Machine Learning

by Stanford University

Week_4

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Contents

1 Neural networks

1.1 Model representation I

Let's examine how we will represent a hypothesis function using neural networks. At a very simple level, neurons are basically computational units that take inputs (**dendrites**) as electrical inputs (called "spikes") that are channeled to outputs (**axons**). In our model, our dendrites are like the input features $x_1 \cdots x_n$, and the output is the result of our hypothesis function. In this model our x_0 input node is sometimes called the "bias unit." It is always equal to 1. In neural networks, we use the same logistic function as in classification, $\frac{1}{1+e^{-\theta^T x}}$, yet we sometimes call it a sigmoid (logistic) **activation** function. In this situation, our "theta" parameters are sometimes called "weights".

Visually, a simplistic representation looks like:

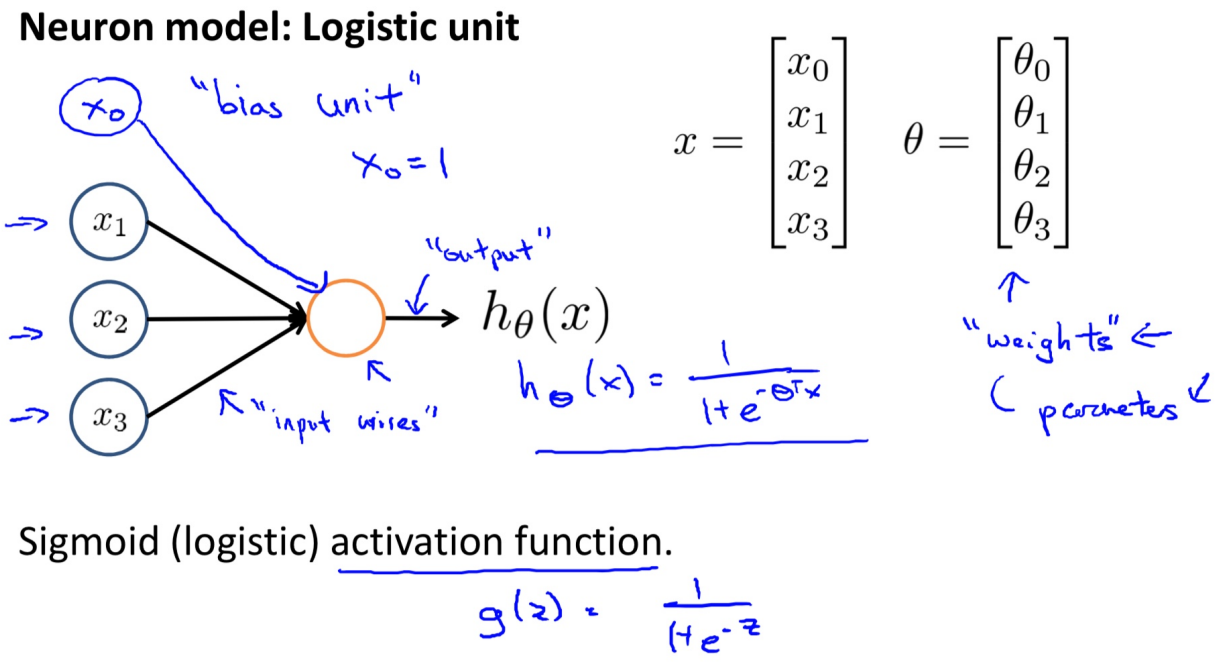
$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow [\quad] \rightarrow h_\theta(x)$$

Our input nodes (layer 1), also known as the "input layer", go into another node (layer 2), which finally outputs the hypothesis function, known as the "output layer".

We can have intermediate layers of nodes between the input and output layers called the "hidden layers."

In this example, we label these intermediate or "hidden" layer nodes $a_0^2 \cdots a_n^2$ and call them "activation units."

$a_i^{(j)}$ = "activation" of unit i in layer j
$\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$



If we had one hidden layer, it would look like:

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \rightarrow \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \end{bmatrix} \rightarrow h_\theta(x)$$

The values for each of the "activation" nodes is obtained as follows:

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

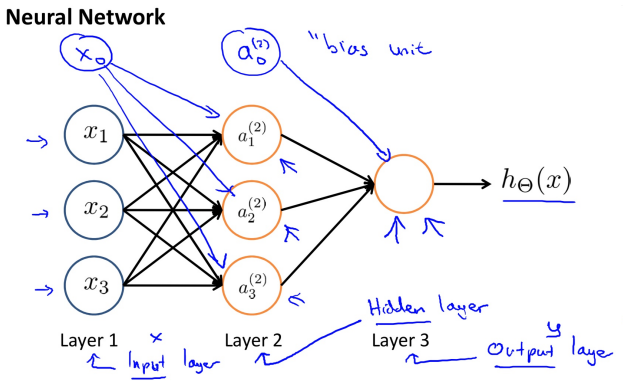
This is saying that we compute our activation nodes by using a 3×4 matrix of parameters. We apply each row of the parameters to our inputs to obtain the value for one activation node. Our hypothesis output is the logistic function applied to the sum of the values of our activation nodes, which have been multiplied by yet another parameter matrix $\Theta^{(2)}$ containing the weights for our second layer of nodes.

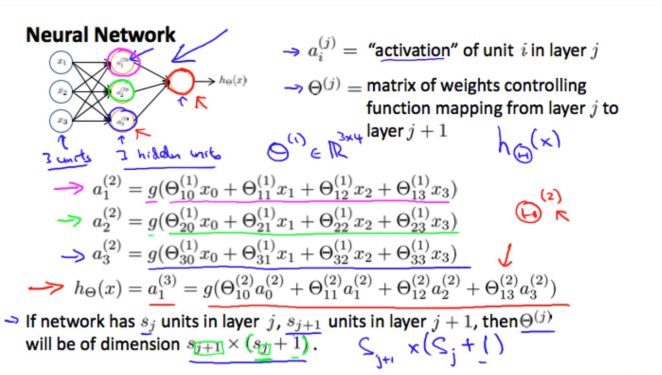
Each layer gets its own matrix of weights, $\Theta^{(j)}$.

The dimensions of these matrices of weights is determined as follows:

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

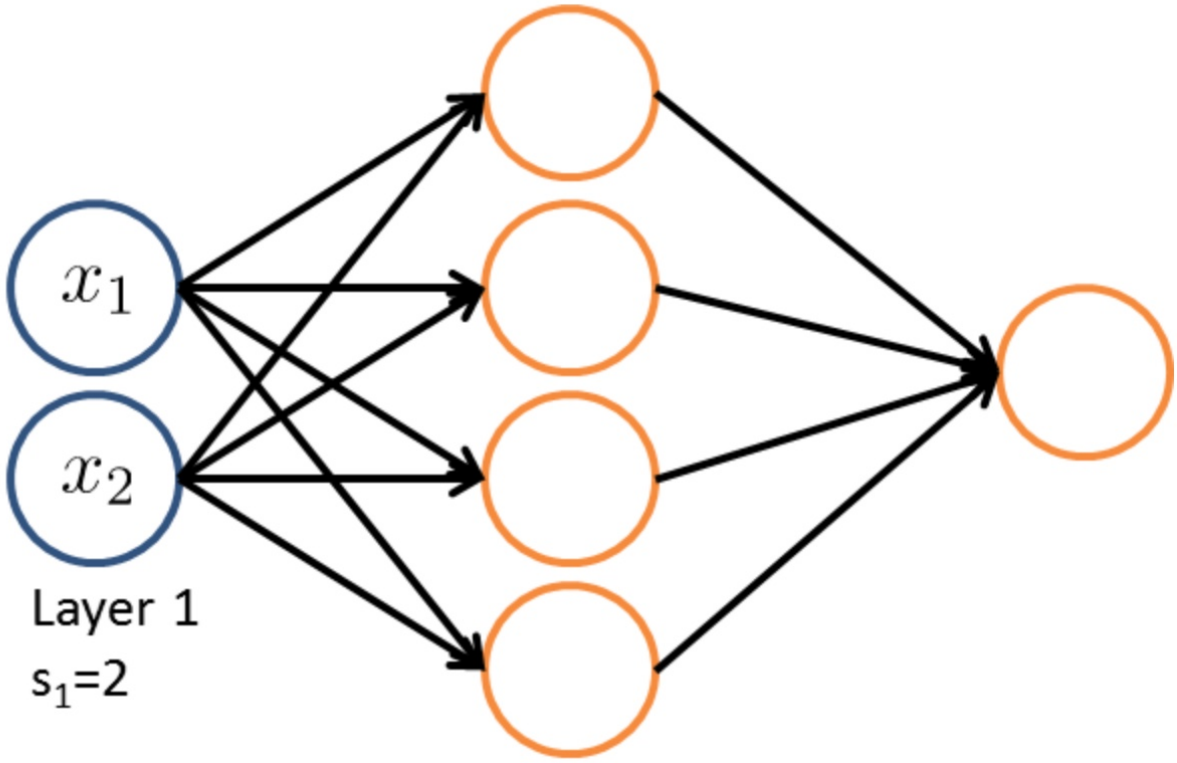
The +1 comes from the addition in $\Theta^{(j)}$ of the "bias nodes," x_0 and $\Theta_0^{(j)}$. In other words the output nodes will not include the bias nodes while the inputs will. The following image summarizes our model representation:





Example: If layer 1 has 2 input nodes and layer 2 has 4 activation nodes. Dimension of $\Theta^{(1)}$ is going to be 4×3 where $s_j = 2$ and $s_{j+1} = 4$, so $s_{j+1} \times (s_j + 1) = 4 \times 3$.

Consider the following neural network:



What is the dimension of $\Theta^{(1)}$ (Hint: add a bias unit to the input and hidden layers)?

- 2×4
- 4×2
- 3×4
- 4×3

Correct

1.2 Model representation II

To re-iterate, the following is an example of a neural network:

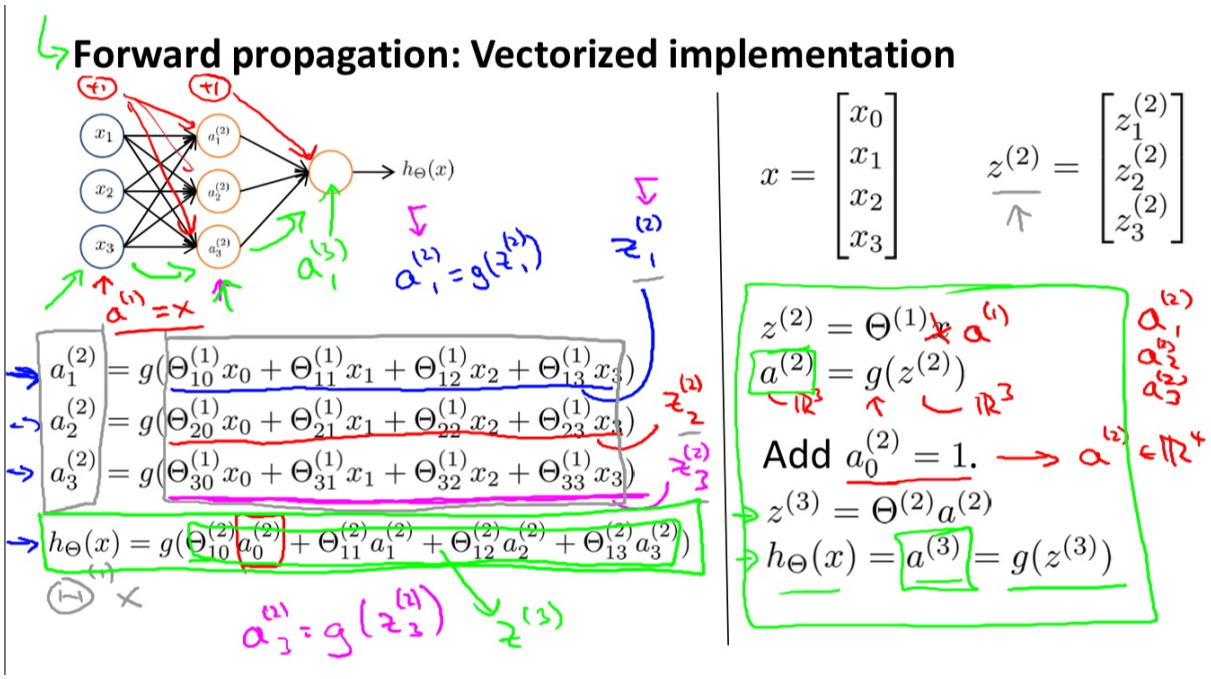
$$
\begin{aligned}
a_1^{(2)} &= g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3) \\
a_2^{(2)} &= g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3) \\
a_3^{(2)} &= g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2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

In this section we'll do a vectorized implementation of the above functions. We're going to define a new variable $z_k^{(j)}$ that encompasses the parameters inside our g function. In our previous example if we replaced by the variable z for all the parameters we would get:

$$
\begin{aligned}
a_1^{(2)} &= g(z_1^{(2)}) \\
a_2^{(2)} &= g(z_2^{(2)}) \\
a_3^{(2)} &= g(z_3^{(2)})
\end{aligned}
$$

In other words, for layer j=2 and node k, the variable z will be:

$$
z_k^{(2)} = \Theta_{k,0}^{(1)}x_0 + \Theta_{k,1}^{(1)}x_1 + \cdots + \Theta_{k,n}^{(1)}x_n
$$



The vector representation of x and z^j is:

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} z^{(j)} = \begin{bmatrix} z_1^{(j)} \\ z_2^{(j)} \\ \cdots \\ z_n^{(j)} \end{bmatrix}$$

Setting $x = a^{(1)}$, we can rewrite the equation as:

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

We are multiplying our matrix $\Theta^{(j-1)}$ with dimensions $s_j \times (n+1)$ (where s_j is the number of our activation nodes) by our vector $a^{(j-1)}$ with height (n+1). This gives us our vector $z^{(j)}$ with height s_j. Now we can get a vector of our activation nodes for layer j as follows:

$$a^{(j)} = g(z^{(j)})$$

Where our function g can be applied element-wise to our vector $z^{(j)}$.

We can then add a bias unit (equal to 1) to layer j after we have computed $a^{(j)}$. This will be element $a_0^{(j)}$ and will be equal to 1. To compute our final hypothesis, let's first compute another z vector:

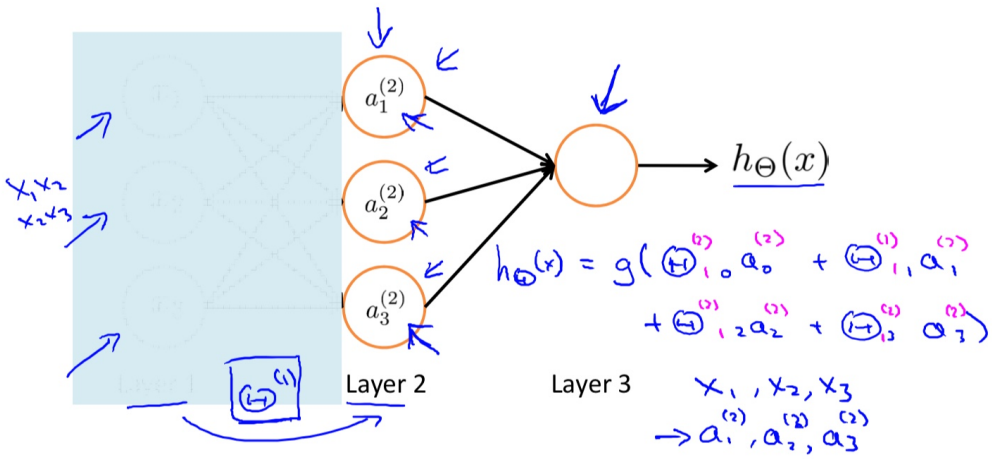
$$z^{(j+1)} = \Theta^{(j)} a^{(j)}$$

We get this final z vector by multiplying the next theta matrix after $\Theta^{(j-1)}$ with the values of all the activation nodes we just got. This last theta matrix $\Theta^{(j)}$ will have only **one row** which is multiplied by one column $a^{(j)}$ so that our result is a single number. We then get our final result with:

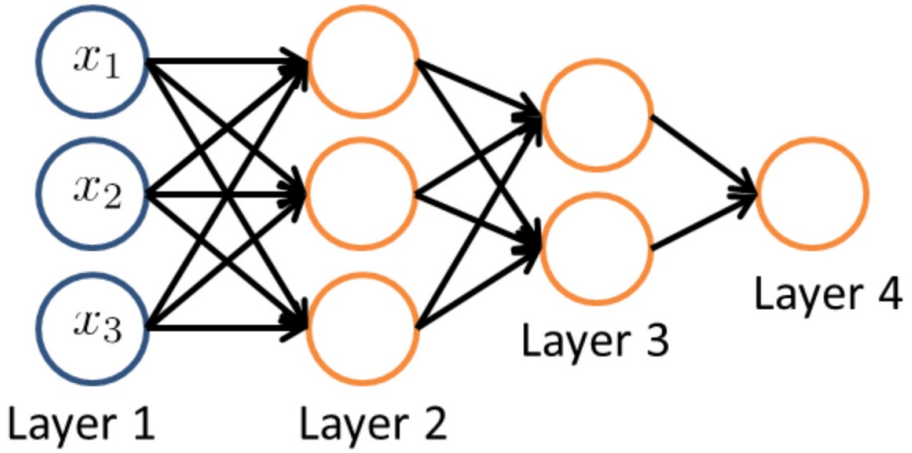
$$h_\Theta(x) = a^{(j+1)} = g(z^{(j+1)})$$

Notice that in this **last step**, between layer j and layer j+1, we are doing **exactly the same thing** as we did in logistic regression. Adding all these intermediate layers in neural networks allows us to more elegantly produce interesting and more complex non-linear hypotheses.

Neural Network learning its own features



Consider the network:



Let $a^{(1)} = x \in \mathbb{R}^{n+1}$ denote the input (with $a_0^{(1)} = 1$).

How would you compute $a^{(2)}$?

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

Correct

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

1.3 Applications

1.3.1 Examples

A simple example of applying neural networks is by predicting x_1 AND x_2, which is the logical 'and' operator and is only true if both x_1 and x_2 are 1.

The graph of our functions will look like:

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \left[g(z^{(2)}) \right] \rightarrow h_\Theta(x)$$

Remember that x_0 is our bias variable and is always 1.

Let's set our first theta matrix as:

$$\Theta^{(1)} = \begin{bmatrix} -30 & 20 & 20 \end{bmatrix}$$

This will cause the output of our hypothesis to only be positive if both x_1 and x_2 are 1. In other words:

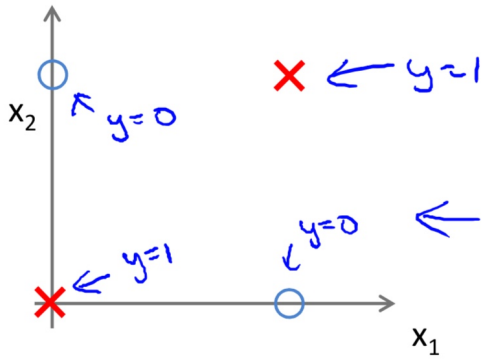
$$h_\Theta(x) = g(-30 + 20x_1 + 20x_2)$$

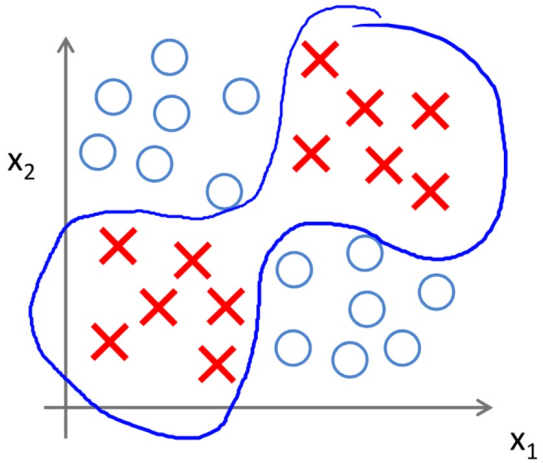
$$\begin{aligned} &x_1 = 0 \ \textit{and} \ x_2 = 0 \ \textit{then} \ g(-30) \approx 0 \\ &x_1 = 0 \ \textit{and} \ x_2 = 1 \ \textit{then} \ g(-10) \approx 0 \\ &x_1 = 1 \ \textit{and} \ x_2 = 0 \ \textit{then} \ g(-10) \approx 0 \\ &x_1 = 1 \ \textit{and} \ x_2 = 1 \ \textit{then} \ g(10) \approx 1 \end{aligned}$$

So we have constructed one of the fundamental operations in computers by using a small neural network rather than using an actual AND gate. Neural networks can also be used to simulate all the other logical gates. The following is an example of the logical operator 'OR', meaning either x_1 is true or x_2 is true, or both:

Non-linear classification example: XOR/XNOR

x_1, x_2 are binary (0 or 1).





$y = x_1 \text{ XOR } x_2$

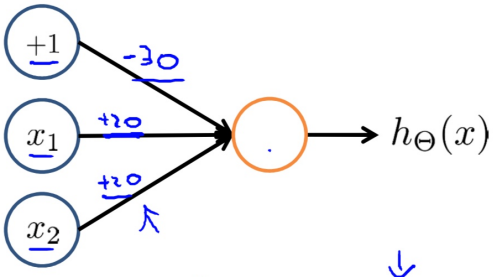
$x_1 \text{ XNOR } x_2$

$\text{NOT } (x_1 \text{ XOR } x_2)$

Simple example: AND

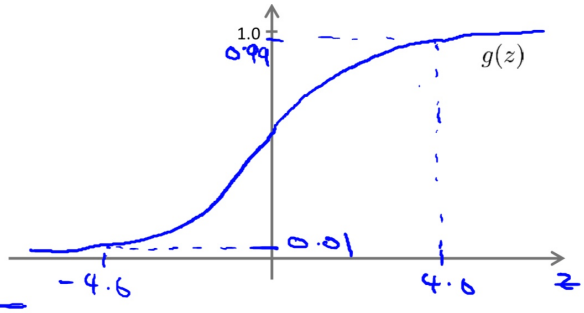
$x_1, x_2 \in \{0, 1\}$

$y = x_1 \text{ AND } x_2$



$h_\Theta(x) = g(-30 + 20x_1 + 20x_2)$

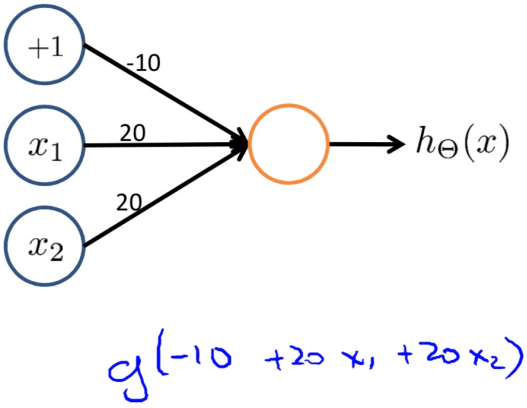
$\Theta^{(1)}_{10}$ $\Theta^{(1)}_{11}$ $\Theta^{(1)}_{12}$



x_1	x_2	$h_\Theta(x)$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

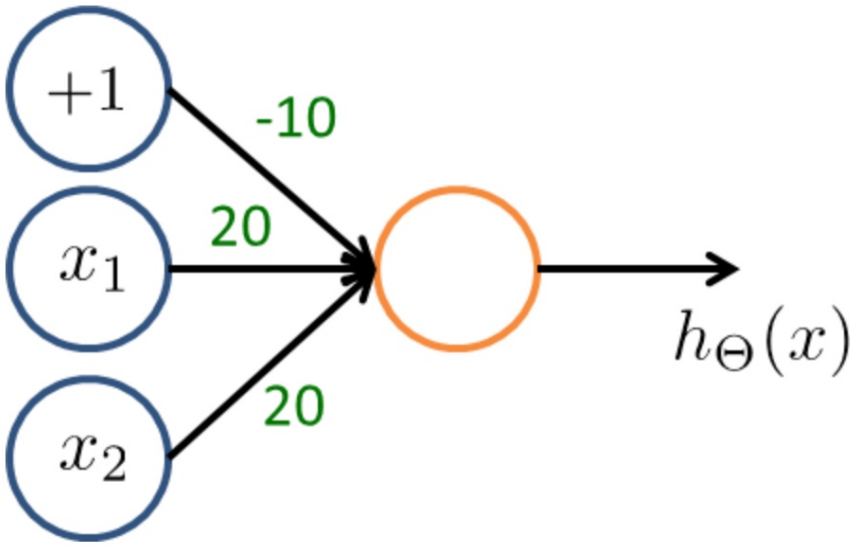
$h_\Theta(x) \approx x_1 \text{ AND } x_2$

Example: OR function



x_1	x_2	$h_\Theta(x)$
0	0	g(-10) ≈ 0
0	1	g(10) ≈ 1
1	0	≈ 1
1	1	≈ 1

Suppose x_1 and x_2 are binary valued (0 or 1). What boolean function does the network shown below (approximately) compute? (Hint: One possible way to answer this is to draw out a truth table, similar to what we did in the video).



- x_1 AND x_2
- (NOT x_1) OR (NOT x_2)
- x_1 OR x_2

  Correct

- (NOT x_1) AND (NOT x_2)

The $\Theta^{(1)}$ matrices for AND, NOR, and OR are:

$$
\begin{aligned}
&AND: \\
&\quad \Theta^{(1)} = \begin{bmatrix} -30 & 20 & 20 \end{bmatrix} \\
&NOR: \\
&\quad \Theta^{(1)} = \begin{bmatrix} 10 & -20 & -20 \end{bmatrix} \\
&OR: \\
&\quad \Theta^{(1)} = \begin{bmatrix} -10 & 20 & 20 \end{bmatrix}
\end{aligned}
$$

We can combine these to get the XNOR logical operator (which gives 1 if x_1 and x_2 are both 0 or both 1).

$$
\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \end{bmatrix} \rightarrow \begin{bmatrix} a^{(3)} \end{bmatrix} \rightarrow h_\Theta(x)
$$

For the transition between the first and second layer, we'll use a $\Theta^{(1)}$ matrix that combines the values for AND and NOR:

$$
\Theta^{(1)} = \begin{bmatrix} -30 & 20 & 20 \\ 10 & -20 & -20 \end{bmatrix}
$$

For the transition between the second and third layer, we'll use a $\Theta^{(2)}$ matrix that uses the value for OR:

$$
\Theta^{(2)} = \begin{bmatrix} -10 & 20 & 20 \end{bmatrix}
$$

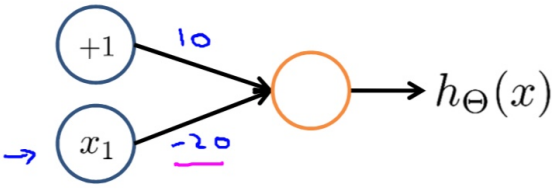
Let's write out the values for all our nodes:

$$
\begin{aligned}
a^{(2)} &= g(\Theta^{(1)} \cdot x) \\
a^{(3)} &= g(\Theta^{(2)} \cdot a^{(2)}) \\
h_\Theta(x) &= a^{(3)}
\end{aligned}
$$

And there we have the XNOR operator using a hidden layer with two nodes! The following summarizes the above algorithm:

→ x_1 AND x_2 → x_1 OR x_2 {0,1}.

Negation: NOT x_1



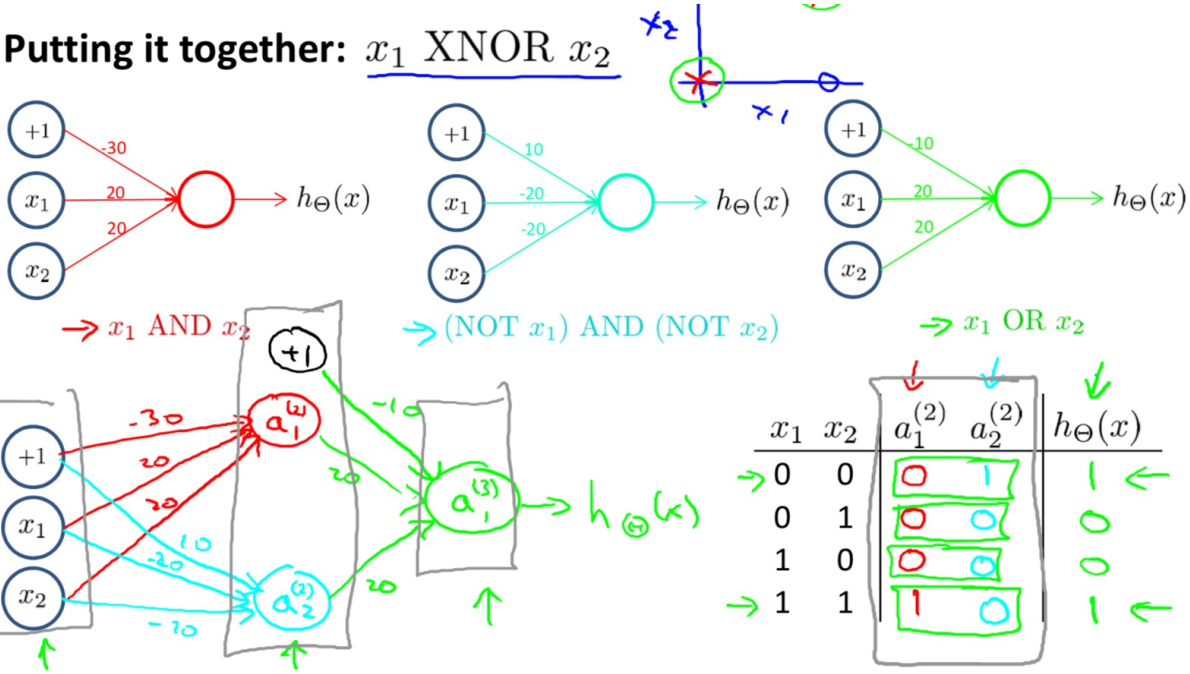
x_1	$h_\Theta(x)$
0	$g(10) \approx 1$
1	$g(-10) \approx 0$

$h_\Theta(x) = g(10 - 20x_1)$

→ (NOT x_1) AND (NOT x_2)

(=1 if and only if → $x_1 = x_2 = 0$

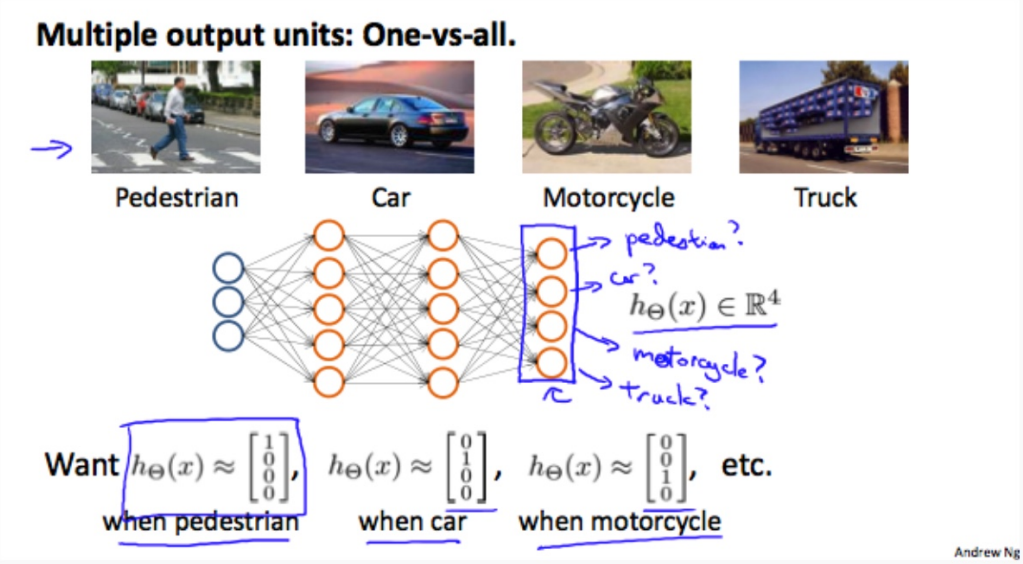
Putting it together: x_1 XNOR x_2



x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
→ 0	0	0	1	1 ←
0	1	0	0	0
1	0	0	0	0
→ 1	1	1	0	1 ←

1.3.2 Multiclass classification

To classify data into multiple classes, we let our hypothesis function return a vector of values. Say we wanted to classify our data into one of four categories. We will use the following example to see how this classification is done. This algorithm takes as input an image and classifies it accordingly:



We can define our set of resulting classes as y:

$$y^{(i)} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\0\\1\end{bmatrix},$$

Each $y^{(i)}$ represents a different image corresponding to either a car, pedestrian, truck, or motorcycle. The inner layers, each provide us with some new information which leads to our final hypothesis function. The setup looks like:

$$\begin{bmatrix}x_0\\x_1\\x_2\\\cdots\\x_n\end{bmatrix} \rightarrow \begin{bmatrix}a_0^{(2)}\\a_1^{(2)}\\a_2^{(2)}\\\cdots\end{bmatrix} \rightarrow \begin{bmatrix}a_0^{(3)}\\a_1^{(3)}\\a_2^{(3)}\\\cdots\end{bmatrix} \rightarrow \cdots \rightarrow \begin{bmatrix}h_\Theta(x)_1\\h_\Theta(x)_2\\h_\Theta(x)_3\\h_\Theta(x)_4\end{bmatrix}$$

Our resulting hypothesis for one set of inputs may look like:

$$h_\Theta(x) = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$

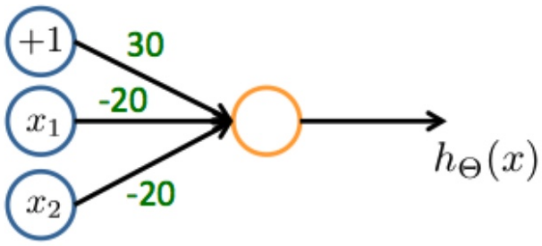
In which case our resulting class is the third one down, or $h_\Theta(x)_3$, which represents the motorcycle.

1.4 Test

1. Which of the following statements are true? Check all that apply.

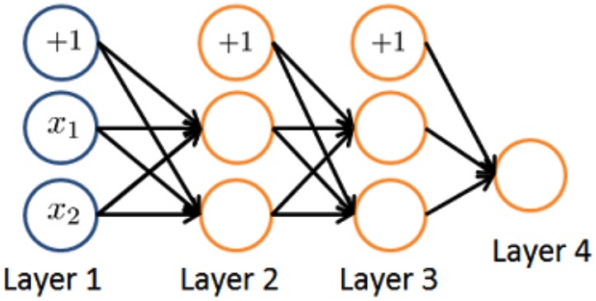
- [x] The activation values of the hidden units in a neural network, with the sigmoid activation function applied at every layer, are always in the range (0, 1).
- [ ] Suppose you have a multi-class classification problem with three classes, trained with a 3 layer network. Let $a_1^{(3)} = (h_\Theta(x))_1$ be the activation of the first output unit, and similarly $a_2^{(3)} = (h_\Theta(x))_2$ and $a_3^{(3)} = (h_\Theta(x))_3$. Then for any input x, it must be the case that $a_1^{(3)} + a_2^{(3)} + a_3^{(3)} = 1$.
- [ ] A two layer (one input layer, one output layer; no hidden layer) neural network can represent the XOR function.
- [x] Any logical function over binary-valued (0 or 1) inputs x_1 and x_2 can be (approximately) represented using some neural network.

2. Consider the following neural network which takes two binary-valued inputs $x_1, x_2 \in \{0, 1\}$ and outputs $h_\Theta(x)$. Which of the following logical functions does it (approximately) compute?



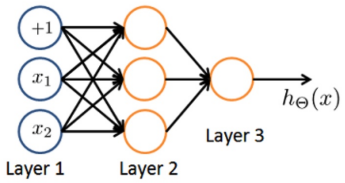
- (●) NAND (meaning "NOT AND")
- ( ) AND
- ( ) OR
- ( ) XOR (exclusive OR)

3. Consider the neural network given below. Which of the following equations correctly computes the activation $a_1^{(3)}$? Note: $g(z)$ is the sigmoid activation function.



- (●) $a_1^{(3)} = g(\Theta_{1,0}^{(2)} a_0^{(2)} + \Theta_{1,1}^{(2)} a_1^{(2)} + \Theta_{1,2}^{(2)} a_2^{(2)})$
- ( ) $a_1^{(3)} = g(\Theta_{1,0}^{(1)} a_0^{(1)} + \Theta_{1,1}^{(1)} a_1^{(1)} + \Theta_{1,2}^{(1)} a_2^{(1)})$
- ( ) $a_1^{(3)} = g(\Theta_{1,0}^{(1)} a_0^{(2)} + \Theta_{1,1}^{(1)} a_1^{(2)} + \Theta_{1,2}^{(1)} a_2^{(2)})$
- ( ) The activation $a_1^{(3)}$ is not present in this network.

4. You have the following neural network:



You'd like to compute the activations of the hidden layer $a^{(2)} \in \mathbb{R}^3$. One way to do so is the following Octave code:

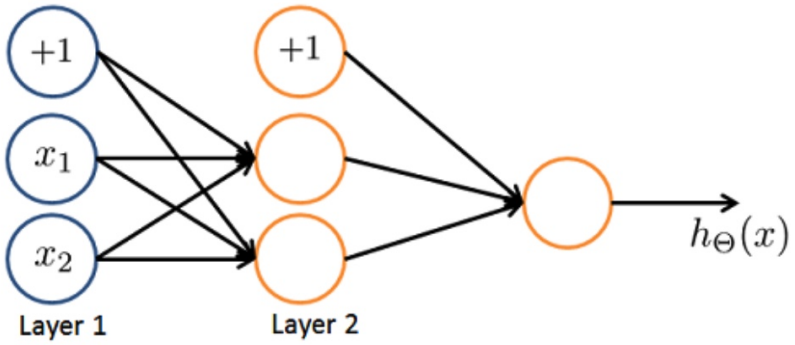
```
% Theta1 is Theta with superscript "(1)" from lecture
% ie, the matrix of parameters for the mapping from layer 1 (input) to layer 2
% Theta1 has size 3x3
% Assume 'sigmoid' is a built-in function to compute 1 / (1 + exp(-z))

a2 = zeros (3, 1);
for i = 1:3
  for j = 1:3
    a2(i) = a2(i) + x(j) * Theta1(i, j);
  end
  a2(i) = sigmoid (a2(i));
end
```

You want to have a vectorized implementation of this (i.e., one that does not use for loops). Which of the following implementations correctly compute $a^{(2)}$? Check all that apply.

- [■] a2 = sigmoid (Theta1 * x);
- [ ] a2 = sigmoid (x * Theta1);
- [ ] a2 = sigmoid (Theta2 * x);
- [ ] z = sigmoid(x); a2 = Theta1 * z;

5. You are using the neural network pictured below and have learned the parameters $\Theta^{(1)} = \begin{bmatrix} 1 & 0.5 & 1.9 \\ 1 & 1.2 & 2.7 \end{bmatrix}$ (used to compute $a^{(2)}$) and $\Theta^{(2)} = \begin{bmatrix} 1 & -0.2 & -1.7 \end{bmatrix}$ (used to compute $a^{(3)}$} as a function of $a^{(2)}$). Suppose you swap the parameters for the first hidden layer between its two units so $\Theta^{(1)} = \begin{bmatrix} 1 & 1.2 & 2.7 \\ 1 & 0.5 & 1.9 \end{bmatrix}$ and also swap the output layer so $\Theta^{(2)} = \begin{bmatrix} 1 & -1.7 & -0.2 \end{bmatrix}$. How will this change the value of the output $h_\Theta(x)$?



- (●) It will stay the same.
- ( ) It will increase.
- ( ) It will decrease
- ( ) Insufficient information to tell: it may increase or decrease.