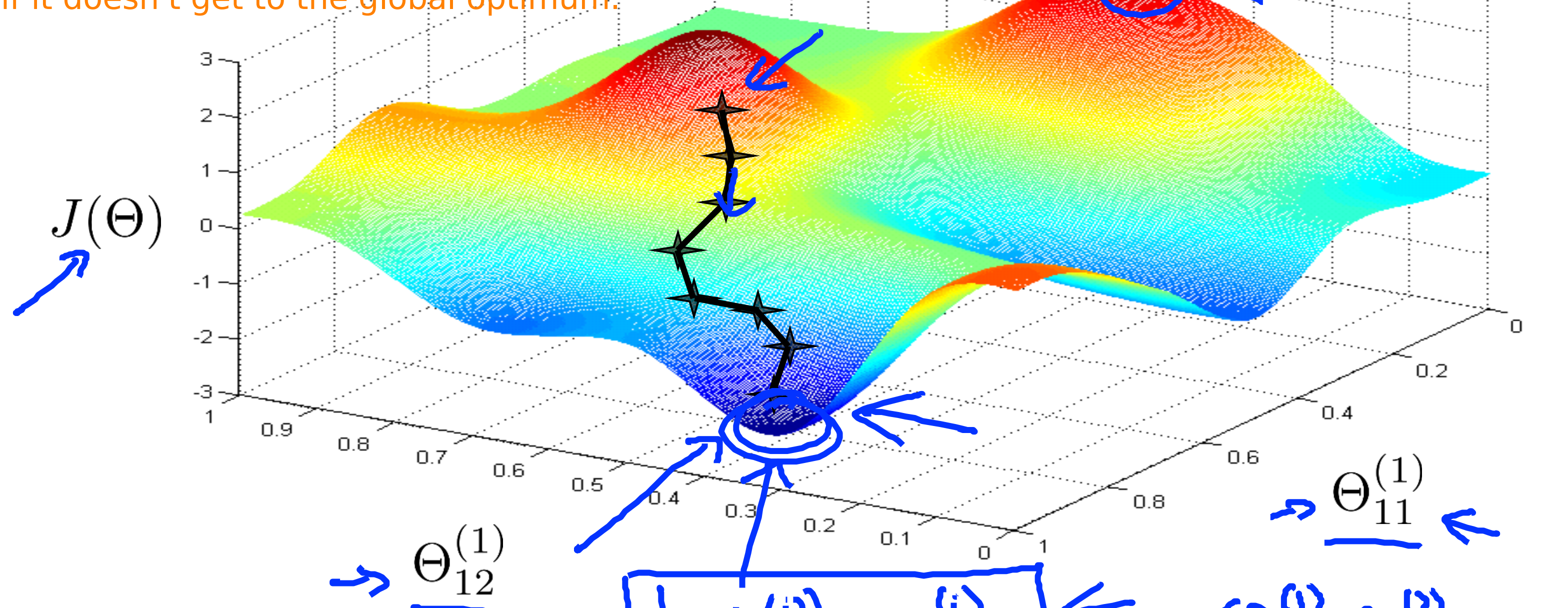
6. Use gradient descent or advanced optimization method with backpropagation to try to minimize $J(\Theta)$ as a function of parameters Θ

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

$J(\Theta)$ – non-convex.

for neural networks, this cost function j of theta is non-convex, or is not convex and so it can theoretically be susceptible to local minima, and in fact algorithms like gradient descent and the advance optimization methods can, in theory, get stuck in local optima, but it turns out that in practice this is not usually a huge problem and even though we can't guarantee that these algorithms will find a global optimum, usually algorithms like gradient descent will do a very good job minimizing this cost function j of theta and get a very good local minimum, even if it doesn't get to the global optimum.

$h_\Theta(x^{(i)})$ far from $y^{(i)}$

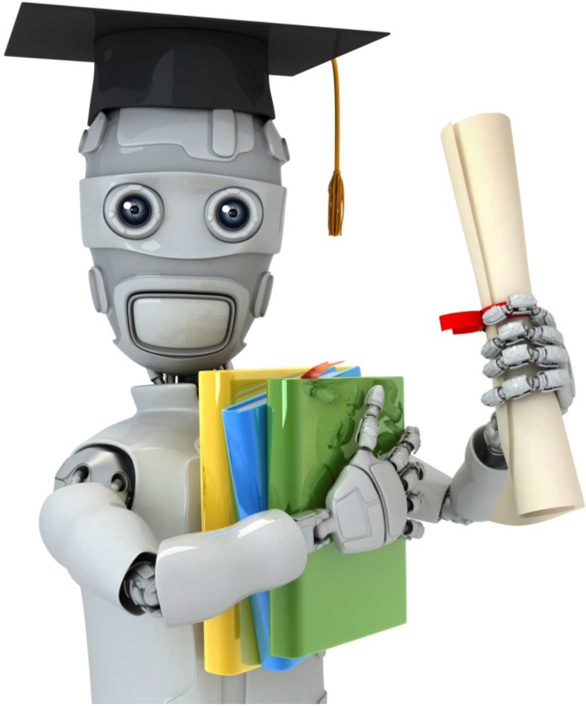


$\boxed{h_\Theta(x^{(i)}) \approx y^{(i)}}$

$\Theta^{(1)}, \Theta^{(2)}, \ldots$

Andrew Ng

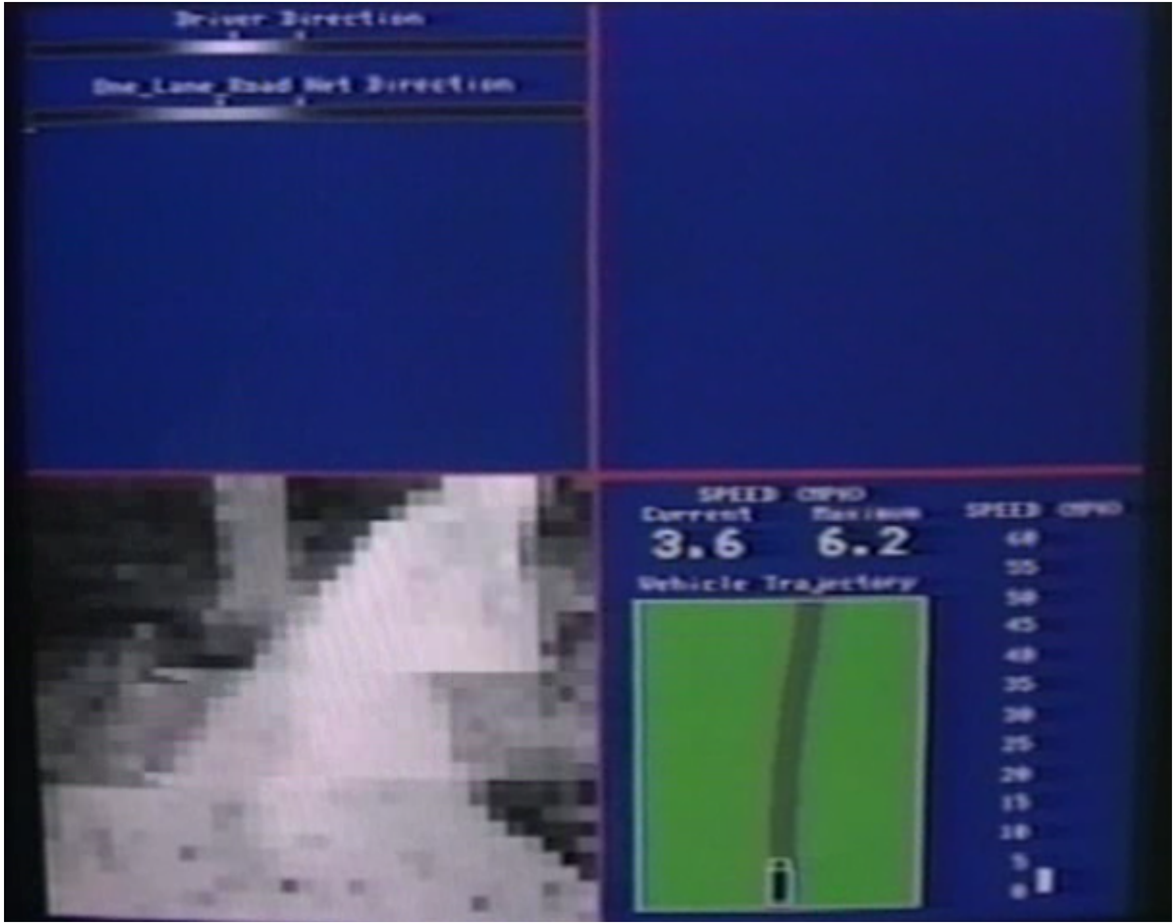
During training, a person drives the vehicle while ALVINN watches. Once every two seconds, ALVINN digitizes a video image of the road ahead, and records the person's steering direction. After about two minutes of training the network learns to accurately imitate the steering reactions of the human driver.



Neural Networks: Learning

Backpropagation example: Autonomous driving (optional)

Machine Learning



[Courtesy of Dean Pomerleau]