

## 1 Foreword

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Disclaimer : This notes is written only for my memorization purpose after I have studied online lecture notes and blogs.

## 2 Confusion Matrix

Predict True, Actual True : True Positive (TP)  
Predict True, Actual False : False Positive (FP)  
Predict False, Actual False : False Negative (FN)  
Predict False, Actual True : True Negative (TN)

Accuracy =  $(TP+TN)/(TP+FP+FN+TN)$ , performance of correct classification

Precision =  $TP / (TP+FP)$  ( correctly classified as positive / Everything classified as positive ), used when Cancer detection. (We don't want to initiate cancer treatment if the person is actually healthy).

Recall =  $TP / (TP + FN)$  ( correctly classified as positive / Actually positive ), FP is more expensive than TN . (e.g. Fraud detection).

Note : Mathematically, Precision and Recall are inverse relationship, there is a trade off between recall and precision.

F1 score =  $2(P*R)/(P+R)$ , a compromised metric

## 3 K-Nearest Neighbour

Description : Choose the \*majority\* class of nearest (e.g. Eclidean Distance ) K data and classify it.

How to Choose K(hyper-parameter) : General rule of thumb :  $\sqrt{\text{number of data}}/2$  or by searching and comparing different k's for highest prediction accuracy.

Normalization of data in preprocessing is a must

## 4 K-Means Clustering

Simple Description : Identify clusters by finding the centroid of data points

Algorithm :

1. Initialize  $\mu_1, \mu_2, \dots, \mu_k$  randomly (k is hyper-parameter)

2. Repeated until converge :

(i)  $c^{(i)} := \arg \min_j \|x^{(i)} - \mu_j\|^2, j \in [1 : k]$  , (i.e.  $c^{(i)}$  denote which  $\mu$  the  $x^{(i)}$  is linked to. Link each data point to nearest  $\mu_j$ . If  $x^{(i)}$  is nearest to  $\mu_s$ , then  $c^{(i)} = j$ . Thus, k partitions are created. )

(ii)  $\mu_j := \frac{\sum_{i=1}^m 1\{c^{(i)}=j\}x^{(i)}}{\sum_{i=1}^m 1\{c^{(i)}=j\}}$  , (i.e. For each data point in each partition from (i) , find the new centroid and assign to  $\mu_k$

Proof of convergence of the algorithm : consider

$$J(c, \mu) = \sum_{i=1}^m \|x^{(i)} - \mu_{c^{(i)}}\|^2$$

Observation : J must be monotonically decreasing. It is because for step (i) It is adjusting  $c^{(i)}$  to reduce J, for step (ii) we are adjusting  $\mu_j$  to reduce J. J is non-convex, it may get to local minimum. To try several random initial values, and choose the lowest J.

## 5 Linear Regression(MSE approach)

Hypothesis :

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

We want to minimize MSE (Mean Square Error)

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

Gradient of J :

$$\frac{\partial J(\theta)}{\partial \theta_j} = \sum_i x_j^{(i)} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)$$

Each  $\theta_j$  is updated for each step by gradient descent algorithm.

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

Practically :

(i) Learning rate  $\alpha$  is hyperparameter and data dependent , larger, fewer steps to get to min. but may miss the minimum. (Monitor the loss curve, J value vs iteration ).

(ii) Batch GD is slow, may be Mini-Batch GD or Stochastic GD.

(iii) If  $\alpha$  is small but the loss oscillate , converged and stop learning.

## 6 Linear Regression(MLE approach)

## 7 Logistic Regression

$$P(y = 1|x) = h_{\theta}(x) = \frac{1}{1 + \exp(-\theta^{\top} x)} \equiv \sigma(\theta^{\top} x)$$
$$P(y = 0|x) = 1 - P(y = 1|x) = 1 - h_{\theta}(x)$$

Loss function is

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

Again , BGD for following gradient of J :

$$\frac{\partial J(\theta)}{\partial \theta_j} = \sum_i x^{(i)}_j \left( h_{\theta}(x^{(i)}) - y^{(i)} \right)$$

Interpretation : For a particular sample : if h return 1/0 and y return 1/0 , the term is 0. if h return 1/0 and y return 0/1 , the term is positive infinity.

## 8 Logistic Regression(MLE approach)

## 9 Softmax Regression(Multi-Class Logistic)

k classes, n x k parameters , and the hypothesis is :

$$h_{\theta}(x) = \begin{bmatrix} P(y = 1|x; \theta) \\ P(y = 2|x; \theta) \\ \vdots \\ P(y = K|x; \theta) \end{bmatrix} = \frac{1}{\sum_{j=1}^K \exp(\theta^{(j)\top} x)} \begin{bmatrix} \exp(\theta^{(1)\top} x) \\ \exp(\theta^{(2)\top} x) \\ \vdots \\ \exp(\theta^{(K)\top} x) \end{bmatrix} \quad (1)$$

Below Loss function is simple to understand : By referencing to previous hypothesis, we want to maximize the y=k associated probability.

$$J(\theta) = - \left[ \sum_{i=1}^m \sum_{k=1}^K 1\{y^{(i)} = k\} \log \left( \frac{\exp(\theta^{(k)\top} x^{(i)})}{\sum_{j=1}^K \exp(\theta^{(j)\top} x^{(i)})} \right) \right]$$

Gradient of J is, we solve the problem by GD :

$$\nabla_{\theta^{(k)}} J(\theta) = - \sum_{i=1}^m \left[ x^{(i)} \left( 1\{y^{(i)} = k\} - P(y^{(i)} = k|x^{(i)}; \theta) \right) \right]$$

Where :

$$P(y^{(i)} = k|x^{(i)}; \theta) = \frac{\exp(\theta^{(k)\top} x^{(i)})}{\sum_{j=1}^K \exp(\theta^{(j)\top} x^{(i)})}$$

## 10 BGD variation : Mini BGD/SGD

BGD use all training data in a single step, which is extremely costly.

## 11 Loss function in Classification(Binary) Problem - General treatment

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

Adjustment for binary classification :

$$\text{sign}(h_{\theta}(x)) = \text{sign}(\theta^T x) = \text{sign}(t) = \begin{cases} 1 & \text{if } t > 0 \\ 0 & \text{if } t = 0 \\ -1 & \text{if } t < 0 \end{cases}$$

Measure of confidence :  $h_{\theta}(x) = x^T \theta$  gives larger value, more confident

Margin (  $y x^T \theta$  ) : (i) if  $h_{\theta}(x)$  classify correctly, margin is positive, otherwise negative.

(ii) Therefore our objective is to maximize the margin ( we want both correct classification and be confident)

Consider the following loss function :

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m \phi \left( y^{(i)} \theta^T x^{(i)} \right)$$

We want penalize wrong classification and encourage correct one , we design  $\phi$  as  $\phi(z) \rightarrow 0$  as  $z \rightarrow \infty$ , while  $\phi(z) \rightarrow \infty$  as  $z \rightarrow -\infty$  where  $z = y x^T \theta$  , and examples are :

logistic loss :  $\phi_{\text{logistic}}(z) = \log(1 + e^{-z})$  ,used in logistic regression

hinge loss :  $\phi_{\text{hinge}}(z) = [1 - z]_+ = \max 1 - z, 0$ , used in SVM

Exponential loss  $\phi_{\text{exp}}(z) = e^{-z}$ , used in boosting

## 12 Kernel Mapping (Special case demo by Linear Regression + Polynominal Kernel)

(I) Purpose : To map from lower higher dimension. Useful when data are non-linearly separable(Transform to a curve)

(II) Computation complexity does not necessarily increase proportionately.

(III) Example : a mapping function  $\varphi : R \rightarrow R^4$  ,  $x \rightarrow [1, x, x^2, x^3]$ , and  $h$  is  $\theta^T x$  having  $\theta = [\theta_1, \theta_2, \theta_3, \theta_4]$

(IV) Terms :  $x$  is called attribute,  $x \rightarrow [1, x, x^2, x^3]$  called feature,  $\varphi$  feature map,  $\varphi : R^1 \rightarrow R^4$  in this case.  $d=1$   $p=4$

(IV) Another Example : a mapping function  $\varphi : R^3 \rightarrow R^{1000}$ ,  $x \rightarrow [1, x_1, x_1^2, x_1^3, x_1x_2, x_1x_2^2, \dots]$

(\*) ,let  $d=3$ ,  $p=1000$ . If we exhaust all possibilities, then  $p=1+d+d^2+d^3$  (\*\*)

Recall GD stepping :

$$\theta := \theta + \alpha \sum_{i=1}^n (y^{(i)} - h_{\theta}(x^{(i)}))x^{(i)}$$

$$\theta := \theta + \alpha \sum_{i=1}^n (y^{(i)} - \theta^T x^{(i)})x^{(i)}$$

Putting kernel mapping to the equation :

$$\theta := \theta + \alpha \sum_{i=1}^n (y^{(i)} - \theta^T \phi(x^{(i)}))\phi(x^{(i)})$$

We pause here to evaluate the cost of computing each of update (Curse of Dimensionality...), considering (\*\*). If we just use the kernel direction, we suffer the curse of dimensionality : Suppose  $d$  (data dimension) = 1000, then by using the mapping in (\*\*) we have  $p=10^9$ .  $\theta^T \phi(x^{(i)})$  need  $O(p)$  (dot product), and  $O(np)$  for summing up all data in each step. Going back to BGD.

$$\theta := \theta + \alpha \sum_{i=1}^n (y^{(i)} - \theta^T \phi(x^{(i)}))\phi(x^{(i)})$$

, assuming  $\theta = \sum_{i=1}^n \beta_i \phi(x^{(i)})$  (\*) at some point, with initialization  $\theta = 0 = \beta$  It becomes

$$\theta := \sum_{i=1}^n \beta_i \phi(x^{(i)}) + \alpha \sum_{i=1}^n (y^{(i)} - \theta^T \phi(x^{(i)}))\phi(x^{(i)})$$

Rearranging :

$$\theta := \sum_{i=1}^n (\beta_i + \alpha(y^{(i)} - \theta^T \phi(x^{(i)})))\phi(x^{(i)})$$

Therefore it is equivalent to updating  $\beta_i$  ( instead of  $\theta_i$  ) by

$$\beta_i := \beta_i + \alpha(y^{(i)} - \theta^T \phi(x^{(i)}))$$

by (\*) above

$$\beta_i := \beta_i + \alpha \left( y^{(i)} - \sum_{j=1}^n \beta_j \phi(x^{(j)})^T \phi(x^{(i)}) \right)$$

Computing of LHS is fast because : (1) we can pre-compute  $\phi(x^{(j)})^T \phi(x^{(i)})$  for all  $i, j$ , and (2)  $\phi(x^{(j)})^T \phi(x^{(i)})$  can be represented by  $\langle x^{(i)}, x^{(j)} \rangle$  :

$$\langle \phi(x), \phi(z) \rangle = 1 + \sum_{i=1}^d x_i z_i + \sum_{i,j \in \{1, \dots, d\}} x_i x_j z_i z_j + \sum_{i,j,k \in \{1, \dots, d\}} x_i x_j x_k z_i z_j z_k = 1 + \langle x, z \rangle + \langle x, z \rangle^2 + \langle x, z \rangle^3 \quad (**)$$

Define  $K$  where  $K$  is  $n \times n$  (  $n$  is the number of training samples) matrix, with  $K(x, z) = \langle \phi(x), \phi(z) \rangle$ , where  $K_{ij}$  is  $\langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$

Therefore, the process is : (1) compute  $K_{ij}$  using  $(**)$ , for all  $i, j \in \{1, \dots, n\}$ . Set  $\beta := 0$ ,  
(2) Loop

$$\forall i \in \{1, \dots, n\}, \quad \beta_i := \beta_i + \alpha \left( y^{(i)} - \sum_{j=1}^n \beta_j K(x^{(i)}, x^{(j)}) \right)$$

in vectorized notation:

$$\beta := \beta + \alpha(\tilde{y} - K\beta)$$

When doing inference :

$$\theta^T \phi(x) = \sum_{i=1}^n \beta_i \phi(x^{(i)})^T \phi(x) = \sum_{i=1}^n \beta_i K(x^{(i)}, x)$$

In practice, we do computation using  $K$  ( at  $O(d)$  cost ) instead of directly from  $\phi(x)$  is much faster. Further, We only need to know  $K$  but "just only need to know" the existence of  $\phi(x)$ . There is no need to be able to write down  $\phi(x)$ . Consider the Kernel applied to bitmap : number of bits as  $d$ . (Great reduction!) Intuitively,  $K$  represents similarity matrix, i.e.  $K$  is small if  $\phi(x^{(j)})^T \phi(x^{(i)})$  is small

Example : Gaussian Kernel, it can support infinitely dimensional space of mapping.

$$K(x, z) = \exp \left( -\frac{\|x - z\|^2}{2\sigma^2} \right)$$

Mercer Theorem : For  $K$  to be a valid Kernel iff  $K$  is PSD.

Application : To SVM, perceptron, linear regression, and other learning algorithms represented only in inner product  $\langle x, z \rangle$ , then Apply  $K(x, z)$

- 13 Entropy
- 14 Decision Tree, with Random Forest, Boosting
- 15 Bootstrapping
- 16 PCA, Principal Component Analysis
- 17 SVD, Singular Value Decomposition
- 18 SVM, Support Vector Machine
- 19 Backpropagation
- 20 EM Algorithm
- 21 Generative Learning Algorithm
- 22 Reinforcement learning
- 23 MAP (Maximum a Posterior) vs MLE (Maximum Likelihood Estimation)
- 24 IDP, Independent Component Analysis
- 25 Bias Variance Analysis
- 26 Hidden Markov Model
- 27 Apriori
- 28 Recommender System
- 29 Anomaly Detection
- 30 Perceptron