Machine Learning
Stanford University Course, by Andrew Ng

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Sumario

What is Machine Learning?

Two definitions of Machine Learning are offered. Arthur Samuel described it as: "*the field of study that gives computers the ability to learn without being explicitly programmed.*" This is an older, informal definition.

Tom Mitchell provides a more modern definition: "*A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.*"

Example: playing checkers.

- E = the experience of playing many games of checkers.
- T = the task of playing checkers.
- P = the probability that the program will win the next game.

In general, any machine learning problem can be assigned to one of two broad classifications:

Supervised learning and Unsupervised learning.

Tipes of ML algorithms

Supervised Learning

In supervised learning, we are given a data set and already know what our correct output should look like, having the idea that there is a relationship between the input and the output.

Supervised learning problems are categorized into "**regression**"(continuous output) and "**classification**"(discrete output) problems. In a regression problem, we are trying to predict results within a continuous output, meaning that we are trying to map input variables to some continuous function. In a classification problem, we are instead trying to predict results in a discrete output. In other words, we are trying to map input variables into discrete categories.

Example 1:

Given data about the size of houses on the real estate market, try to predict their price. Price as a function of size is a continuous output, so this is a regression problem.

We could turn this example into a classification problem by instead making our output about whether the house "sells for more or less than the asking price." Here we are classifying the houses based on price into two discrete categories.

Example 2:

(a) Regression - Given a picture of a person, we have to predict their age on the basis of the given picture

(b) Classification - Given a patient with a tumor, we have to predict whether the tumor is malignant or benign.

Unsupervised Learning

Unsupervised learning allows us to approach problems with little or no idea what our results should look like. We can derive structure from data where we don't necessarily know the effect of the variables.

We can derive this structure by clustering the data based on relationships among the variables in the data.

With unsupervised learning there is no feedback based on the prediction results.

Example:

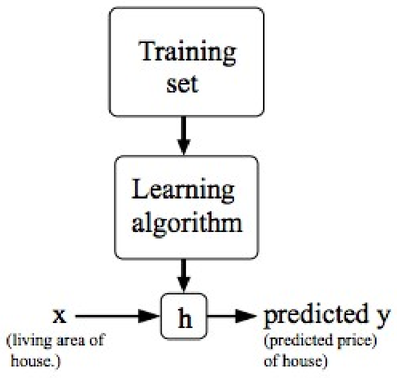
Clustering: Take a collection of 1,000,000 different genes, and find a way to automatically group these genes into groups that are somehow similar or related by different variables, such as lifespan, location, roles, and so on.

Non-clustering: The "Cocktail Party Algorithm", allows you to find structure in a chaotic environment. (i.e. identifying individual voices and music from a mesh of sounds at a cocktail party).

Model Representation

To establish notation for future use, we'll use $x^{(i)}$ to denote the "input" variables (living area in this example), also called input features, and $y^{(i)}$ to denote the "output" or target variable that we are trying to predict (price). A pair $(x^{(i)}, y^{(i)})$ is called a **training example**, and the dataset that we'll be using to learn—a list of m training examples $(x^{(i)}, y^{(i)}); i=1,\dots,m$ —is called a training set. Note that the superscript "(i)" in the notation is simply an index into the training set, and has nothing to do with exponentiation. We will also use X to denote the space of input values, and Y to denote the space of output values. In this example, X = Y = ℝ.

To describe the supervised learning problem slightly more formally, our goal is, given a training set, to learn a function h : X → Y so that h(x) is a "good" predictor for the corresponding value of y. For historical reasons, this **function h is called a hypothesis**. Seen pictorially, the process is therefore like this:



When the target variable that we're trying to predict is continuous, such as in our housing example, we call the learning problem a regression problem. When y can take on only a small number of discrete values (such as if, given the living area, we wanted to predict if a dwelling is a house or an apartment, say), we call it a classification problem.

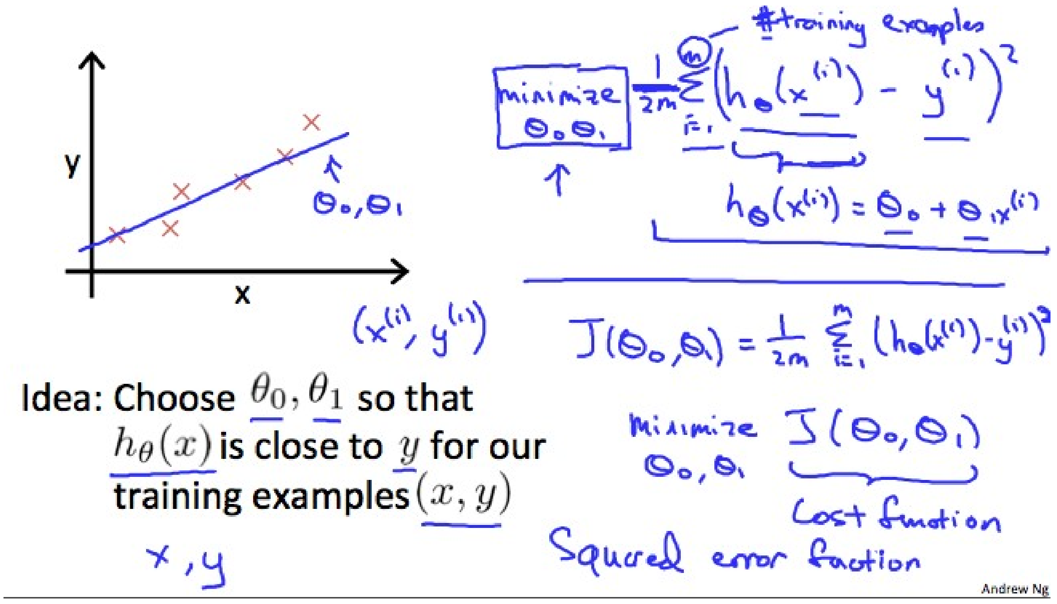
Cost Function

We can measure the accuracy of our hypothesis function by using a **cost function**. This takes an average difference (actually a fancier version of an average) of all the results of the hypothesis with inputs from x's and the actual output y's.

$$J(\theta_0,\theta_1)=\frac{1}{2m}\sum_{i=1}^{m}(\hat{y}_i-y_i)^2=\frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x_i)-y_i)^2$$

To break it apart, it is $\frac{1}{2}\bar{x}$ where $\bar{x}$ is the mean of the squares of $h_\theta(x_i)-y_i$, or the difference between the predicted value and the actual value.

This function is otherwise called the "Squared error function", or "Mean squared error". The mean is halved $\left(\frac{1}{2}\right)$ as a convenience for the computation of the gradient descent, as the derivative term of the square function will cancel out the $\frac{1}{2}$ term. The following image summarizes what the cost function does:

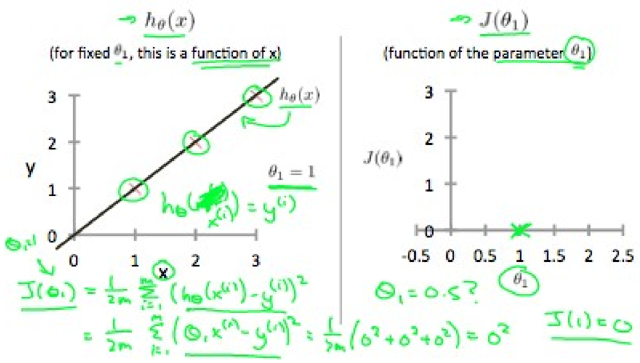


y
x
θ_0, θ_1
$(x^{(i)}, y^{(i)})$
Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ is close to y for our training examples (x, y)
x, y
# training examples
minimize $\theta_0\theta_1$ $\frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2$
$h_\theta(x^{(i)})=\theta_0+\theta_1x^{(i)}$
$J(\theta_0,\theta_1)=\frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2$
minimize θ_0,θ_1 $J(\theta_0,\theta_1)$
Cost function
Squared error function
Andrew Ng

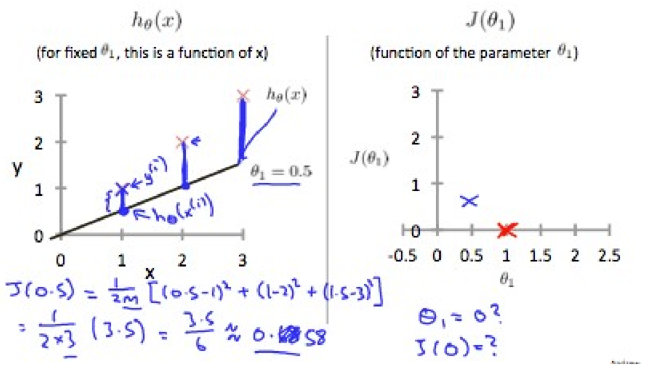
Cost Function - Intuition I

If we try to think of it in visual terms, our training data set is scattered on the x-y plane. We are trying to make a straight line (defined by $h_\theta(x)$) which passes through these scattered data points.

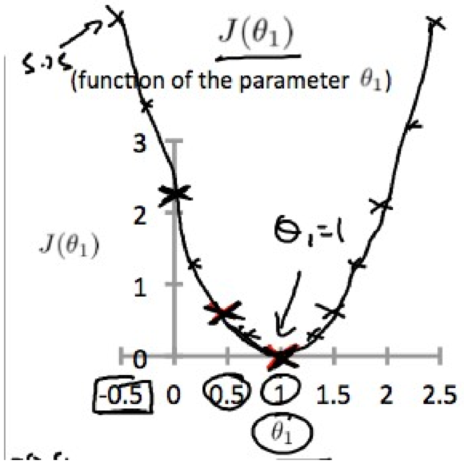
Our objective is to get the best possible line. The best possible line will be such so that the average squared vertical distances of the scattered points from the line will be the least. Ideally, the line should pass through all the points of our training data set. In such a case, the value of $J(\theta_0,\theta_1)$ will be 0. The following example shows the ideal situation where we have a cost function of 0.



When $\theta_1 = 1$, we get a slope of 1 which goes through every single data point in our model. Conversely, when $\theta_1 = 0.5$, we see the vertical distance from our fit to the data points increase.



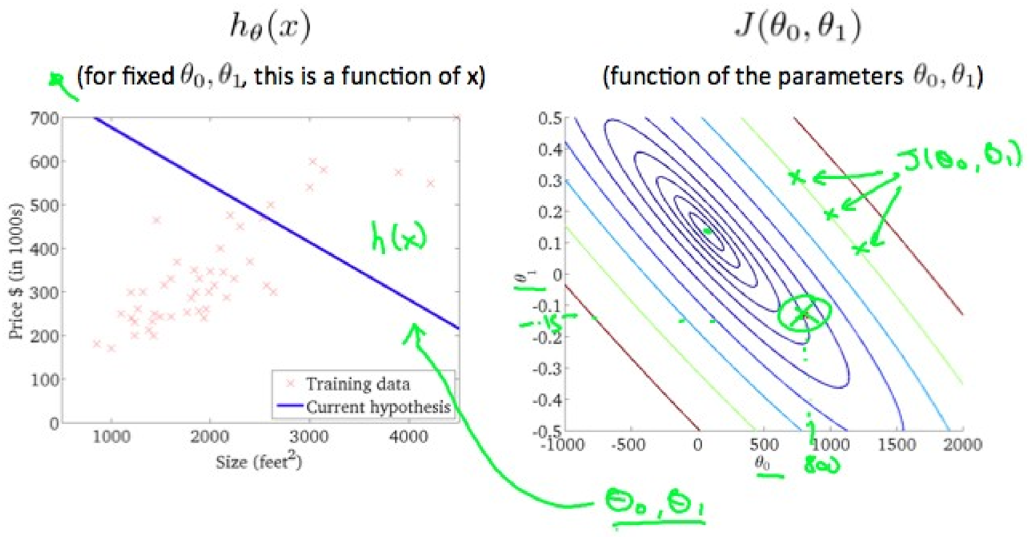
This increases our cost function to 0.58. Plotting several other points yields to the following graph:



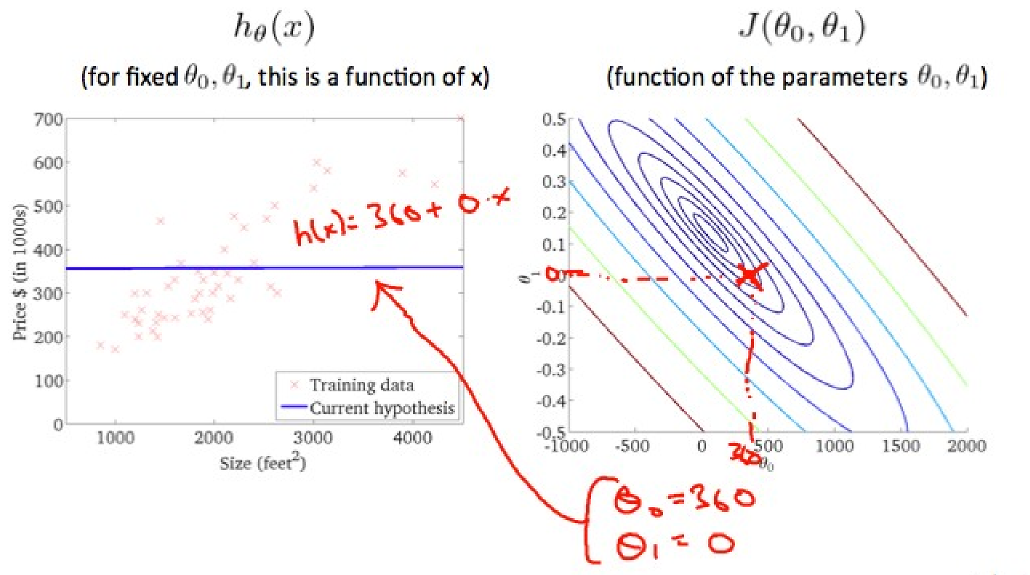
Thus as a goal, we should try to minimize the cost function. In this case, $\theta_1 = 1$ is our global minimum.

Cost Function - Intuition II

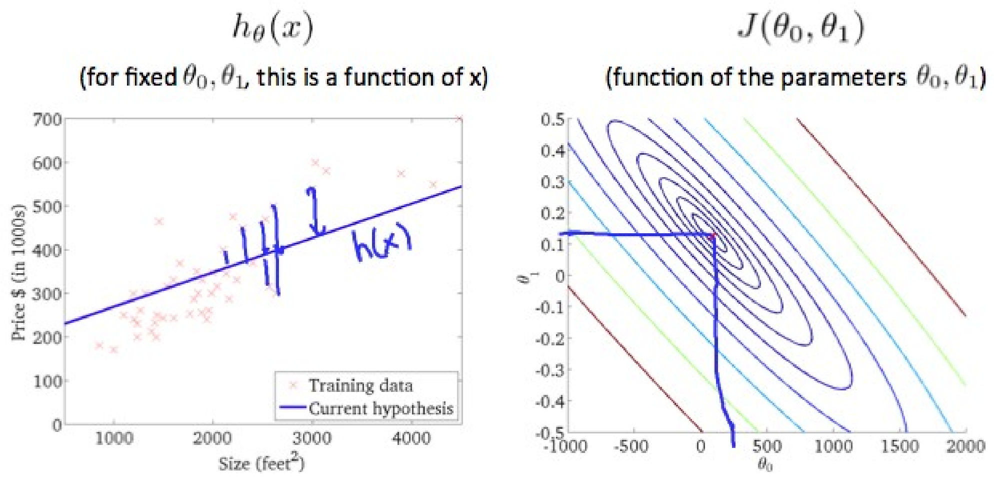
A contour plot is a graph that contains many contour lines. A contour line of a two variable function has a constant value at all points of the same line. An example of such a graph is the one to the right below.



Taking any color and going along the 'circle', one would expect to get the same value of the cost function. For example, the three green points found on the green line above have the same value for $J(\theta_0, \theta_1)$ and as a result, they are found along the same line. The circled x displays the value of the cost function for the graph on the left when $\theta_0 = 800$ and $\theta_1 = -0.15$. Taking another h(x) and plotting its contour plot, one gets the following graphs:



When $\theta_0 = 360$ and $\theta_1 = 0$, the value of $J(\theta_0, \theta_1)$ in the contour plot gets closer to the center thus reducing the cost function error. Now giving our hypothesis function a slightly positive slope results in a better fit of the data.



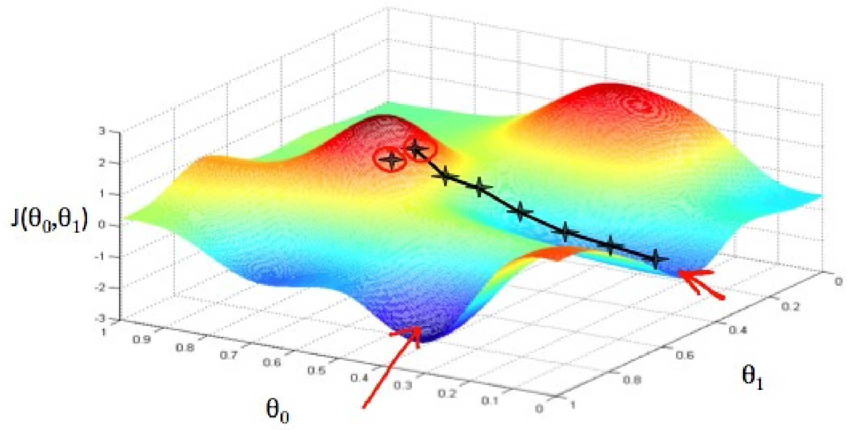
The graph above minimizes the cost function as much as possible and consequently, the result of θ_1, and θ_0 tend to be around 0.12 and 250 respectively. Plotting those values on our graph to the right seems to put our point in the center of the inner most 'circle'.

Regression problems: Linear regression

So we have our hypothesis function and we have a way of measuring how well it fits into the data. Now we need to estimate the parameters in the hypothesis function. That's where gradient descent comes in.

Imagine that we graph our hypothesis function based on its fields θ_0 and θ_1 (actually we are graphing the cost function as a function of the parameter estimates). We are not graphing x and y itself, but the parameter range of our hypothesis function and the cost resulting from selecting a particular set of parameters.

We put θ_0 on the x axis and θ_1 on the y axis, with the cost function on the vertical z axis. The points on our graph will be the result of the cost function using our hypothesis with those specific theta parameters. The graph below depicts such a setup.



We will know that we have succeeded when our cost function is at the very bottom of the pits in our graph, i.e. when its value is the minimum. The red arrows show the minimum points in the graph.

The way we do this is by taking the derivative (the tangential line to a function) of our cost function. The slope of the tangent is the derivative at that point and it will give us a direction to move towards. We make steps down the cost function in the direction with the steepest descent. The size of each step is determined by the parameter α, which is called the learning rate.

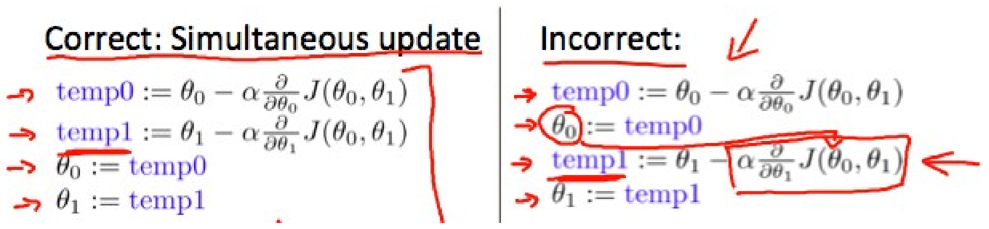
For example, the distance between each 'star' in the graph above represents a step determined by our parameter α. A smaller α would result in a smaller step and a larger α results in a larger step. The direction in which the step is taken is determined by the partial derivative of $J(\theta_0,\theta_1)$. Depending on where one starts on the graph, one could end up at different points. The image above shows us two different starting points that end up in two different places.

The gradient descent algorithm is:

repeat until convergence:

$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ where j=0,1 represents the feature index number.

At each iteration j, one should simultaneously update the parameters $\theta_1, \theta_2, \cdots, \theta_n$. Updating a specific parameter prior to calculating another one on the $j^{(th)}$ iteration would yield to a wrong implementation.



Correct: Simultaneous update

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$

$\theta_0 := \text{temp0}$

$\theta_1 := \text{temp1}$

Incorrect:

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

$\theta_0 := \text{temp0}$

$\text{temp1} := \theta_1 - \boxed{\alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)}$

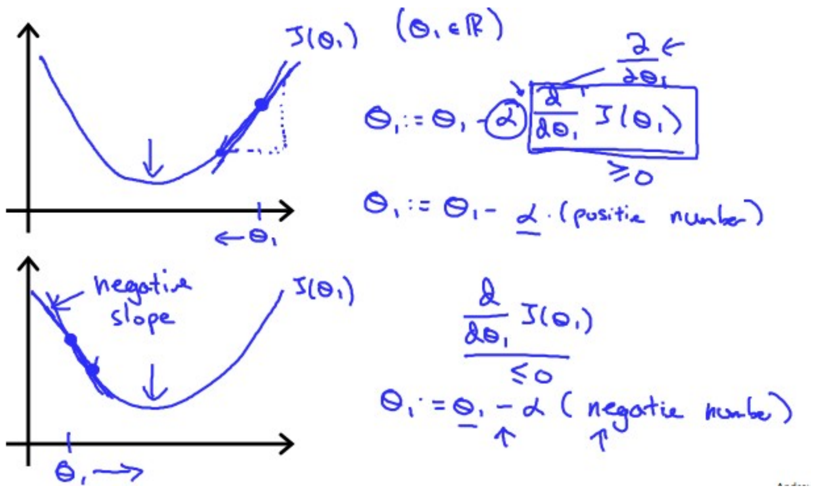
$\theta_1 := \text{temp1}$

Gradient Descent Intuition

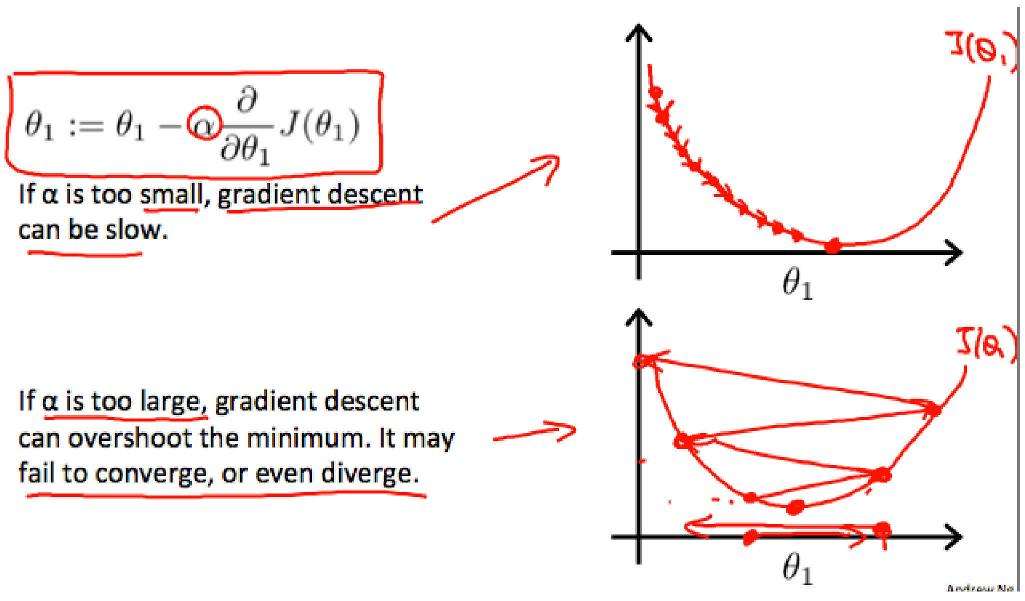
In this video we explored the scenario where we used one parameter θ_1 and plotted its cost function to implement a gradient descent. Our formula for a single parameter was:

Repeat until convergence: $\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$

Regardless of the slope's sign for $\frac{d}{d\theta_1} J(\theta_1)$, it eventually converges to its minimum value. The following graph shows that when the slope is negative, the value of θ_1 increases and when it is positive, the value of θ_1 decreases.



On a side note, we should adjust our parameter α to ensure that the gradient descent algorithm converges in a reasonable time. Failure to converge or too much time to obtain the minimum value imply that our step size is wrong.



$$\boxed{\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)}$$

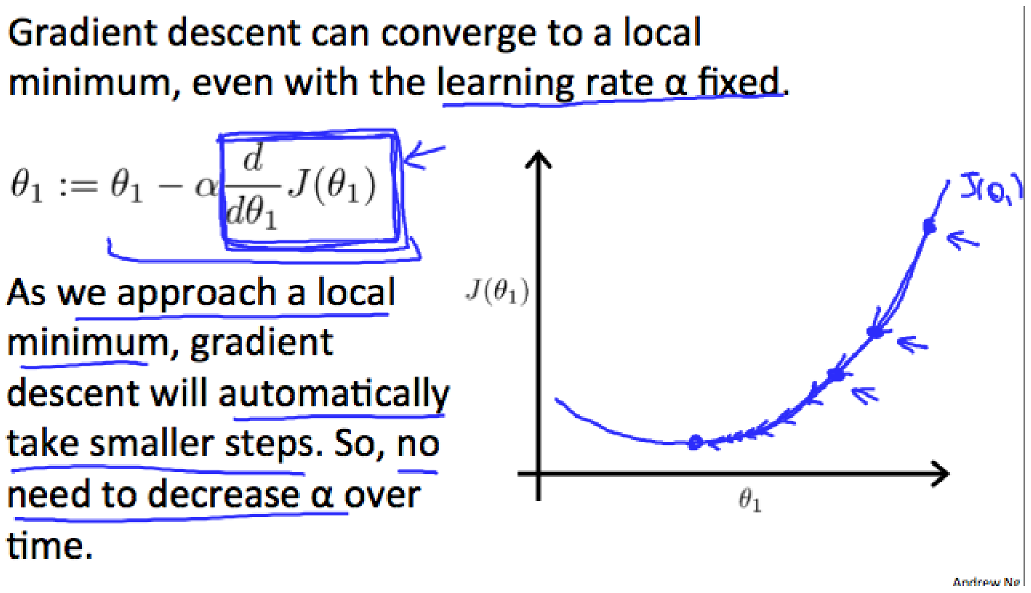
If α is too small, gradient descent can be slow.

If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.

How does gradient descent converge with a fixed step size α?

The intuition behind the convergence is that $\frac{d}{d\theta_1} J(\theta_1)$ approaches 0 as we approach the bottom of our convex function. At the minimum, the derivative will always be 0 and thus we get:

$$\theta_1 := \theta_1 - \alpha * 0$$



Gradient descent can converge to a local minimum, even with the learning rate α fixed.

$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$

As we approach a local minimum, gradient descent will automatically take smaller steps. So, no need to decrease α over time.

Gradient Descent For Linear Regression

When specifically applied to the case of linear regression, a new form of the gradient descent equation can be derived. We can substitute our actual cost function and our actual hypothesis function and modify the equation to:

repeat until convergence: {

$$\theta_0 = \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)$$

$$\theta_1 = \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i) x_1$$

}

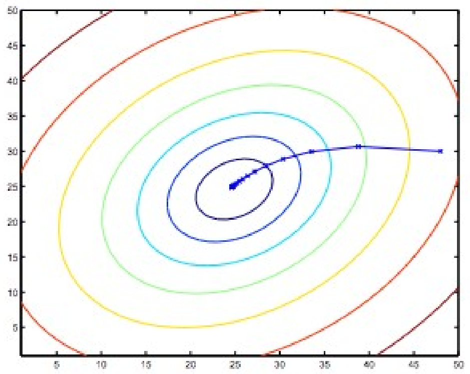
where *m* is the size of the training set, θ_0 a constant that will be changing simultaneously with θ_1 and x_i, y_i are values of the given training set (data).

Note that we have separated out the two cases for θ_j into separate equations for θ_0 and θ_1 ; and that for θ_1 we are multiplying x_i at the end due to the derivative. The following is a derivation of $\frac{\partial}{\partial \theta_j} J(\theta)$ for a single example:

$$\begin{aligned} \frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\ &= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\ &= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right) \\ &= (h_\theta(x) - y) x_j \end{aligned}$$

The point of all this is that if we start with a guess for our hypothesis and then repeatedly apply these gradient descent equations, our hypothesis will become more and more accurate.

So, this is simply gradient descent on the original cost function J. This method looks at every example in the entire training set on every step, and is called **batch gradient descent**. Note that, while gradient descent can be susceptible to local minima in general, the optimization problem we have posed here for linear regression has only one global, and no other local, optima; thus gradient descent always converges (assuming the learning rate α is not too large) to the global minimum. Indeed, J is a convex quadratic function. Here is an example of gradient descent as it is run to minimize a quadratic function.



The ellipses shown are the contours of a quadratic function. Also shown is the trajectory taken by gradient descent, which was initialized at (48,30). The x's in the figure (joined by straight lines) mark the successive values of θ that gradient descent went through as it converged to its minimum.

Multiple Features

Linear regression with multiple variables is also known as "multivariate linear regression".

We now introduce notation for equations where we can have any number of input variables:

- $x_j^{(i)}$ = value of feature *j* in the i^{th} training example
- $x^{(i)}$ = the input (features) of the i^{th} training example
- m = the number of training examples
- n = the number of features

The multivariable form of the hypothesis function accommodating these multiple features is as follows:

$$h_\theta(x)=\theta_0+\theta_1 x_1+\theta_2 x_2+\theta_3 x_3+\cdots+\theta_n x_n$$

In order to develop intuition about this function, we can think about θ_0 as the basic price of a house, θ_1 as the price per square meter, θ_2 as the price per floor, etc. x_1 will be the number of square meters in the house, x_2 the number of floors, etc.

Using the definition of matrix multiplication, our multivariable hypothesis function can be concisely represented as:

$$h_\theta(x)=[\theta_0 \;\; \theta_1 \;\; \theta_2 \;\; \cdots \;\; \theta_n]\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}=\theta^T x$$

This is a vectorization of our hypothesis function for one training example; see the lessons on vectorization to learn more.

Remark: Note that for convenience reasons in this course we assume $x_0^{(i)}=1 \, for(i\in 1,\ldots,m)$. This allows us to do matrix operations with theta and x. Hence making the two vectors 'θ' and $x^{(i)}$ match each other element-wise (that is, have the same number of elements: n+1).]

Gradient Descent for Multiple Variables

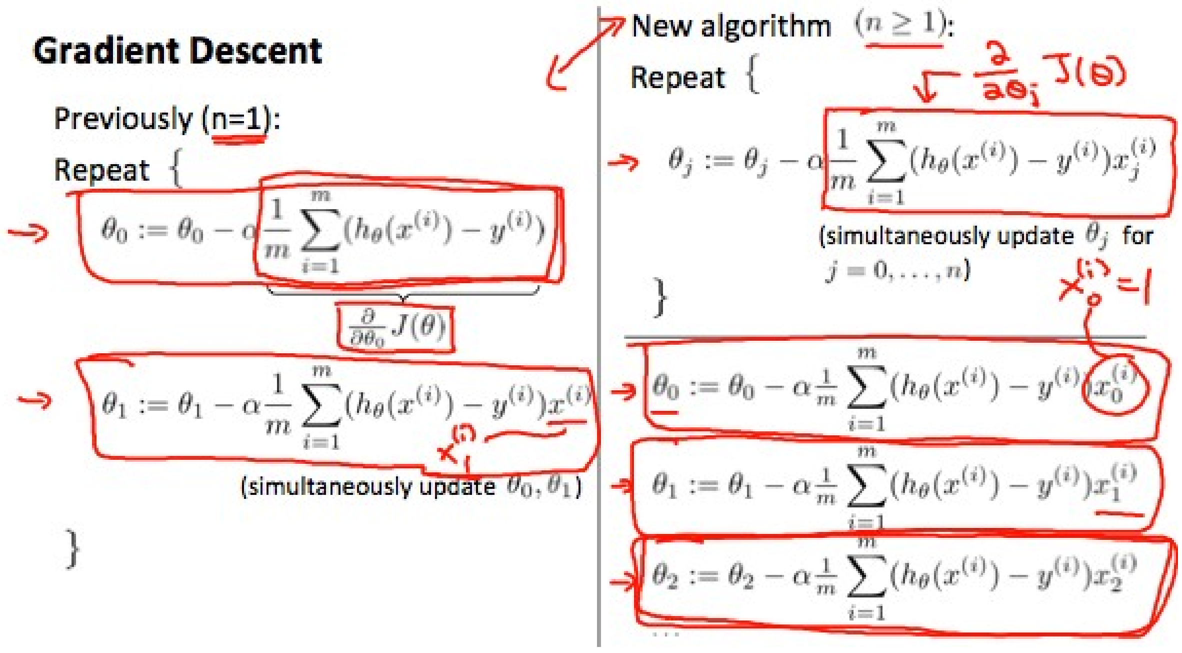
The gradient descent equation itself is generally the same form; we just have to repeat it for our 'n' features:

$$
\begin{aligned}
&\text{repeat until convergence: } \{ \\
&\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_0^{(i)} \\
&\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_1^{(i)} \\
&\theta_2 := \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_2^{(i)} \\
&\cdots \\
&\}
\end{aligned}
$$

In other words:

$$
\begin{aligned}
&\text{repeat until convergence: } \{ \\
&\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)} \qquad \text{for j := 0...n} \\
&\}
\end{aligned}
$$

The following image compares gradient descent with one variable to gradient descent with multiple variables:



Gradient Descent

Previously (n=1):

Repeat {

$$\theta_0 := \theta_0 - \underbrace{\alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})}_{\frac{\partial}{\partial \theta_0} J(\theta)}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$$

(simultaneously update θ_0, θ_1)

}

New algorithm $(n \geq 1)$:

Repeat { $\quad \frac{\partial}{\partial \theta_j} J(\theta)$

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update θ_j for $j = 0, \ldots, n$)

}

$x_0^{(i)} = 1$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

$$\theta_2 := \theta_2 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

...

Gradient Descent in Practice I - Feature Scaling

We can speed up gradient descent by having each of our input values in roughly the same range. This is because θ will descend quickly on small ranges and slowly on large ranges, and so will oscillate inefficiently down to the optimum when the variables are very uneven.

The way to prevent this is to modify the ranges of our input variables so that they are all roughly the same. Ideally:

$-1 \leqslant x_{(i)} \leqslant 1$ or $-0.5 \leqslant x_{(i)} \leqslant -0.5$

These aren't exact requirements; we are only trying to speed things up. The goal is to get all input variables into roughly one of these ranges, give or take a few.

Two techniques to help with this are **feature scaling** and **mean normalization**. Feature scaling involves dividing the input values by the range (i.e. the maximum value minus the minimum value) of the input variable, resulting in a new range of just 1. Mean normalization involves subtracting the average value for an input variable from the values for that input variable resulting in a new average value for the input variable of just zero. To implement both of these techniques, adjust your input values as shown in this formula:

$$x_i := \frac{x_i - \mu_i}{s_i}$$

Where μ_i is the **average** of all the values for feature (i) and s_i is the **range of values (max - min), or** s_i is **the standard deviation**.

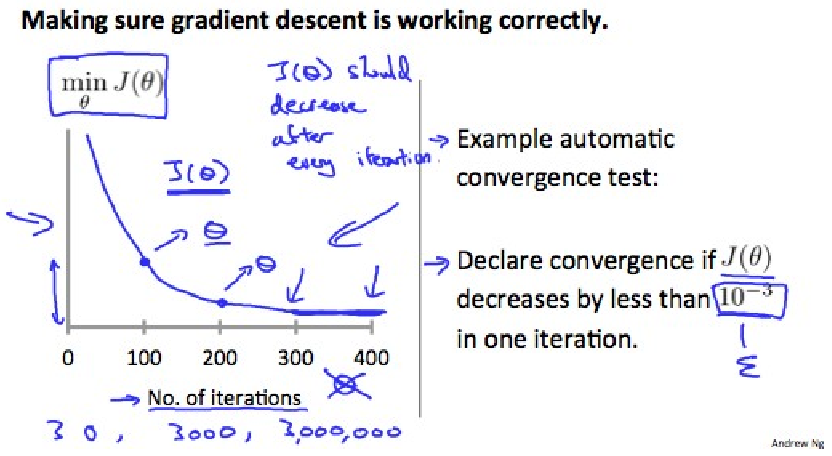
Note that dividing by the range, or dividing by the standard deviation, give different results. The quizzes in this course use range - the programming exercises use standard deviation.

For example, if x_i represents housing prices with a range of 100 to 2000 and a mean value of 1000, then, $x_i := \frac{price - 1000}{1900}$

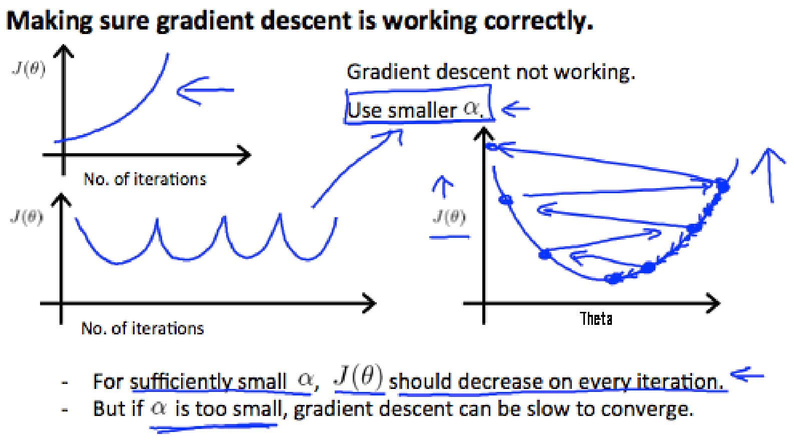
Gradient Descent in Practice II - Learning Rate

Debugging gradient descent. Make a plot with *number of iterations* on the x-axis. Now plot the cost function, J(θ) over the number of iterations of gradient descent. If J(θ) ever increases, then you probably need to decrease α.

Automatic convergence test. Declare convergence if J(θ) decreases by less than E in one iteration, where E is some small value such as 10^{-3}. However in practice it's difficult to choose this threshold value.



It has been proven that if learning rate α is sufficiently small, then J(θ) will decrease on every iteration.



To summarize:

<u>If α is too small: slow convergence.</u>

<u>If α is too large: may not decrease on every iteration and thus may not converge.</u>

Features and Polynomial Regression

We can improve our features and the form of our hypothesis function in a couple different ways.

We can **combine** multiple features into one. For example, we can combine x_1 and x_2 into a new feature x_3 by taking $x_1 \cdot x_2$.

Polynomial Regression

Our hypothesis function need not be linear (a straight line) if that does not fit the data well.

We can **change the behavior or curve** of our hypothesis function by making it a quadratic, cubic or square root function (or any other form).

For example, if our hypothesis function is $h_\theta(x) = \theta_0 + \theta_1 x_1$ then we can create additional features based on x_1 , to get the quadratic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$ or the cubic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x^3$.

In the cubic version, we have created new features x_2 and x_3 where $x_2 = x_1^2$ and $x_3 = x_1^3$.

To make it a square root function, we could do: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 \sqrt{x_1}$

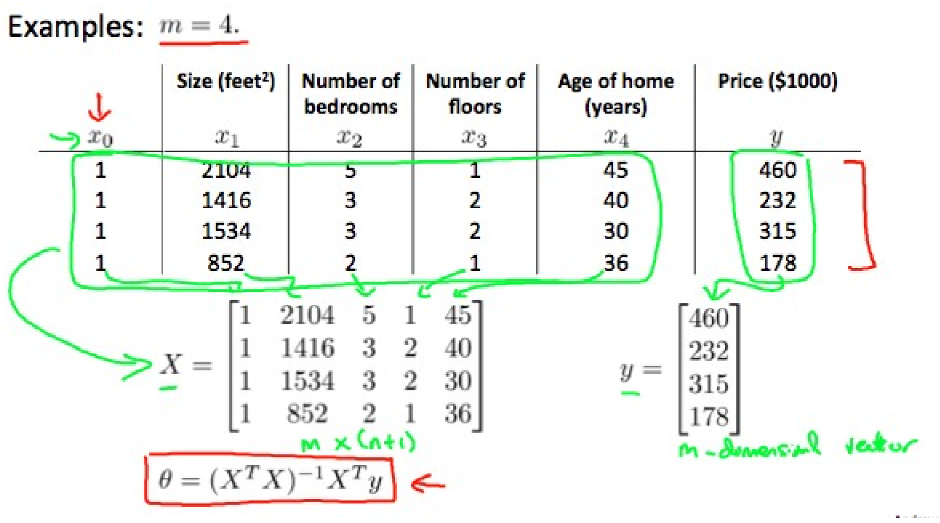
One important thing to keep in mind is, **if you choose your features this way then feature scaling becomes very important**.

eg. if x_1 has range 1 - 1000 then range of x_1^2 becomes 1 - 1000000 and that of x_1^3 becomes 1 - 1000000000

Normal Equation for linear regression

Gradient descent gives one way of minimizing J. Let's discuss a second way of doing so, this time performing the minimization explicitly and without resorting to an iterative algorithm. In the "Normal Equation" method, we will minimize J by explicitly taking its derivatives with respect to the θj 's, and setting them to zero. This allows us to find the optimum theta without iteration. The normal equation formula is given below:

$$\theta = (X^T X)^{-1} X^T y$$



Examples: $\underline{m = 4.}$

	Size (feet²)	Number of bedrooms	Number of floors	Age of home (years)	Price ($1000)
x_0	x_1	x_2	x_3	x_4	y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178

$$\underline{X} = \underbrace{\begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}}_{m \times (n+1)} \qquad \underline{y} = \underbrace{\begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}}_{m\text{-dimensional vector}}$$

$$\boxed{\theta = (X^T X)^{-1} X^T y} \leftarrow$$

There is **no need** to do feature scaling with the normal equation.

The following is a comparison of gradient descent and the normal equation:

Gradient Descent	Normal Equation
Need to choose alpha	No need to choose alpha
Needs many iterations	No need to iterate
O (kn^2)	O (n^3), need to calculate inverse of $X^T X$
Works well when n is large	Slow if n is very large

With the normal equation, computing the inversion has complexity $O(n^3)$. So if we have a very large number of features, the normal equation will be slow. In practice, when n exceeds 10,000 it might be a good time to go from a normal solution to an iterative process.

Normal Equation Noninvertibility

When implementing the normal equation in octave we want to use the 'pinv' function rather than 'inv.' The 'pinv' function will give you a value of θ even if $X^T X$ is not invertible.

If $X^T X$ is **noninvertible,** the common causes might be having:

- Redundant features, where two features are very closely related (i.e. they are linearly dependent)
- Too many features for too little trainings (e.g. m ≤ n). In this case, delete some features or use "regularization" (to be explained in a later lesson).

Solutions to the above problems include deleting a feature that is linearly dependent with another or deleting one or more features when there are too many features.

Classification problems: Logistic regression

To attempt classification, one method is to use linear regression and map all predictions greater than 0.5 as a 1 and all less than 0.5 as a 0. However, this method doesn't work well because classification is not actually a linear function.

The classification problem is just like the regression problem, except that the values we now want to predict take on only a small number of discrete values. For now, we will focus on the **binary classification problem** in which *y* can take on only two values, 0 and 1. (Most of what we say here will also generalize to the multiple-class case.) For instance, if we are trying to build a spam classifier for email, then $x^{(i)}$ may be some features of a piece of email, and *y* may be 1 if it is a piece of spam mail, and 0 otherwise. Hence, $y \in \{0,1\}$. 0 is also called the negative class, and 1 the positive class, and they are sometimes also denoted by the symbols "-" and "+." Given $x^{(i)}$, the corresponding $y^{(i)}$ is also called the label for the training example.

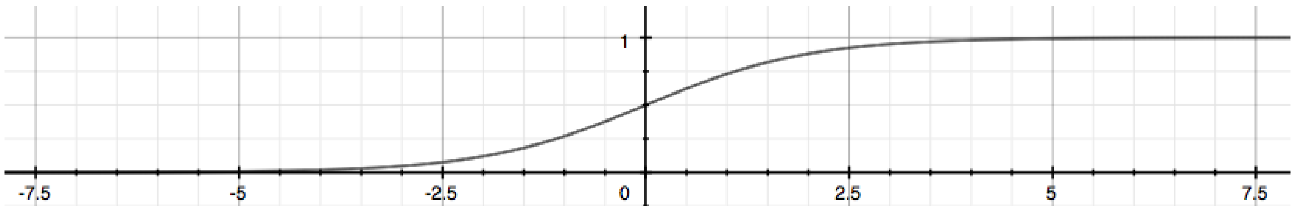
Hypothesis Representation

We could approach the classification problem ignoring the fact that y is discrete-valued, and use our old linear regression algorithm to try to predict y given x. However, it is easy to construct examples where this method performs very poorly. Intuitively, it also doesn't make sense for $h_\theta(x)$ take values larger than 1 or smaller than 0 when we know that y ∈ {0, 1}. To fix this, let's change the form for our hypotheses $h_\theta(x)$ to satisfy $0 \leq h_\theta(x) \leq 1$. This is accomplished by plugging $\theta^T x$ into the Logistic Function.

Our new form uses the "Sigmoid Function," also called the "Logistic Function":

$$h_\theta(x) = g(\theta^T x)$$
$$z = \theta^T x$$
$$g(z) = \frac{1}{1+e^{-z}}$$

The following image shows us what the sigmoid function looks like:



The function g(z), shown here, maps any real number to the (0, 1) interval, making it useful for transforming an arbitrary-valued function into a function better suited for classification.

will give us the **probability** that our output is 1. For example $h_\theta(x)=0.7$, gives us a probability of 70% that our output is 1. Our probability that our prediction is 0 is just the complement of our probability that it is 1 (e.g. if probability that it is 1 is 70%, then the probability that it is 0 is 30%).

$$h_\theta(x)=P(\ y=1\,|\,x\ ;\ \theta\ )=1-P(\ y=0\,|\,x\ ;\ \theta\ )\Rightarrow P(\ y=1\,|\,x\ ;\ \theta\ )+P(\ y=0\,|\,x\ ;\ \theta\ )=1$$

Decision Boundary

In order to get our discrete 0 or 1 classification, we can translate the output of the hypothesis function as follows:

$$h_\theta(x)\geq 0.5 \rightarrow y=1$$
$$h_\theta(x)\leq 0.5 \rightarrow y=0$$

The way our logistic function g behaves is that when its input is greater than or equal to zero, its output is greater than or equal to 0.5: $g(z)\geq 0.5\, when\, z\geq 0$.

Remember:
$$If\ z=0, then\, e^0=1\Rightarrow g(z)=1/2$$
$$If\ z\rightarrow\infty, then\, e^{-\infty}\rightarrow 0\Rightarrow g(z)=1$$
$$If\ z\rightarrow-\infty, then\, e^{\infty}\rightarrow\infty\Rightarrow g(z)=0$$

So if our input to g is $\theta^T X$, then that means: $h_\theta(x)=g(\theta^T x)\geq 0.5\, when\, \theta^T x\geq 0$

From these statements we can now say: $\theta^T x\geq 0\Rightarrow y=1\ ;\ \theta^T x<0\Rightarrow y=0$

The **decision boundary** is the line that separates the area where y = 0 and where y = 1. It is created by our hypothesis function.

Example:

$$\theta=\begin{matrix}5\\-1\\0\end{matrix}$$
$$y=1\ if\ 5+(-1)x_1+0x_2\geq 0$$
$$5-x_1\geq 0$$
$$-x_1\geq -5$$
$$x_1\leq 5$$

In this case, our decision boundary is a straight vertical line placed on the graph where $x_1=5$, and everything to the left of that denotes y = 1, while everything to the right denotes y = 0.

Again, the input to the sigmoid function g(z) (e.g. $\theta^T X$) doesn't need to be linear, and could be a function that describes a circle (e.g. $z=\theta_0+\theta_1 x_1^2+\theta_2 x_2^2$) or any shape to fit our data.

Cost Function

We cannot use the same cost function that we use for linear regression because the Logistic Function will cause the output to be wavy, causing many local optima. In other words, it will not be a convex function.

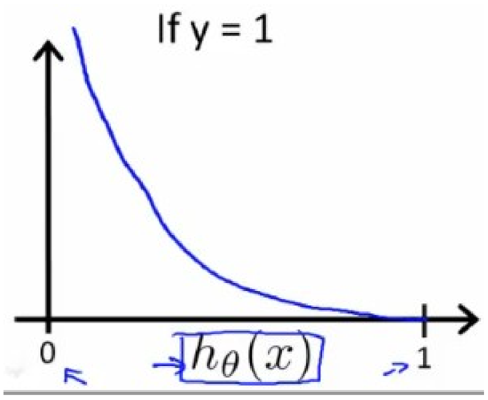
Instead, our cost function for logistic regression looks like:

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

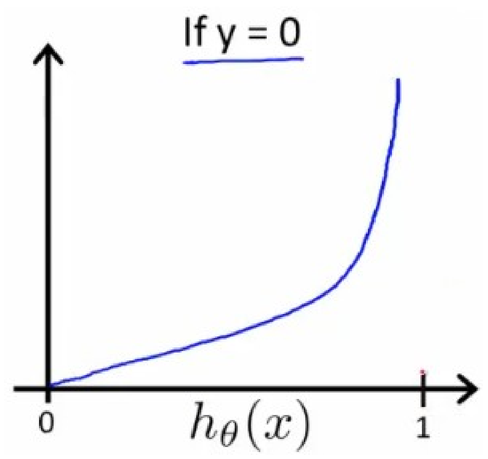
$$\mathrm{Cost}(h_\theta(x), y) = -\log(h_\theta(x)) \qquad \text{if } y = 1$$

$$\mathrm{Cost}(h_\theta(x), y) = -\log(1 - h_\theta(x)) \qquad \text{if } y = 0$$

When y = 1, we get the following plot for $J(\theta)\, vs\, h_\theta(x)$:



Similarly, when y = 0, we get the following plot for $J(\theta)\, vs\, h_\theta(x)$:



$$\mathrm{Cost}(h_\theta(x), y) = 0 \text{ if } h_\theta(x) = y$$

$$\mathrm{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 0 \text{ and } h_\theta(x) \to 1$$

$$\mathrm{Cost}(h_\theta(x), y) \to \infty \text{ if } y = 1 \text{ and } h_\theta(x) \to 0$$

If our correct answer 'y' is 0, then the cost function will be 0 if our hypothesis function also outputs 0. If our hypothesis approaches 1, then the cost function will approach infinity.

If our correct answer 'y' is 1, then the cost function will be 0 if our hypothesis function outputs 1. If our hypothesis approaches 0, then the cost function will approach infinity.

Note that writing the cost function in this way guarantees that J(θ) is convex for logistic regression.

Simplified Cost Function and Gradient

We can compress our cost function's two conditional cases into one case:

$$Cost(h_\theta(x), y) = -y\log(h_\theta(x)) - (1-y)\log(1-h_\theta(x))$$

Notice that when y is equal to 1, then the second term $(1-y)\log(1-h_\theta(x))$ will be zero and will not affect the result. If y is equal to 0, then the first term $-y\log(h_\theta(x))$ will be zero and will not affect the result.

We can fully write out our entire cost function as follows:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\log(h_\theta(x^{(i)})) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))]$$

A vectorized implementation is:

$$h = g(X\theta)$$
$$J(\theta) = \frac{1}{m}\cdot -y^T\log(h) - (1-y^T)\log(1-h)$$

Gradient Descent for logistic regression

Remember that the general form of gradient descent is:

```
Repeat {
  $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$
}
```

We can work out the derivative part using calculus to get:

```
Repeat {
  $\theta_j := \theta_j - \frac{\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$
}
```

Notice that this algorithm is identical to the one we used in linear regression. We still have to simultaneously update all values in theta.

A vectorized implementation is:

$$\theta := \theta - \frac{\alpha}{m}X^T(g(X\theta) - \vec{y})$$

Advanced Optimization

"Conjugate gradient", "BFGS", and "L-BFGS" are more sophisticated, faster ways to optimize θ that can be used instead of gradient descent. We suggest that you should not write these more sophisticated algorithms yourself (unless you are an expert in numerical computing) but use the libraries instead, as they're already tested and highly optimized. Octave provides them.

We first need to provide a function that evaluates the following two functions for a given input value θ:

$$J(\theta)$$
$$\frac{\partial}{\partial j} J(\theta)$$

We can write a single function that returns both of these:

```
function [jVal, gradient] = costFunction(theta)
  jVal = [...code to compute J(theta)...];
  gradient = [...code to compute derivative of J(theta)...];
end
```

Then we can use octave's "fminunc()" optimization algorithm along with the "optimset()" function that creates an object containing the options we want to send to "fminunc()".

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
   [optTheta, functionVal, exitFlag] = fminunc(@costFunction, initialTheta, options);

```

We give to the function "fminunc()" our cost function, our initial vector of theta values, and the "options" object that we created beforehand.

Multiclass Classification: Ove-vs-all

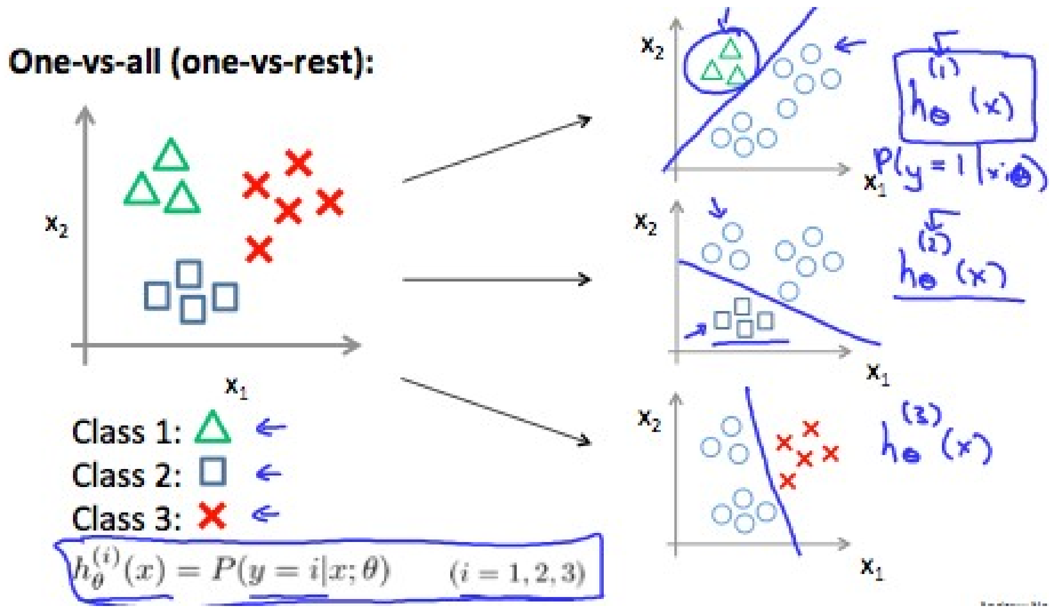
Now we will approach the classification of data when we have more than two categories. Instead of y = {0,1} we will expand our definition so that y = {0,1..., n}.

Since y = {0,1..., n}, we divide our problem into n+1 (+1 because the index starts at 0) binary classification problems; in each one, we predict the probability that 'y' is a member of one of our classes.

$$\begin{aligned}
&y \in \{0, 1 \ldots n\} \\
&h_\theta^{(0)}(x) = P(y = 0 | x; \theta) \\
&h_\theta^{(1)}(x) = P(y = 1 | x; \theta) \\
&\cdots \\
&h_\theta^{(n)}(x) = P(y = n | x; \theta) \\
&\text{prediction} = \max_i (h_\theta^{(i)}(x))
\end{aligned}$$

We are basically choosing one class and then lumping all the others into a single second class. We do this repeatedly, applying binary logistic regression to each case, and then use the hypothesis that returned the highest value as our prediction.

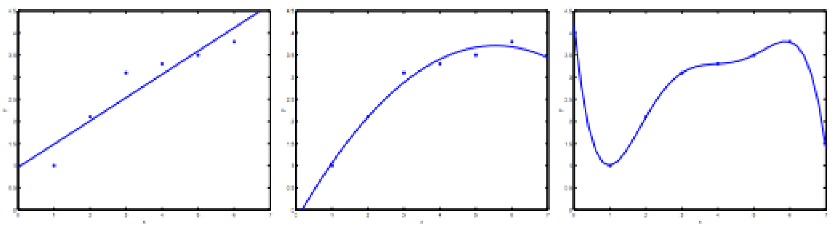
The following image shows how one could classify 3 classes:



Regularization

The Problem of Overfitting

Consider the problem of predicting y from x ∈ R. The leftmost figure below shows the result of fitting a $y=\theta_0+\theta_1 x$ to a dataset. We see that the data doesn't really lie on straight line, and so the fit is not very good.



Instead, if we had added an extra feature x^2 and fit $y=\theta_0+\theta_1 x+\theta_2 x^2$, then we obtain a slightly better fit to the data (See middle figure). Naively, it might seem that the more features we add, the better. However, there is also a danger in adding too many features: The rightmost figure is the result of fitting a 5th order polynomial $y=\sum_{j=0}^{m}\theta_j x^j$. We see that even though the fitted curve passes through the data perfectly, we would not expect this to be a very good predictor of, say, housing prices (y) for different living areas (x). Without formally defining what these terms mean, we'll say the figure on the left shows an instance of **underfitting**—in which the data clearly shows structure not captured by the model—and the figure on the right is an example of **overfitting**.

Underfitting, or high bias, is when the form of our hypothesis function h maps poorly to the trend of the data. It is usually caused by a function that is too simple or uses too few features. At the other extreme, overfitting, or high variance, is caused by a hypothesis function that fits the available data but does not generalize well to predict new data. It is usually caused by a complicated function that creates a lot of unnecessary curves and angles unrelated to the data.

This terminology is applied to both linear and logistic regression. There are two main options to address the issue of overfitting:

1) Reduce the number of features:

- Manually select which features to keep.
- Use a model selection algorithm (studied later in the course).

2) Regularization

- Keep all the features, but reduce the magnitude of parameters θ_j .
- Regularization works well when we have a lot of slightly useful features.

Cost Funtion

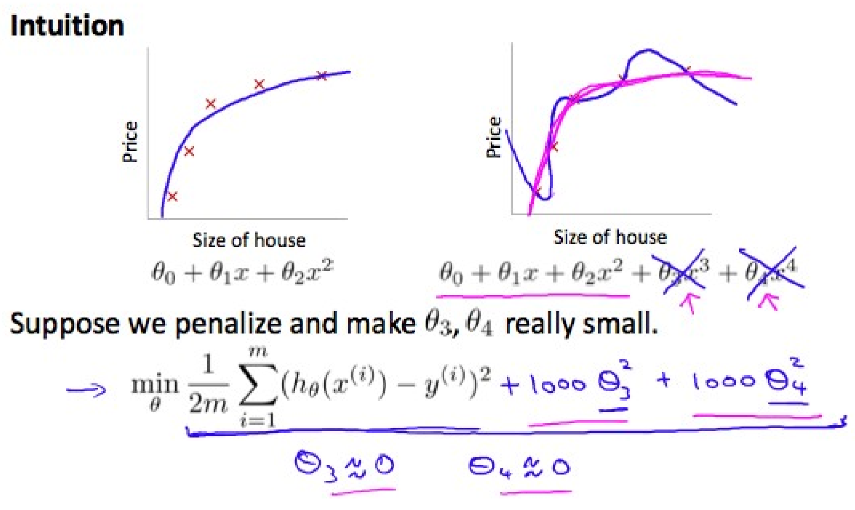
If we have overfitting from our hypothesis function, we can reduce the weight that some of the terms in our function carry by increasing their cost.

Say we wanted to make the following function more quadratic: $\theta_0+\theta_1x+\theta_2x^2+\theta_3x^3+\theta_4x^4$

We'll want to eliminate the influence of θ_3x^3 and θ_4x^4 . Without actually getting rid of these features or changing the form of our hypothesis, we can instead modify our **cost function**:

$$min\theta \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2+1000\cdot\theta_3^2+1000\cdot\theta_4^2$$

We've added two extra terms at the end to inflate the cost of θ_3 and θ_4 . Now, in order for the cost function to get close to zero, we will have to reduce the values of θ_3 and θ_4 to near zero. This will in turn greatly reduce the values of θ_3x^3 and θ_4x^4 in our hypothesis function. As a result, we see that the new hypothesis (depicted by the pink curve) looks like a quadratic function but fits the data better due to the extra small terms θ_3x^3 and θ_4x^4 .


Intuition

$\theta_0+\theta_1x+\theta_2x^2$

$\underline{\theta_0+\theta_1x+\theta_2x^2}+\cancel{\theta_3x^3}+\cancel{\theta_4x^4}$

Suppose we penalize and make θ_3, θ_4 really small.

$$\rightarrow \underline{\min_\theta \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2 + 1000\,\theta_3^2 + 1000\,\theta_4^2}$$

$\underline{\theta_3 \approx 0}$ $\underline{\theta_4 \approx 0}$

We could also regularize all of our theta parameters in a single summation as:

$$min\theta \ \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2+\lambda\sum_{j=1}^{m}\theta_j^2$$

The λ, or lambda, is the **regularization parameter**. It determines how much the costs of our theta parameters are inflated.

Using the above cost function with the extra summation, we can smooth the output of our hypothesis function to reduce overfitting. If lambda is chosen to be too large, it may smooth out the function too much and cause underfitting. Hence, what would happen if λ=0 is too small ?

Regularized Linear Regression

We can apply regularization to both linear regression and logistic regression. We will approach linear regression first.

Gradient Descent

We will modify our gradient descent function to separate out θ_0 from the rest of the parameters because we do not want to penalize θ_0 .

```
Repeat {
    $\theta_0 := \theta_0 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$
    $\theta_j := \theta_j - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j$        $j \in \{1, 2...n\}$
}
```

The term $\frac{\lambda}{m}\theta_j$ performs our regularization. With some manipulation our update rule can also be represented as:

$$\theta_j := \theta_j(1-\alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})x_j^{(i)}$$

The first term in the above equation, $1-\alpha\frac{\lambda}{m}$, will always be less than 1. Intuitively you can see it as reducing the value of θ_j by some amount on every update. Notice that the second term is now exactly the same as it was before.

Normal Equation

Now let's approach regularization using the alternate method of the non-iterative normal equation.

To add in regularization, the equation is the same as our original, except that we add another term inside the parentheses:

$$\theta = X^T X + \lambda \cdot L^{-1} X^T y$$

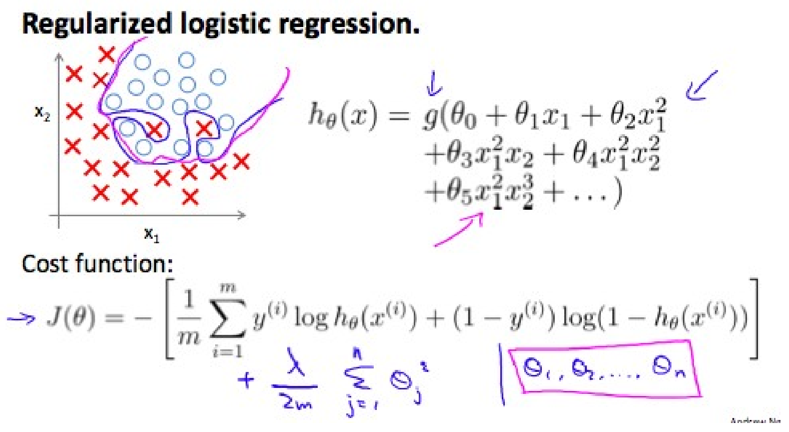
$$\text{where } L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

L is a matrix with 0 at the top left and 1's down the diagonal, with 0's everywhere else. It should have dimension (n+1)×(n+1). Intuitively, this is the identity matrix (though we are not including x_0 , multiplied with a single real number λ.

Recall that if m < n, then $X^T X$ is non-invertible. However, when we add the term λ⋅L, then $X^T X + \lambda \cdot L$ becomes invertible.

Regularized Logistic Regression

We can regularize logistic regression in a similar way that we regularize linear regression. As a result, we can avoid overfitting. The following image shows how the regularized function, displayed by the pink line, is less likely to overfit than the non-regularized function represented by the blue line:


Regularized logistic regression.
x_2
x_1
$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$
Cost function:
$J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log(1-h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$
$\theta_1, \theta_2, \dots, \theta_n$
Andrew Ng

Cost Function

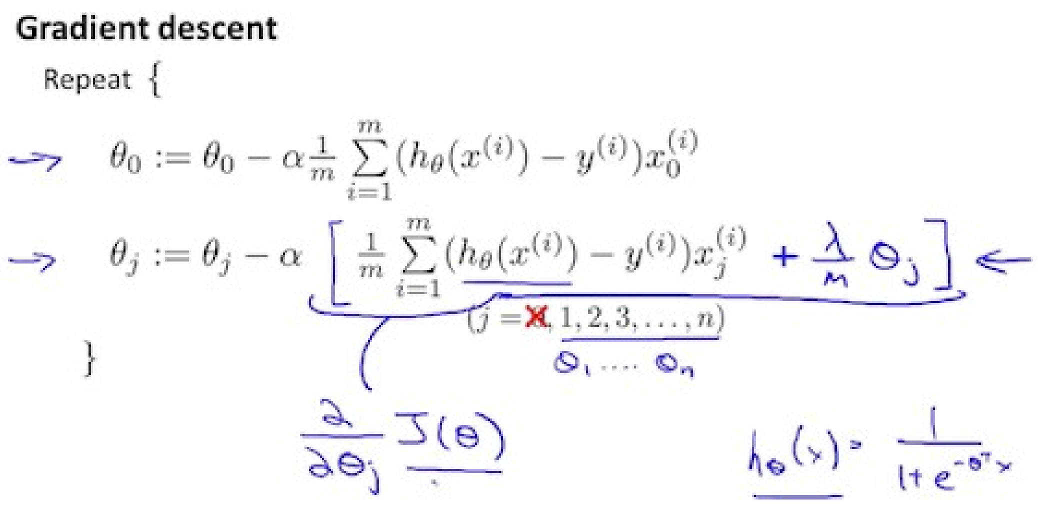
Recall that our cost function for logistic regression was:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)} \log(h_\theta(x^{(i)})) + (1-y^{(i)}) \log(1-h_\theta(x^{(i)}))]$$

We can regularize this equation by adding a term to the end:

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

The second sum, $\sum_{j=1}^{n}\theta_j^2$ **means to explicitly exclude** the bias term, θ_0 : i.e. the θ vector is indexed from 0 to n (holding n+1 values, θ_0 through θ_n , and this sum explicitly skips θ_0 by running from 1 to n, skipping 0. Thus, when computing the equation, we should continuously update the two following equations:



Gradient descent

Repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j \right]$$

$$(j = \cancel{0}, 1, 2, 3, \dots, n)$$

$$\theta_1 \dots \theta_n$$

}

$$\frac{\partial}{\partial \theta_j} J(\theta) \qquad h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

Neural networks

Model Representation

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: $[x_0 x_1 x_2] \rightarrow [\ ] \rightarrow h_\theta(x)$

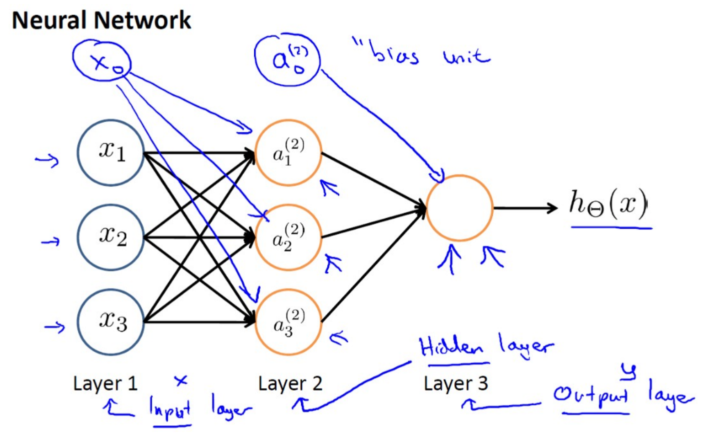
Our input nodes (layer 1), also known as the "input layer", go into another node (layer 2), which finally outputs the hypothesis function, known as the "output layer".

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:

$$[x_0 x_1 x_2 x_3] \rightarrow [a_1^{(2)} a_2^{(2)} a_3^{(3)}] \rightarrow h_\theta(x)$$



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

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

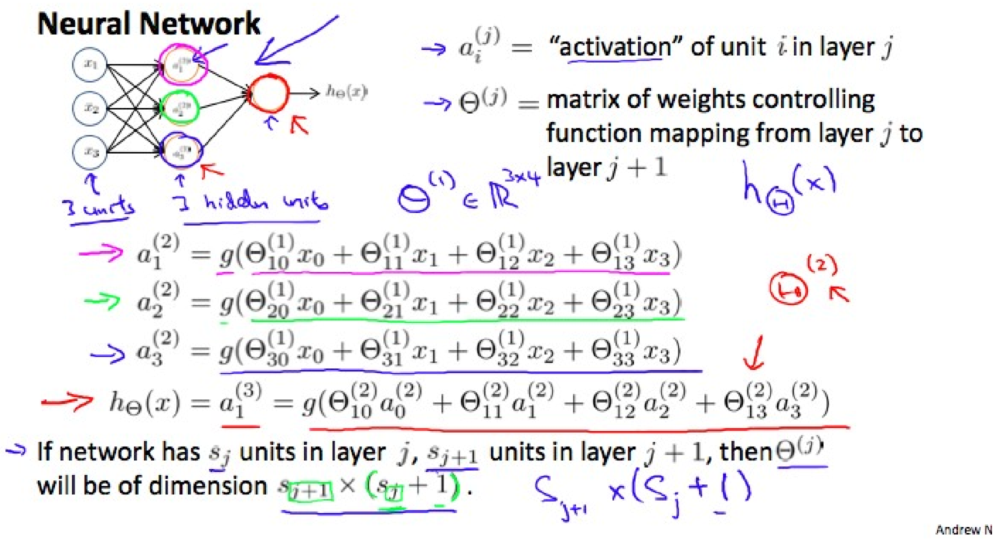
This is saying that we compute our activation nodes by using a 3×4 matrix of parameters. We apply each row of the parameters to our inputs to obtain the value for one activation node. Our hypothesis output is the logistic function applied to the sum of the values of our activation nodes, which have been 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

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

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

x_1
x_2
x_3
$h_\Theta(x)$
3 units
3 hidden units
$\Theta^{(1)} \in \mathbb{R}^{3\times4}$
$h_\Theta(x)$
$\Theta^{(2)}$

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

→ 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 $s_{j+1}\times(s_j+1)=4\times3$.

Now we'll do a vectorized implementation of the functions:

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

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:

$$a_1^{(2)}=g\left(z_1^{(2)}\right)$$
$$a_2^{(2)}=g\left(z_2^{(2)}\right)$$
$$a_3^{(2)}=g\left(z_3^{(2)}\right)$$

In other words, for layer j=2 and node k, the variable z will be: $z_k^{(2)}=\Theta_{k,0}^{(1)}x_0^{(1)}+\Theta_{k,1}^{(1)}x_1^{(1)}+\cdots+\Theta_{k,n}^{(1)}x_n^{(1)}$

The vector representation of x and z^j is:

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

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:

$$a^{(j)}=g\left(z^{(j)}\right)$$

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:

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

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

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.

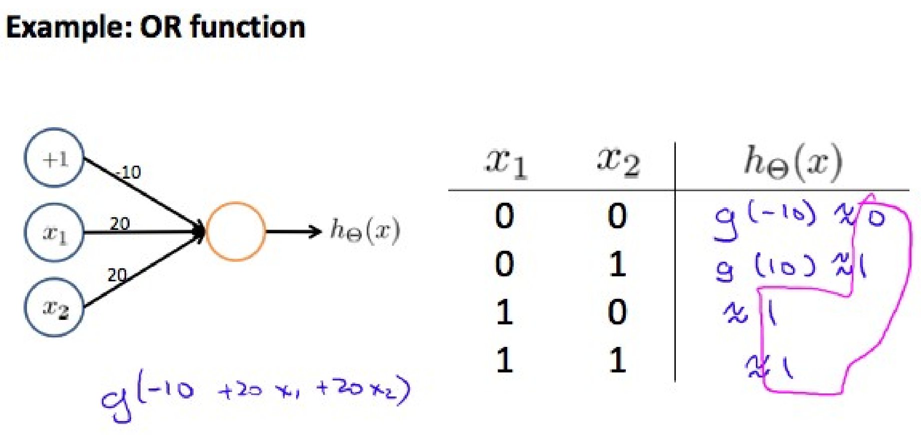
The graph of our functions will look like: $\begin{array}{l} x_0 \\ x_1 \rightarrow g(z^{(2)}) \rightarrow h_\Theta(x) \\ x_2 \end{array}$

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

Let's set our first theta matrix as: $\Theta^{(1)} = [-30 \quad 20 \quad 20]$

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

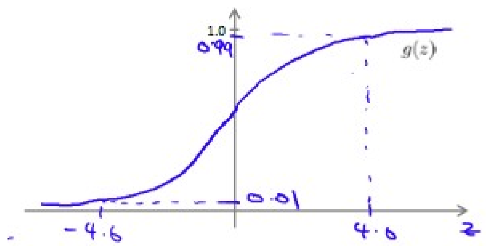
So we have constructed one of the fundamental operations in computers by using a small neural network rather than using an actual AND gate. Neural networks can also be used to simulate all the other logical gates. The following is an example of the logical operator 'OR', meaning either x_1 is true or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



Example: OR function

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

Where g(z) is the following:



Observe that $\begin{array}{l} g(-4.6) = 0.01 \approx 0 \\ g(4.6) = 0.99 \approx 1 \end{array}$, so that's the reason we consider $\begin{array}{l} g(10) \approx 1 \\ g(-10) \approx 0 \end{array}$

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

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

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): $\begin{array}{c} x_0 \\ x_1 \\ x_2 \end{array} \rightarrow \begin{array}{c} a_1^{(2)} \\ a_2^{(2)} \end{array} \rightarrow h_\Theta(x)$.

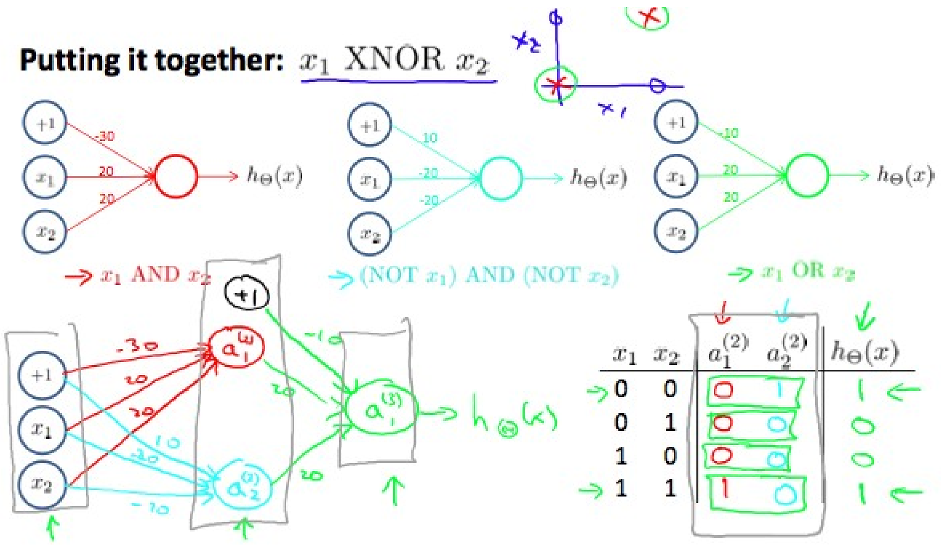
For the transition between the first and second layer, we'll use a $\Theta^{(1)}$ matrix that combines the values for AND and NOR: $\Theta^{(1)} = \begin{bmatrix} -30 & 20 & 20 \\ 10 & -20 & -20 \end{bmatrix}$

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

$\Theta^{(2)} = [-10 \quad 20 \quad 20]$

Let's write out the values for all our nodes: $\begin{array}{l} a^{(2)} = g(\Theta^{(1)} \cdot x) \\ a^{(3)} = g(\Theta^{(2)} \cdot a^{(2)}) \\ h_\Theta(x) = a^{(3)} \end{array}$

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

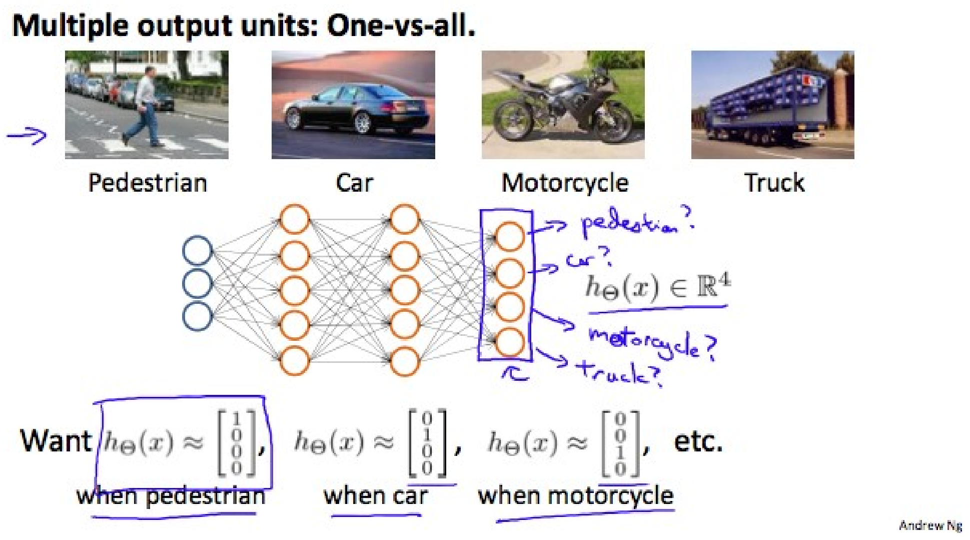


Putting it together: x_1 XNOR x_2
x_2
x_1
+1
x_1
x_2
-30
20
20
$h_\Theta(x)$
10
-20
-20
-10
$\rightarrow$ x_1 AND x_2
$\rightarrow$ (NOT x_1) AND (NOT x_2)
$\rightarrow$ x_1 OR x_2
$a_1^{(2)}$
$a_2^{(2)}$
$a_1^{(3)}$
$h_\Theta(x)$

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

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:



Multiple output units: One-vs-all.
Pedestrian
Car
Motorcycle
Truck
pedestrian?
car?
$h_\Theta(x) \in \mathbb{R}^4$
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
Andrew Ng

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:

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

Our resulting hypothesis for one set of inputs may look like: $h_\Theta(x) = [0010]$, in which case our resulting class is the third one down, or $h_\Theta(x)_3$ which represents the motorcycle.

Cost function

Let's first define a few variables that we will need to use:

- L = total number of layers in the network
- s_l = number of units (not counting bias unit) in layer l
- K = number of output units/classes

Recall that in neural networks, we may have many output nodes. We denote $h_\Theta(x)_k$ as being a hypothesis that results in the k^{th} output. Our cost function for neural networks is going to be a generalization of the one we used for logistic regression. Recall that the cost function for regularized logistic regression was:

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

For neural networks, it is going to be slightly more complicated:

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

We have added a few nested summations to account for our multiple output nodes. In the first part of the equation, before the square brackets, we have an additional nested summation that loops through the number of output nodes.

In the regularization part, after the square brackets, we must account for multiple theta matrices. The number of columns in our current theta matrix is equal to the number of nodes in our current layer (including the bias unit). The number of rows in our current theta matrix is equal to the number of nodes in the next layer (excluding the bias unit). As before with logistic regression, we square every term.

Note:

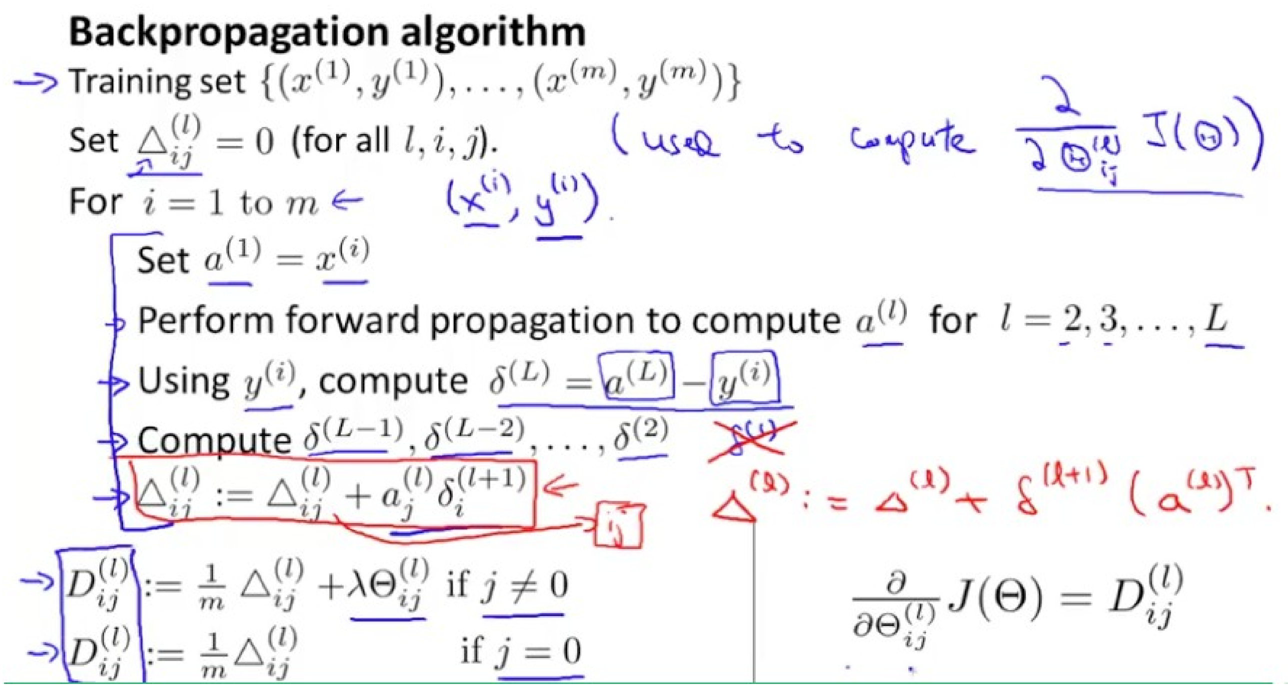
- the double sum simply adds up the logistic regression costs calculated for each cell in the output layer
- the triple sum simply adds up the squares of all the individual Θs in the entire network.
- the *i* in the triple sum does **not** refer to training example *i*

Backpropagation Algorithm

"Backpropagation" is neural-network terminology for minimizing our cost function, just like what we were doing with gradient descent in logistic and linear regression. Our goal is to compute: $\min_{\Theta} J(\Theta)$

That is, we want to minimize our cost function J using an optimal set of parameters in theta. In this section we'll look at the equations we use to compute the partial derivative of J(Θ): $\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta)$

To do so, we use the following algorithm:



Backpropagation algorithm

```
→ Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$
  Set $\triangle_{ij}^{(l)} = 0$ (for all $l, i, j$).     (used to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$)
  For $i = 1$ to $m$ ←     $(x^{(i)}, y^{(i)})$.
      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 $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$   $\cancel{\delta^{(1)}}$
      → $\boxed{\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}}$ ←   $\boxed{ij}$   $\triangle^{(l)} := \triangle^{(l)} + \delta^{(l+1)} (a^{(l)})^T$.
→ $D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)}$ if $j \neq 0$
→ $D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)}$   if $j = 0$
```

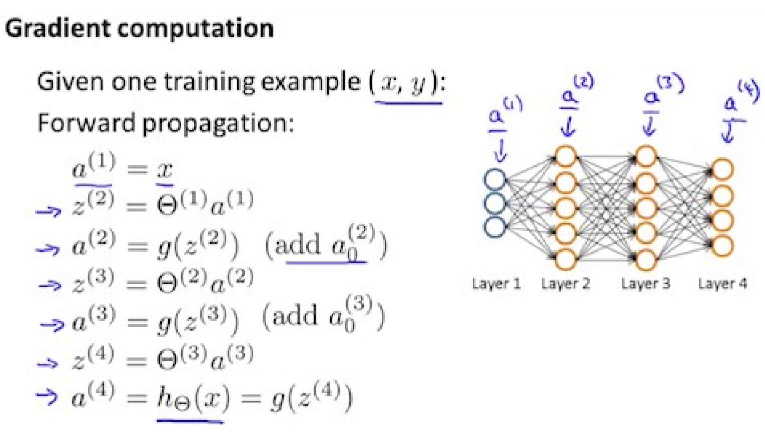
$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)}$$

So, for the back propagation Algorithm, given the training set $\{(x^{(1)}, y^{(1)}) \cdots (x^{(m)}, y^{(m)})\}$

- Set $\Delta_{i,j}^{(l)} := 0$ for all (l,i,j), (hence you end up having a matrix full of zeros)

For training example t =1 to m:

1. Set $a^{(1)} := x^{(t)}$
2. Perform forward propagation to compute $a^{(l)}$ for l=2,3,…,L



Gradient computation

Given one training example (x, y):

Forward propagation:

$a^{(1)} = x$

→ $z^{(2)} = \Theta^{(1)} a^{(1)}$

→ $a^{(2)} = g(z^{(2)})$ (add $a_0^{(2)}$)

→ $z^{(3)} = \Theta^{(2)} a^{(2)}$

→ $a^{(3)} = g(z^{(3)})$ (add $a_0^{(3)}$)

→ $z^{(4)} = \Theta^{(3)} a^{(3)}$

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

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

Where L is our total number of layers and $a^{(L)}$ is the vector of outputs of the activation units for the last layer. So our "error values" for the last layer are simply the differences of our actual results in the last layer and the correct outputs in y. To get the delta values of the layers before the last layer, we can use an equation that steps us back from right to left:

4. Compute $\delta^{(L-1)},\delta^{(L-2)},\cdots,\delta^{(2)}$ using $\delta^{(l)}=((\Theta^{(l)})^T\delta^{(l+1)}).*a^{(l)}.*(1-a^{(l)})$

The delta values of layer l are calculated by multiplying the delta values in the next layer with the theta matrix of layer l. We then element-wise multiply that with a function called g', or g-prime, which is the derivative of the activation function g evaluated with the input values given by $z^{(l)}$.

The g-prime derivative terms can also be written out as: $g'(z^{(l)})=a^{(l)}.*(1-a^{(l)})$

5. $\Delta_{i,j}^{(l)}:=\Delta_{i,j}^{(l)}+a_j^{(l)}\delta_i^{(l+1)}$ or with vectorization, $\Delta^{(l)}:=\Delta^{(l)}+\delta^{(l+1)}(a^{(l)})^T$

Hence we update our new Δ matrix.

- $D_{i,j}^{(l)}:=\frac{1}{m}(\Delta_{i,j}^{(l)}+\lambda\Theta_{i,j}^{(l)}), if\ j\neq 0.$
- $D_{i,j}^{(l)}:=\frac{1}{m}\Delta_{i,j}^{(l)}, if\ j=0$

The capital-delta matrix D is used as an "accumulator" to add up our values as we go along and eventually compute our partial derivative. Thus we get $\frac{\partial}{\partial\Theta_{ij}^{(l)}}J(\Theta)=D_{ij}^{(l)}$

Backpropagation Intuition

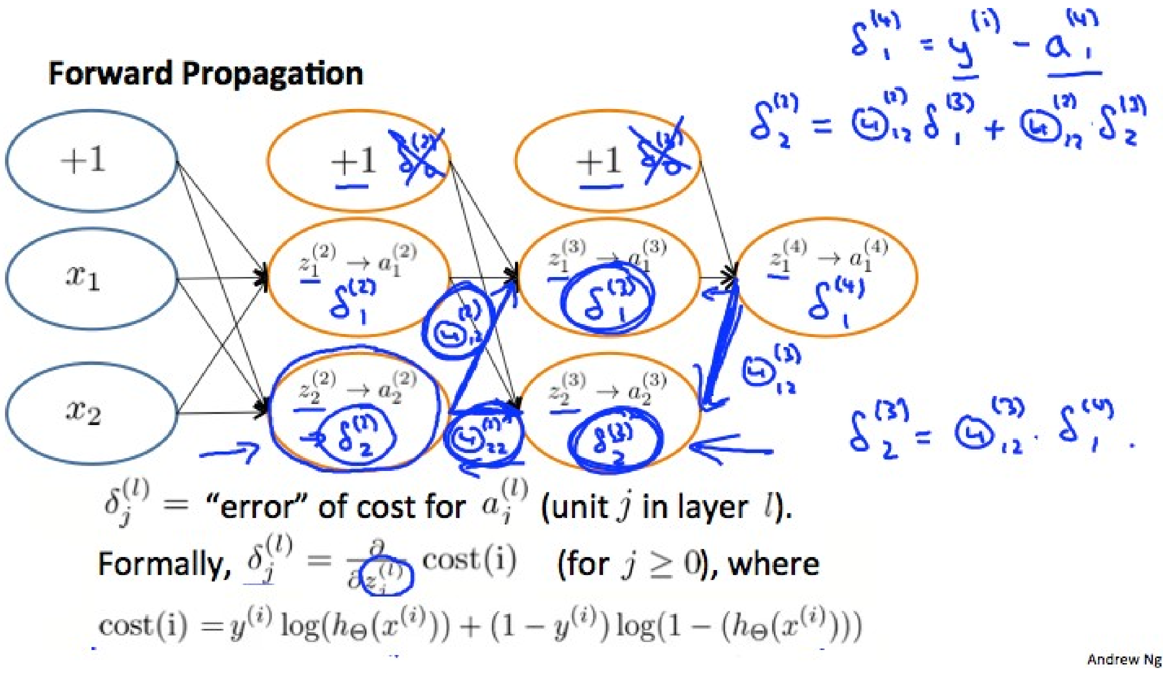
Recall that the cost function for a neural network is:

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

Intuitively, $\delta_j^{(l)}$ is the "error" for $a_j^{(l)}$ (unit j in layer l). More formally, the delta values are actually the derivative of the cost function:

$$\delta_j^{(l)}=\frac{\partial}{\partial z_j^{(l)}}cost(t)$$

Recall that our derivative is the slope of a line tangent to the cost function, so the steeper the slope the more incorrect we are. Let us consider the following neural network below and see how we could calculate some $\delta_j^{(l)}$:


Forward Propagation
+1
x_1
x_2
+1
$z_1^{(2)} \to a_1^{(2)}$
$z_2^{(2)} \to a_2^{(2)}$
+1
$z_1^{(3)} \to a_1^{(3)}$
$z_2^{(3)} \to a_2^{(3)}$
$z_1^{(4)} \to a_1^{(4)}$
$\delta_1^{(2)}$
$\delta_2^{(2)}$
$\delta_1^{(3)}$
$\delta_2^{(3)}$
$\delta_1^{(4)}$
$\Theta_{12}^{(2)}$
$\Theta_{22}^{(2)}$
$\Theta_{12}^{(3)}$
$\delta_1^{(4)} = y^{(i)} - a_1^{(4)}$
$\delta_2^{(2)} = \Theta_{12}^{(2)}\delta_1^{(3)} + \Theta_{22}^{(2)}\delta_2^{(3)}$
$\delta_2^{(3)} = \Theta_{12}^{(3)} \cdot \delta_1^{(4)}.$
Andrew Ng

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

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

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

In the image above, to calculate $\delta_2^{(2)}$, we multiply the weights $\Theta_{12}^{(2)}$ and $\Theta_{22}^{(2)}$ by their respective δ values found to the right of each edge. So we get $\delta_2^{(2)} = \Theta_{12}^{(2)} * \delta_1^{(3)} + \Theta_{22}^{(2)} * \delta_2^{(3)}$. To calculate every single possible $\delta_j^{(l)}$ we could start from the right of our diagram. We can think of our edges as our Θ_{ij}. Going from right to left, to calculate the value of $\delta_j^{(l)}$ you can just take the over all sum of each weight times the δ it is coming from. Hence, another example would be $\delta_2^{(3)} = \Theta_{12}^{(3)} * \delta_1^{(4)}$.

Implementation Notes

Unrolling Parameters

With neural networks, we are working with sets of matrices: $\Theta^{(1)}, \Theta^{(2)}, \dots, D^{(1)}, D^{(2)}, \dots$

In order to use optimizing functions such as "fminunc()", we will want to "unroll" all the elements and put them into one long vector:

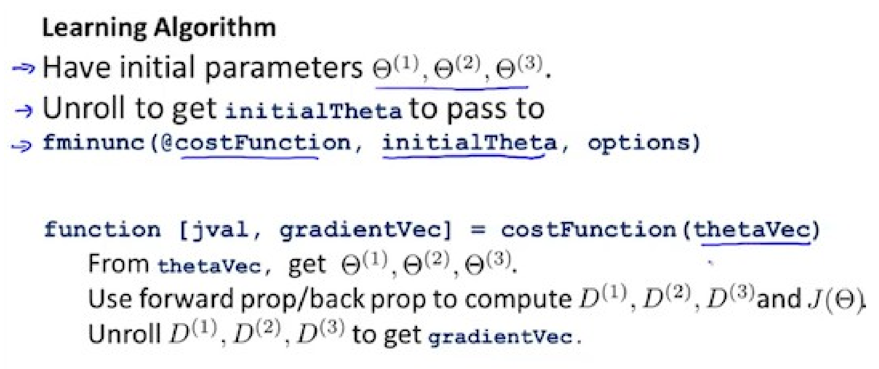
```
thetaVector = [ Theta1(:); Theta2(:); Theta3(:); ]
deltaVector = [ D1(:); D2(:); D3(:) ]
```

If the dimensions of Theta1 is 10x11, Theta2 is 10x11 and Theta3 is 1x11, then we can get back our original matrices from the "unrolled" versions as follows:

```
Theta1 = reshape(thetaVector(1:110),10,11)
Theta2 = reshape(thetaVector(111:220),10,11)
Theta3 = reshape(thetaVector(221:231),1,11)

```

To summarize:



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 $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$.
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`.

Gradient Checking

Gradient checking will assure that our backpropagation works as intended. We can approximate the derivative of our cost function with:

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

With multiple theta matrices, we can approximate the derivative **with respect to** Θ_j as follows:

$$\frac{\partial}{\partial \Theta_j} J(\Theta) \approx \frac{J(\Theta_1, \dots, \Theta_j + \epsilon, \dots, \Theta_n) - J(\Theta_1, \dots, \Theta_j - \epsilon, \dots, \Theta_n)}{2\epsilon}$$

A small value for ϵsuch as $\epsilon = 10^{-4}$, guarantees that the math works out properly. If the value for ϵ is too small, we can end up with numerical problems.

Hence, we are only adding or subtracting epsilon to the Θ_j matrix. In octave we can do it as follows:

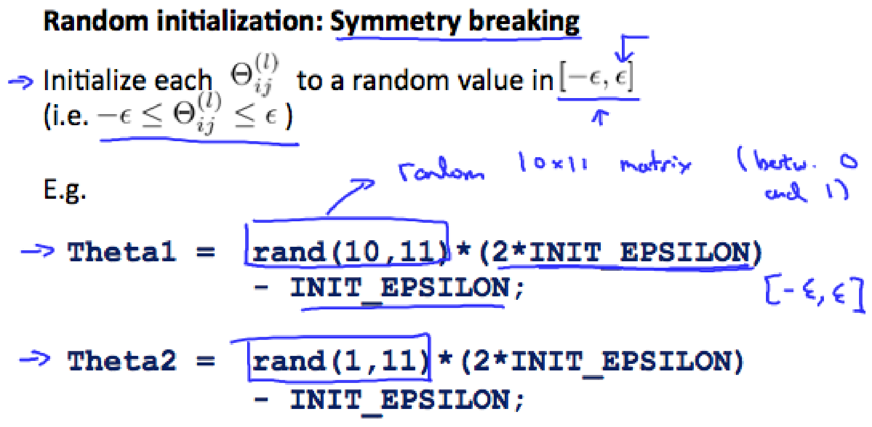
```
epsilon = 1e-4;
for i = 1:n,
  thetaPlus = theta;
  thetaPlus(i) += epsilon;
  thetaMinus = theta;
  thetaMinus(i) -= epsilon;
  gradApprox(i) = (J(thetaPlus) - J(thetaMinus))/(2*epsilon)
end;
```

We previously saw how to calculate the deltaVector. So once we compute our gradApprox vector, we can check that gradApprox ≈ deltaVector.

Once you have verified once that your backpropagation algorithm is correct, you don't need to compute gradApprox again. The code to compute gradApprox can be very slow.

Random Initialization

Initializing all theta weights to zero does not work with neural networks. When we backpropagate, all nodes will update to the same value repeatedly. Instead we can randomly initialize our weights for our Θ matrices using the following method:


Random initialization: Symmetry breaking

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

E.g. random 10×11 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;
```

Hence, we initialize each $\Theta_{ij}^{(l)}$ to a random value between$[-\epsilon,\epsilon]$. Using the above formula guarantees that we get the desired bound. The same procedure applies to all the Θ's. Below is some working code you could use to experiment.

```
If the dimensions of Theta1 is 10x11, Theta2 is 10x11 and Theta3 is 1x11.

Theta1 = rand(10,11) * (2 * INIT_EPSILON) - INIT_EPSILON;
Theta2 = rand(10,11) * (2 * INIT_EPSILON) - INIT_EPSILON;
Theta3 = rand(1,11) * (2 * INIT_EPSILON) - INIT_EPSILON;

```

rand(x,y) is just a function in octave that will initialize a matrix of random real numbers between 0 and 1.

(Note: the epsilon used above is unrelated to the epsilon from Gradient Checking)

Putting all together

First, pick a network architecture; choose the layout of your neural network, including how many hidden units in each layer and how many layers in total you want to have.

- Number of input units = dimension of features $x^{(i)}$
- Number of output units = number of classes
- Number of hidden units per layer = usually more the better (must balance with cost of computation as it increases with more hidden units)
- Defaults: 1 hidden layer. If you have more than 1 hidden layer, then it is recommended that you have the same number of units in every hidden layer.

Training a Neural Network

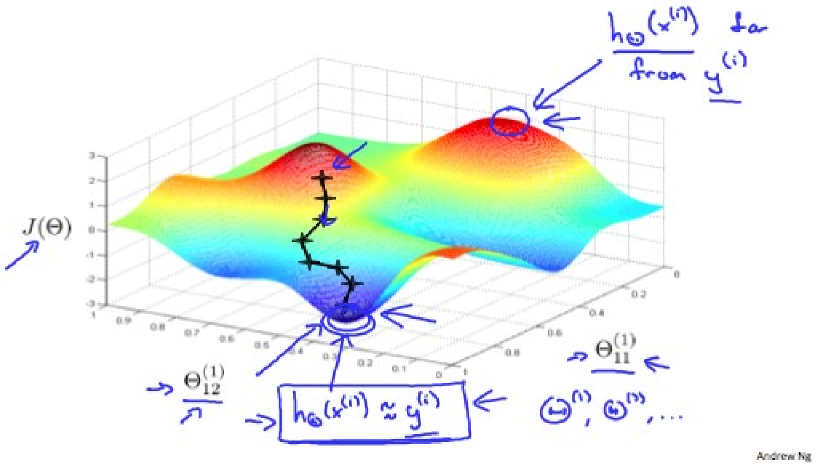
1. Randomly initialize the weights
2. Implement forward propagation to get $h_\Theta(x^{(i)})$ for any $x^{(i)}$
3. Implement the cost function
4. Implement backpropagation to compute partial derivatives

5. Use gradient checking to confirm that your backpropagation works. Then disable gradient checking.
6. Use gradient descent or a built-in optimization function to minimize the cost function with the weights in theta.

When we perform forward and back propagation, we loop on every training example:

```
for i = 1:m,
   Perform forward propagation and backpropagation using example (x(i),y(i))
   (Get activations a(l) and delta terms d(l) for l = 2,...,L
```

The following image gives us an intuition of what is happening as we are implementing our neural network:



Ideally, you want $h_\Theta(x^{(i)}) \approx y^{(i)}$. This will minimize our cost function. However, keep in mind that J(Θ)is not convex and thus we can end up in a local minimum instead.

Evaluating a Learning algorithm

Evaluating a Hypothesis

Once we have done some troubleshooting for errors in our predictions by:

- Getting more training examples
- Trying smaller sets of features
- Trying additional features
- Trying polynomial features
- Increasing or decreasing λ

We can move on to evaluate our new hypothesis.

A hypothesis may have a low error for the training examples but still be inaccurate (because of overfitting). Thus, to evaluate a hypothesis, given a dataset of training examples, we can split up the data into two sets: a **training set** and a **test set**. Typically, the training set consists of 70 % of your data and the test set is the remaining 30 %.

The new procedure using these two sets is then:

1. Learn Θ and minimize $J_{train}(\Theta)$ using the training set
2. Compute the test set error $J_{test}(\Theta)$

The test set error

1. For linear regression: J $J_{test}(\Theta)=\frac{1}{2m_{test}}\sum_{i=1}^{m_{test}}(h\Theta(x_{test}^{(i)})-y_{test}^{(i)})^2$
2. For classification ~ Misclassification error (aka 0/1 misclassification error):

$$err(h\Theta(x),y)=\begin{matrix}1: if\ h\Theta(x)\geq 0.5, y=0\ \ or\ \ h\Theta(x)<0.5, y=1\\ 0: Otherwise\end{matrix}$$

This gives us a binary 0 or 1 error result based on a misclassification. The average test error for the test set is:

$$Test_{Error}=\frac{1}{m_{test}}\sum_{i=1}^{m_{test}}err(h_\Theta(x_{test}^{(i)}),y_{test}^{(i)})$$

This gives us the proportion of the test data that was misclassified.

Model Selection and Train/ Validation/ Test Sets

Just because a learning algorithm fits a training set well, that does not mean it is a good hypothesis. It could over fit and as a result your predictions on the test set would be poor. The error of your hypothesis as measured on the data set with which you trained the parameters will be lower than the error on any other data set.

Given many models with different polynomial degrees, we can use a systematic approach to identify the 'best' function. In order to choose the model of your hypothesis, you can test each degree of polynomial and look at the error result.

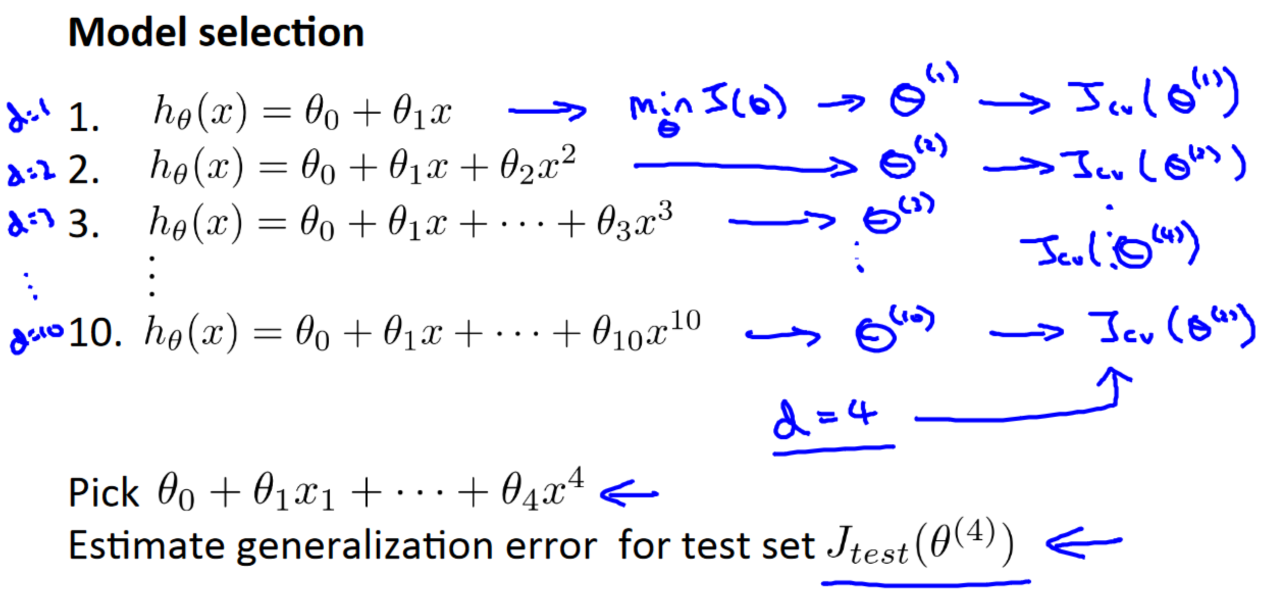
One way to break down our dataset into the three sets is:

- Training set: 60%
- Cross validation set: 20%
- Test set: 20%

We can now calculate three separate error values for the three different sets using the following method:

1. Optimize the parameters in Θ using the training set for each polynomial degree.
2. Find the polynomial degree d with the least error using the cross validation set.
3. Estimate the generalization error using the test set with $J_{test}(\Theta^{(d)})$, (d = theta from polynomial with lower error);

This way, the degree of the polynomial d has not been trained using the test set.



Model selection

1. $h_\theta(x) = \theta_0 + \theta_1 x$
2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$
3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3$

$\vdots$

10. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$

Pick $\theta_0 + \theta_1 x_1 + \cdots + \theta_4 x^4$

Estimate generalization error for test set $J_{test}(\theta^{(4)})$

Diagnosing Bias vs. Variance

In this section we examine the relationship between the degree of the polynomial d and the underfitting or overfitting of our hypothesis.

- We need to distinguish whether **bias** or **variance** is the problem contributing to bad predictions.
- High bias is underfitting and high variance is overfitting. Ideally, we need to find a golden mean between these two.

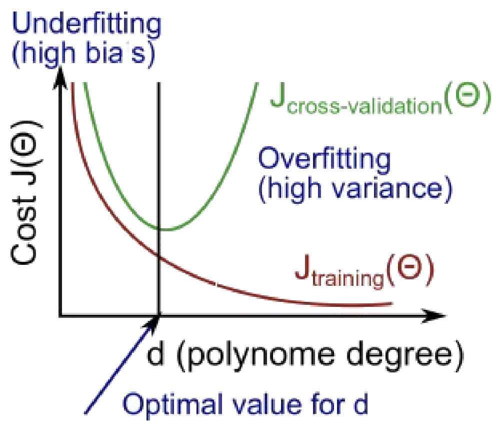
The training error will tend to **decrease** as we increase the degree d of the polynomial.

At the same time, the cross validation error will tend to **decrease** as we increase d up to a point, and then it will **increase** as d is increased, forming a convex curve.

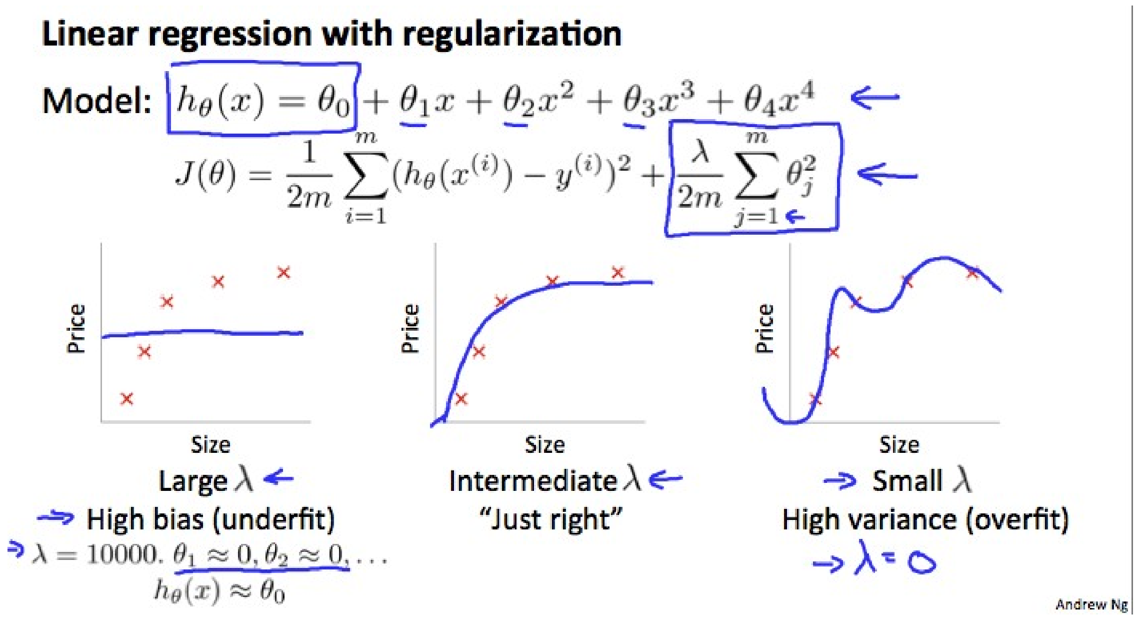
High bias (underfitting): both $J_{train}(\Theta)$ and $J_{CV}(\Theta)$ will be high. Also, $J_{CV}(\Theta) \approx J_{train}(\Theta)$

High variance (overfitting): $J_{train}(\Theta)$ will be low and $J_{CV}(\Theta)$ will be much greater than $J_{train}(\Theta)$

The is summarized in the figure below:



Regularization and Bias/ Variance



Linear regression with regularization

Model: $\boxed{h_\theta(x) = \theta_0} + \underline{\theta_1} x + \underline{\theta_2} x^2 + \underline{\theta_3} x^3 + \theta_4 x^4 \leftarrow$

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

Large $\lambda \leftarrow$

$\rightarrow$ High bias (underfit)

$\rightarrow \lambda = 10000.\ \underline{\theta_1 \approx 0, \theta_2 \approx 0}, \ldots$

$h_\theta(x) \approx \theta_0$

Intermediate $\lambda \leftarrow$

"Just right"

$\rightarrow$ Small λ

High variance (overfit)

$\rightarrow \lambda = 0$

Andrew Ng

In the figure above, we see that as λ increases, our fit becomes more rigid. On the other hand, as λ approaches 0, we tend to overfit the data. So how do we choose our parameter λto get it 'just right' ? In order to choose the model and the regularization term λ, we need to:

1. Create a list of lambdas (i.e. λ∈{0,0.01,0.02,0.04,0.08,0.16,0.32,0.64,1.28,2.56,5.12,10.24});
2. Create a set of models with different degrees or any other variants.
3. Iterate through the λs and for each λ go through all the models to learn some Θ.
4. Compute the cross validation error using the learned Θ (computed with λ) on the $J_{CV}(\Theta)$ **without** regularization or λ = 0.
5. Select the best combo that produces the lowest error on the cross validation set.

6. Using the best combo Θ and λ, apply it on $J_{test}(\Theta)$ to see if it has a good generalization of the problem.

Learning Curves

Training an algorithm on a very few number of data points (such as 1, 2 or 3) will easily have 0 errors because we can always find a quadratic curve that touches exactly those number of points. Hence:

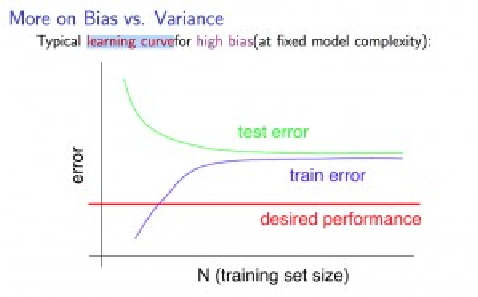
- As the training set gets larger, the error for a quadratic function increases.
- The error value will plateau out after a certain m, or training set size.

Experiencing high bias:

Low training set size: causes J_{train} to be low and $J_{CV}(\Theta)$ to be high.

Large training set size: causes both $J_{train}(\Theta)$ and $J_{CV}(\Theta)$ to be high with $J_{train}(\Theta) \approx J_{CV}(\Theta)$.

If a learning algorithm is suffering from **high bias**, getting more training data will not **(by itself)** help much.

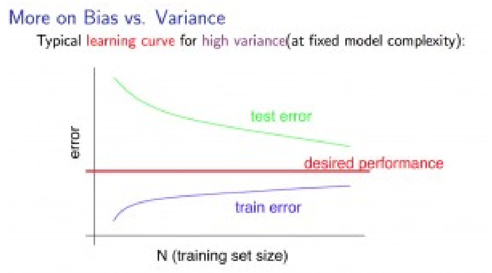


Experiencing high variance:

Low training set size: $J_{train}(\Theta)$ will be low and $J_{CV}(\Theta)$ will be high.

Large training set size: $J_{train}(\Theta)$ increases with training set size and $J_{CV}(\Theta)$ continues to decrease without leveling off. Also, $J_{train}(\Theta) < J_{CV}(\Theta)$ but the difference between them remains significant.

If a learning algorithm is suffering from **high variance**, getting more training data is likely to help.



Deciding What to Do Next - Revisited!

Our decision process can be broken down as follows:

- **Getting more training examples:** Fixes high variance
- **Trying smaller sets of features:** Fixes high variance
- **Adding features:** Fixes high bias
- **Adding polynomial features:** Fixes high bias
- **Decreasing λ:** Fixes high bias
- **Increasing λ:** Fixes high variance.

Diagnosing Neural Networks

- A neural network with fewer parameters is **prone to underfitting**. It is also **computationally cheaper**.
- A large neural network with more parameters is **prone to overfitting**. It is also **computationally expensive**. In this case you can use regularization (increase λ) to address the overfitting.

Using a single hidden layer is a good starting default. You can train your neural network on a number of hidden layers using your cross validation set. You can then select the one that performs best.

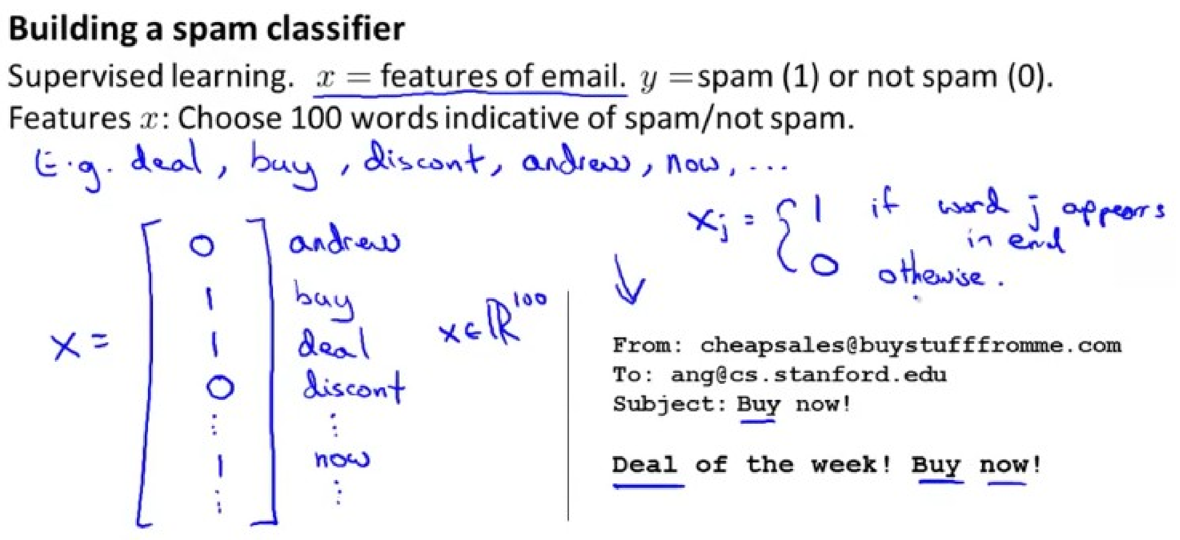
Model Complexity Effects:

- Lower-order polynomials (low model complexity) have high bias and low variance. In this case, the model fits poorly consistently.
- Higher-order polynomials (high model complexity) fit the training data extremely well and the test data extremely poorly. These have low bias on the training data, but very high variance.
- In reality, we would want to choose a model somewhere in between, that can generalize well but also fits the data reasonably well.

Prioritizing What to Work On

System Design Example:

Given a data set of emails, we could construct a vector for each email. Each entry in this vector represents a word. The vector normally contains 10,000 to 50,000 entries gathered by finding the most frequently used words in our data set. If a word is to be found in the email, we would assign its respective entry a 1, else if it is not found, that entry would be a 0. Once we have all our x vectors ready, we train our algorithm and finally, we could use it to classify if an email is a spam or not.



Building a spam classifier

Supervised learning. x = features of email. y = spam (1) or not spam (0).

Features x: Choose 100 words indicative of spam/not spam.

E.g. deal, buy, discount, andrew, now, ...

$$x = \begin{array}{c|c} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ \vdots \\ 1 \\ \vdots \end{bmatrix} & \begin{array}{l} \text{andrew} \\ \text{buy} \\ \text{deal} \\ \text{discount} \\ \vdots \\ \text{now} \\ \vdots \end{array} \end{array} \qquad x \in \mathbb{R}^{100}$$

$$x_j = \begin{cases} 1 & \text{if word } j \text{ appears in email} \\ 0 & \text{otherwise.} \end{cases}$$

```
From: cheapsales@buystufffromme.com
To: ang@cs.stanford.edu
Subject: Buy now!

Deal of the week! Buy now!
```

So how could you spend your time to improve the accuracy of this classifier?

- Collect lots of data (for example "honeypot" project but doesn't always work)
- Develop sophisticated features (for example: using email header data in spam emails)
- Develop algorithms to process your input in different ways (recognizing misspellings in spam).

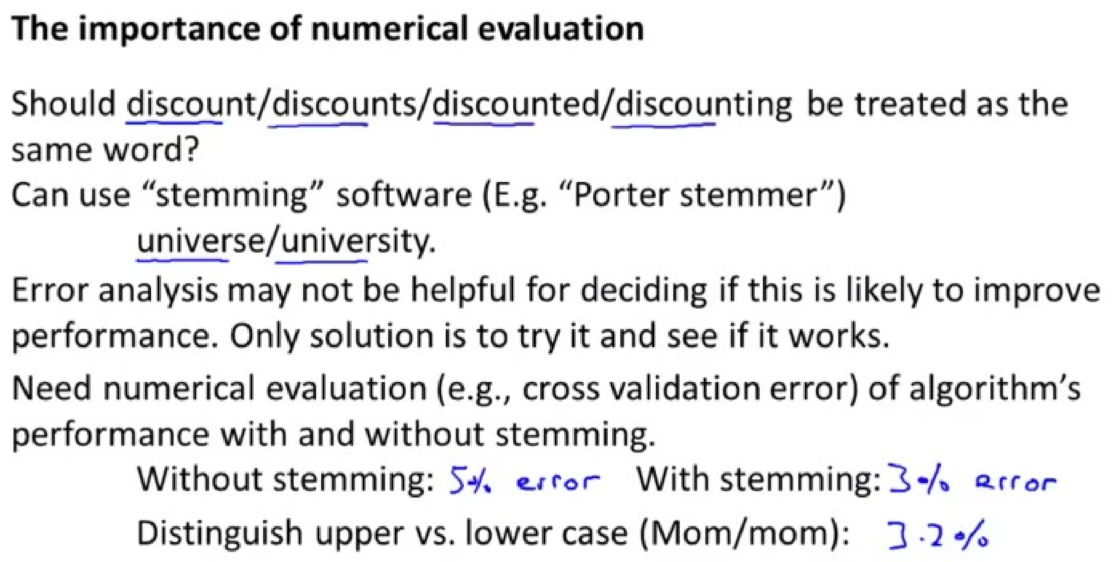
It is difficult to tell which of the options will be most helpful.

Error Analysis

The recommended approach to solving machine learning problems is to:

- Start with a **simple algorithm, implement it quickly, and test it early** on your cross validation data.
- **Plot learning curves** to decide if more data, more features, etc. are likely to help.
- **Manually examine the errors** on examples in the cross validation set and try to spot a trend where most of the errors were made.

For example, assume that we have 500 emails and our algorithm misclassifies a 100 of them. We could manually analyze the 100 emails and categorize them based on what type of emails they are. We could then try to come up with new cues and features that would help us classify these 100 emails correctly. Hence, if most of our misclassified emails are those which try to steal passwords, then we could find some features that are particular to those emails and add them to our model. We could also see how classifying each word according to its root changes our error rate:



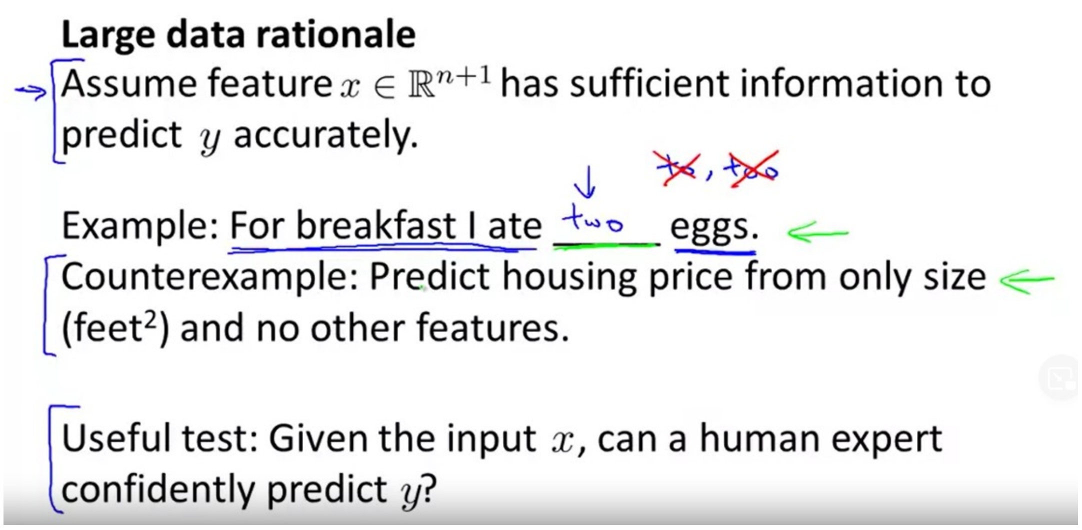
The importance of numerical evaluation

Should discount/discounts/discounted/discounting be treated as the same word?
Can use "stemming" software (E.g. "Porter stemmer")
universe/university.
Error analysis may not be helpful for deciding if this is likely to improve performance. Only solution is to try it and see if it works.
Need numerical evaluation (e.g., cross validation error) of algorithm's performance with and without stemming.
Without stemming: 5% error With stemming: 3% error
Distinguish upper vs. lower case (Mom/mom): 3.2%

It is very important to get error results as a single, numerical value. Otherwise it is difficult to assess your algorithm's performance. For example if we use stemming, which is the process of treating the same word with different forms (fail/failing/failed) as one word (fail), and get a 3% error rate instead of 5%, then we should definitely add it to our model. However, if we try to distinguish between upper case and lower case letters and end up getting a 3.2% error rate instead of 3%, then we should avoid using this new feature. Hence, we should try new things, get a numerical value for our error rate, and based on our result decide whether we want to keep the new feature or not.

Using large data sets

When asking ourselves if we have enough data, a useful question to ask is: **Given the input *x* to a human expert on the particular field of the algorithm, can he or she confidently predict *y*?** For example, if we try to predict house prices only based on their size, any expert would say there is not enough information (we would probably need location, rooms, age, etc.). That means we would need more features.



Large data rationale

Assume feature $x \in \mathbb{R}^{n+1}$ has sufficient information to predict y accurately.

~~to~~, ~~too~~

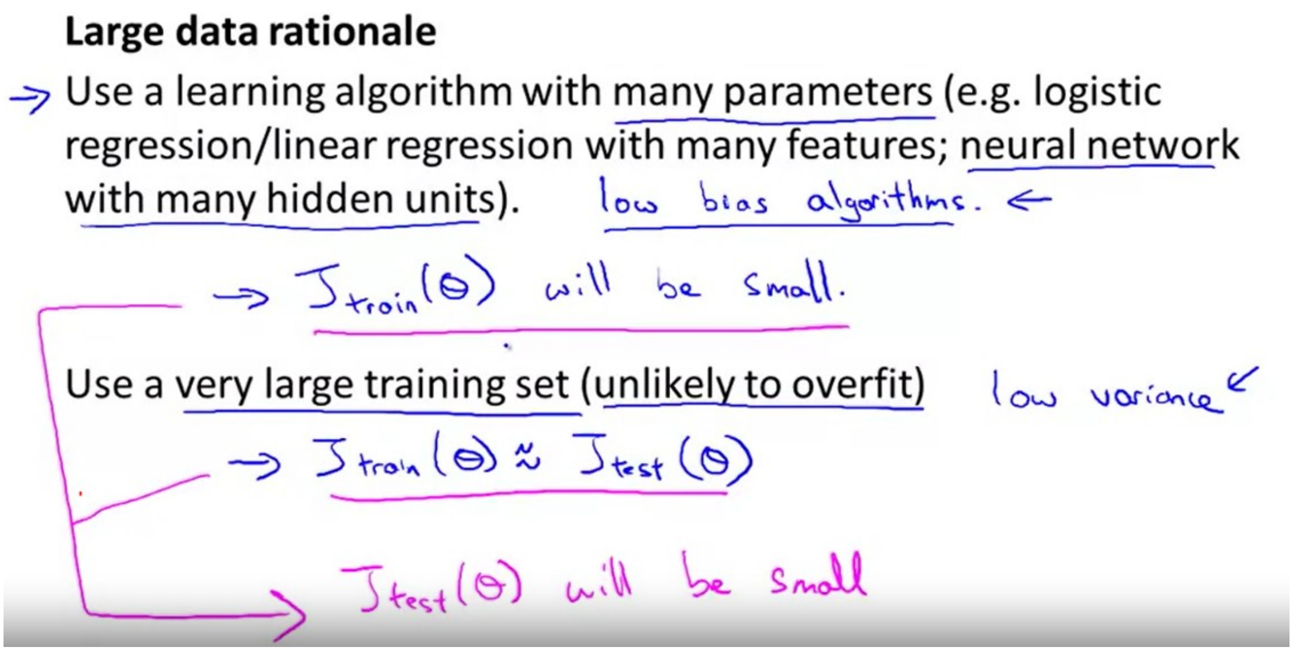
Example: For breakfast I ate two eggs.
Counterexample: Predict housing price from only size (feet^2) and no other features.

Useful test: Given the input x, can a human expert confidently predict y?

When is it relevant to aim for big training sets? A way to think about this is that:

- In order to have a high performance learning algorithm we want it not to have high bias and not to have high variance.
    - **Bias problem:** We make sure we have a learning algorithm with many parameters.
    - **Variance problem:** We use a very large training set.

By pulling these two together, that we end up with a low bias and a low variance learning algorithm and this allows us to do well on the test set.



Large data rationale

→ Use a learning algorithm with many parameters (e.g. logistic regression/linear regression with many features; neural network with many hidden units). low bias algorithms. ←

→ $J_{train}(\theta)$ will be small.

Use a very large training set (unlikely to overfit) low variance ↙

→ $J_{train}(\theta) \approx J_{test}(\theta)$

→ $J_{test}(\theta)$ will be small

And fundamentally these are the key ingredients: features that have enough information and a rich class of functions which guarantees low bias, and then having a massive training set that guarantees low variance.

Support Vector Machines (SVM)

SVM as alternative to logistic regression

(x,y)

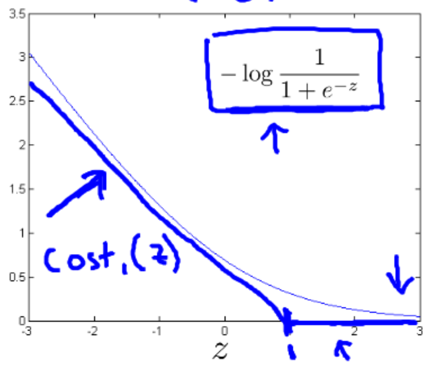
Alternative view of logistic regression

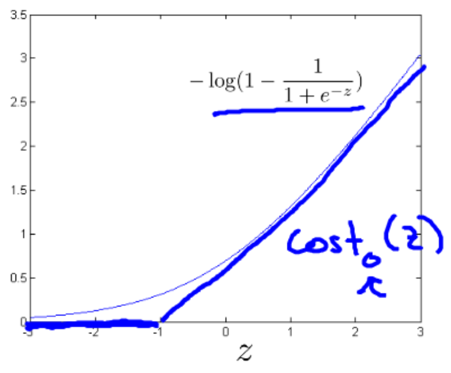
Cost of example: $-(y\log \underline{h_\theta(x)} + (1-y)\log(1-\underline{h_\theta(x)}))$

$$= \boxed{-y\log\underline{\frac{1}{1+e^{-\theta^T x}}}} - \boxed{\underline{(1-y)}\log(1-\underline{\frac{1}{1+e^{-\theta^T x}}})}$$

If $\underline{y=1}$ (want $\theta^T x \gg 0$): $z=\theta^T x$

If $y=0$ (want $\theta^T x \ll 0$):





Support vector machine

Logistic regression:

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

Support vector machine:

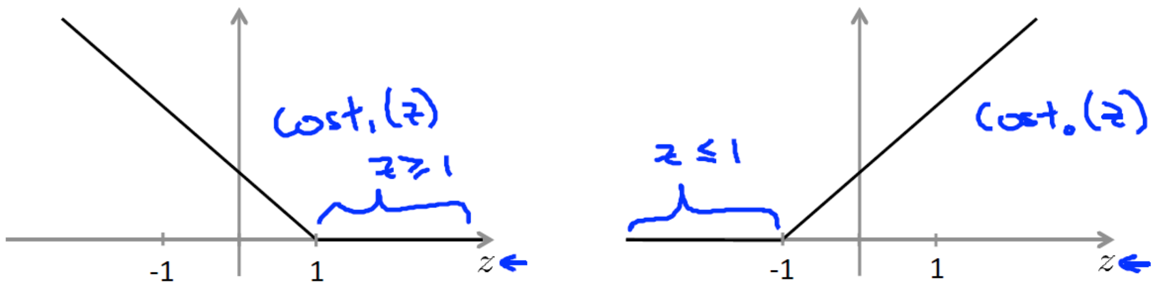
$$\min_\theta C\sum_{i=1}^{m}\left[y^{(i)}cost_1(\theta^T x^{(i)}) + (1-y^{(i)})cost_0(\theta^T x^{(i)})\right] + \frac{1}{2}\sum_{i=1}^{n}\theta_j^2$$

Andrew

Large Margin Intuition

Support Vector Machine

$$\rightarrow \quad \min_\theta \underset{\uparrow}{C} \sum_{i=1}^{m} \left[y^{(i)} \underline{cost_1(\theta^T x^{(i)})} + (1 - y^{(i)}) \underline{cost_0(\theta^T x^{(i)})} \right] + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$



$\rightarrow$ If $\underline{y = 1}$, we want $\underline{\theta^T x \geq 1}$ (not just ≥ 0) $\qquad \theta^T x \geq \cancel{0}\ 1$

$\rightarrow$ If $\underline{y = 0}$, we want $\underline{\theta^T x \leq -1}$ (not just < 0) $\qquad \theta^T x \leq \cancel{0}\ -1$

$C = 100{,}000$

SVM Decision Boundary

$$\min_\theta \underset{\nearrow}{C} \underbrace{\boxed{\sum_{i=1}^{m} \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T x^{(i)}) \right]}}_{= 0} + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

Whenever $y^{(i)} = 1$:

$\theta^T x^{(i)} \geq 1$

$$\min_\theta \cancel{C \times 0} + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$$

s.t. $\theta^T x^{(i)} \geq 1$ if $y^{(i)} = 1$

$\theta^T x^{(i)} \leq -1$ if $y^{(i)} = 0$.

Whenever $y^{(i)} = 0$:

$\theta^T x^{(i)} \leq -1$

More on SVMs

Have a good look at the PDFs of lectures 11 and 12!