

Linear Regression with Multiple Variables

Multivariate Linear Regression

- Multiple features (variables)
 - n = number of features
 - $\mathbf{x}^{(i)}$ = input (features) of i^{th} training example.
 - $x_j^{(i)}$ = value of feature j in i^{th} training example.
- Hypothesis
 - Previously: $h_{\theta}(x) = \theta_0 + \theta_1 x$
 - $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$

- For convenience of notation, define $x_0 = 1$

- $$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}, h_{\theta}(x) = \theta^T x$$

Gradient Descent for Multiple Variables

- Hypothesis: $h_{\theta}(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$
- Parameters: $\theta_0, \theta_1, \dots, \theta_n$
- Cost function: $J(\theta_0, \theta_1, \dots, \theta_n) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$
 - or $J(\theta) = \frac{1}{2m} \sum_{i=1}^m (\theta^T x^{(i)} - y^{(i)})^2$
- Gradient descent

```
repeat {  
     $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n)$   
    (simultaneously update for every  $j = 0, \dots, n$ )  
}
```

or

```
repeat {  
     $\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$   
    (simultaneously update for every  $j = 0, \dots, n$ )  
}
```

Gradient Descent in Practice

Feature Normalization

Idea: Make sure features are on a similar scale.

- 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.

Example

- x_1 = size (0-2000 *feet*²)
- x_2 = number of bedrooms (1-5)

x_1 has a much larger range of values than x_2 . So the $J(\theta_1, \theta_2)$ can be a very very skewed elliptical shape. And if you run gradient descents on this cost function, your gradients may end up taking a long time and can oscillate back and forth and take a long time before it can finally find its way to the global minimum.

Feature scaling

Get every feature into approximately $-1 \leq x_i \leq 1$ range.

- 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.
- These aren't exact requirements; we are only trying to speed things up.
- $-3 \leq x_i \leq 3$ or $-\frac{1}{3} \leq x_i \leq \frac{1}{3}$ just is fine.

Mean normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$)

- E.g. $x_1 = \frac{\text{size} - 1000}{2000}$, $x_2 = \frac{\text{bedrooms} - 2}{5}$
- $x_i = \frac{x_i - \mu_i}{s_i}$
 - μ_i is the average value of x_i in training set.
 - s_i is the range ($x_{i\max} - x_{i\min}$) or standard deviation (σ)

Learning Rate

- "Debugging": **How to make sure gradient descent is working correctly**
 - Make a plot with *number of iterations* on the x-axis. Now plot the cost function, $J(\theta)$ over the number of iterations of gradient descent.
 - For sufficient small α , $J(\theta)$ should decrease on every iteration.
 - But if α is too small, gradient descent can be slow to converge.

- If $J(\theta)$ ever increases, then you probably need to use smaller α .
- Example automatic convergence test
 - Declare convergence if $J(\theta)$ decreases by less than ϵ (e.g., 10^{-3}) in one iteration.
- **How to choose learning rate α**
 - So just try running gradient descent with a range of values for α , like 0.001 and 0.01. And for these different values of α are just plot $J(\theta)$ as a function of number of iterations, and then pick the value of α that seems to be causing $J(\theta)$ to decrease rapidly.
 - Andrew Ng recommends decreasing α by multiples of 3. And then try to pick the largest possible value, or just something slightly smaller than the largest reasonable value.
 - E.g. . . . , 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, . . .

Features and Polynomial Regression

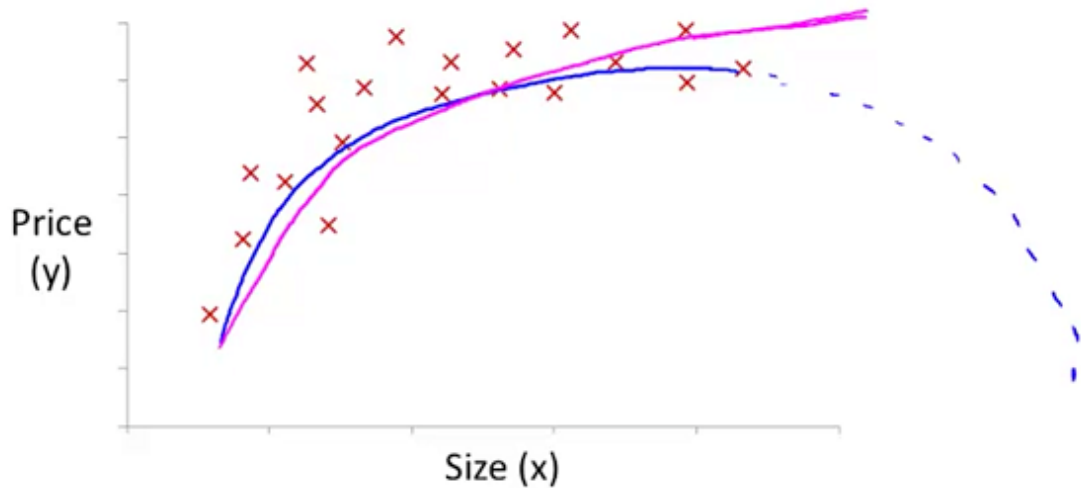
Choice of features

- 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 $x_1 \cdot x_2$. (E.g. $HouseArea = Frontage \times Depth$)

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: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 \sqrt{x_1}$
 - Note that at 2:52 and through 6:22 in the "Features and Polynomial Regression" video, the curve that Prof Ng discusses about "doesn't ever come back down" is in reference to the hypothesis function that uses the `sqrt()` function (shown by the solid purple line), not the one that uses $size^2$ (shown with the dotted blue line). The quadratic form of the hypothesis function would have the shape shown with the blue dotted line if θ_2 was negative.



- One important thing to keep in mind is, if you choose your features this way then **feature scaling becomes very important**.
 - E.g. if x_1 has range $1 - 1000$ then range of x_1^2 becomes $1 - 1000000$ and that of x_1^3 becomes $1 - 1000000000$
 - So you should scale x_1 before using polynomial regression.

Computing Parameters Analytically

Normal Equation

The "Normal Equation" (正规方程) is a method of finding the optimum θ **without iteration**.

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

Intuition

- $\theta \in \mathbb{R}^{n+1}, J(\theta_0, \theta_1, \dots, \theta_m) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$
- Set $\frac{\partial}{\partial \theta_j} J(\theta) = \dots = 0$ (for every j), solve for $\theta_0, \theta_1, \dots, \theta_m$

Method

We have m examples $(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})$ and n features. (Note that $x_0^{(i)} = 0$)

$$x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}$$

And construct the $m \times (n + 1)$ matrix X

$$X = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ (\mathbf{x}^{(2)})^T \\ \vdots \\ (\mathbf{x}^{(m)})^T \end{bmatrix}$$

And the m -dimension vector \mathbf{y}

$$\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

Finally, we can get

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

Example

Suppose you have the training in the table below:

age (x_1)	height in cm (x_2)	weight in kg (y)
4	89	16
9	124	28
5	103	20

You would like to predict a child's weight as a function of his age and height with the model

$$weight = \theta_0 + \theta_1 age + \theta_2 height$$

Then you can construct X and \mathbf{y}

$$X = \begin{bmatrix} 1 & 4 & 89 \\ 1 & 9 & 124 \\ 1 & 5 & 103 \end{bmatrix}$$

$$Y = \begin{bmatrix} 16 \\ 28 \\ 20 \end{bmatrix}$$

Usage in Octave

```
pinv (X'*X)*X'*y
```

Comparison of gradient descent and the normal equation

m training examples and n features.

Gradient Descent	Normal Equation
Need to choose α	No need to choose α
Needs many iterations	No need to iterate
$O(kn^2)$	$O(n^3)$, need to calculate $(X^T X)^{-1}$
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

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

- What if $X^T X$ is non-invertible (不可逆的)? (singular/ degenerate)
- Octave: `pinv(X'*X)*X'*y`
 - There's two functions in Octave for inverting matrices, `pinv` (pseudo-inverse, 伪逆) and `inv` (inverse).
 - As long as you use the `pinv` function then this will actually compute the value of data that you want even if $X^T X$ is non-invertible.
 - So when implementing the normal equation in octave we want to use the `pinv` function rather than `inv`.
- $X^T X$ may be **noninvertible**. The common causes are:
 - Redundant features, where two features are very closely related (i.e. they are linearly dependent)
 - E.g. x_1 = size in *feet*², and x_2 = size in *m*². So you'll always have $x_1 = (3.28)^2 x_2$
 - Too many features (e.g. $m \leq n$).
 - In this case, delete some features or use "regularization".

Octave/Matlab Tutorial

Basic Operations

- Print specific decimals: `disp(sprintf('6 decimals: %0.6f', a)) // 6 decimals:`

3.141593

- `v = 1:0.2:2` // [1.0 1.2 1.4 1.6 1.8 2.0]
- `ones`, `zeros`, `rand`, `randn` (生成正态分布的随机数矩阵), `eye` (生成单位矩阵)
- `hist` (直方图, 第二个参数自定义条数)
- `size` (返回矩阵的行数与列数 [m n])
- `length` (返回向量的维数)

Moving Data Around

- Use `load` to load data set.

```
load featureX.dat
load('priceY.dat')
```

- Use `who` to show all variables in Octave workspace
 - `whos` for detail information
 - `clear` to delete a variable

```
clear featureX
```

- Get first ten elements of a matrix

```
v = priceY(1:10)
```

- Use `save` to save your variable

```
save hello.mat v
```

- By default the data is saved in binary. You can save it to ASCII by

```
save hello.txt v -ascii
```

- Use `A(3, 2)` to get A_{32} , or `A(2, :)` to get every element along the second row
 - `A([1, 3], :)` to get everything in the first and third rows
 - `A(:, 2) = [10; 11; 12]` to change the value of elements in second column.
 - `A = [A, [100; 101; 102]]` to append another column vector to right
 - `A(:)` to put all elements of A into a single vector

Computing on Data

- Use `max` to get the largest element in a vector

```
a = [1 15 2 0.5];  
[val, ind] = max(a); // val = 15, ind = 2
```

- If you do `max(A)`, where **A** is a matrix, what this actually does is the column wise maximum.

```
A = [1 2; 3 4; 5 6];  
max(A) // [5 6]  
  
A = [8 1 6; 3 5 7; 4 9 2];  
max(A, [], 1) // [8 9 7] (get the column wise maximum)  
max(A, [], 2) // [8 7 9] (get the row wise maximum)  
max(max(A)) // 9  
max(A(:)) // 9
```

- `a < 3` does the element wise operation, you'll get `[1 0 1 1]`
 - `find(a<3)` gets `[1 3 4]`
- `magic(3)` gets a 3x3 magic matrix
- `sum`, `prod`, `floor`, `ceil`, `flipud`

Plotting Data

- `plot`
- `hold on`, `figure`, `subplot`
- `xlabel`, `ylabel`, `legend`, `title`, `axis`
- `print -dpng 'myPlot.png'`
- `imagesc(A)` to visualize a matrix
 - `imagesc(A)`, `colorbar`, `colormap gray` to be in gray scale.

Control Statements: for, while, if statement

Vectorization

Vectorization is the process of taking code that relies on **loops** and converting it into **matrix operations**. It is more efficient, more elegant, and more concise.

As an example, let's compute our prediction from a hypothesis. Theta is the vector of fields for the hypothesis and x is a vector of variables.

With loops ($h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$):


```
prediction = 0.0;
for j = 1:n+1,
    prediction += theta(j) * x(j);
end;
```

With vectorization ($h_{\theta}(x) = \theta^T x$):

```
prediction = theta' * x;
```