Notes

Machine Learning by Andrew Ng on Coursera

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Contents

Chapter 1

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.

Chapter 2

Linear Regression with One Variable

2.1 Notations

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

2.2 Supervised Learning

We have a data set (*Training Set*).

Training Set → Learning Algorithm → h (*hypothesis*, a function $X \to Y$)

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

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

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

2.3 Gradient Descent

Finds local optimum:

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

Algorithm

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

where α = 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.

Chapter 3

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:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$
$$A_{ij} = \text{“}i, j \text{ entry” in the } i^{th} \text{ row, } j^{th} \text{ col}$$

3.2 Vector

An $n \times 1$ matrix.

$$y = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$
$$y_i = i^{th} \text{ element}$$

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 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.

Chapter 4

Linear Regression with Multiple Variables

4.1 Notations

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

4.2 Hypothesis

Previously:

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

Now:

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

For convinience, define $x_0 = 1$. So

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

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

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

4.3 Gradient Descent

$$\begin{aligned} \text{Hypothesis} : h_\theta(x) = \theta^T x & & = \theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_n x_n \\ \text{Parameters} : \theta & & = \theta_0, \theta_1, \ldots, \theta_n \\ \text{Cost Function} : J(\theta) = J(\theta_0, \theta_1, \ldots, \theta_n) & & = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \end{aligned}$$

Gradient Descent :

$$\begin{aligned} & \text{Repeat}\{ \\ \theta_j & := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \\ & = \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1, \ldots, \theta_n) \\ & = \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)} - y^{(i)}) x_j^{(i)}) \\ & \}(\text{simultaneously update } \forall j = 0, 1, \ldots, n) \end{aligned}$$

4.3.1 Feature Scaling

Idea: Make sure features are on a similar scale.

Get every feature into approximately a $-1 \leq x_i \leq 1$ 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

$$\begin{aligned} \mu_i &= \text{average value of } x_i \\ S_i &= \text{range (max - min)} && \textit{or} \\ &= \sigma (\text{standard deviation}) \end{aligned}$$

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 $\ldots,\ 0.001,\ 0.003,\ 0.01,\ 0.03,\ 0.1,\ 0.3,\ 1,\ \ldots$

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 → breadth.

4.4.2 Polynomial Regression

Ex:

$$\begin{aligned} x_1 &= size \\ x_2 &= size^2 \\ x_3 &= size^3 \end{aligned}$$

4.5 Normal Equation

Solve for θ analytically!

$$
\begin{aligned}
x^{(i)} &= \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} && \in \mathbb{R}^{n+1} \\
X &= \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} && \in \mathbb{R}^{m\times(n+1)} \\
&= \begin{bmatrix} x_0 & x_1 & \dots & x_n \end{bmatrix} && \in \mathbb{R}^{m\times(n+1)} \\
y &= \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} && \in \mathbb{R}^{m} \\
\theta &= (X^T X)^{-1} X^T y
\end{aligned}
$$

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

4.5.1 Non Invertibility of $X^T X$

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

If $X^T X$ is non-invertible, common causes are

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

Check Lecture4.pdf for more details.

Chapter 5

Octave Tutorial

Check Lecture5.pdf for more details.

Chapter 6

Classification

Classify into categories (binary or multiple).

6.1 Logistic Regression

$$
\begin{aligned}
0 \leq h_\theta(x) &\leq 1 \\
h_\theta(x) &= g(\theta^T x) \\
g(z) &= \frac{1}{1+e^{-z}} \qquad g \text{ is called a } \textit{sigmoid} \text{ function or a } \textit{logistic} \text{ function.} \\
h_\theta(x) &= \frac{1}{1+e^{\theta^T x}}
\end{aligned}
$$

Interpretation of Hypothesis Output

$h_\theta(x)$ = estimated probability that $y = 1$ on input x
$h_\theta(x) = P(y = 1|x;\theta)$ = probability that $y = 1$, given x, parameterized by θ

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

6.2 Decision Boundary

$$\begin{aligned}
\text{Predict: } y = 1 & \qquad \text{if } h_\theta(x) \geq 0.5 \\
& \qquad (\theta^T x \geq 0) \\
\text{Predict: } y = 0 & \qquad \text{if } h_\theta(x) < 0.5 \\
& \qquad (\theta^T x < 0) \\
\theta^T x = 0 & \qquad \text{is the } \textit{decision boundary.}
\end{aligned}$$

Non-linear Decision Boundaries

Use same technique as polynomial regression for features.

6.3 Cost Function

$$\begin{aligned}
\text{Training Set} &: \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ./dots, (x^{(m)}, y^{(m)})\} \\
x &= \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1} \\
x_0 &= 1 \\
y &\in \{0, 1\} \\
h_\theta(x) &= \frac{1}{1 + e^{-\theta^T x}}
\end{aligned}$$

How to choose parameter θ?

Linear Regression:

$$\begin{aligned} J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}(h_\theta(x^{(i)}) - y^{(i)})^2 \\ J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)}) \\ \mathrm{Cost}(h_\theta(x), y) &= \frac{1}{2}(h_\theta(x) - y)^2 \end{aligned}$$

Logistic Regression:

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

Note: $y = 0$ or 1 always.

$$\begin{aligned} \mathrm{Cost}(h_\theta(x), y) &= -y\log(h_\theta(x)) - (1-y)\log(1 - h_\theta(x)) \\ J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\mathrm{Cost}\left(h_\theta(x^{(i)}), y^{(i)}\right) \\ &= -\frac{1}{m}\left[\sum_{i=1}^{m}\left(y^{(i)}\log(h_\theta(x^{(i)})) + (1 - y^{(i)})\log(1 - h_\theta(x^{(i)}))\right)\right] \end{aligned}$$

To fit parameters θ:

$$\underset{\theta}{\text{minimize}}\, J(\theta)$$

To make a prediction given a new x:

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

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

```
% We can write a single function that can return 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()*.

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
        [optTheta, functionVal, exitFlag] = fminunc(@costFunction,
                initialTheta, options);
```

6.5 Multi-Class Classification

6.5.1 One vs All

Build a separate binary classifier $h_\theta^{(i)}(x)$ for each class against all other classes.

$$h\theta^{(i)} = P(y = i|x; \theta)\ \forall i$$

On a new input x, to make a prediction, pick the class i that maximizes $h_\theta^{(i)}(x)$

Check Lecture6.pdf for more details.

Chapter 7

Regularization

7.1 Problem of Overfitting

1. Underfitting (High Bias)
2. Right Fit
3. Overfitting (High Variance)

Overfitting: If we have too many features, the learned hypothesis may fit the training set very well $\left(J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h\theta(x^{(i)}) - y^{(i)})^2 \approx 0\right)$, but fail to generalize to new examples (predict prices on new examples).

7.2 Addressing Overfitting

Options:

1. Reduce the number of features
   - Manually select which features to keep
   - Model selection algorithm (later)
2. Regularization
   - Keep all the features, but reduce the magnitude/values of parameters θ_j
   - Works well when we have a lot of features, each of which contributes a bit to predicting y

7.3 Cost Function

Say our overfitting hypothesis is $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$. Suppose, we penalize and make θ_3, θ_4 very small

$$\underset{\theta}{\text{minimize}} \left(\frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 + 1000\theta_3^2 + 1000\theta_4^2 \right)$$

Regularization

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$.

- *Simpler* hypothesis
- Less prone to overfitting

Which parameters to penalize?

- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

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

Note: The convention, we don't regularize θ_0 but it doesn't make very much difference.

λ here is *regularization parameter.*

What if λ is set too high (say 10^{10})? Underfitting!

7.4 Regularized Linear Regression

Updated $J(\theta)$:

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

$$\underset{\theta}{\text{minimize}}\, J(\theta)$$

Gradient Descent:

Repeat{

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

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

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

}

Normal Equation:

$$X = \begin{bmatrix} \left(x^{(1)}\right)^T \\ \left(x^{(2)}\right)^T \\ \vdots \\ \left(x^{(m)}\right)^T \end{bmatrix} \qquad \in \mathbb{R}^{m\times(n+1)}$$

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \qquad \in \mathbb{R}^{m}$$

$$\theta = \left(X^TX + \lambda \begin{bmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \left(\in \mathbb{R}^{(n+1)\times(n+1)}\right) \right)^{-1} - X^Ty \quad \in \mathbb{R}^{n+1}$$

Non-Invertibility

Suppose $m \leq n$,

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

If $\lambda > 0$,

$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \right)^{-1} - X^T y$$

Not a problem!

7.5 Regularized Logistic Regression

Cost Function:

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

Gradient Descent:

Repeat{

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

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

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

}

Advanced Optimization:

```
function [jVal, gradient] = costFunction(theta)
        jVal = [...code to compute J(theta)...];
        gradient = [...code to compute derivative of J(theta)...];
```

Check Lecture7.pdf for more details.