Week 2

Multivariate Linear Regression

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:

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

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 $x_0(i) = 1$ for $(i \in 1, \dots, m)$

[**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 θ 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 R^{n+1} or in $R^{(n+1)\times 1}$, the cost function is:

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

The vectorized version is:

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

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 $i = 1, \ldots, m$, represents the m elements of the j-th column, $\vec{x}_j$, of the training set X.

The other term $(h_\theta(x^{(i)}) - y^{(i)})$ 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:

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

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

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

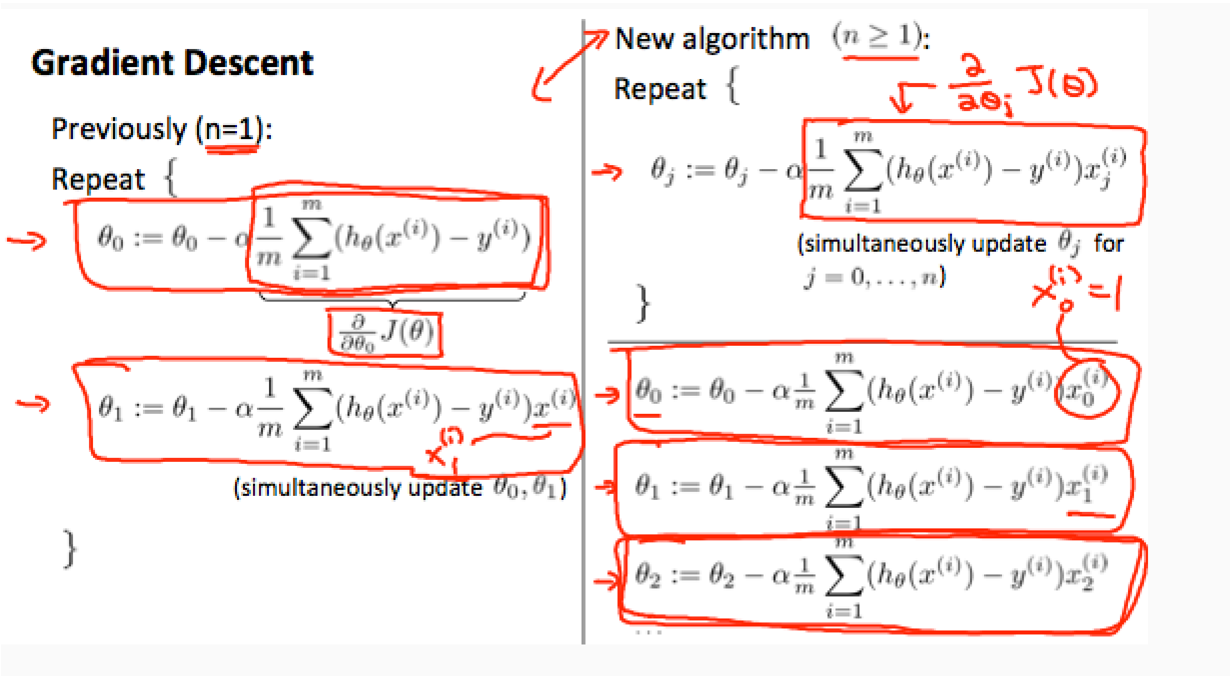
$$\theta := \theta - \frac{\alpha}{m} X^T (X\theta - \vec{y})$$

Algorithm: Gradient Descent

Repeat until convergence:

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

Context of gradient descent w.r.t. n=1



Note $x_0^i = 1$ and the partial derivative of the cost function for $n \geq 1$

Feature Normalization - Speeding up Gradient Descent

We can speed up our algorithm by having our input values in roughly the same ranges. θ will descent quickly on small ranges and slowly on large ranges. i.e oscillation occurs on the uneven surface.

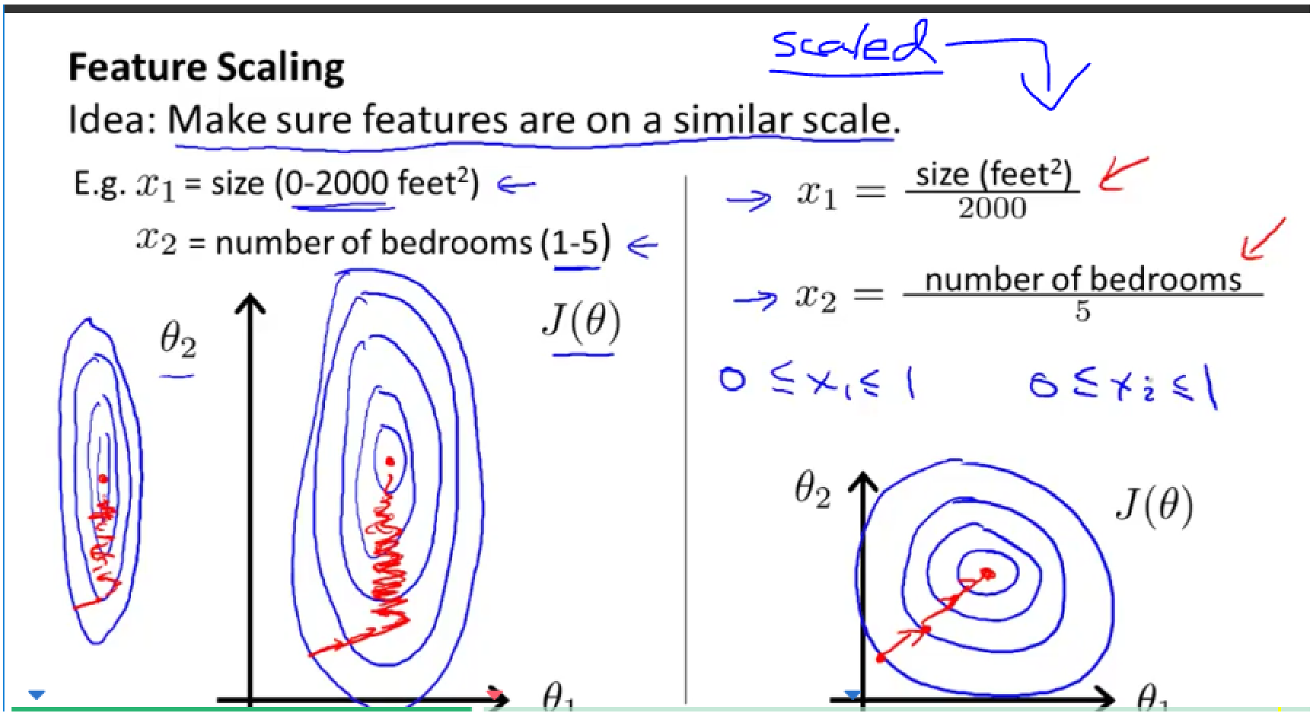
Two techniques to help with this are **feature scaling** and **mean normalization**. Feature scaling involves dividing the input values by the range (i.e. the maximum value minus the minimum value) of the input variable, resulting in a new range of just 1. *Mean normalization* involves subtracting the 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.

Feature Scaling

> Make sure features are on a **similar scale**
>
> Get every feature into approximately a $a \le x_i \le b$ range

Naïve Method:

$$x_i := \frac{x_i}{\max(x_i)}$$



Mean Normalization

> Replace x_i with $x_i - \mu_i$ to make features have approximately **zero mean**

NOTE do not apply to $x_0 = 1$

Method: - This method will normalize and feature scale.

$$x_i := \frac{x_i - \mu_i}{s_i}$$
$$\mu_i - \text{average of all values of feature i}$$
$$s_i - \text{range of values (min-max) or its the standard deviation}$$

NOTE The quizzes in this course use range - the programming exercises use standard deviation.

Learning Rate & Debugging

- If α is to small: slow convergence
- If α is to large: $J(\theta)$ may not decrease on every iteration; may not converge

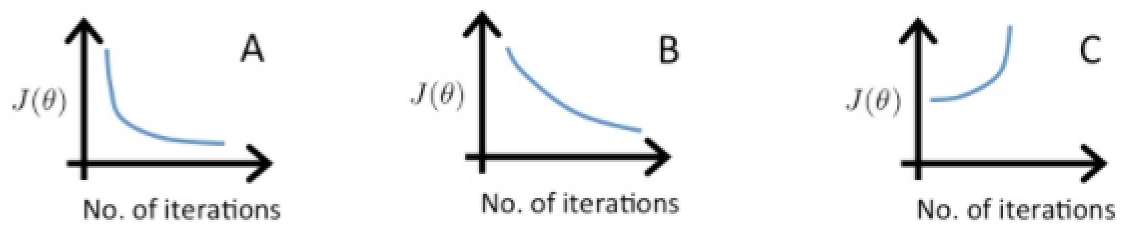
Debugging gradient descent.

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.

Example 1: Different Learning Rates

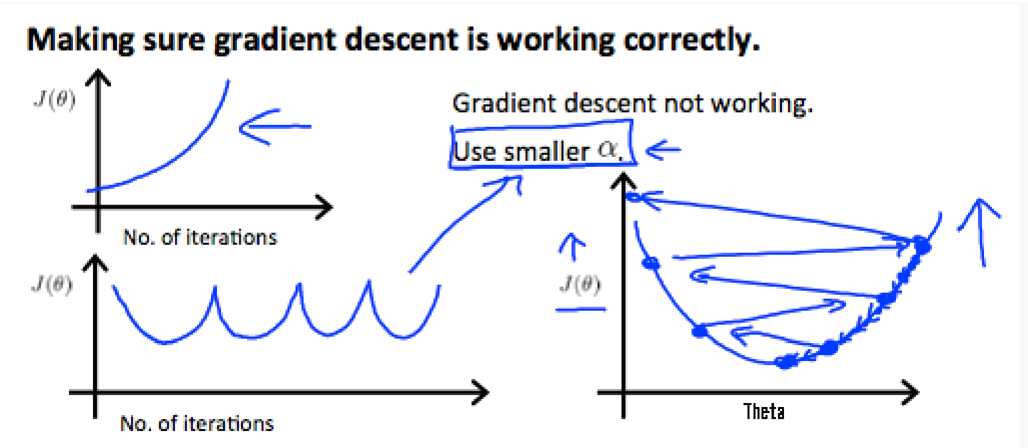


The learning rates: $\alpha_B << \alpha_A << \alpha_C$

In graph C, the cost function is increasing- the learning rate is to high. Graph A,B converge to an optimum of the cost function, but graph B does so much slower due to how small α is.

Example 2: Oscillation

Observe what the cost function plot looks like when overshooting occurs:



Vectorized: Gradient Descent

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

Derivation

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 $i = 1, \ldots, m$, represents the m elements of the j-th column, $\vec{x}_j$, of the training set X.

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

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

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

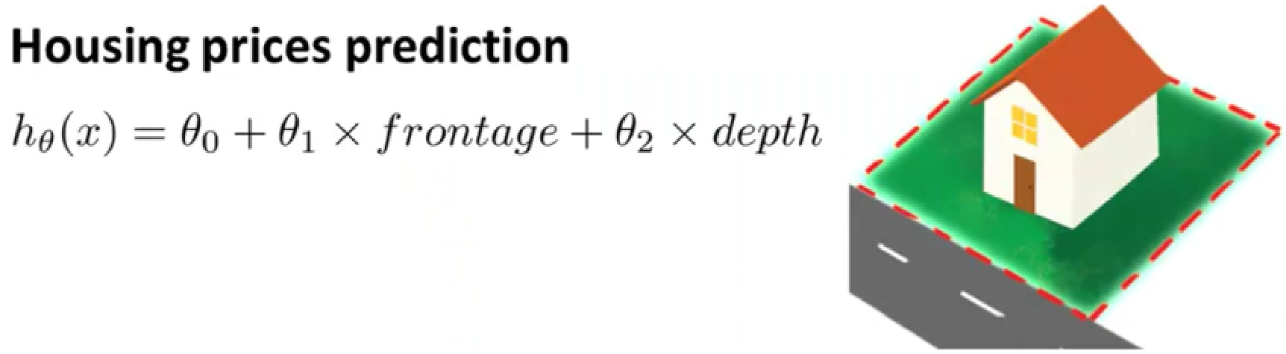
$$\theta := \theta - \frac{\alpha}{m} X^T (X\theta - \vec{y})$$

Features

We can **combine** multiple features into one.

For example:

We can combine x_1 and x_2 into a new feature $x_3 = x_1 x_2$ i.e frontage x depth, no need for two separate parameters.



Polynomial Regression

> 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).

If our hypothesis functions is $h_\theta(x) = \theta_0 + \theta_1 x_1$, we can create additional features based on x_1.

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

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

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

NOTE Scaling becomes very important when dealing with polynomials terms

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

NOTE: We will look algorithms later that can determine what kind of polynomial to use

Normal Equation - Computing Parameters Analytically

> Method for solving for θ analytically

NOTE Feature scaling is not needed

Formula: Normal Equation

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

Where θ is a vector containing the parameter values

Terminology:

- X - design matrix

Example:

Examples: $m = 4.$

x_0	Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) 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

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

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

Octave Code

```
pinv(x'*x)*x'*y
```

Intuition

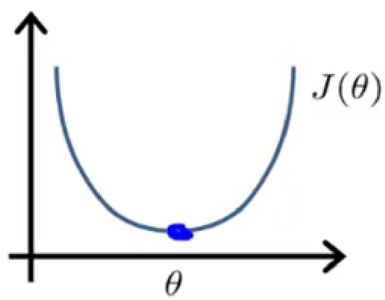
Here we consider the **1D** case. essentially we find the 1st derivative of the cost function and equate it to zero - as is done to find the optimal solution of the curve.

Intuition: If 1D $(\theta \in \mathbb{R})$

$$J(\theta) = a\theta^2 + b\theta + c$$

$$\frac{\partial}{\partial \theta} J(\theta) = \dots \overset{\text{set}}{=} 0$$

Solve for θ



n dimensional extension

$$\theta \in \mathbb{R}^{n+1} \qquad J(\theta_0, \theta_1, \dots, \theta_m) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \dots = 0 \qquad \text{(for every } j\text{)}$$

Solve for $\theta_0, \theta_1, \dots, \theta_n$

Pros & Cons

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^TX
Works well when n is large	Slow if n is very large

With the normal equation, computing the inversion has complexity O(n3). 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.

Recap:

Matrix identity

$(X^TX)^{-1}$ is inverse of matrix $\underline{X^TX}$.

Set $A = X^TX$

$$\boxed{(X^TX)^{-1}} = A^{-1}$$

Non-Inevitability

> What if X^TX is non-invertible?

NOTE Octave already considers this situation with `pinv`

Common Causes

- 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.