Notes Machine Learning by Andrew Ng on Coursera

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Contents

1	Introduction 3				
	1.1	Supervised Learning	3		
		1.1.1 Regression Problem	3		
		1.1.2 Classification Problems	3		
	1.2	Unsupervised Learning	3		
2	Lin	ear Regression with One Variable	4		
	2.1	Notations	4		
	2.2	Supervised Learning	4		
	2.3	Gradient Descent	5		
	2.4	Gradient Descent for Linear Regression	5		
3	Lin	ear Algebra	6		
	3.1	Matrix	6		
	3.2	Vector	6		
	3.3	Addition and Scalar Multiplication	7		
	3.4	Matrix Multiplication	7		
	3.5	Inverse and Transpose	7		
4	Lin	ear Regression with Multiple Variables	9		
	4.1	Notations	9		
	4.2	Hypothesis	9		
	4.3		10		
		4.3.1 Feature Scaling	10		
			11		
		4.3.3 Learning Rate	11		
	4.4		11		
		4.4.1 Features	11		
			11		
	4.5		12		
		4.5.1 Non Invertibility of X^TX			

5	Oct	ave Tutorial	13
6	Cla	ssification	14
	6.1	Logistic Regression	14
	6.2	Decision Boundary	15
	6.3	Cost Function	15
	6.4	Advanced Optimization:	17
\mathbf{A}	ppen	dices	19

Introduction

Machine learning (task, experience, performance) can be classified into Supervised and Unsupervised learning.

1.1 Supervised Learning

Supervised learning can be basically classified into *Regression* and *Classification* problems.

1.1.1 Regression Problem

Regression problems work loosely on continuous range of outputs.

1.1.2 Classification Problems

Classification problems work loosely on discrete range of outputs.

1.2 Unsupervised Learning

An example is *Clustering Problem*.

Check Lecture1.pdf for more details.

Linear Regression with One Variable

2.1 Notations

m = number of training examples x's = 'input' variables / features y's = 'output' variables / 'target' variables (x,y) = single training example $(x^{(i)}, y^{(i)}) = i^{th} \text{ example}$

2.2 Supervised Learning

We have a data set (*Training Set*). Training Set \rightarrow Learning Algorithm \rightarrow h (hypothesis, a function $X \rightarrow Y$)

To Represent h

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

Cost

$$\underset{\theta_0, \ \theta_1}{\text{minimize}} \frac{1}{2m} \sum_{1}^{m} (h_{\theta}(x) - y)^2$$

Cost Function

Squared Error Cost Function

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{1}^{m} (h_{\theta}(x) - y)^2$$

$$\underset{\theta_0, \ \theta_1}{\operatorname{minimize}} J(\theta_0, \theta_1)$$

2.3 Gradient Descent

Finds local optimum:

- 1. Start with some value
- 2. Get closer to optimum

Algorithm

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_i} J(\theta) \ \forall j$$

where $\alpha = \text{learning rate}$

Important!

Simultaneous Update!

$$temp_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \ \forall j$$
$$\theta_j := temp_j \ \forall j$$

2.4 Gradient Descent for Linear Regression

Cost function for linear regression is convex!

Batch Gradient Descent: Each step of gradient descent uses all training examples.

Check Lecture2.pdf for more details.

Linear Algebra

3.1 Matrix

Rectangular array of numbers:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Dimension of the matrix: #rows x #cols (2 x 3)

Elements of the matrix:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

$$A_{ij} = "i, j \text{ entry" in the } i^{th} \text{ row, } j^{th} \text{ col}$$

3.2 Vector

An $n \times 1$ matrix.

$$y = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

 $y_i = i^{th}$ element

Note: Uppercase for matrices, lowercase for vectors.

3.3 Addition and Scalar Multiplication

Add/Subtract (element by element) matrices of same dimention only! Multiply/Divide (all elements) a matrix by scalar!

3.4 Matrix Multiplication

 $m \times n$ matrix multiplied by $n \times o$ matrix gives a $m \times o$ matrix.

Properties

- 1. Matrix Multiplication is *not* Commutative.
- 2. Matrix Multiplication is Associative.
- 3. Identity Matrix (I): 1's along diagonal, 0's everywhere else in an $n \times n$ matrix. AI = IA = A.

3.5 Inverse and Transpose

Inverse

Only square $(n \times n)$ matrices may have an inverse.

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

Matrices that don't have an inverse are *singular* or *degenerate* matrices.

Transpose

Let A be an $m \times n$ matrix and let $B = A^T$, then

$$B_{ij} = A_{ji}$$

Example:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$
$$B = A^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

Check Lecture3.pdf for more details.

Linear Regression with Multiple Variables

4.1 Notations

n = number of features $x^{(i)} = \text{input (features) of } i^{th} \text{ training example}$ $x_j^{(i)} = \text{value of feature } j \text{ of } i^{th} \text{ training example}$

4.2 Hypothesis

Previously:

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

Now:

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

For convinience, define $x_0 = 1$. So

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

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1} \qquad \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

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

4.3 Gradient Descent

Hypothesis: $h_{\theta}(x) = \theta^{T}x$ $= \theta_{0}x_{0} + \theta_{1}x_{1} + \dots + \theta_{n}x_{n}$ Parameters: θ $= \theta_{0}, \theta_{1}, \dots, \theta_{n}$ Cost Function: $J(\theta) = J(\theta_{0}, \theta_{1}, \dots, \theta_{n})$ $= \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2}$

Gradient Descent:

Repeat {
$$\theta_{j} := \theta_{j} - \alpha \frac{\partial}{\partial \theta_{j}} J(\theta)$$

$$= \theta_{j} - \alpha \frac{\partial}{\partial \theta_{j}} J(\theta_{0}, \theta_{1}, \dots, \theta_{n})$$

$$= \theta_{j} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)} - y^{(i)}) x_{j}^{(i)})$$
}(simultaneously update $\forall j = 0, 1, \dots, n$)

4.3.1 Feature Scaling

Idea: Make sure features are on a similar scale.

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

4.3.2 Mean Normalization

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

General Rule

$$x_i \leftarrow \frac{x_i - \mu_i}{S_i}$$

where

$$\mu_i = \text{average value of } x_i$$

$$S_i = \text{range (max - min)} \qquad or$$

$$= \sigma(\text{standard deviation})$$

4.3.3 Learning Rate

 $J(\theta)$ should decrease after every iteration. #iterations vary a lot.

Example Automatic Convergence Test: Declare convergence if $J(\theta)$ decreases by less than ϵ (say 10^{-3}) in one iteration.

If $J(\theta)$ increases, use smaller α . Too small α means slow convergence.

To choose α , try ..., 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, ...

4.4 Features and Polynomial Regression

4.4.1 Features

Get an insight in your problem and choose better features (may even combine/separate features).

Ex: size = length \rightarrow breadth.

4.4.2 Polynomial Regression

Ex:

$$x_1 = size$$

$$x_2 = size^2$$

$$x_3 = size^3$$

4.5 Normal Equation

Solve for θ analytically!

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

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

$$= \begin{bmatrix} x_0 & x_1 & \dots & x_n \end{bmatrix}$$

$$Y = \begin{bmatrix} y_1^{(1)} \\ y_2^{(2)} \\ \vdots \\ y_m^{(m)} \end{bmatrix}$$

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

$$\in \mathbb{R}^{m+1}$$

$$\theta \in \mathbb{R}^m$$

Inverse of a matrix grows as $O(n^3)$, use wisely.

4.5.1 Non Invertibility of X^TX

Use 'pinv' function in Octave (pseudo-inverse) instead of 'inv' function (inverse).

If X^TX is non-invertible, common causes are

- 1. Redundant features (linearly dependent)
- 2. Too many features $(m \le n)$. In this case, delete some features or use regularization

Check Lecture4.pdf for more details.

Chapter 5 Octave Tutorial

Check Lecture 5.pdf for more details.

Classification

Classify into categories (binary or multiple).

6.1 Logistic Regression

$$0 \le h_{\theta}(x) \le 1$$
 $h_{\theta}(x) = g(\theta^T x)$
 $g(z) = \frac{1}{1 + e^{-z}}$ g is called a sigmoid function or a logistic function.
$$h_{\theta}(x) = \frac{1}{1 + e^{\theta^T x}}$$

Interpretation of Hypothesis Output

$$h_{\theta}(x) = \text{estimated probability that } y = 1 \text{ on input } x$$

 $h_{\theta}(x) = P(y = 1|x; \theta) = \text{probability that } y = 1, \text{ given } x, \text{ parameterized by } \theta$

$$P(y = 0|x; \theta) + P(y = 1|x; \theta) = 1$$

6.2 Decision Boundary

Predict:
$$y = 1$$
 if $h_{\theta}(x) \ge 0.5$
$$(\theta^{T} x \ge 0)$$
Predict: $y = 0$ if $h_{\theta}(x) < 0.5$
$$(\theta^{T} x < 0)$$

$$\theta^{T} x = 0$$
 is the decision boundary.

Non-linear Decision Boundaries

Use same technique as polynomial regression for features.

6.3 Cost Function

Training Set :
$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ./dots, (x^{(m)}, y^{(m)})\}$$

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

$$x_0 = 1$$

$$y \in \{0, 1\}$$

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

How to choose parameter θ ?

Linear Regression:

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

Logistic Regression:

$$\operatorname{Cost}(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & y = 1\\ -\log(1 - h_{\theta}(x)) & y = 0 \end{cases}$$
$$\operatorname{Cost}(h_{\theta}(x), y) = 0 \text{ if } h_{\theta}(x) = y$$
$$\operatorname{Cost}(h_{\theta}(x), y) \to \inf \text{ if } y = 0 \text{ and } h_{\theta}(x) \to 1$$
$$\operatorname{Cost}(h_{\theta}(x), y) \to \inf \text{ if } y = 1 \text{ and } h_{\theta}(x) \to 0$$

Note: y = 0 or 1 always.

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

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

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

To fit parameters θ :

$$\underset{\theta}{\operatorname{minimize}} J(\theta)$$

To make a prediction given a new x:

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

Gradient Descent:

Simultaneously update all θ_j

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

Plug in the derivative

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

Don't forget feature scaling!

6.4 Advanced Optimization:

Something better than gradient descent:

- 1. Conjugate Gradient
- 2. BFGS
- 3. L-BFGS

Advantages:

- 1. No need to manually pick α
- 2. Often faster than gradient descent

Disadvantages:

1. More complex

Use libraries! Beware of bad implementations!

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

- 1. $J(\theta)$
- 2. $\frac{\partial}{\partial \theta_j} J(\theta)$

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().

Check Lecture 6.pdf for more details.

Appendices