

Machine Learning

Week 4

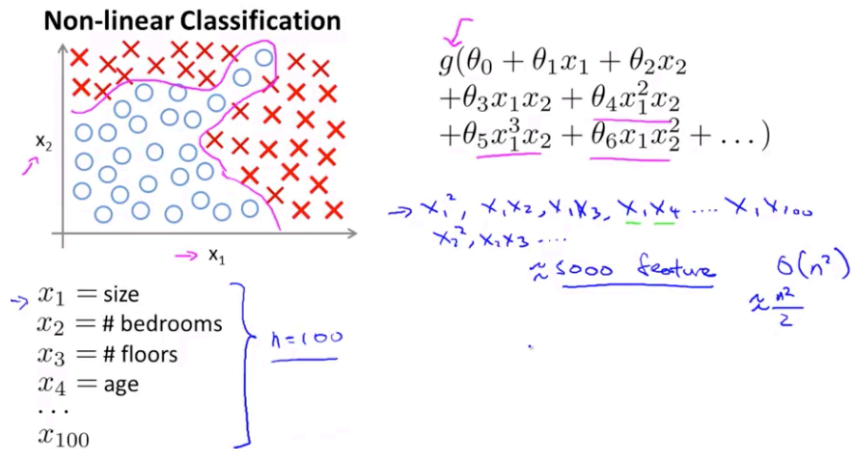
Section 1

Neural Networks: Representation

Non-linear Hypothesis

Neural Networks are good for problems where we need to create a complex non-linear hypothesis

Ex. For lots of features, logistic regression would become really complicated with 5000 polynomial terms.

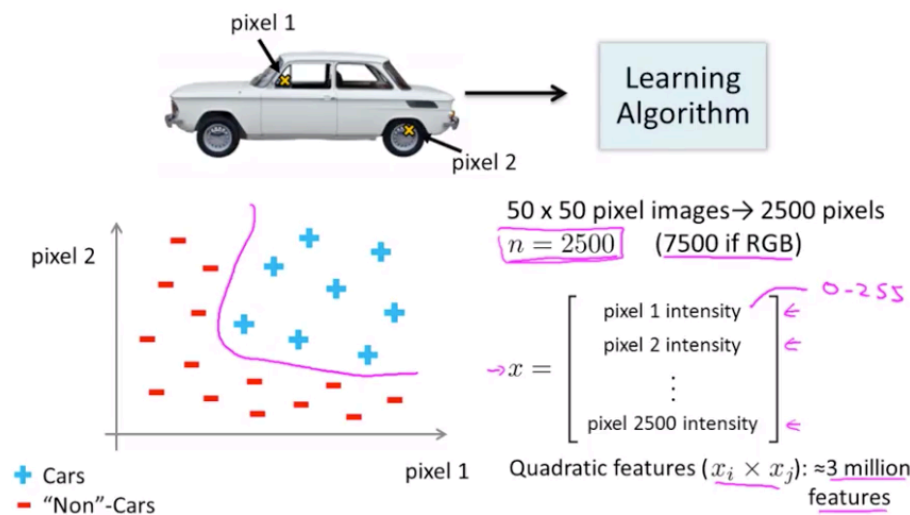


TLDR Logistic Regression isn't create for lots of features, and there are a lot of ML problems that have a lot of features.

What is the dimension of the feature space?

For grayscale a 50x50 pixel image = 2500 pixels = n is 2500 (7500 if RGB pixels)

Using logistic regression we would need 3 million polynomial terms. ($x_i \times x_j$) = 3 million



Neurons and the Brain

Neural Networks are a pretty old algorithm that was created to mimic the brain.

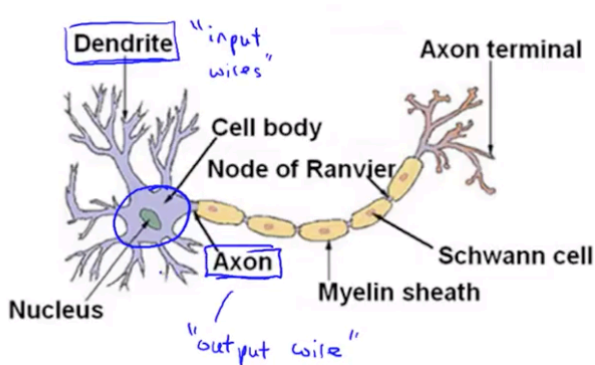
Neural Networks are computationally expensive algorithms.

The "one learning algorithm" hypothesis of the brain

Model Representation 1

How we represent Neural Networks, our hypothesis

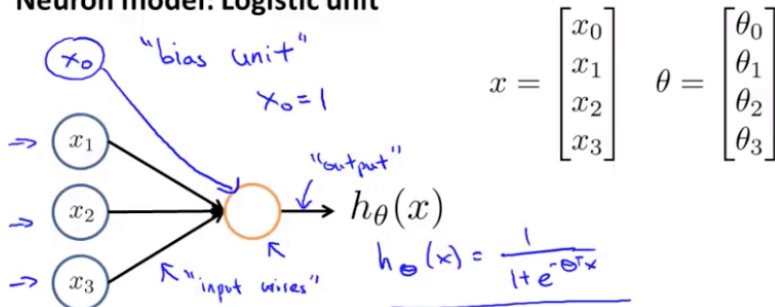
Neuron in the brain



Input -> Computation -> Output

We will create a very simply model of this process:

Neuron model: Logistic unit



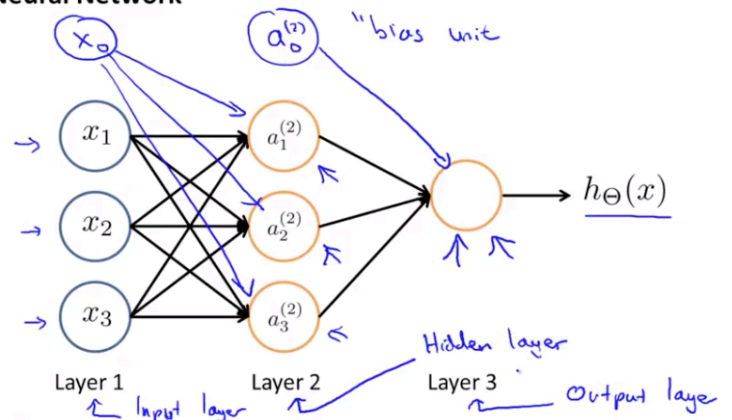
Sigmoid (logistic) activation function.

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

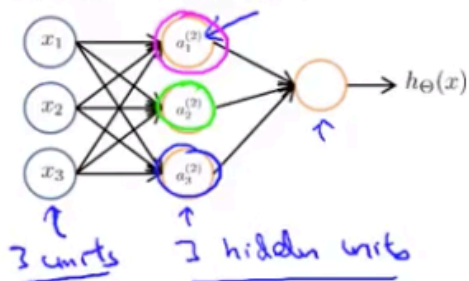
Our parameters theta are also called the weights of the model (parameters == weights)

A Neural Network is just a group of these logistic units put together.

Neural Network



Neural Network



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

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

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

$$\rightarrow a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$

$$\rightarrow a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$

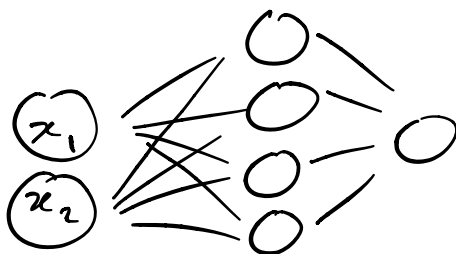
$$\rightarrow a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$

$$h_{\Theta}(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

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

$$s_{j+1} \times (s_j + 1)$$

Note g is still the sigmoid activation function



Layer 1
 $s_1 = 2$

Layer 2
 $s_2 = 4$

$$\Theta^1 = 4 \times (2 + 1) = 4 \times 3$$

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.

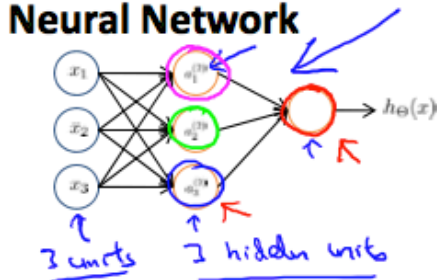
Each layer gets its own matrix of weights, $\Theta^{(j)}$.

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:

Neural Network



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

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

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

$$h_{\Theta}(x)$$

$$\rightarrow a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$

$$\rightarrow a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$

$$\rightarrow a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$

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

$$\rightarrow h_{\Theta}(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

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

$$s_{j+1} \times (s_j + 1)$$

Andrew N

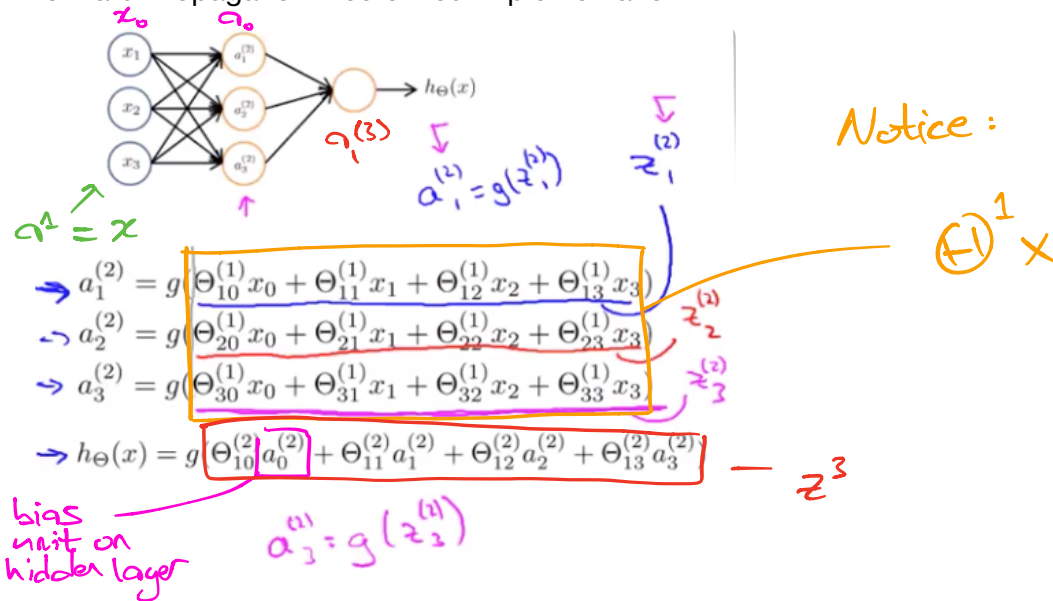
Example: If layer 1 has 2 input nodes and layer 2 has 4 activation nodes. Dimension of $\Theta^{(1)}$ is going to be 4×3 where $s_j = 2$ and $s_{j+1} = 4$, so $s_{j+1} \times (s_j + 1) = 4 \times 3$.

Model Representation 2

In the last section we saw the mathematical definition of how to represent and compute the hypotheses used by a Neural Network

In this section we will look at how to carry out the computation efficiently and a vectorized implementation.

Forward Propagation: Vectorized Implementation



Concretely:

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad z^{(2)} = \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix}$$

$$z^{(2)} = \Theta^{(1)} x \rightarrow \mathbb{R}^1 \mathbb{R}^1$$

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

Add $a_0^{(2)} = 1$. $\rightarrow a^{(2)} \in \mathbb{R}^4$

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

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

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:

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

The vector representation of x and z^j is:

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

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.

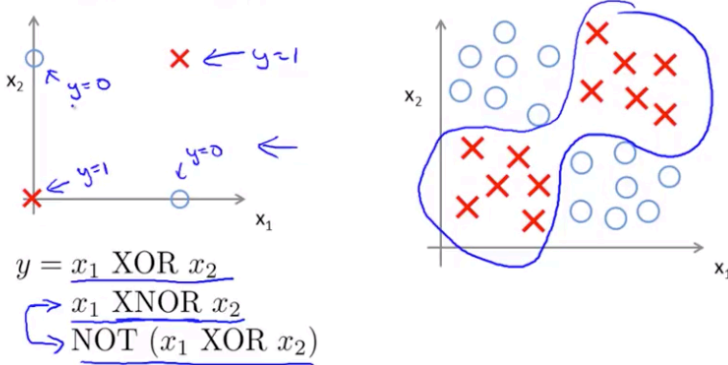
Examples and Intuitions 1

Neural Networks can compute a complex non-linear function of the input.

Lets investigate why neural networks can be used to learn complex non-linear hypotheses.

Non-linear classification example: XOR/XNOR

→ x_1, x_2 are binary (0 or 1).

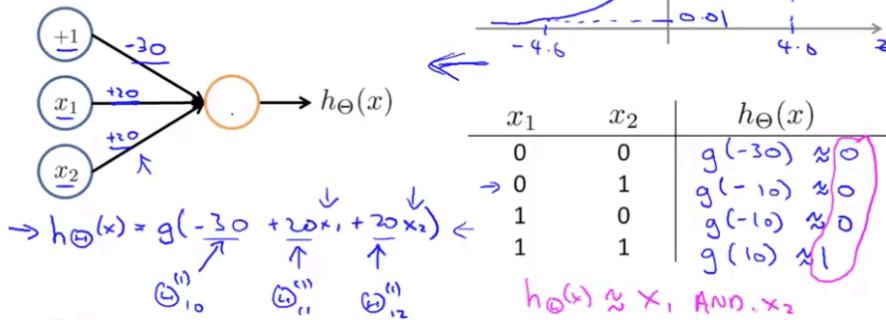


Before we start with the XNOR example above, let's first look at a simpler case:

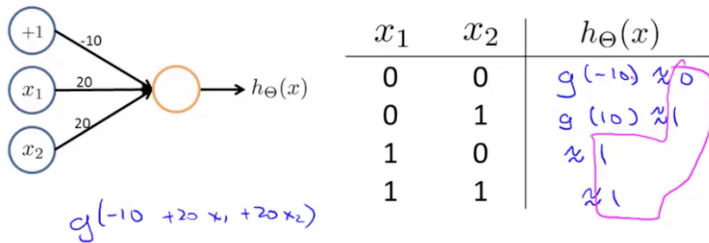
Simple example: AND

→ $x_1, x_2 \in \{0, 1\}$

→ $y = x_1 \text{ AND } x_2$



Example: OR function



A simple example of applying neural networks is by predicting $x_1 \text{ AND } x_2$, 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:

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

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:

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

$$x_1 = 0 \text{ and } x_2 = 0 \text{ then } g(-30) \approx 0$$

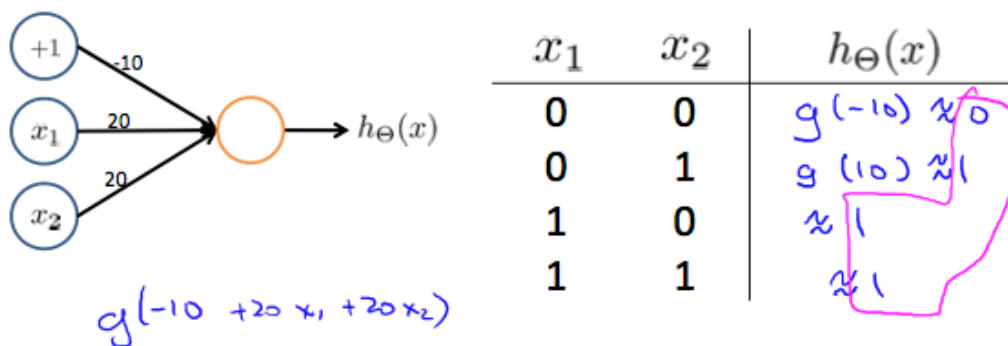
$$x_1 = 0 \text{ and } x_2 = 1 \text{ then } g(-10) \approx 0$$

$$x_1 = 1 \text{ and } x_2 = 0 \text{ then } g(-10) \approx 0$$

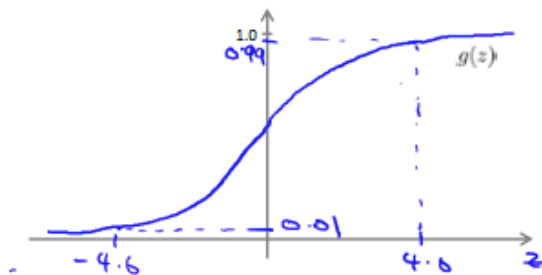
$$x_1 = 1 \text{ and } x_2 = 1 \text{ then } g(10) \approx 1$$

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:

Example: OR function

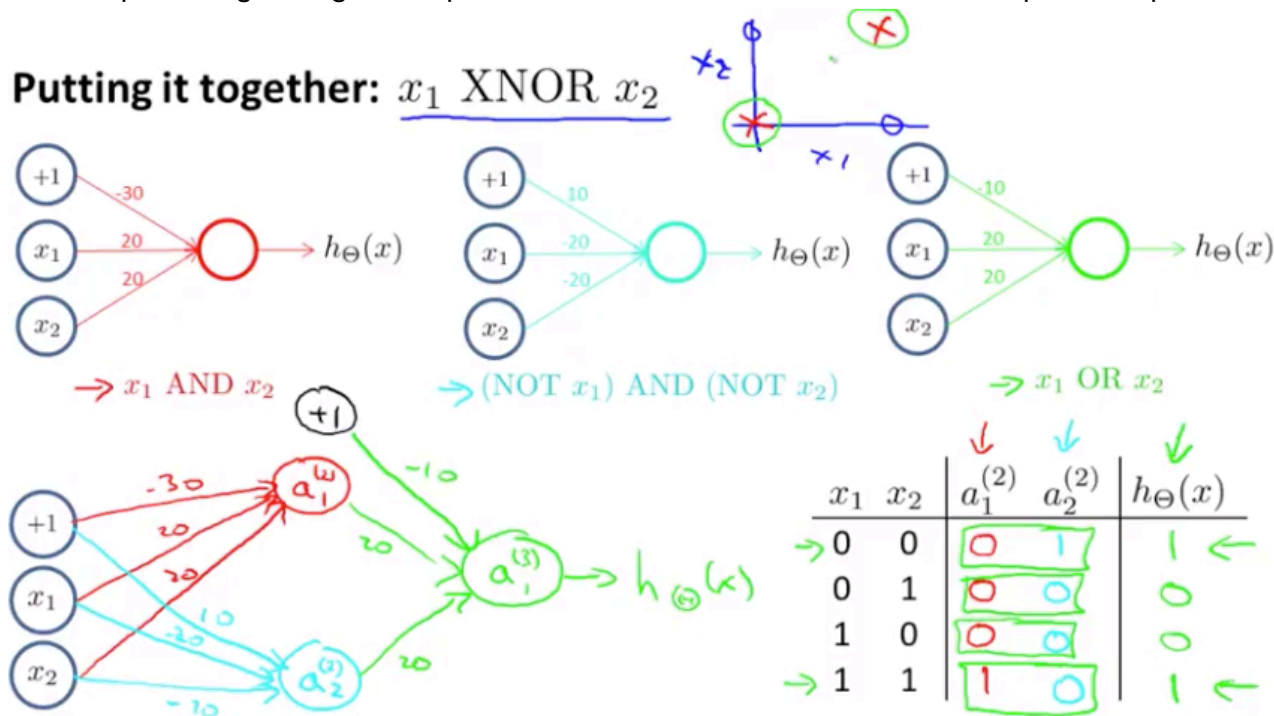


Where $g(z)$ is the following:



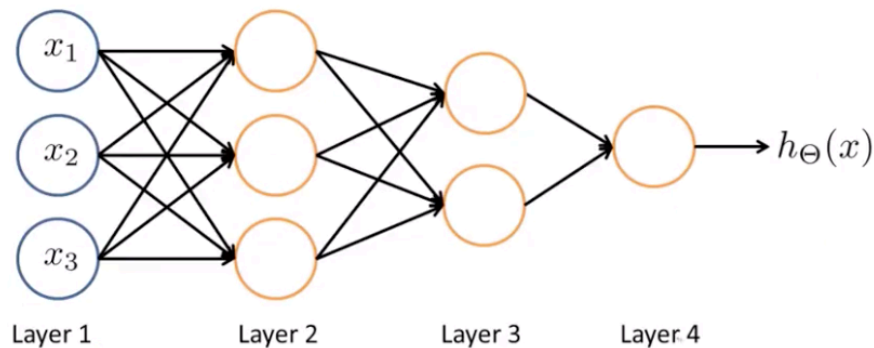
Examples and Intuitions 2

Lets keep working through examples to see how a Neural Network can compute complex non-linear hypotheses.



As you can see from above we are able to compute a complex non-linear decision boundary.

The intuition is that as we add more hidden layers, more complex functions can be computed.



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

AND :

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

NOR :

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

OR :

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

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).

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

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

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

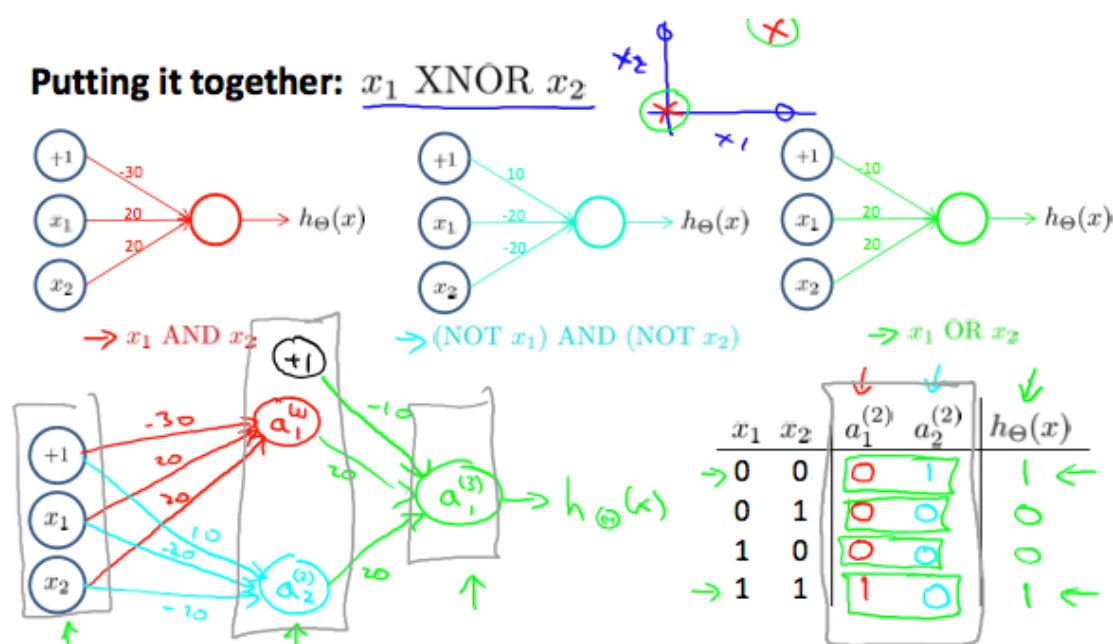
For the transition between the second and third layer, we'll use a $\Theta^{(2)}$ matrix that uses the value for OR:

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

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:



Multi-class Classification

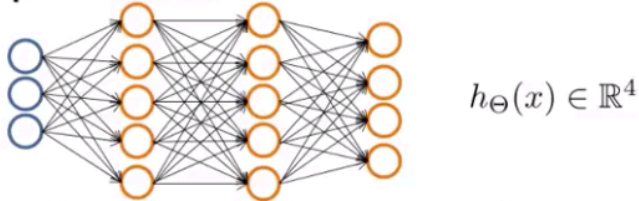
How to use Neural Networks to do multi-class classification

Ex. Handwritten digit recognition.

We use an extension of the 'One vs. All' method

We output a vector w/ dimension of the amount of predictions we want to make:

Multiple output units: One-vs-all.



Want $h_{\theta}(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, etc.
when pedestrian when car when motorcycle

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

$\rightarrow y^{(i)}$ one of $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$
pedestrian car motorcycle truck

~~Previously~~
 ~~$y \in \{1, 2, 3, 4\}$~~

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:

Multiple output units: One-vs-all.

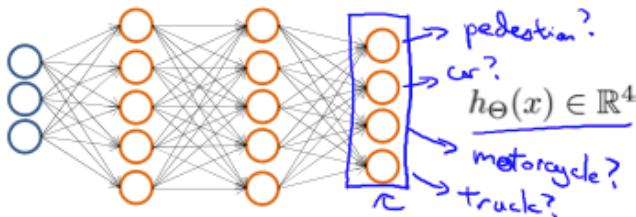


Pedestrian

Car

Motorcycle

Truck



Want $h_{\theta}(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, etc.
when pedestrian when car when motorcycle

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:

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

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.