Week 2 Lecture Notes

ML: Linear Regression with Multiple Variables

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.

$$\begin{aligned} x_j^{(i)} &= \text{value of feature } j \text{ in the } i^{th} \text{ training example} \\ x^{(i)} &= \text{the column vector of all the feature inputs of the } i^{th} \text{ training example} \\ m &= \text{the number of training examples} \\ n &= \left| x^{(i)} \right| ; (\text{the number of features}) \end{aligned}$$

Now define the multivariable form of the hypothesis function as follows, accommodating these multiple features:

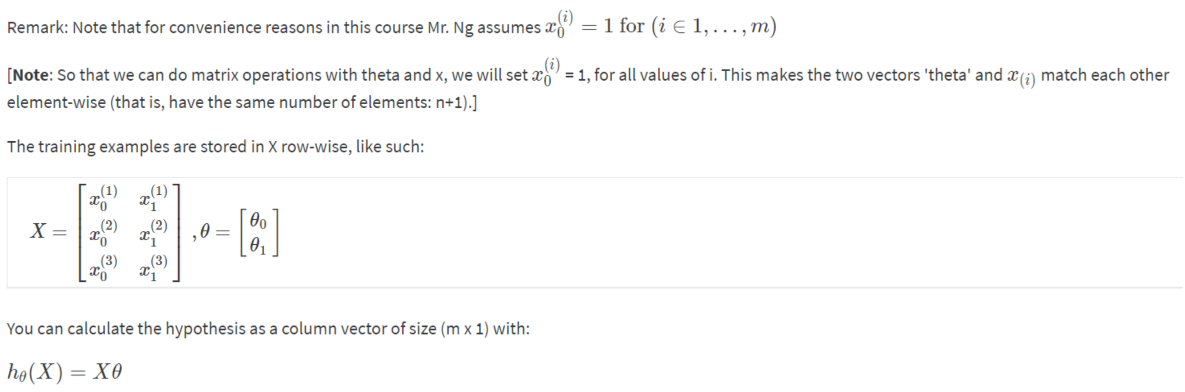
$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \cdots + \theta_n x_n$$

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:

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

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

[**Note**: So that we can do matrix operations with theta and x, we will set $x_0^{(i)}$ = 1, for all values of i. This makes the two vectors 'theta' and $x_{(i)}$ match each other element-wise (that is, have the same number of elements: n+1).]

The training examples are stored in X row-wise, like such:

$$X = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} \\ x_0^{(2)} & x_1^{(2)} \\ x_0^{(3)} & x_1^{(3)} \end{bmatrix}, \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$$

You can calculate the hypothesis as a column vector of size (m x 1) with:

$h_\theta(X) = X\theta$

For the rest of these notes, and other lecture notes, X will represent a matrix of training examples $x_{(i)}$ stored row-wise.

Cost Function

For the parameter vector θ (of type $\mathbb{R}^{n+1}$ or in $\mathbb{R}^{(n+1)\times 1}$, the cost function is:

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

The vectorized version is:

$$J(\theta) = \frac{1}{2m} (X\theta - \vec{y})^T (X\theta - \vec{y})$$

Where $\vec{y}$ denotes the vector of all y values.

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:

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

Matrix Notation

The Gradient Descent rule can be expressed as:

$$\theta := \theta - \alpha \nabla J(\theta)$$

Where $\nabla J(\theta)$ is a column vector of the form:

$$\nabla J(\theta) = \begin{bmatrix} \frac{\partial J(\theta)}{\partial \theta_0} & \frac{\partial J(\theta)}{\partial \theta_1} & \vdots & \frac{\partial J(\theta)}{\partial \theta_n} \end{bmatrix}$$

The j-th component of the gradient is the summation of the product of two terms:

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

Sometimes, the summation of the product of two terms can be expressed as the product of two vectors.

Here, $x_j^{(i)}$, for i = 1,...,m, represents the m elements of the j-th column, $\vec{x_j}$, of the training set X.

The other term $\left(h_\theta(x^{(i)}) - y^{(i)} \right)$ is the vector of the deviations between the predictions $h_\theta(x^{(i)})$ and the true values $y^{(i)}$. Re-writing $\frac{\partial J(\theta)}{\partial \theta_j}$, we have:

$$\begin{aligned} \frac{\partial J(\theta)}{\partial \theta_j} &= \frac{1}{m} \vec{x_j}^{T} (X\theta - \vec{y}) \\ \nabla J(\theta) &= \frac{1}{m} X^T (X\theta - \vec{y}) \end{aligned}$$

Finally, the matrix notation (vectorized) of the Gradient Descent rule is:

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

Feature Normalization

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（震荡） inefficiently down to the optimum when the variables are very uneven.（非均衡）

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

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

or

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

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.

Gradient Descent Tips

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. Andrew Ng recommends decreasing α by multiples of 3.

Features and Polynomial Regression

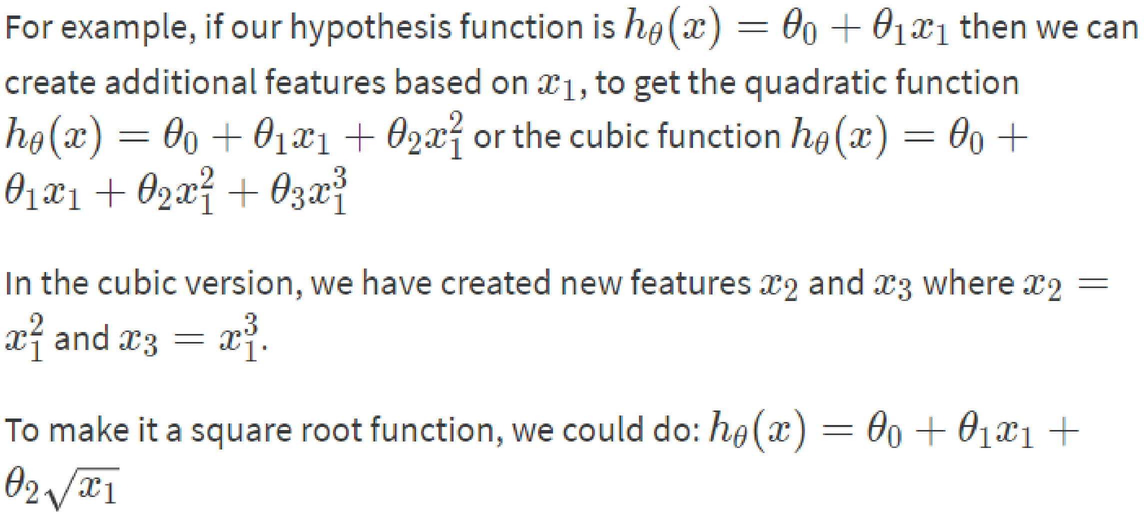
We can improve our features and the form of our hypothesis function in a couple different ways.

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⋅*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).

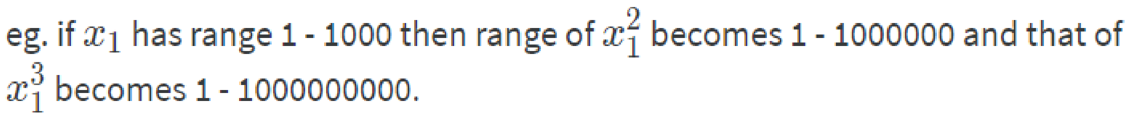


For example, if our hypothesis function is $h_\theta(x) = \theta_0 + \theta_1 x_1$ then we can create additional features based on x_1, to get the quadratic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2$ or the cubic function $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_1^2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

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.

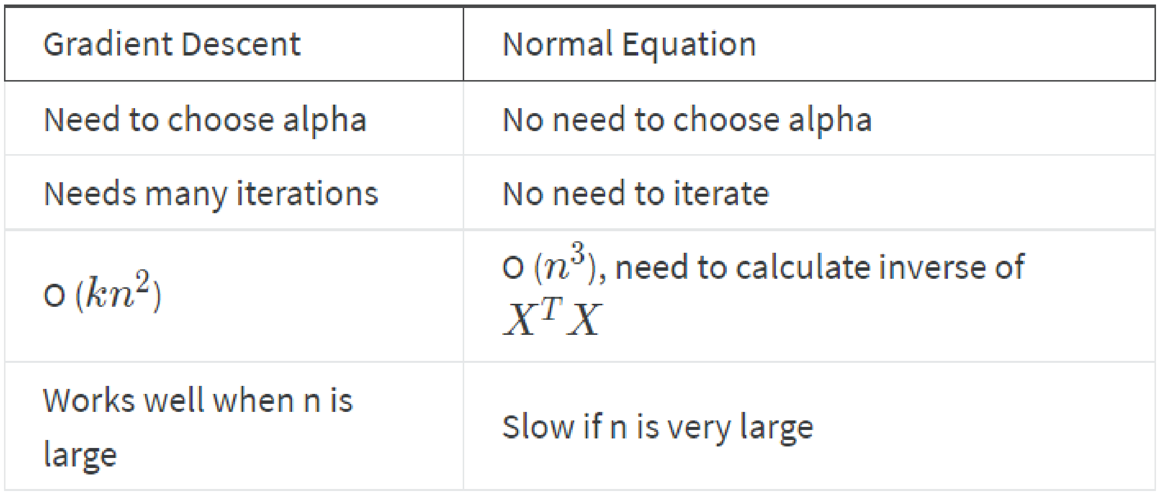
Normal Equation

The "Normal Equation" is a method of finding the optimum theta **without iteration.**

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

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)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.'

X^TX may be **noninvertible**. The common causes are:

- Redundant(多余的) 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.

ML:Octave Tutorial

Basic Operation

```
%% Change Octave prompt
PS1('>> ');
%% Change working directory in windows example:
cd 'c:/path/to/desired/directory name'
%% Note that it uses normal slashes and does not use escape characters for the empty spaces.

%% elementary operations
5+6
3-2
5*8
1/2
2^6
1 == 2 % false
1 ~= 2 % true.  note, not "!="
1 && 0
1 || 0
xor(1,0)


%% variable assignment
a = 3; % semicolon suppresses output
b = 'hi';
c = 3>=1;

% Displaying them:
a = pi
disp(a)
disp(sprintf('2 decimals: %0.2f', a))
disp(sprintf('6 decimals: %0.6f', a))
format long
a
format short
a


%%  vectors and matrices
A = [1 2; 3 4; 5 6]
```

```
v = [1 2 3]
v = [1; 2; 3]
v = 1:0.1:2   % from 1 to 2, with stepsize of 0.1. Useful for plot axes
v = 1:6       % from 1 to 6, assumes stepsize of 1 (row vector)

C = 2*ones(2,3) % same as C = [2 2 2; 2 2 2]
w = ones(1,3)   % 1x3 vector of ones
w = zeros(1,3)
w = rand(1,3) % drawn from a uniform distribution
w = randn(1,3)% drawn from a normal distribution (mean=0, var=1)
w = -6 + sqrt(10)*(randn(1,10000));  % (mean = -6, var = 10) - note: add the semicolon
hist(w)    % plot histogram using 10 bins (default)
hist(w,50) % plot histogram using 50 bins
% note: if hist() crashes, try "graphics_toolkit('gnu_plot')"

I = eye(4)   % 4x4 identity matrix

% help function
help eye
help rand
help help
```

etc.matlab uses