Week 1

Cost Function and Parameter Learning

Mean squared error cost function for regression problems

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

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: {

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

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

}

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. (The cost function for linear regression is always going to be a bow shaped function-convex.)

Linear Algebra Review

Matrix Multiplication Properties:

Not commutative -> A x B != B x A

Associative -> A x B x C = A x (B x C)

Identity Matrix I -> A x I = I x A = A

If A is an m x m matrix, and if it has an inverse,

$$AA^{-1} = A^{-1}A = I$$

Matrices that don't have an inverse are "singular" or "degenerate". E.g. A = [0, 0; 0, 0].

Let A be an m x n matrix, and let $B = A^T$. Then B is an n x m matrix and $B_{ij} = A_{ji}$.

Week 2

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:

$$h_\theta(x) = \begin{bmatrix}\theta_0 & \theta_1 & \cdots & \theta_n\end{bmatrix} \begin{bmatrix}x_0 \\ x_1 \\ \vdots \\ x_n\end{bmatrix} = \theta^T x$$

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 $x_0^{(i)} = 1 \text{ for } (i \in 1, \ldots, m)$. 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:

repeat until convergence: {

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

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

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

...

}

In other words:

repeat until convergence: {

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

}

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:

$-1 \le x_{(i)} \le 1$

or

$-0.5 \le x_{(i)} \le 0.5$

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:

If α is too small: slow convergence.

If α is too large: J(θ) may not decrease on every iteration and thus may not converge.

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 $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^3$

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: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 \sqrt{x_1}$

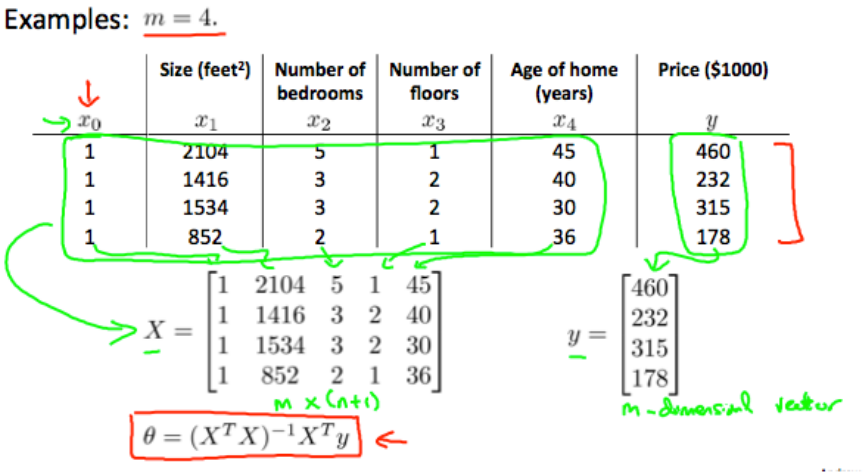
One important thing to keep in mind is, if you choose your features this way then feature scaling becomes very important.

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

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:

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



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 $\mathcal{O}(n^3)$. 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 (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.

Week 3

Classification

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∈{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.

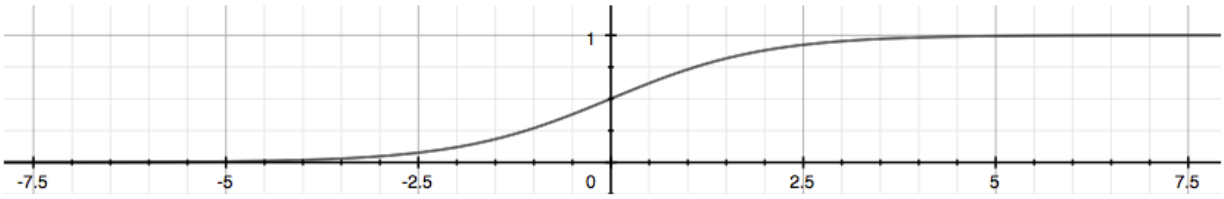
Hypothesis Representation

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 $h_\theta(x)$ to 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.

$h_\theta(x)$ 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%).

$$h_\theta(x) = P(y = 1 \mid x; \theta) = 1 - P(y = 0 \mid x; \theta)$$
$$P(y = 0 \mid x; \theta) + P(y = 1 \mid x; \theta) = 1$$

Decision Boundary

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

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

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.

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

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.

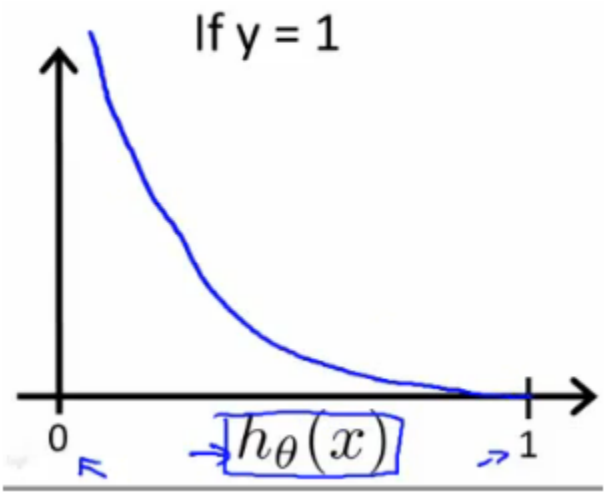
Instead, our cost function for logistic regression looks like:

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

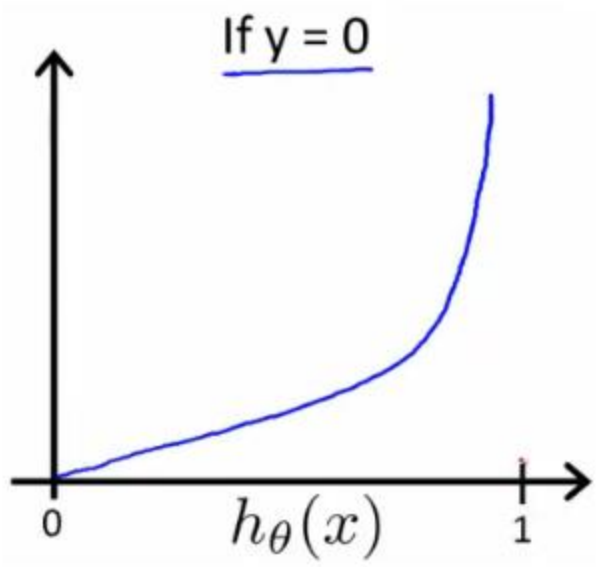
$$\text{Cost}(h_\theta(x), y) = -\log(h_\theta(x)) \qquad \text{if } y = 1$$

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

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 $h_\theta(x)$:



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

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

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

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

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

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

Remember that the general form of gradient descent is:

$$\begin{aligned}&Repeat\ \{\\ &\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta)\\ &\}\end{aligned}$$

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

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

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:

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

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()". (Note: the value for MaxIter should be an integer, not a character string - errata in the video at 7:30)

```
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: One-vs-all

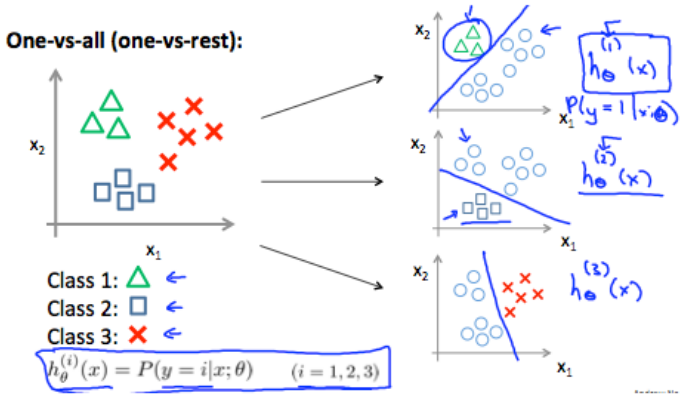
Now we will approach the classification of data when we have more than two categories. Instead of y = {0,1} we will expand our definition so that y = {0,1...n}.

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.

$$y \in \{0, 1 \ldots n\}$$
$$h_\theta^{(0)}(x) = P(y = 0 \mid x; \theta)$$
$$h_\theta^{(1)}(x) = P(y = 1 \mid x; \theta)$$
$$\ldots$$
$$h_\theta^{(n)}(x) = P(y = n \mid x; \theta)$$
$$\text{prediction} = \max_i (h_\theta^{(i)}(x))$$

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:



The Problem 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 θj .
- Regularization works well when we have a lot of slightly useful features.

Cost Function

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

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

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

Regularized Linear Regression

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 {

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

$$\theta_j := \theta_j - \alpha\left[\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j\right] \qquad j \in \{1, 2...n\}$$

}

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:

$$\theta = X^TX + \lambda \cdot L^{-1}X^Ty$$

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

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^TX is non-invertible. However, when we add the term λ·L, then X^TX + λ·L becomes invertible.

Regularized Logistic Regression

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 $\{$

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

$$\theta_j := \theta_j - \alpha\left[\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j\right] \quad (j = 1, 2, 3, \ldots, n)$$

$\theta_1 \ldots \theta_n$

$\}$

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

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

Week 4

Model Representation

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:

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

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

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

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 $\Theta_0^{(j)}$.

Examples and Intuitions I

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:

$$x_0$$
$$x_1 \rightarrow g(z^{(2)}) \rightarrow h_\Theta(x)$$
$$x_2$$

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

Let's set our first theta matrix as:

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

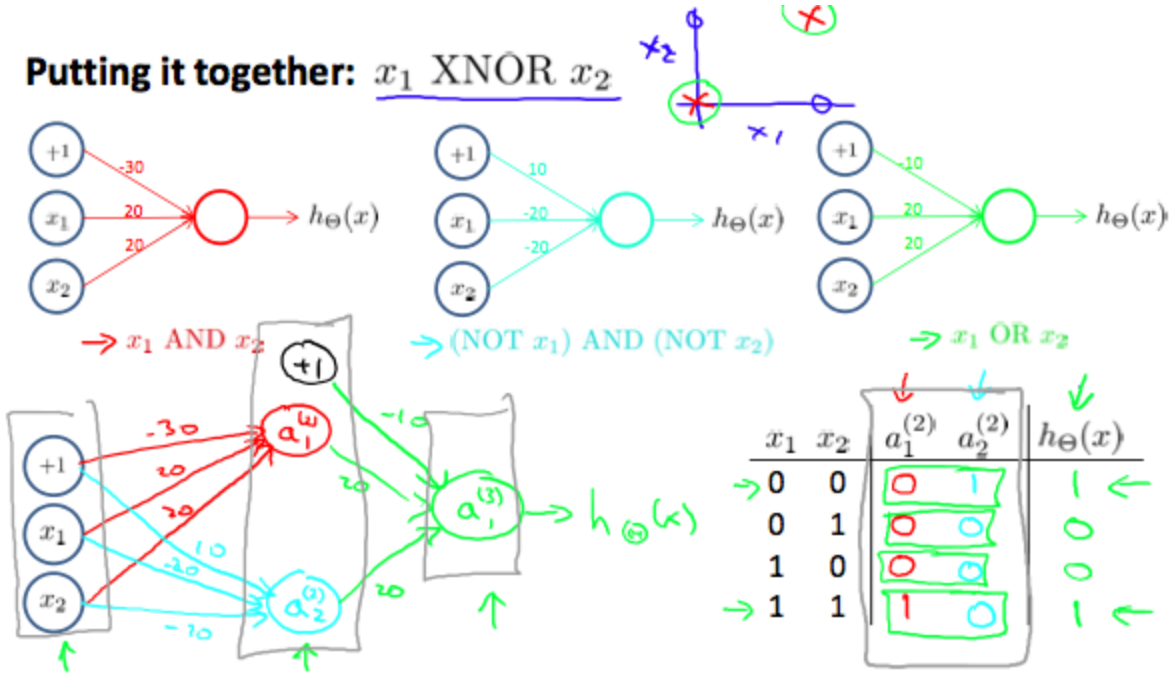
This will cause the output of our hypothesis to only be positive if both x_1 and x_2 are 1. In other words:

$$h_\Theta(x) = g(-30 + 20x_1 + 20x_2)$$
$$x_1 = 0 \ and \ x_2 = 0 \ then \ g(-30) \approx 0$$
$$x_1 = 0 \ and \ x_2 = 1 \ then \ g(-10) \approx 0$$
$$x_1 = 1 \ and \ x_2 = 0 \ then \ g(-10) \approx 0$$
$$x_1 = 1 \ and \ x_2 = 1 \ then \ g(10) \approx 1$$

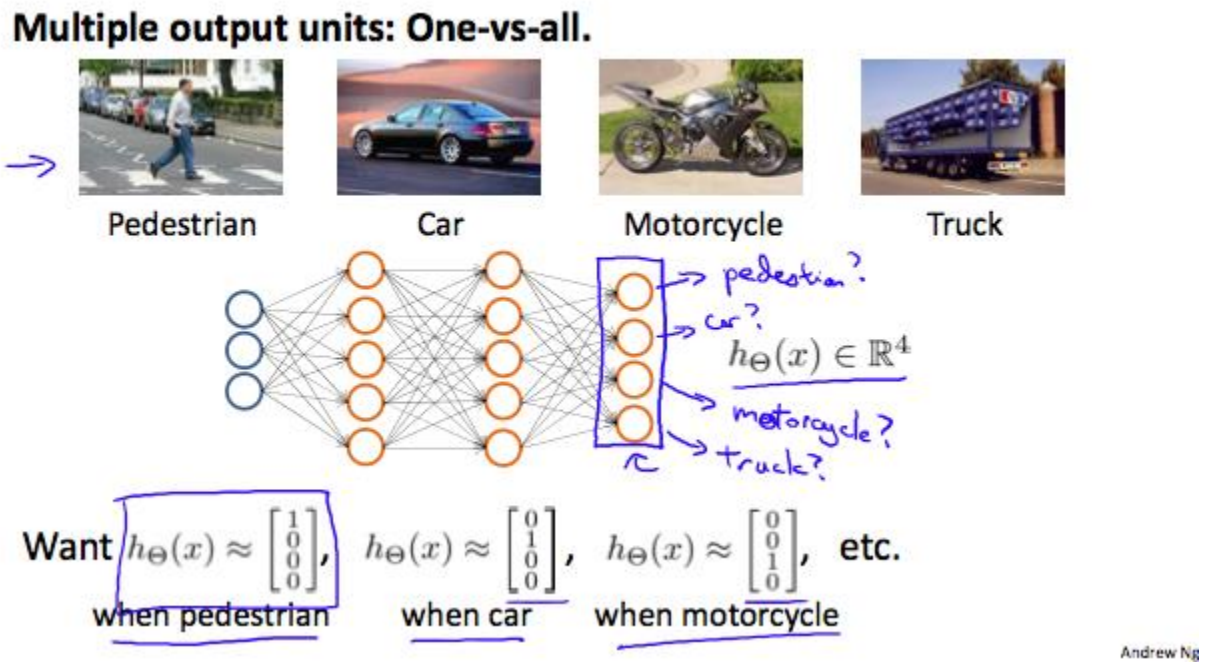
So we have constructed one of the fundamental operations in computers by using a small neural network rather than using an actual AND gate. Neural networks can also be used to simulate all the other logical gates. The following is an example of the logical operator 'OR', meaning either x_1 is true or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

Examples and Intuitions II

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



Multiclass Classification



Week 5

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:

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

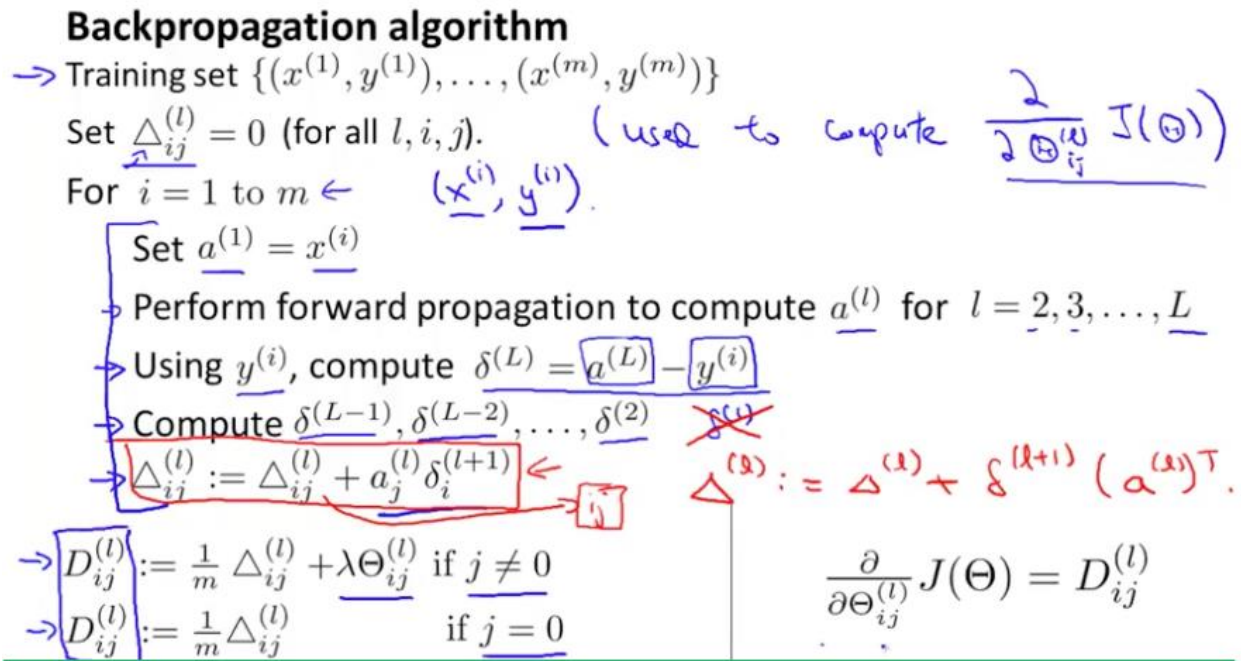
We have added a few nested summations to account for our multiple output nodes. In the first part of the equation, before the square brackets, we have an additional nested summation that loops through the number of output nodes.

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



Back propagation Algorithm

Given 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:

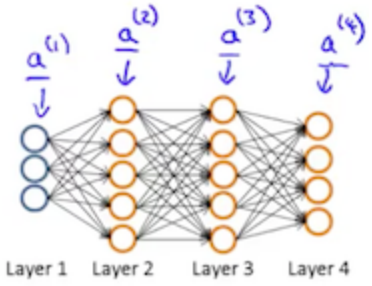
1. Set $a^{(1)} := x^{(t)}$
2. Perform forward propagation to compute $a^{(l)}$ for l=2,3,…,L

Gradient computation

Given one training example (x, y):

Forward propagation:

$$a^{(1)} = x$$
$$z^{(2)} = \Theta^{(1)} a^{(1)}$$
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$
$$z^{(3)} = \Theta^{(2)} a^{(2)}$$
$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$
$$z^{(4)} = \Theta^{(3)} a^{(3)}$$
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



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 $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$ 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.

- $D_{i,j}^{(l)} := \frac{1}{m} \left(\Delta_{i,j}^{(l)} + \lambda \Theta_{i,j}^{(l)} \right)$, if j≠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:

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

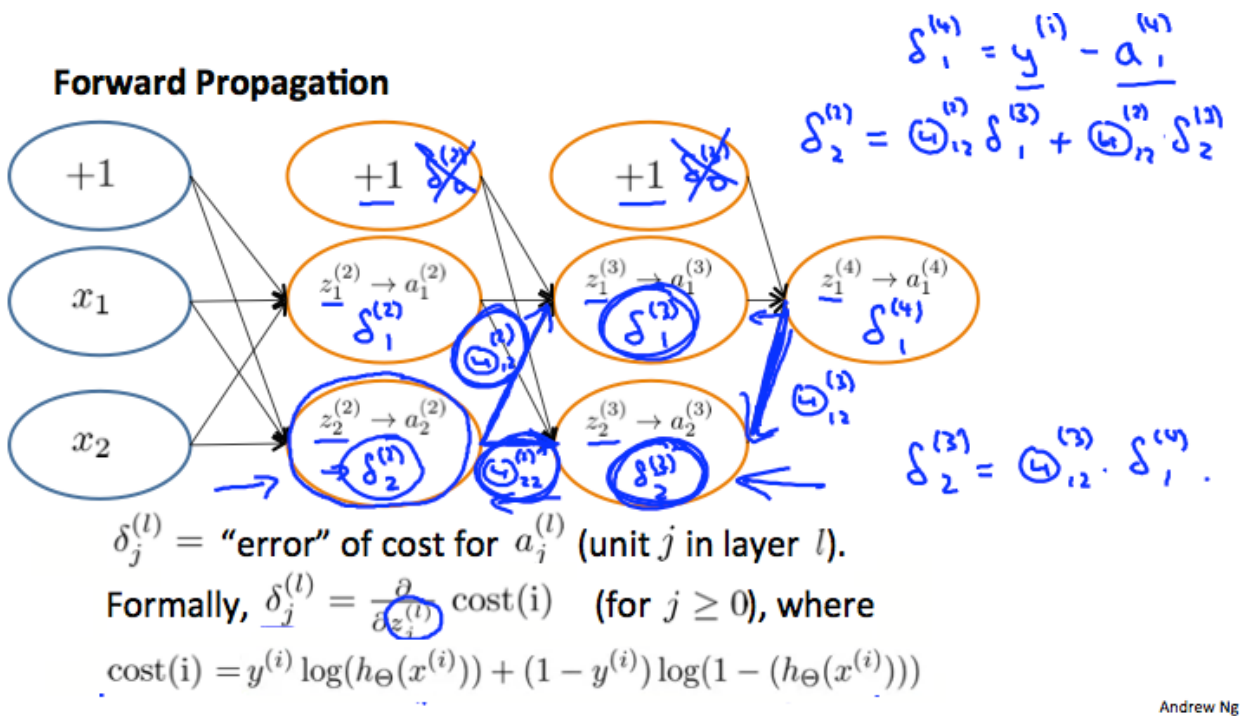
If we consider simple non-multiclass classification (k = 1) and disregard regularization, the cost is computed with:

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

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 $\delta_j^{(l)}$:



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 Note: Unrolling Parameters

With neural networks, we are working with sets of matrices:

$$\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}, \ldots$$
$$D^{(1)}, D^{(2)}, D^{(3)}, \ldots$$

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)
```

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:

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

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 ϵ (epsilon) such 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:

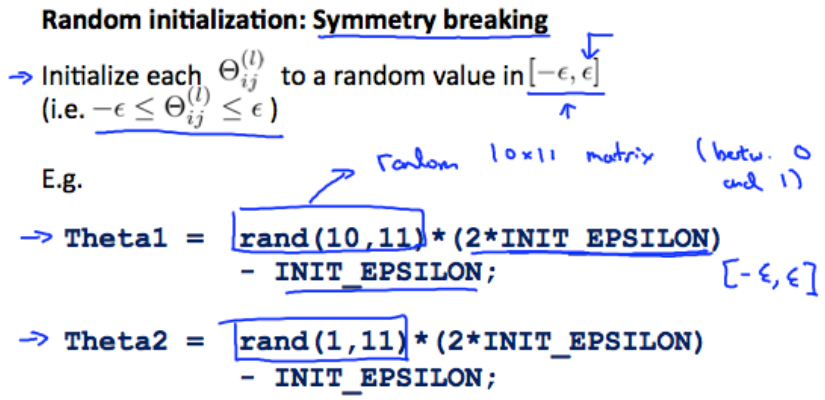
```
epsilon = 1e-4;
for i = 1:n,
  thetaPlus = theta;
  thetaPlus(i) += epsilon;
  thetaMinus = theta;
  thetaMinus(i) -= epsilon;
  gradApprox(i) = (J(thetaPlus) - J(thetaMinus))/(2*epsilon)
end;
```

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:



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 it 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.

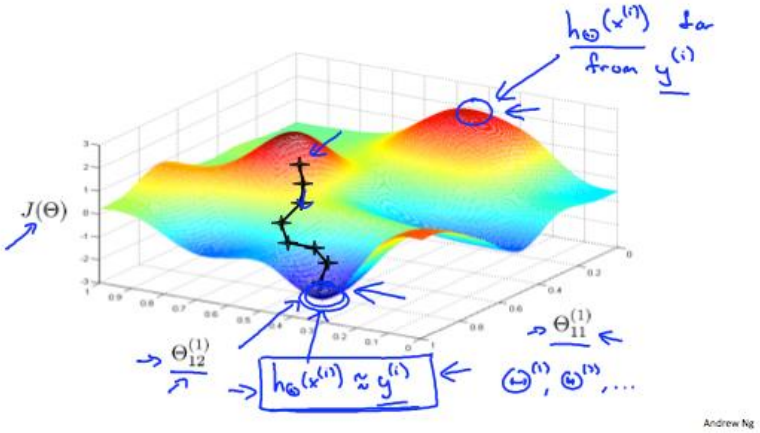
Training a Neural Network

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 $J(\Theta)$ is not convex and thus we can end up in a local minimum instead.

Derivation

https://www.coursera.org/learn/machine-learning/discussions/all/threads/cfIooMsjEemH9w4Og_zfOg

Backpropagation is essentially repeated applications of the chain rule in calculus to compute the derivatives (gradients) used for gradient descent. The $\delta_i^{(l)}$ are actually $\frac{\partial}{\partial z_i^{(l)}} J$. The $\Delta_{j,i}^{(l)}$, after being scaled by m and regularized to get $D_{j,i}^{(l)}$, are actually the $\frac{\partial}{\partial \Theta_{j,i}^{(l)}} J$ that are used to update the $\Theta_{j,i}^{(l)}$ in gradient descent. The recurrence relations allow you to move backwards from $l = L$, where the derivatives can be calculated directly from the cost function J, to the hidden layers and then compute the gradients.

- Here's a backpropagation $\delta^{(L)}$ derivation for the logistic regression J, ignoring superscripts ($l = L$) and subscripts (and bias) for clarity.

$$
\begin{aligned}
\sigma(z) &= \frac{1}{1+e^{-z}} = (1+e^{-z})^{-1} \implies \\
\frac{\partial \sigma}{\partial z} &= \sigma'(z) = (-1)(1+e^{-z})^{-2}\frac{\partial}{\partial z}(1+e^{-z}) \\
&= \cancel{(-1)}(1+e^{-z})^{-2}(e^{-z})\cancel{(-1)} \\
&= \frac{1}{1+e^{-z}}\frac{1+e^{-z}-1}{1+e^{-z}} \\
&= \sigma(z)(1-\sigma(z)) \qquad \square \\
a &= \sigma(z) \implies \frac{\partial a}{\partial z} = \sigma'(z) = a(1-a) \qquad \square
\end{aligned}
$$

$$
\begin{aligned}
J(\Theta) &= -[y\log(a) + (1-y)\log(1-a)] \implies \\
\frac{\partial J}{\partial a} &= -[y(\tfrac{1}{a}) + (1-y)\tfrac{(-1)}{1-a}] \\
&= -[(\tfrac{y}{a}) - (\tfrac{1-y}{1-a})] \\
&= -\frac{1}{a(1-a)}[(1-a)y - a(1-y)] \\
&= -\frac{1}{a(1-a)}[y - \cancel{ay} - a + \cancel{ay}] \\
&= \frac{1}{a(1-a)}[a-y] \qquad \square
\end{aligned}
$$

$$
\begin{aligned}
\delta^{(L)} &\equiv \frac{\partial}{\partial z} J = \frac{\partial J}{\partial a}\frac{\partial a}{\partial z} = \frac{1}{a(1-a)}[a-y]\, a(1-a) \\
&= a - y = a^{(L)} - y \qquad \blacksquare
\end{aligned}
$$

- The $\delta^{(l)}$ recurrence is independent of the particular cost function and depends only on the structure of the neural network. Here's a derivation:

$$\begin{aligned}\delta^{(l-1)} &\equiv \frac{\partial}{\partial z^{(l-1)}} J = \frac{\partial J}{\partial z^{(l)}} \frac{\partial z^{(l)}}{\partial z^{(l-1)}} = \delta^{(l)} \frac{\partial}{\partial z^{(l-1)}} z^{(l)} \\ &= \delta^{(l)} \frac{\partial}{\partial z^{(l-1)}} \Theta^{(l-1)} g(z^{(l-1)}) \\ &= \delta^{(l)} \Theta^{(l-1)} g'(z^{(l-1)}) \end{aligned}$$ ■

  Please read the week 2 Programming Tips from Mentors for questions about matrix order or transposes.

- The chain rule gives the derivative with respect to $\Theta^{(l)}$:

$$\begin{aligned}\Delta^{(l)} &\equiv \frac{\partial}{\partial \Theta^{(l)}} J = \frac{\partial z^{(l+1)}}{\partial \Theta^{(l)}} \frac{\partial J}{\partial z^{(l+1)}} \\ &= \frac{\partial (\Theta^{(l)} a^{(l)})}{\partial \Theta^{(l)}} \delta^{(l+1)} = a^{(l)} \delta^{(l+1)}\end{aligned}$$ ■

  $a^{(l)}$ only depends on $\Theta^{(l-1)}$ and below so, as far as differentiation by $\Theta^{(l)}$ is concerned, it's multiplication by a constant.

- The derivations above are for individual members of the training set. Remember that the slide for the Backpropagation Algorithm shows the steps inside a loop from one to m. You first get the $\delta^{(L)}$ for a member of the training set. You then use the recurrence relationship to get all the $\delta^{(l)}$s for that member; that's the "backpropagation" part. Finally, you combine those $\delta^{(l)}$ vectors with the $a^{(l-1)}$s to obtain the $\Delta^{(l)}$ matrices for each member of the training set. You then average those $\Delta^{(l)}$s over the entire training set the same way you averaged gradients in the previous cost functions. That's all the "accumulation" part of the backpropagation algorithm in the lectures does; it averages the gradients.

Backpropagation Intuition

The cost function is:

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

If we consider simple non-multiclass classification (k = 1) and disregard regularization, the cost is computed with:

$$cost(t) = y^{(t)}\ \log(h_\theta(x^{(t)})) + (1 - y^{(t)})\ \log(1 - h_\theta(x^{(t)}))$$

More intuitively you can think of that equation roughly as:

$$cost(t) \approx (h_\theta(x^{(t)}) - y^{(t)})^2$$

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.

Note: In lecture, sometimes i is used to index a training example. Sometimes it is used to index a unit in a layer. In the Back Propagation Algorithm described here, t is used to index a training example rather than overloading the use of i.

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.

Week 6

Evaluating a Hypothesis

Once we have done some trouble shooting 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: $J_{test}(\Theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_\Theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$
2. For classification ~ Misclassification error (aka 0/1 misclassification error):

$$err(h_\Theta(x), y) = \begin{matrix} 1 & \text{if } h_\Theta(x) \geq 0.5 \; and \; y = 0 \; or \; h_\Theta(x) < 0.5 \; and \; y = 1 \\ 0 & otherwise \end{matrix}$$

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

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

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.

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.

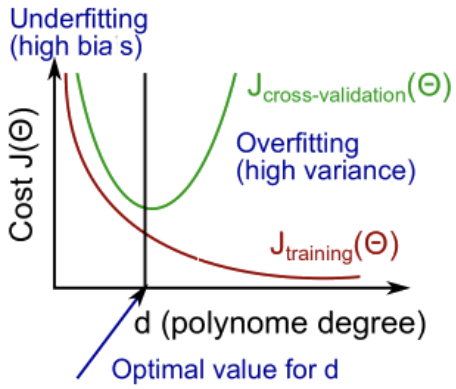
The training error will tend to **decrease** as we increase the degree d of the polynomial.

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, $J_{CV}(\Theta) \approx J_{train}(\Theta)$.

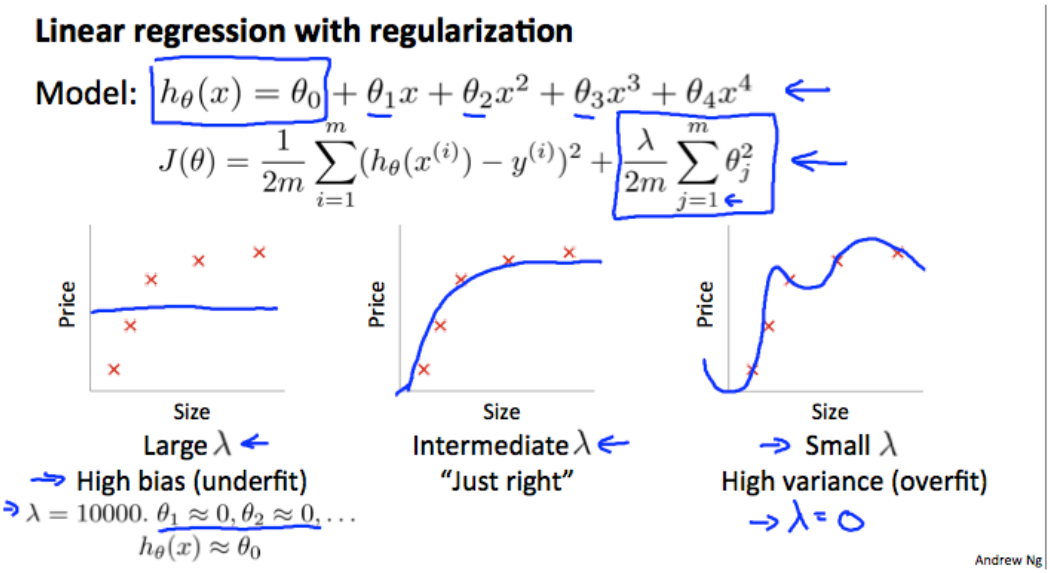
High variance (overfitting): $J_{train}(\Theta)$ will be low and $J_{CV}(\Theta)$ will be much greater than $J_{train}(\Theta)$.

The is summarized in the figure below:



Regularization and Bias/Variance

Note: [The regularization term below and through out the video should be $\frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$ and **NOT** $\frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$]



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 over overfit the data. So how do we choose our parameter λ to 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:

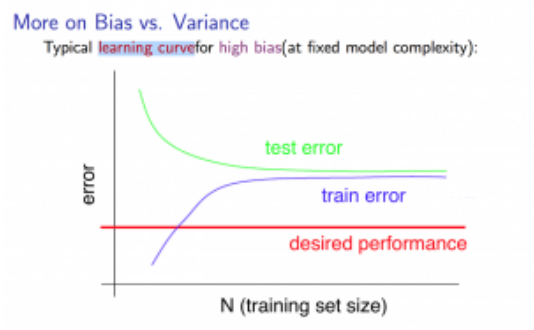
- As the training set gets larger, the error for a quadratic function increases.
- The error value will plateau out after a certain m, or training set size.

Experiencing high bias:

Low training set size: causes $J_{train}(\Theta)$ 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.

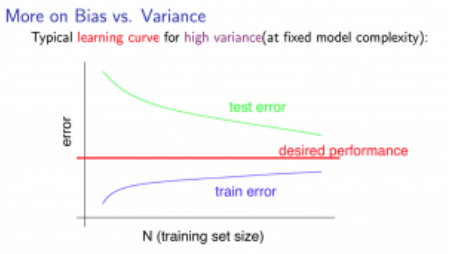


Experiencing high variance:

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.

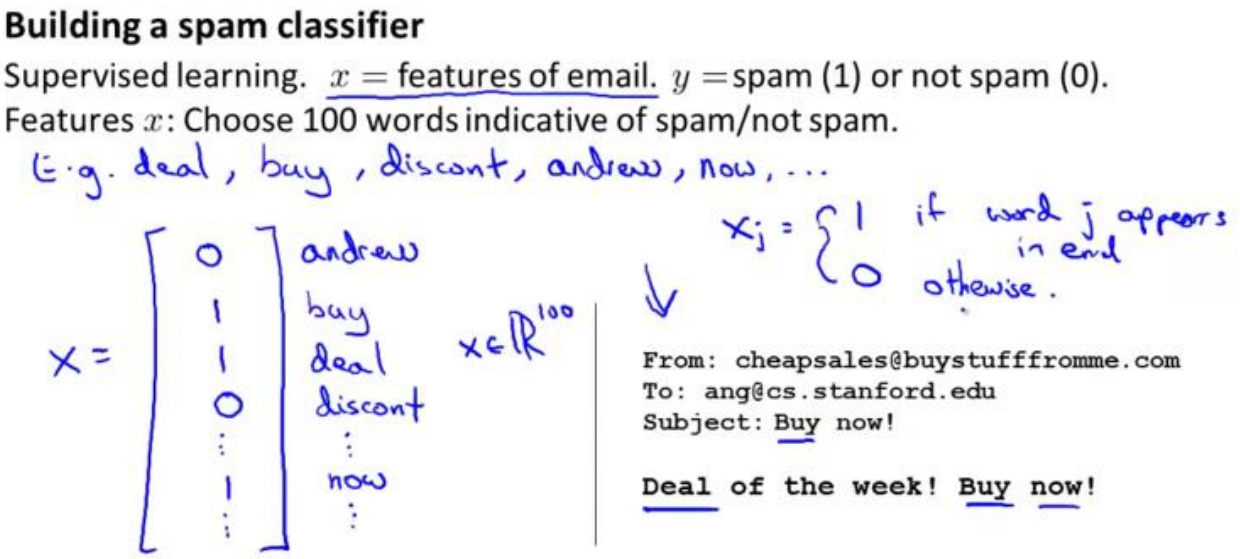
Using a single hidden layer is a good starting default. You can train your neural network on a number of hidden layers using your cross validation set. You can then select the one that performs best.

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

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.



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.