CS4220: Machine Learning

Yuhang Tian[1]

[1]Technology University of Delft

y.tian-13@student.tudelft.nl

1. Bayesian Classifier Theorem

1.1. Decision Boundary

$$p(x|w_1)p(w_1) \gtrless p(x|w_2)p(x|w_2) \tag{1}$$

1.2. Minimizing the Classification Error Probability (Bayes Error)

$$P_e = p(w_2)\int_{-\infty}^{x_0} p(x|w_2)dx + p(w_1)\int_{x_0}^{\infty} p(x|w_1)dx \tag{2}$$

where $p(x_0|w_1)p(w_1) = p(x_0|w_2)p(x|w_2)$

1.3. Minimizing the Average Risk

Loss Matrix

$$L = \begin{bmatrix} 0 & \lambda_{12} \\ \lambda_{21} & 0 \end{bmatrix} \tag{3}$$

Risk Function

$$r = \lambda_{21}p(w_2)\int_{-\infty}^{x_0} p(x|w_2)dx + \lambda_{12}p(w_1)\int_{x_0}^{\infty} p(x|w_1)dx \tag{4}$$

1.4. Gaussian pdf in the l-dimensional space

$$p(x) = \frac{1}{(2\pi)^{l/2}|\Sigma|^{l/2}} exp(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)) \tag{5}$$

where $\Sigma = E[(x-\mu)(x-\mu)^T]$

1.5. Bayesian Classifier

discriminant functions

$$g_i(x) = ln(p(x|w_i)p(w_i)) = lnp(x|w_i) + lnp(w_i) \tag{6}$$

Normally Distributed Classifier

$$g_i(x) = -\frac{1}{2}x^T\Sigma_i^{-1}x + \frac{1}{2}x^T\Sigma_i^{-1}\mu_i - \frac{1}{2}\mu_i^T\Sigma_i^{-1}\mu_i + \frac{1}{2}\mu_i^T\Sigma_i^{-1}x + lnp(w_i) + c_i \tag{7}$$

where $c_i = -(l/2)ln2\pi - (1/2)ln(det(\Sigma_i))$

- if l=2, corelation=0

$$g_i(x) = -\frac{1}{2\sigma_i^2}(x_1^2 + x_2^2) + \frac{1}{\sigma_i^2}(\mu_i 1x_1 + \mu_i 2x2) - \frac{1}{2\sigma_i^2}(\mu_{i1}^2 + \mu_{i2}^2) + lnp(w_i) + c_i \tag{8}$$

$g_i(x) - g_j(x) = 0$ are quadratics (i.e., ellipsoids, parabolas, hyperbolas, pairs of lines)

- if covariance matrix is the same in all classes

$$g_i(x) = w_i^T x + b \tag{9}$$

where $w_i = \Sigma^{-1}\mu_i$ and $b = lnp(w_i) - \frac{1}{2}\mu_i^T\Sigma^{-1}\mu_i$

- if Diagonal covariance matrix with equal elements ($\Sigma = \sigma^2 I$)

$$g_i(x) = \frac{1}{\sigma^2}\mu_i^T x + b \tag{10}$$

2. ESTIMATION OF UNKNOWN PROBABILITY DENSITY FUNCTIONS

2.1. ML

we considered θ as an unknown parameter.

$$\hat{\theta}_{ML} = arg\ max_\theta \prod_{k=1}^{N} p(x_k;\theta) \tag{11}$$

ML estimate of σ^2

$$\hat{\sigma}^2_{ML} = \frac{1}{N}\sum_{k=1}^{N}(x_k - \mu)^2 \tag{12}$$

ML estimate of μ

$$\hat{\mu}_{ML} = \frac{1}{N}\sum_{k=1}^{N} x_k \tag{13}$$

2.2. MAP

we considered θ as a random vector.

$$p(\theta|X) = \frac{p(\theta)p(X|\theta)}{P(X)} \tag{14}$$

then,

$$\hat{\theta}_{MAP} : \frac{\partial}{\partial\theta}p(\theta|X) = 0\ or\ \frac{\partial}{\partial\theta}p(X|\theta)p(\theta) = 0 \tag{15}$$

2.3. Bayesian Inference

Given the set X of the N training vectors and the *a priori information* about the pdf $p(\theta)$, the goal is to compute the conditional pdf $p(x|X)$.

$$p(x|X) = \int p(x|\theta)p(\theta|X)d\theta \tag{16}$$

with

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} \tag{17}$$

$$p(X|\theta) = \prod_{k=1}^{N} p(x_k|\theta) \tag{18}$$

3. Normal-based Classifier: Quadratic Discriminant, Linear Discriminant and Nearest Mean

Let's assume that we have two classes:

3.1. Quadratic Discriminant

by eq.7, the quadratic classifier,

$$f(x) = x^T W x + w^T + w_0 \tag{19}$$

with

$$W = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1}) \tag{20}$$

$$w = \mu_1^T \Sigma_1^{-1} - \mu_2^T \Sigma_2^{-1} \tag{21}$$

$$w_0 = -\frac{1}{2} ln(det(\Sigma_1)) - \frac{1}{2}\mu_1^T \Sigma_1^{-1} \mu_1 + lnp(y_1) + \frac{1}{2} ln(det(\Sigma_2)) + \frac{1}{2}\mu_2^T \Sigma_2^{-1} \mu_2 - lnp(y_2) \tag{22}$$

(i.e., ellipsoids, parabolas, hyperbolas, pairs of lines)

3.2. Linear Discriminant

by eq.9, the linear classifier,

$$f(x) = w^T x + w_0 \tag{23}$$

with

$$w = \Sigma^{-1}(\mu_2 - \mu_1) \tag{24}$$

$$w_0 = \frac{1}{2}\mu_1^T \Sigma^{-1} \mu_1 - \frac{1}{2}\mu_2^T \Sigma^{-1} \mu_2 + ln\frac{p(y_1)}{p(y_2)} \tag{25}$$

Therefore, the Linear Discriminant has a **strong assumption** on that $\Sigma_1 = \Sigma_2$

3.3. Nearest Mean Classifier

by eq.10, the nearest mean classifier,

$$f(x) = w^T x + w_0 = \sigma^2(g_1(x) - g_2(x)) \tag{26}$$

with

$$w = \mu_2 - \mu_1 \tag{27}$$

$$w_0 = \frac{1}{2}\mu_1^T \mu_1 - \frac{1}{2}\mu_2^T \mu_2 + \sigma^2 ln\frac{p(y_1)}{p(y_2)} \tag{28}$$

Therefore, the Nearest Mean has a **strong assumption** on mutually uncorrelated and of the same variance ($\Sigma_1 = \Sigma_2 = \sigma^2 I$)

4. More Parametric Classifiers

4.1. Logistic Classifier

$$\begin{cases} p(y_1|x) = \frac{1}{e^{-(w^T x + w_0)}+1} \\ p(y_2|x) = \frac{1}{e^{(w^T x + w_0)}+1} \end{cases} \tag{29}$$

Maximize Log Likelihood

$$lnp(y|x) = \sum_{i=1}^{N} ln(\frac{1}{e^{-y_i(w^T x_i + w_0)} + 1}) \tag{30}$$

4.2. Fisher Classifier

$$y_i = w^T x_i \begin{cases} \geq 0 & \text{if class 1} \\ < 0 & \text{if class 2} \end{cases} \tag{31}$$

Minimize Square Loss

$$L(w) = \sum_{i=1}^{N} (w^T x_i - y_i)^2 \tag{32}$$

4.3. The Perception

Forward&backward propagation and update w

$$w \leftarrow w + \eta y x \tag{33}$$

5. Non-parametric Classification

In the above sections, all the classifiers are based on **Parametric Classification** method, more precisely, based on normal distribution and Bayes Theorem. In this section, it will mainly demonstrate two non-parametric classifiers - Parzen Classifier and Nearest Neighbour Classifier (Both methods are sensitive to the scaling of the features).

5.1. Parametric vs. Non-parametric

- Parametric: Assumptions can greatly simplify the learning process, but can also limit what can be learned. Algorithms that simplify the function to a known form are called parametric machine learning algorithms.
- Non-parametric: Algorithms that do not make strong assumptions about the form of the mapping function are called non-parametric machine learning algorithms. By not making assumptions, they are free to learn any functional form from the training data.

5.2. Histogram method

it's easy, so I just skip it.

5.3. Parzen Density Estimation

- Kernel

$$f(x) = \begin{cases} 0 & \text{if |r|>h} \\ \frac{1}{V} & \text{if |r|} \leq \text{h} \end{cases} \tag{34}$$

- Parzen Classifier

$$p(z|h) = \frac{1}{n}\sum_{i=1}^{n} K(||z - x_i||, h) \tag{35}$$

- Parzen plugs in the Gaussian density:

$$p(x|w_i) = \frac{1}{n_i}\sum_{j=1}^{n_i} N(x|x_j^{(i)}, hI) \tag{36}$$

5.4. Nearest Neighbour Classification

$$p(x) = p(x|w_m)p(w_m) = \frac{k_m}{n_m V_k} \cdot \frac{n_m}{n} \tag{37}$$

where V_k is the volume of the sphere centered at x with radius r (the distance to the k-th nearest neighbor)

6. More Non-parametric Classifiers

GitHub Markdown

6.1. SVM

By putting some constraints on the linear classifier, the VC dimension can be reduced. Why do that? Ans: When h is small, the true error is close to the apparent error

$$\begin{cases} w^T x_i + b \geq +1 & \text{for } y_i = +1 \\ w^T x_i + b \leq -1 & \text{for } y_i = -1 \end{cases} \tag{38}$$

Core Idea of SVM: Find the decision boundary, while maximize the margin

1. The above two equation can be merged into one

$$y_i(w^T x_i + b) - 1 \geq 0 \tag{39}$$

2. The distance between the two boundaries

$$maximize \frac{2}{||w||} \rightarrow minimize \frac{1}{2}||w||^2 \tag{40}$$

3. by Lagrange Multiplier

$$L = \frac{1}{2}||w||^2 - \sum \alpha_i[y_i(wx_i + b) - 1] \tag{41}$$

4. by $\frac{\partial L}{\partial w} = 0$

$$w = \sum \alpha_i y_i x_i \tag{42}$$

5. by $\frac{\partial L}{\partial b} = 0$

$$\sum \alpha_i y_i = 0 \tag{43}$$

6. put eq.42 back to eq.41

$$L = \sum \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j x_i \cdot x_j \tag{44}$$

7. put eq.42 back to decision rule

$$\begin{cases} \sum \alpha_i y_i x_i \cdot u_i + b - 1 \geq 0 & \text{Then, +} \\ \sum \alpha_i y_i x_i \cdot u_i + b - 1 \leq 0 & \text{Then, -} \end{cases} \tag{45}$$

8. kernelize

$$K(x_i, x_j) = \phi(x_i) \cdot \phi(x_j) \tag{46}$$

6.2. Agglomerative Hierarchical Clustering

1. Determine distances between all clusters
   - Two nearest objects in the clusters: single linkage
   - Two most remote objects in the clusters: complete linkage
   - Cluster centers: average linkage
2. Merge clusters that are closes
3. IF #clusters>1 THEN GOTO 1

- Dendrogram: Cut at "largest jump"$\rightarrow$ Clustering
- Fusion Graph: Cut at "largest drop"$\rightarrow$ Clustering

7. Regression

7.1. Intuitively Understanding

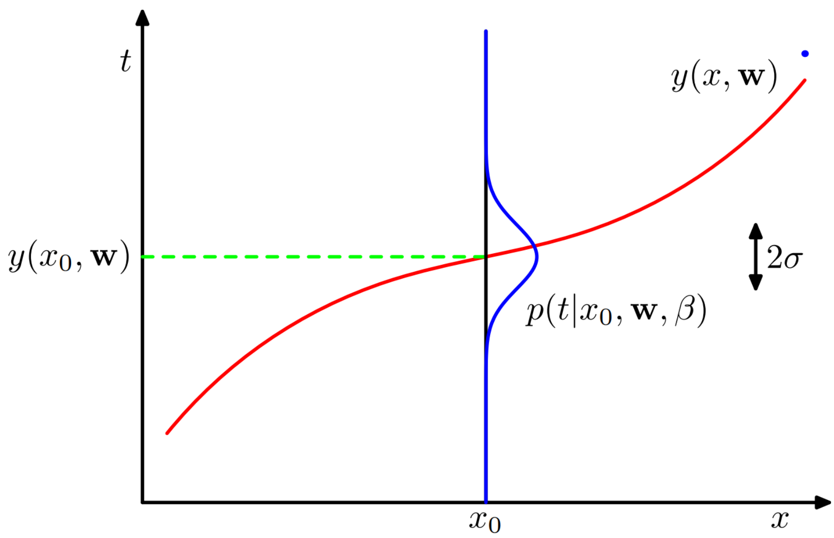


Figura 1. Regression Curve

Suppose that there is a fixed x_0 and a bunch of choices of θ (here are μ and $\sigma^2(\beta^{-1})$). If we expect the predicted value $\hat{y}(x_0, w)$ to locate on the true value t_0, the probability of this occurrence $p(t_0|x_0, w, \beta)$ should be maximized.

7.2. Maximum Likelihood Regression

$$p(t|x, w, \beta) = \prod_{n=1}^{N} N(t_n|y(x_n, w), \beta^{-1}) \tag{47}$$

Log Likelihood function

$$lnp(t|x, w, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N} y(x_n, w) - {t_n}^2 + \frac{N}{2}ln\beta - \frac{N}{2}ln(2\pi) \tag{48}$$

To solve

$$\frac{\partial}{\partial w} lnp(t|x_0, w, \beta) = 0 \tag{49}$$

and

$$\frac{\partial}{\partial \beta^{-1}} lnp(t|x_0, w, \beta) = 0 \tag{50}$$

If we use linear regression, the solutions of eq.49 and eq.50

$$w_{ML} = (X^T X)^{-1} X^T Y \ \beta_{ML}^{-1} = \frac{1}{N}(w_{ML}^T X - Y) \tag{51}$$

7.3. Max a Posterior Regression

Suppose that we have some knowledge about $w\ N(0, \alpha I)$

$$w_{MAP} : (\prod_{i=1}^{N} p(y_i|w^T x_i, \sigma^2))p(w|0, \alpha I) \tag{52}$$

$$\frac{\partial}{\partial w}(\prod_{i=1}^{N} p(y_i|w^T x_i, \sigma^2))p(w|0, \alpha I) = 0 \rightarrow w_{MAP} = (X^T X + \frac{\sigma^2}{\alpha} I)^{-1} X^T Y \tag{53}$$

8. Regularization

8.1. Keep Eigenvalues Away From Zero

Add identity to XX^T

$$\hat{w} = (X^T X + \lambda I)^{-1} X^T Y \tag{54}$$

8.2. LASSO, L1 Norm

$$min_{\beta} \frac{1}{N}\sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda||w|| \tag{55}$$

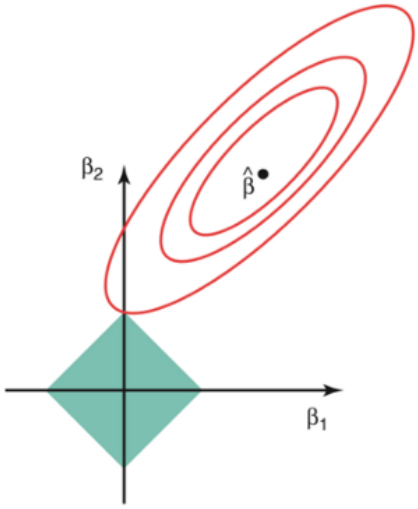


Figura 2. LASSO/L1 Regularization

$\lambda \propto \frac{1}{\tau}$

8.3. Ridge, L2 Norm

$$min_{\beta}\frac{1}{N}\sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda ||w||^2 \tag{56}$$

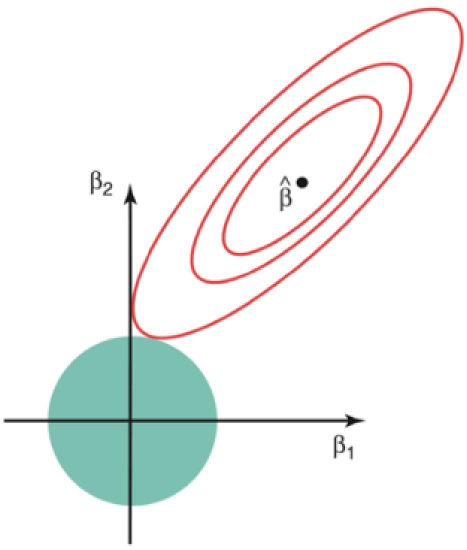


Figura 3. Ridge/L2 Regularization

$\lambda \propto \frac{1}{\tau}$

8.4. L1 vs. L2

- L1 is for feature selection

- L2 is for avoiding overfitting

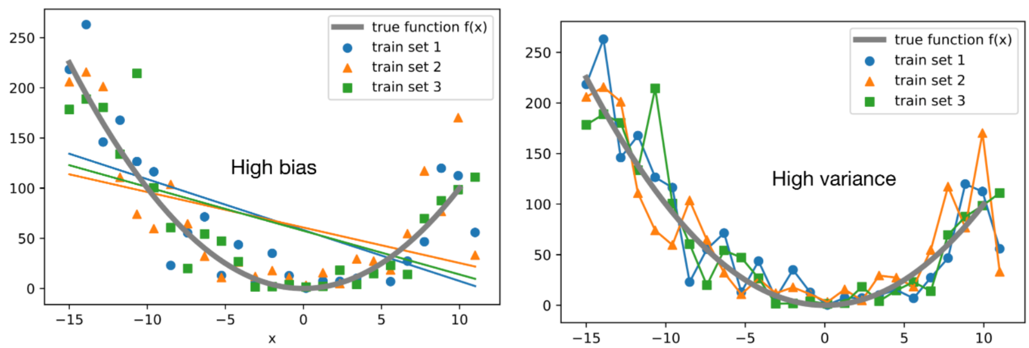
Read More

9. Data Pre-processing

9.1. LDA vs. PCA

10. Curves

10.1. Bias-Variance Decomposition



(a) High Bias (b) High Variance

Figura 4. High Bias vs. High Variance

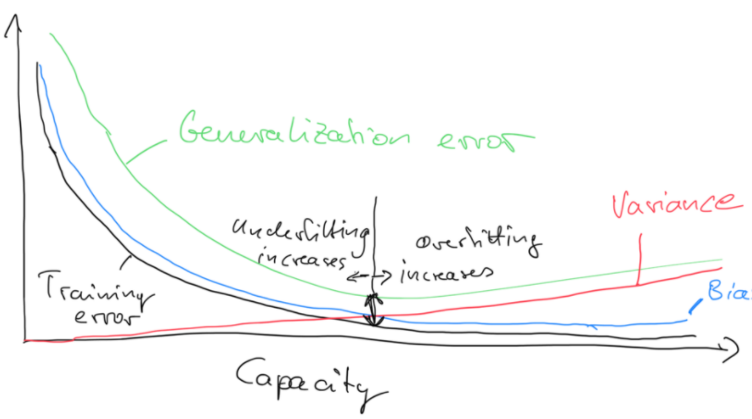


Figura 5. Decomposition Of Loss

10.2. Cross Validation Curve

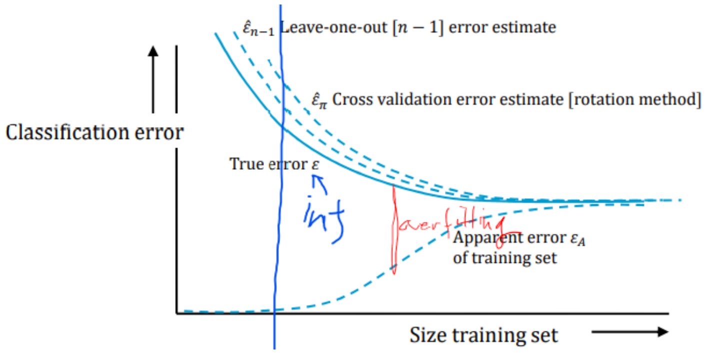


Figura 6. Cross Validation Curve

10.3. Learning Curve

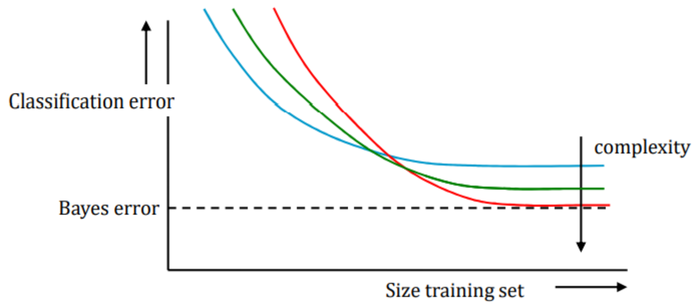


Figura 7. Learning Curve

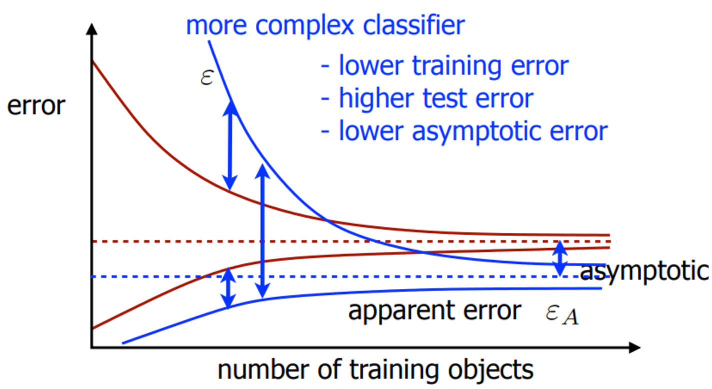


Figura 8. Learning Curve 2

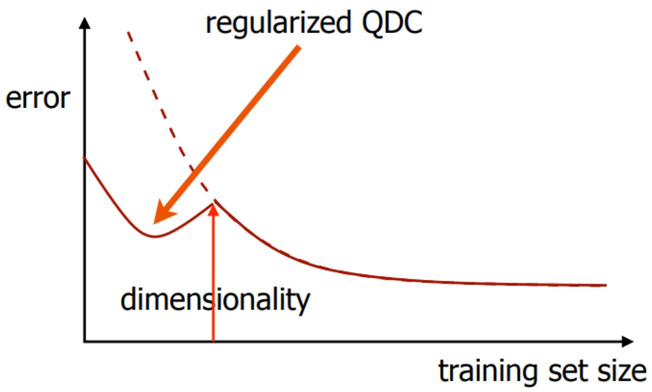


Figura 9. Regularized QDC

10.4. Feature Curve

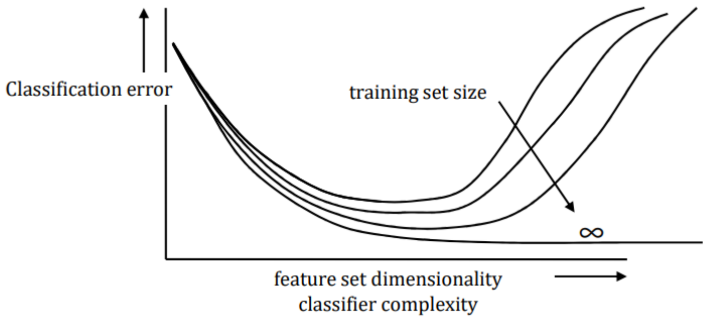


Figura 10. Feature Curve

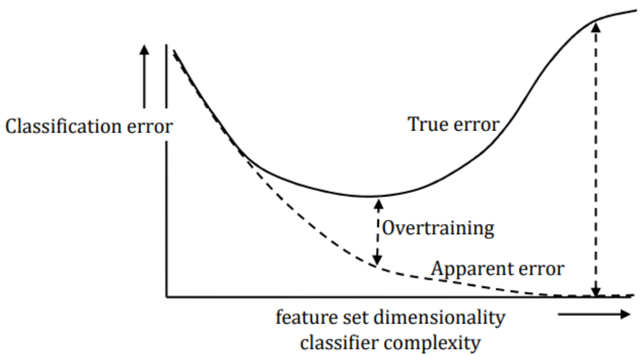


Figura 11. Curse of Dimensionality

10.5. ROC: receiver operating characteristic curve

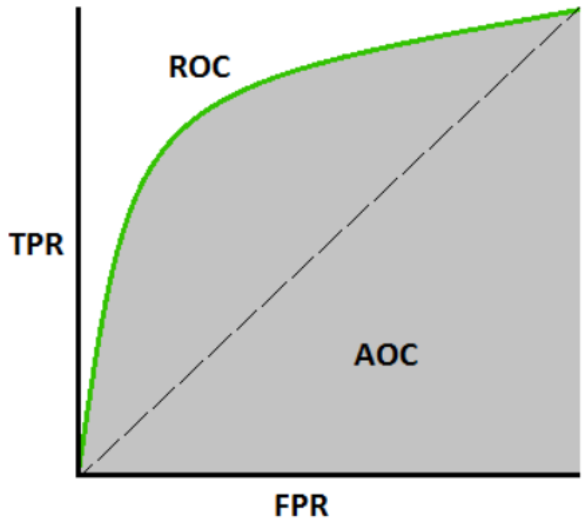
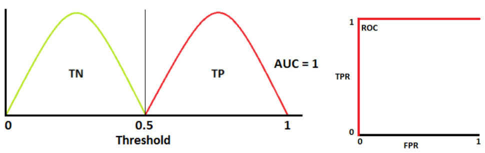


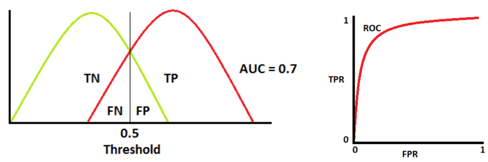
Figura 12. ROC Curve

$$TPR/Recall/Senstivity = \frac{TP}{TP + FN} \tag{57}$$

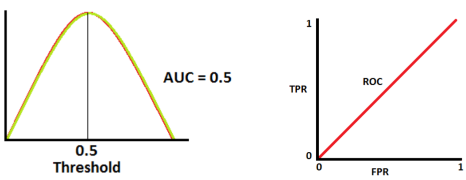
$$FPR = \frac{FP}{TN + FP} \tag{58}$$



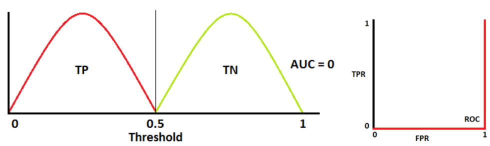
(a) AUC=1



(b) AUC=0.7



(c) AUC=0.5



(d) AUC=0

Figura 13. Different ROCs

Area under the Curve of ROC (AUC ROC)