



Day 15/100 of Data Science

Model Evaluation Techniques

What is a Confusion Matrix?

- A confusion matrix is a matrix that summarizes the performance of a machine learning model on a set of test data.
- It is a means of displaying the number of accurate and inaccurate instances based on the model's predictions.
- A Confusion matrix is an N x N matrix used for evaluating the performance of a classification model, where N is the number of target classes.
- The matrix compares the actual target values with those predicted by the machine learning model.

		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) Type II Error	Sensitivity $\frac{TP}{(TP + FN)}$
	Negative	False Positive (FP) Type I Error	True Negative (TN)	Specificity $\frac{TN}{(TN + FP)}$
		Precision $\frac{TP}{(TP + FP)}$	Negative Predictive Value $\frac{TN}{(TN + FN)}$	Accuracy $\frac{TP + TN}{(TP + TN + FP + FN)}$

The matrix displays the number of instances produced by the model on the test data.

- True positives (TP): occur when the model accurately predicts a positive data point.
- True negatives (TN): occur when the model accurately predicts a negative data point.
- True positives (FP): occur when the model predicts a positive data point incorrectly.

- False negatives (FN): occur when the model mispredicts a negative data point.

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Accuracy

- Accuracy is a metric that measures how often a machine learning model correctly predicts the outcome

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

Precision

- Precision is one indicator of a machine learning model's performance – the quality of a positive prediction made by the model.
- Precision refers to the number of true positives divided by the total number of positive predictions

$$\text{Precision} = \frac{TP}{TP + FP}$$

Recall or Sensitivity

- The recall is the measure of our model correctly identifying True Positives.

$$\text{Recall} = \frac{TP}{TP + FN}$$

F1 score

- F1 score is a measure of the harmonic mean of precision and recall.
- Commonly used as an evaluation metric in binary and multi-class classification

$$\begin{aligned}\text{F1 Score} &= \frac{2}{\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}} \\ &= \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}\end{aligned}$$

$$\text{F1 Score} = \frac{TP}{TP + \frac{1}{2}(FP + FN)}$$

Specificity

- Specificity itself can be described as the algorithm/model's ability to predict a true negative of each category available.

Specificity Formula

$$\text{Specificity} = \frac{TN}{TN + FP}$$

ROC curve

An ROC curve (receiver operating characteristic curve) is a graph showing the performance of a classification model at all classification thresholds. This curve plots two parameters:

- True Positive Rate
- False Positive Rate

True Positive Rate (TPR) is a synonym for recall and is therefore defined as follows:

$$TPR = \frac{TP}{TP + FN}$$

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

False Positive Rate (FPR) is defined as follows:

- An ROC curve plots TPR vs. FPR at different classification thresholds.
- Lowering the classification threshold classifies more items as positive, thus increasing both False Positives and True Positives.
- The following figure shows a typical ROC curve.

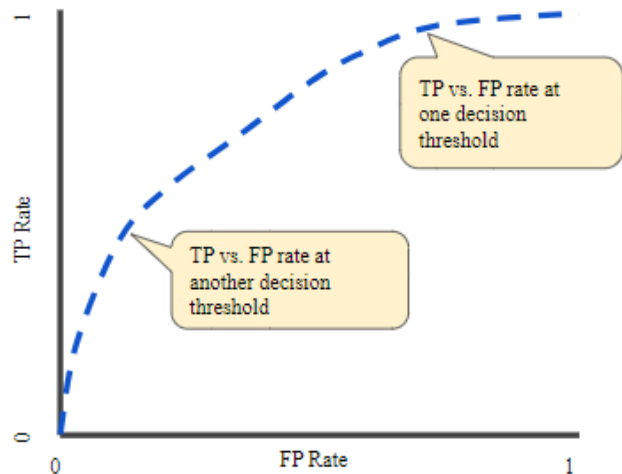


Figure 4. TP vs. FP rate at different classification thresholds.

AUC: Area Under the ROC Curve

- AUC stands for "Area under the ROC Curve."
- That is, AUC measures the entire two-dimensional area underneath the entire ROC curve (think integral calculus) from (0,0) to (1,1).

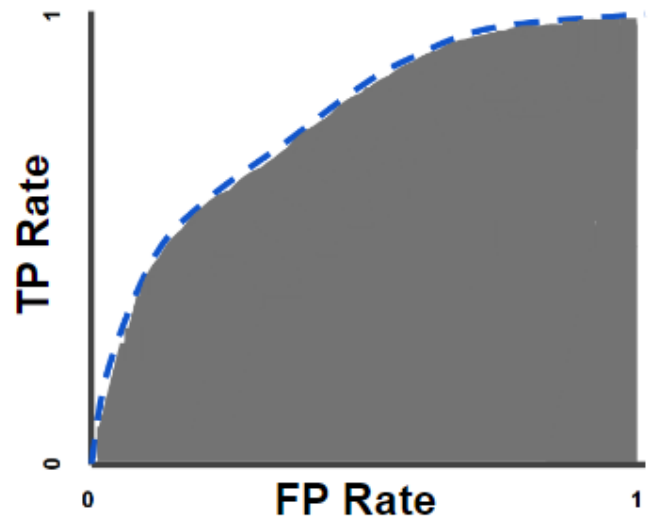


Figure 5. AUC (Area under the ROC Curve).

Mean Squared Error

- In Statistics, Mean Squared Error (MSE) is defined as Mean or Average of the square of the difference between actual and estimated values.

MSE Formula

The formula for MSE is the following.

$$MSE = \frac{\sum (y_i - \hat{y}_i)^2}{n}$$

Where:

- y_i is the i th observed value.
- \hat{y}_i is the corresponding predicted value.
- n = the number of observations.

The Root Mean Squared Error (RMSE)

- The Root Mean Squared Error (RMSE) is one of the two main performance indicators for a regression model.

- It measures the average difference between values predicted by a model and the actual values.
- It provides an estimation of how well the model is able to predict the target value (accuracy).

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^N (x_i - \hat{x}_i)^2}{N}}$$

RMSE = root-mean-square deviation

i = variable i

N = number of non-missing data points

x_i = actual observations time series

\hat{x}_i = estimated time series

R squared (R2)

- R squared (R2) is a regression error metric that justifies the performance of the model.
- It represents the value of how much the independent variables are able to describe the value for the response/target variable.

$$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

Where:

- $SS_{\text{regression}}$ is the sum of squares due to regression (explained sum of squares)
- SS_{total} is the total sum of squares

Mean Absolute Error (MAE)

- It is the arithmetic average of the absolute difference between predicted and actual values

$$\text{MAE} = \frac{\sum_{i=1}^n |y_i - x_i|}{n}$$

MAE = mean absolute error

y_i = prediction

x_i = true value

n = total number of data points

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