INTRODUCTION TO DATA ANALYTICS

Class # 23

Sensitivity Analysis – Performance Estimation

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Performance Estimation

PERFORMANCE ESTIMATION OF A CLASSIFIER

- Predictive accuracy works fine, when the classes are balanced
  - That is, every class in the data set are equally important
- In fact, data sets with imbalanced class distributions are quite common in many real life applications
- When the classifier classified a test data set with imbalanced class distributions then, predictive accuracy on its own is not a reliable indicator of a classifier's effectiveness.

Example 22.1: Effectiveness of Predictive Accuracy

- Given a data set of stock markets, we are to classify them as "good" and "worst". Suppose, in the data set, out of 100 entries, 98 belong to "good" class and only 2 are in "worst" class.
  - With this data set, if classifier's predictive accuracy is 0.98, a very high value!
    - Here, there is a high chance that 2 "worst" stock markets may incorrectly be classified as "good"
  - On the other hand, if the predictive accuracy is 0.02, then none of the stock markets may be classified as "good"

PERFORMANCE ESTIMATION OF A CLASSIFIER

- Thus, when the classifier classified a test data set with imbalanced class distributions, then predictive accuracy on its own is not a reliable indicator of a classifier's effectiveness.

- This necessitates an alternative metrics to judge the classifier.

- Before exploring them, we introduce the concept of Confusion matrix.

CONFUSION MATRIX

- A confusion matrix for a two classes (+, -) is shown below.

	C1	C2
C1	True positive	False negative
C2	False positive	True negative

	+	-
+	++	+-
-	-+	--

- There are four quadrants in the confusion matrix, which are symbolized as below.
  - True Positive (TP: f_{++}) : The number of instances that were positive (+) and correctly classified as positive (+v).
  - False Negative (FN: f_{+-}): The number of instances that were positive (+) and incorrectly classified as negative (-). It is also known as **Type 2 Error**.
  - False Positive (FP: f_{-+}): The number of instances that were negative (-) and incorrectly classified as (+). This also known as **Type 1 Error**.
  - True Negative (TN: f_{--}): The number of instances that were negative (-) and correctly classified as (-).

CONFUSION MATRIX

Note:

- $N_p = TP\ (f_{++}) + FN\ (f_{+-})$

  $=$ is the total number of positive instances.

- $N_n = FP(f_{-+}) + TN(f_{--})$

  $=$ is the total number of negative instances.

- $N = N_p + N_n$

  $=$ is the total number of instances.

- (TP + TN) denotes the number of correct classification

- (FP + FN) denotes the number of errors in classification.

- For a perfect classifier FP = FN = 0, that is, there would be no Type 1 or Type 2 errors.

CONFUSION MATRIX

Example 22.2: Confusion matrix

A classifier is built on a dataset regarding Good and Worst classes of stock markets. The model is then tested with a test set of 10000 unseen instances. The result is shown in the form of a confusion matrix. The result is self explanatory.

Class	Good	Worst	Total
Good	6954	46	7000
Worst	412	2588	3000
Total	**7366**	**2634**	**10000**

Predictive accuracy?

CONFUSION MATRIX FOR MULTICLASS CLASSIFIER

- Having m classes, confusion matrix is a table of size $m \times m$, where, element at (i, j) indicates the number of instances of class i but classified as class j.

- To have good accuracy for a classifier, ideally most diagonal entries should have large values with the rest of entries being close to zero.

- Confusion matrix may have additional rows or columns to provide total or recognition rates per class.

CONFUSION MATRIX FOR MULTICLASS CLASSIFIER

Example 22.3: Confusion matrix with multiple class

Following table shows the confusion matrix of a classification problem with six classes labeled as C_1, C_2, C_3, C_4, C_5 and C_6.

Class	C1	C2	C3	C4	C5	C_6
C1	52	10	7	0	0	1
C2	15	50	6	2	1	2
C3	5	6	6	0	0	0
C4	0	2	0	10	0	1
C5	0	1	0	0	7	1
C_6	1	3	0	1	0	24

Predictive accuracy?

CONFUSION MATRIX FOR MULTICLASS CLASSIFIER

- In case of multiclass classification, sometimes one class is important enough to be regarded as positive with all other classes combined together as negative.
- Thus a large confusion matrix of m*m can be concised into 2*2 matrix.

Example 22.4: *m*×*m* CM to 2×2 CM

- For example, the CM shown in the above Example is transformed into a CM of size 2×2 considering the class C_1 as the positive class and classes C_2, C_3, C_4, C_5 and C_6 combined together as negative.

Class	+	-
+	52	18
-	21	123

How we can calculate the predictive accuracy of the classifier model in this case?

Are the predictive accuracy same in both Example 22.3 and Example 22.4?

PERFORMANCE EVALUATION METRICS

- We now define a number of metrics for the measurement of a classifier.
  - In our discussion, we shall make the assumptions that there are only two classes: + (positive) and – (negative)
  - Nevertheless, the metrics can easily be extended to multi-class classifiers (with some modifications)

- **True Positive Rate** (**TPR**)**:** It is defined as the fraction of the positive examples predicted correctly by the classifier.

$$TPR = \frac{TP}{P} = \frac{TP}{TP+FN} = \frac{f_{++}}{f_{++}+f_{+-}}$$

  - This metrics is also known as ***Recall***, ***Sensitivity*** or ***Hit rate***.

- **False Positive Rate** (**FPR**)**:** It is defined as the fraction of negative examples classified as positive class by the classifier.

$$FPR = \frac{FP}{N} = \frac{FP}{FP+TN} = \frac{f_{-+}}{f_{-+}+f_{--}}$$

  - This metric is also known as ***False Alarm Rate***.

PERFORMANCE EVALUATION METRICS

- **False Negative Rate (FNR):** It is defined as the fraction of positive examples classified as a negative class by the classifier.

$$FNR = \frac{FN}{P} = \frac{FN}{TP + FN} = \frac{f_{+-}}{f_{++} + f_{+-}}$$

- **True Negative Rate (TNR):** It is defined as the fraction of negative examples classified correctly by the classifier

$$TNR = \frac{TN}{N} = \frac{TN}{TN + FP} = \frac{f_{--}}{f_{--} + f_{-+}}$$

  - This metric is also known as ***Specificity***.

PERFORMANCE EVALUATION METRICS

- **Positive Predictive Value (PPV):** It is defined as the fraction of the positive examples classified as positive that are really positive

$$PPV = \frac{TP}{TP + FP} = \frac{f_{++}}{f_{++} + f_{-+}}$$

  - It is also known as *Precision*.

- **F_1 Score (F_1):** Recall (r) and Precision (p) are two widely used metrics employed in analysis, where detection of one of the classes is considered more significant than the others.

  - It is defined in terms of (r or TPR) and (p or PPV) as follows.

$$F_1 = \frac{2r.p}{r + p} = \frac{2TP}{2TP + FP + FN}$$

$$= \frac{2f_{++}}{2f_{++} + f_{\mp} + f_{+-}} = \frac{2}{\frac{1}{r} + \frac{1}{p}}$$

Note

- F_1 represents the harmonic mean between recall and precision
- High value of F_1 score ensures that both Precision and Recall are reasonably high.

PERFORMANCE EVALUATION METRICS

- More generally, F_β score can be used to determine the trade-off between Recall and Precision as

$$F_\beta = \frac{(\beta + 1)rp}{r + \beta p} = \frac{(\beta + 1)TP}{(\beta + 1)TP + \beta FN + FP}$$

- Both, Precision and Recall are special cases of F_β when $\beta = 0$ and $\beta = 1$, respectively.

$$F_\beta = \frac{TP}{TP + FP} = Precision$$

$$F_\alpha = \frac{TP}{TP + FN} = Recall$$

PERFORMANCE EVALUATION METRICS

- A more general metric that captures Recall, Precision is defined in the following.

$$F_\omega = \frac{\omega_1 TP + \omega_4 TN}{\omega_1 TP + \omega_2 FP + \omega_3 FN + \omega_4 TN}$$

Metric				
Recall	1	1	0	1
Precision	1	0	1	0
			1	0

Note

- In fact, given *TPR*, *FPR*, *p* and *r*, we can derive all others measures.
- That is, these are the universal metrics.

PREDICTIVE ACCURACY (E)

- It is defined as the fraction of the number of examples that are correctly classified by the classifier to the total number of instances.

$$\varepsilon = \frac{TP + TN}{P + N}$$

$$= \frac{TP + TN}{TP + FP + FN + TN}$$

$$= \frac{f_{++} + f_{--}}{f_{++} + f_{+-} + f_{\mp} + f_{--}}$$

- This accuracy is equivalent to F_w with $w_1 = w_2 = w_3 = w_4 = 1$.

ERROR RATE ($\bar{\text{E}}$)

- The error rate $\bar{\varepsilon}$ is defined as the fraction of the examples that are incorrectly classified.

$$\bar{\varepsilon} = \frac{FP + FN}{P + N}$$

$$= \frac{FP + FN}{TP + TN + FP + FN}$$

$$= \frac{f_{+-} + f_{-+}}{f_{++} + f_{+-} + f_{-+} + f_{--}}$$

Note

$$\bar{\varepsilon} = 1 - \varepsilon.$$

ACCURACY, SENSITIVITY AND SPECIFICITY

- Predictive accuracy (ε) can be expressed in terms of sensitivity and specificity.

- We can write

$$\varepsilon = \frac{TP + TN}{TP + FP + FN + TN}$$

$$= \frac{TP + TN}{P + N}$$

$$\varepsilon = \frac{TP}{P} \times \frac{P}{P + N} + \frac{TN}{N} \times \frac{N}{P + N}$$

Thus, $\varepsilon = \text{Sensitivity} \times \frac{P}{P+N} + \text{Specificity} \times \frac{N}{P+N}$

ANALYSIS WITH PERFORMANCE MEASUREMENT METRICS

- Based on the various performance metrics, we can characterize a classifier.
- We do it in terms of TPR, FPR, Precision and Recall and Accuracy
- **Case 1: Perfect Classifier**

When every instance is correctly classified, it is called the perfect classifier. In this case, $TP = P$, $TN = N$ and CM is

$$TPR = \frac{P}{P} = 1$$

$$FPR = \frac{0}{N} = 0$$

$$Precision = \frac{P}{P} = 1$$

$$F_1\ Score = \frac{2\times1}{1+1} = 1$$

$$Accuracy = \frac{P+N}{P+N} = 1$$

		Predicted Class	
		+	-
Actual class	+	P	0
	-	0	N

- **Case 2: Worst Classifier**

When every instance is wrongly classified, it is called the worst classifier. In this case, $TP = 0$, $TN = 0$ and the CM is

$$TPR = \frac{0}{P} = 0$$

$$FPR = \frac{N}{N} = 1$$

$$Precision = \frac{0}{N} = 0$$

F_1 $Score$ = Not applicable as $Recall + Precision = 0$

$$\text{Accuracy} = \frac{0}{P+N} = 0$$

		Predicted Class	
		+	-
Actual class	+	0	P
	-	N	0

- **Case 3: Ultra-Liberal Classifier**

The classifier always predicts the + class correctly. Here, the False Negative (FN) and True Negative (TN) are zero. The CM is

		Predicted Class	
		+	-
Actual class	+	P	0
	-	N	0

$$TPR = \frac{P}{P} = 1$$

$$FPR = \frac{N}{N} = 1$$

$$Precision = \frac{P}{P+N}$$

$$F_1\ Score = \frac{2P}{2P+N}$$

$$\text{Accuracy} = \frac{P}{P+N}$$

- **Case 4: Ultra-Conservative Classifier**

This classifier always predicts the - class correctly. Here, the False Negative (FN) and True Negative (TN) are zero. The CM is

$$TPR = \frac{0}{P} = 0$$

$$FPR = \frac{0}{N} = 0$$

$$Precision = \text{Not applicable}$$

$$(\text{as } TP + FP = 0)$$

$$F_1\ Score = \text{Not applicable}$$

$$\text{Accuracy} = \frac{N}{P+N}$$

		Predicted Class	
		+	**-**
Actual class	**+**	**0**	**p**
	-	**0**	**N**

PREDICTIVE ACCURACY VERSUS TPR AND FPR

- One strength of characterizing a classifier by its *TPR* and *FPR* is that they do not depend on the relative size of *P* and *N*.
  - The same is also applicable for *FNR* and *TNR* and others measures from CM.
- In contrast, the *Predictive Accuracy*, *Precision*, *Error Rate*, F_1 *Score*, etc. are affected by the relative size of *P* and *N*.
- *FPR*, *TPR*, *FNR* and *TNR* are calculated from the different rows of the CM.
  - On the other hand Predictive Accuracy, etc. are derived from the values in both rows.
- This suggests that *FPR*, *TPR*, *FNR* and TNR are more effective than *Predictive Accuracy*, etc.

ROC Curves

ROC CURVES

- ROC is an abbreviation of Receiver Operating Characteristic come from the signal detection theory, developed during World War 2 for analysis of radar images.

- In the context of classifier, ROC plot is a useful tool to study the behaviour of a classifier or comparing two or more classifiers.

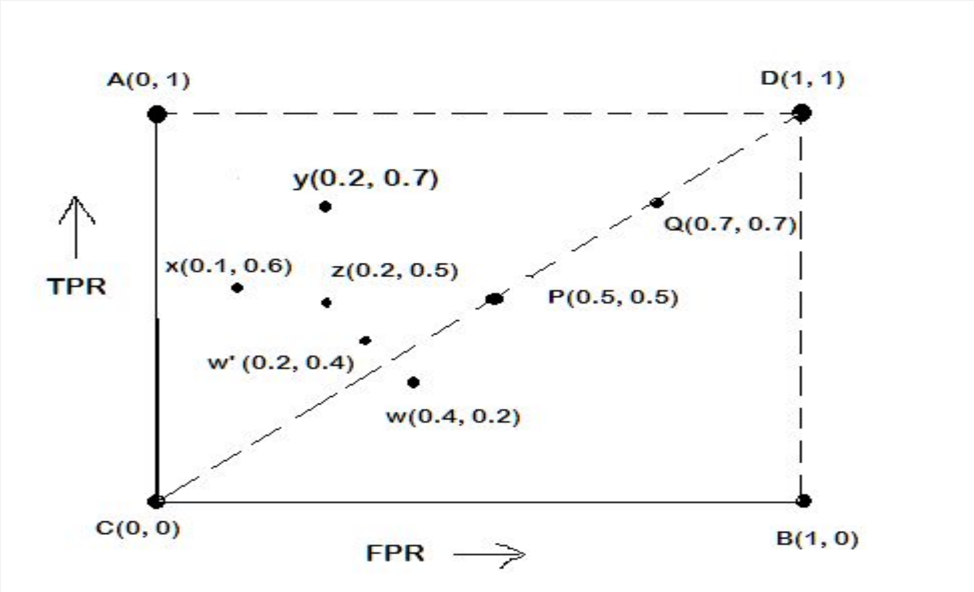
- A ROC plot is a two-dimensional graph, where, X-axis represents FP rate (FPR) and Y-axis represents TP rate (TPR).

- Since, the values of FPR and TPR varies from 0 to 1 both inclusive, the two axes thus from 0 to 1 only.

- Each point *(x, y)* on the plot indicating that the FPR has value *x* and the TPR value *y*.

ROC PLOT

- A typical look of ROC plot with few points in it is shown in the following figure.

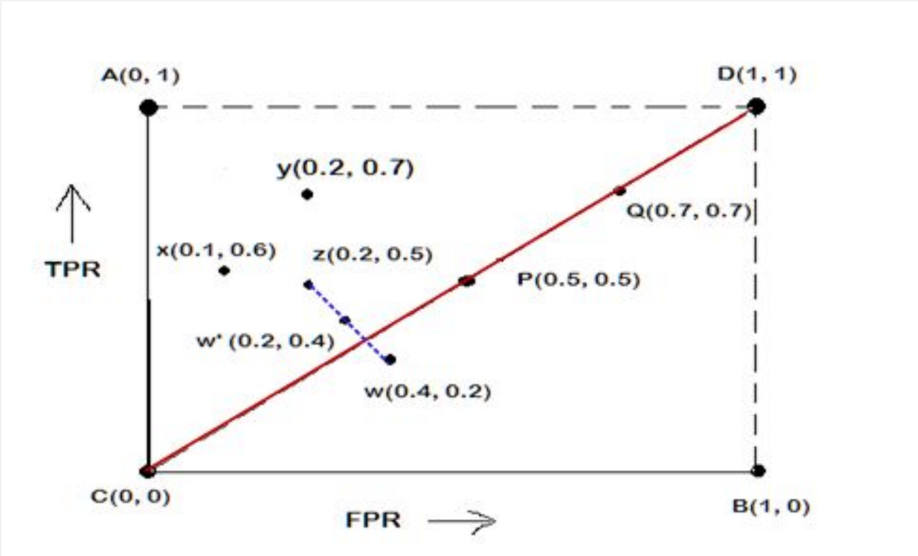


- Note the four cornered points are the four extreme cases of classifiers

Identify the four extreme classifiers.

INTERPRETATION OF DIFFERENT POINTS IN ROC PLOT

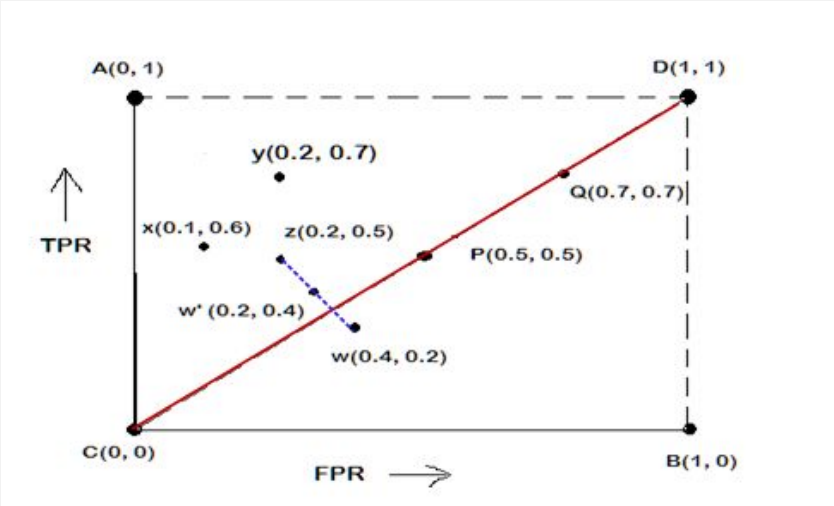
- Le us interpret the different points in the ROC plot.



- The four points (A, B, C, and D)
  - A: TPR = 1, FPR = 0, the ideal model, i.e., the perfect classifier, no false results
  - B: TPR = 0, FPR = 1, the worst classifier, not able to predict a single instance
  - C: TPR = 0, FPR = 0, the model predicts every instance to be a Negative class, i.e., it is an ultra-conservative classifier
  - D: TPR = 1, FPR = 1, the model predicts every instance to be a Positive class, i.e., it is an ultra-liberal classifier

INTERPRETATION OF DIFFERENT POINTS IN ROC PLOT

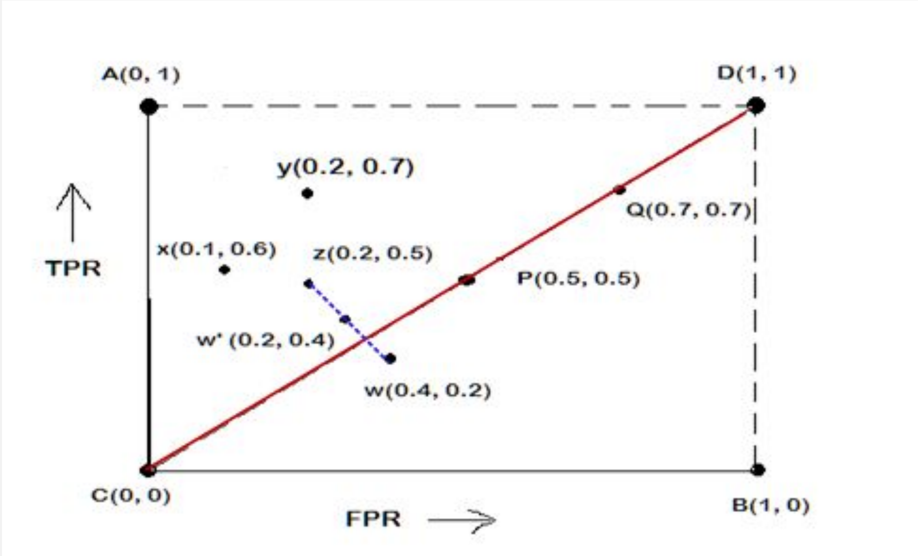
- Let us interpret the different points in the ROC plot.



- The points on diagonals
  - The diagonal line joining point C(0,0) and D(1,1) corresponds to random guessing
    - Random guessing means that a record is classified as positive (or negative) with a certain probability
    - Suppose, a test set contacting N_+ positive and N_- negative instances. Suppose, the classifier guesses any instances with probability p
    - Thus, the random classifier is expected to correctly classify $p.N_+$ of the positive instances and $p.N_-$ of the negative instances
    - Hence, $TPR = FPR = p$
    - Since $TPR = FPR$, the random classifier results reside on the main diagonals

INTERPRETATION OF DIFFERENT POINTS IN ROC PLOT

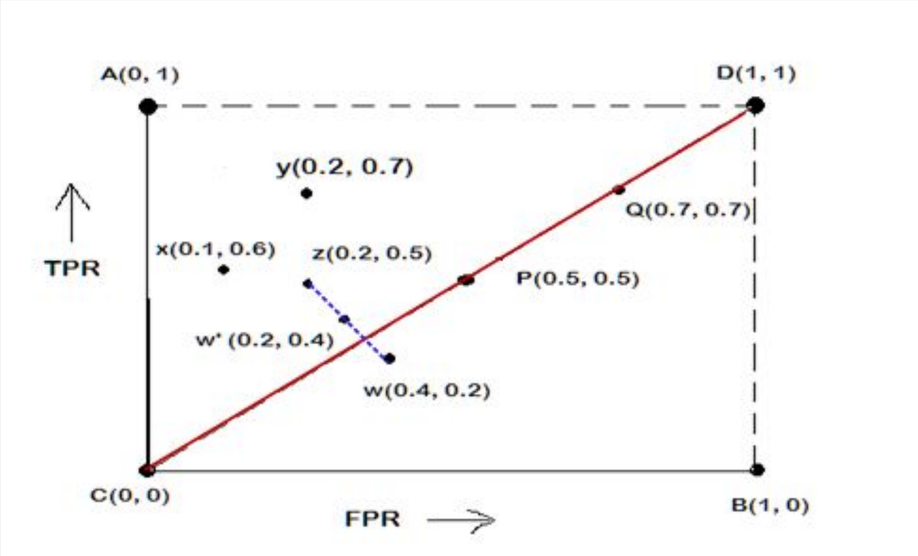
- Let us interpret the different points in the ROC plot.



- The points on the upper diagonal region
  - All points, which reside on upper-diagonal region are corresponding to classifiers "good" as their TPR is as good as FPR (i.e., FPRs are lower than TPRs)
  - Here, X is better than Z as X has higher TPR and lower FPR than Z.
  - If we compare X and Y, neither classifier is superior to the other

INTERPRETATION OF DIFFERENT POINTS IN ROC PLOT

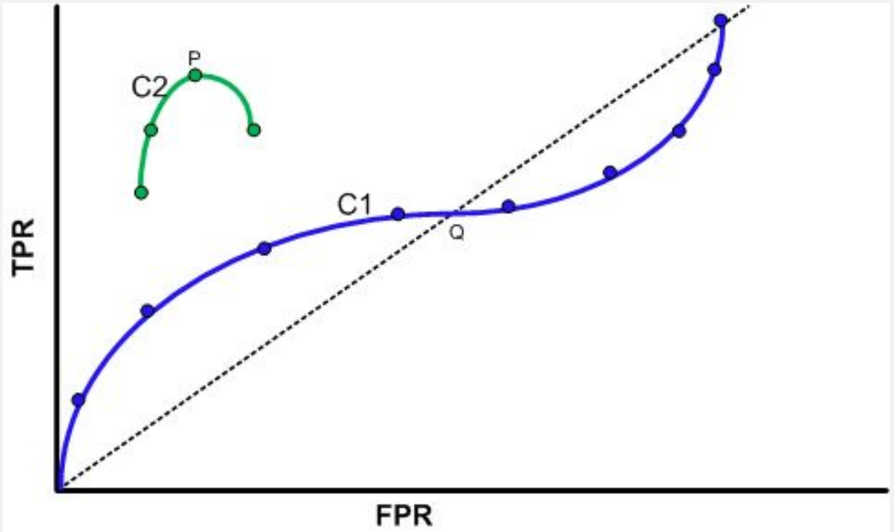
- Let us interpret the different points in the ROC plot.



- The points on the lower diagonal region
  - The Lower-diagonal triangle corresponds to the classifiers that are worst than random classifiers
  - Note: A classifier that is worst than random guessing, simply by reversing its prediction, we can get good results.
    - W'(0.2, 0.4) is the better version than W(0.4, 0.2), W' is a mirror reflection of W

TUNING A CLASSIFIER THROUGH ROC PLOT

- Using ROC plot, we can compare two or more classifiers by their TPR and FPR values and this plot also depicts the trade-off between TPR and FPR of a classifier.

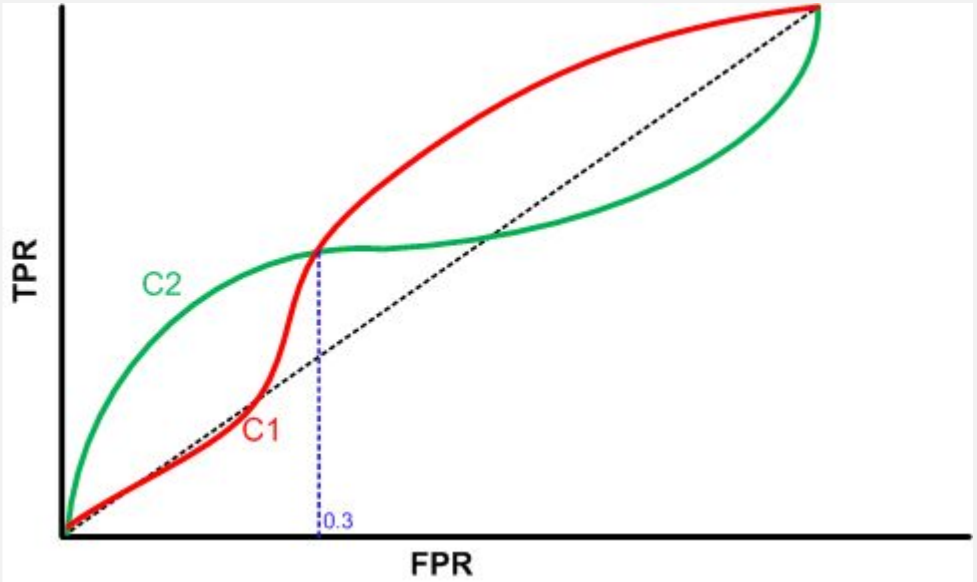


- Examining ROC curves can give insights into the best way of tuning parameters of classifier.

- For example, in the curve C2, the result is degraded after the point P. Similarly for the observation C1, beyond Q the settings are not acceptable.

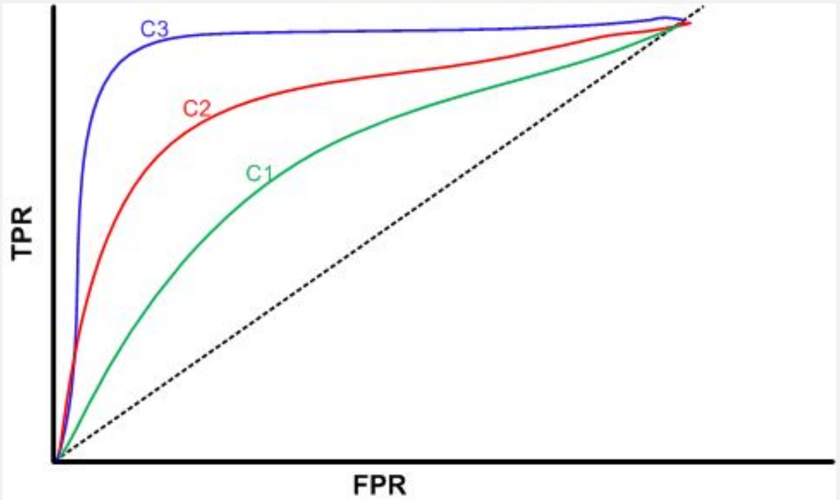
COMPARING CLASSIFIERS TROUGH ROC PLOT

- Two curves C1 and C2 are corresponding to the experiments to choose two classifiers with their parameters.
- Here, C2 is better than C1 when FPR is less than 0.3.
- However, C1 is better, when FPR is greater than 0.3.
- Clearly, neither of these two classifiers dominates the other.



COMPARING CLASSIFIERS TROUGH ROC PLOT

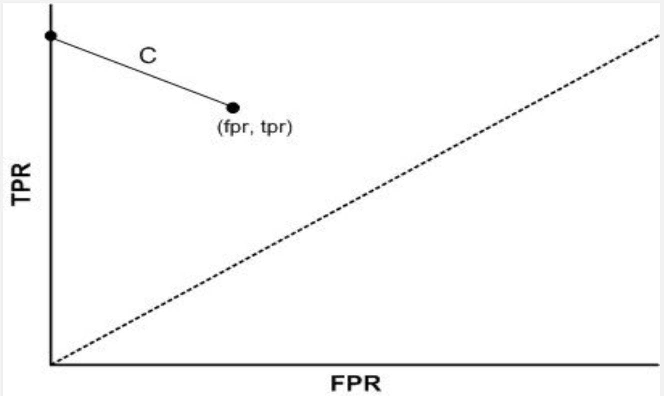
- We can use the concept of "area under curve" (AUC) as a better method to compare two or more classifiers.
- If a model is perfect, then its AUC = 1.
- If a model simply performs random guessing, then its AUC = 0.5
- A model that is strictly better than other, would have a larger value of AUC than the other.



- Here, C3 is best, and C2 is better than C1 as AUC(C3)>AUC(C2)>AUC(C1).

A QUANTITATIVE MEASURE OF A CLASSIFIER

- The concept of ROC plot can be extended to compare quantitatively using Euclidean distance measure.
- See the following figure for an explanation.



- Here, *C(fpr, tpr)* is a classifier and $\boldsymbol{\delta}$ denotes the Euclidean distance between the best classifier (0, 1) and C. That is,
  - $\boldsymbol{\delta} = \sqrt{fpr^2 + (1 - tpr)^2}$
- The smallest possible value of $\boldsymbol{\delta}$ is 0
- The largest possible values of $\boldsymbol{\delta}$ is $\sqrt{2}$ (when (fpr = 1 and tpr = 0).

REFERENCE

- The detail material related to this lecture can be found in

  Data Mining: Concepts and Techniques, (3rd Edn.), Jiawei Han, Micheline Kamber, Morgan Kaufmann, 2015.

  Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach, and Vipin Kumar, Addison-Wesley, 2014

Any question?