Evaluation Metrics

Classification Related Metrics

Classification is one of the most widely used problems in machine learning with various industrial applications, from face recognition, Youtube video categorization, content moderation, medical diagnosis, to text classification, hate speech detection on Twitter.

Models such as support vector machine (SVM), logistic regression, decision trees, random forest, XGboost, convolutional neural network[1], recurrent neural network are some of the most popular classification models[2].

There are various ways to evaluate a classification model, and I am covering some of the most popular ones below.

1- Confusion Matrix (not a metric, but important to know!)

Let's first make sure we know the basic terminologies used in classification problems before going through the detail of each metric. **You can skip this section if you are already familiar with the terminologies.**

One of the key concept in classification performance is **confusion matrix** (AKA error matrix), which is a tabular visualization of the model predictions versus the ground-truth labels. Each row of confusion matrix represents the instances in

a predicted class and each column represents the instances in an actual class.

Let's go through this with an example. Let's assume we are building a binary classification to classify cat images from non-cat images. And let's assume our test set has 1100 images (1000 non-cat images, and 100 cat images), with the below confusion matrix.

		Actual Class	
		Cat	Non-Cat
Predicted Class	Cat	90	60
	Non-Cat	10	940

- **Out of 100 cat images** the model has predicted 90 of them correctly and has mis-classified 10 of them. If we refer to the "cat" class as positive and the non-cat class as negative class, then 90 samples predicted as cat are considered as as **true-positive**, and the 10 samples predicted as non-cat are **false negative**.
- **Out of 1000 non-cat images**, the model has classified 940 of them correctly, and mis-classified 60 of them. The 940 correctly classified samples are referred as **true-negative**, and those 60 are referred as **false-positive**.

As we can see diagonal elements of this matrix denote the correct prediction for different classes, while the off-diagonal elements denote the samples which are mis-classified.

Now that we have a better understanding of the confusion matrix, let's get into the actual metrics.

2- Classification Accuracy

Classification accuracy is perhaps the simplest metrics one can imagine, and is defined as the **number of correct predictions divided by the total number of predictions,** multiplied by 100**.** So in the above example, out of 1100 samples 1030 are predicted correctly, resulting in a classification accuracy of:

Classification accuracy= (90+940)/(1000+100)= 1030/1100= 93.6%

3- Precision

There are many cases in which classification accuracy is not a good indicator of your model performance. One of these scenarios is when your class distribution is imbalanced (one class is more frequent than others). In this case, even if you predict all samples as the most frequent class you would get a high accuracy rate, which does not make sense at all (because your model is not learning anything, and is just predicting everything as the top class). For example in our cat vs non-cat classification above, if the model predicts all samples as non-cat, it would result in a 1000/1100= 90.9%.

Therefore we need to look at class specific performance metrics too. Precision is one of such metrics, which is defined as:

Precision= True_Positive/ (True_Positive+ False_Positive)

The precision of Cat and Non-Cat class in above example can be calculated as:

Precision_cat= #samples correctly predicted cat/#samples predicted as cat = **90/(90+60) = 60%**

Precision_NonCat= 940/950= 98.9%

As we can see the model has much higher precision in predicting non-cat samples, versus cats. This is not surprising, as model has seen more examples of non-cat images during training, making it better in classifying that class.

4- Recall

Recall is another important metric, which is defined as the fraction of samples from a class which are correctly predicted by the model. More formally:

Recall= True_Positive/ (True_Positive+ False_Negative)

Therefore, for our example above, the recall rate of cat and non-cat classes can be found as:

Recall_cat= 90/100= 90%

Recall_NonCat= 940/1000= 94%

5- F1 Score

Depending on application, you may want to give higher priority to recall or precision. But there are many applications in which both recall and precision are important. Therefore, it is natural to think of a way to combine these two into a single metric. **One popular metric which combines precision and recall is called F1-score**, which is the harmonic mean of precision and recall defined as:

F1-score= 2*Precision*Recall/(Precision+Recall)

So for our classification example with the confusion matrix in Figure 1, the F1-score can be calculated as:

F1_cat= 2*0.6*0.9/(0.6+0.9)= 72%

The generalized version of F-score is defined as below. As we can see F1-score is special case of F_$\mathcal{B}$ when $\mathcal{B}$= 1.

$$F_\beta = (1+\beta^2)\cdot\frac{\text{precision}\cdot\text{recall}}{\beta^2\cdot\text{precision}+\text{recall}}$$

It is good to mention that there is always a trade-off between precision and recall of a model, if you want to make the precision too high, you would end up seeing a drop in the recall rate, and vice versa.

6- Sensitivity and Specificity

Sensitivity and specificity are two other popular metrics mostly used in medical and biology related fields, and are defined as:

Sensitivity= Recall= TP/(TP+FN)

Specificity= True Negative Rate= TN/(TN+FP)

7- ROC Curve

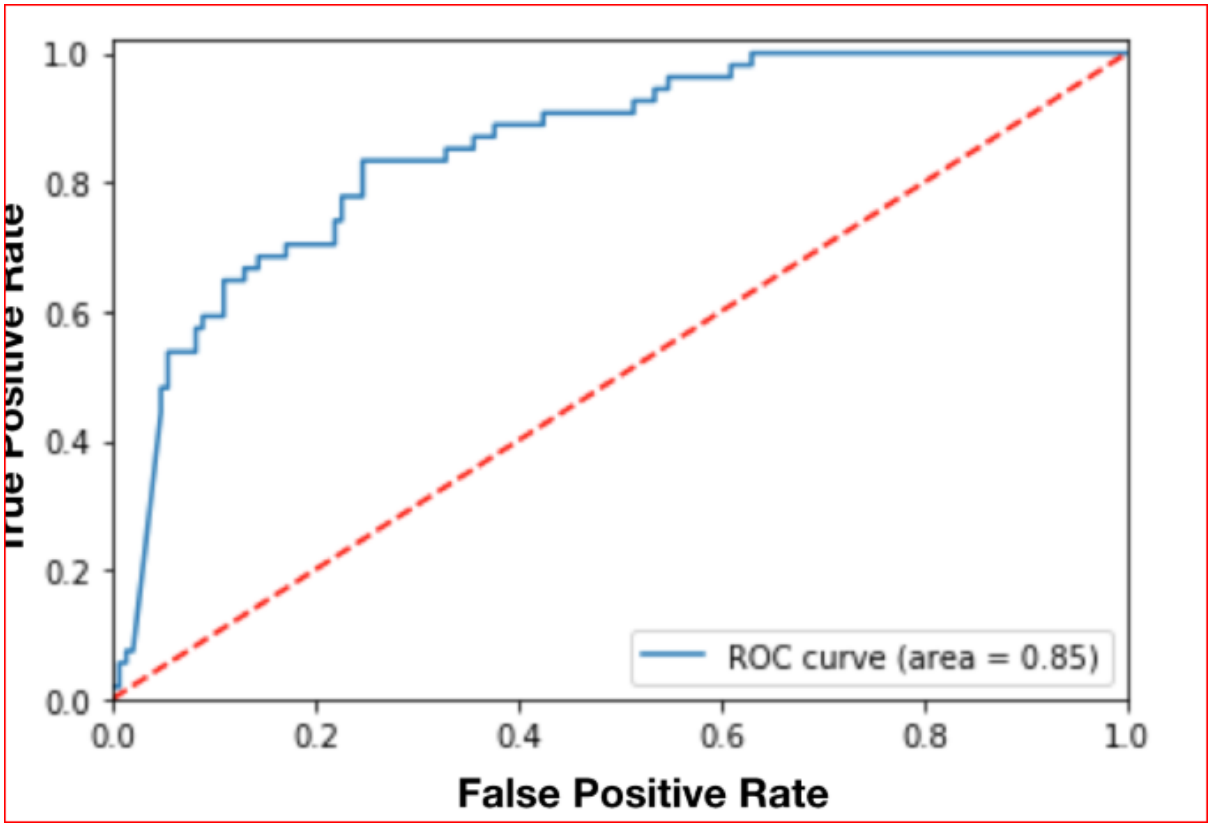
The **receiver operating characteristic curve** is plot which shows the performance of a binary classifier as function of its cut-off threshold. **It essentially shows the true positive rate (TPR) against the false positive rate (FPR) for various threshold values. Let's explain more.**

Many of the classification models are probabilistic, i.e. they predict the probability of a sample being a cat. They then compare that output probability with some cut-off threshold and if it is larger than the threshold they predict its label as cat, otherwise as non-cat. As an example your model may predict the below probabilities for 4 sample images: **[0.45, 0.6, 0.7, 0.3]**. Then depending on the threshold values below, you will get different labels:

cut-off= 0.5: predicted-labels= [0,1,1,0] (default threshold)
cut-off= 0.2: predicted-labels= [1,1,1,1]
cut-off= 0.8: predicted-labels= [0,0,0,0]

As you can see by varying the threshold values, we will get completely different labels. And as you can imagine each of these scenarios would result in a different precision and recall (as well as TPR, FPR) rates.

ROC curve essentially finds out the TPR and FPR for various threshold values and plots TPR against the FPR. A sample ROC curve is shown in Figure 2.



As we can see from this example, the lower the cut-off threshold on positive class, the more samples predicted as positive class, i.e. higher true positive rate (recall) and also higher false positive rate (corresponding to the right side of this curve). Therefore, there is a trade-off between how high the recall could be versus how much we want to bound the error (FPR).

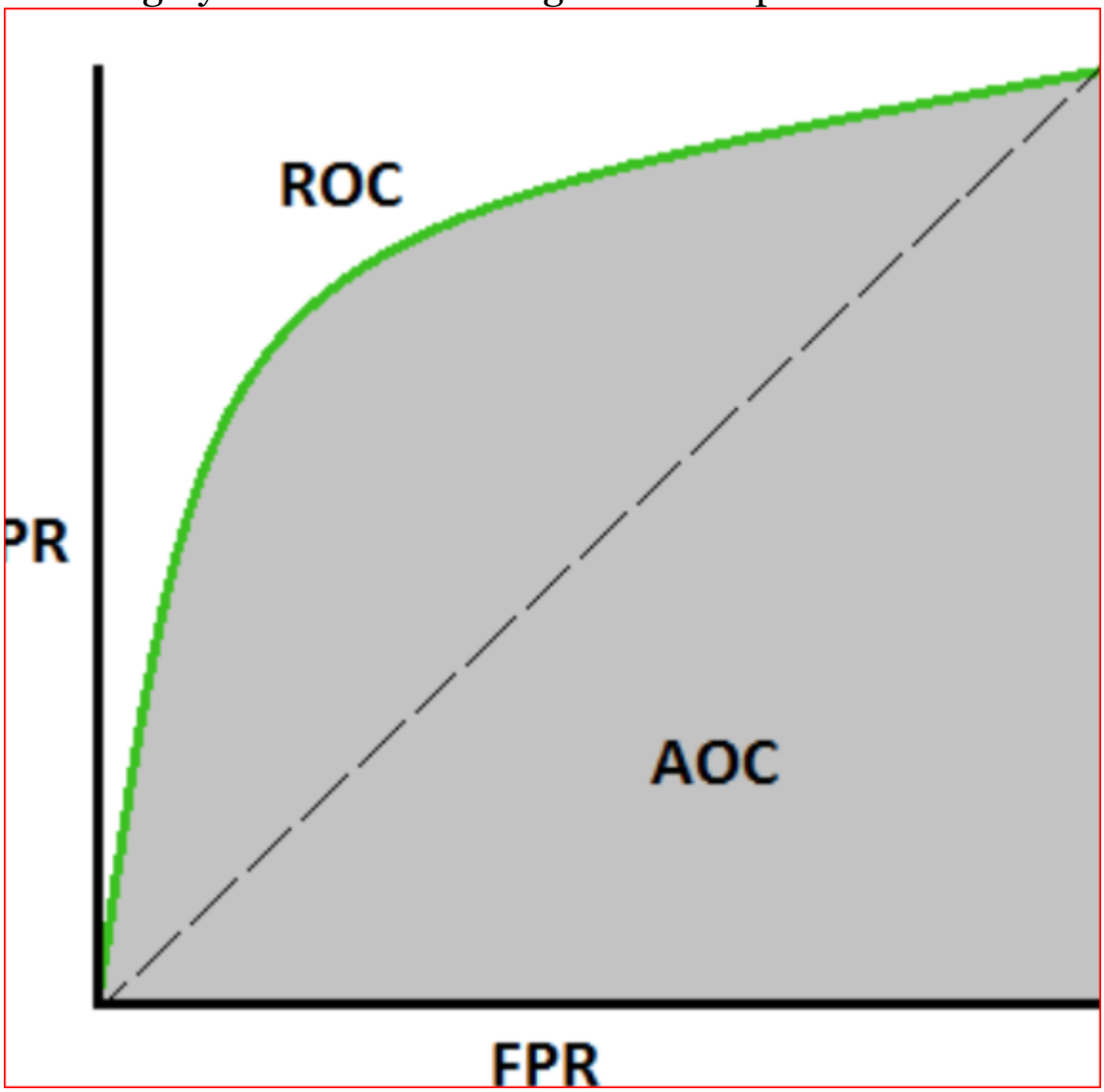
ROC curve is a popular curve to look at overall model performance and pick a good cut-off threshold for the model.

8- AUC

The **area under the curve** (AUC), is an aggregated measure of performance of a binary classifier on all possible threshold values (and therefore it is threshold invariant**)**.

AUC calculates the area under the ROC curve, and therefore it is between 0 and 1. One way of interpreting AUC is as the

probability that the model ranks a random positive example more highly than a random negative example.



On high-level, the higher the AUC of a model the better it is. But sometimes threshold independent measure is not what you want, e.g. you may care about your model recall and require that to be higher than 99% (while it has a reasonable precision or FPR). In that case, you may want to tune your model threshold such that it meets your minimum requirement on those metrics (and you may not care even if you model AUC is not too high).

Therefore in order to decide how to evaluate your classification model performance, perhaps you want to have a good understanding of the business/problem requirement and the impact of low recall vs. low precision, and decide what metric to optimize for.

From a practical standpoint, a classification model which outputs probabilities is preferred over a single label output, as it provides the flexibility of tuning the threshold such that it meets your minimum recall/precision requirements. Not all models provide this nice probabilistic outputs though, e.g. SVM does not provide a simple probability as an output (although it provides margin which can be used to tune the decision, but it is not as straightforward and interpretable as having output probabilities).

Regression Related Metrics

Regression models are another family of machine learning and statistical models, which are used to predict a continuous target values[3]. They have a wide range of applications, from house price prediction, E-commerce pricing systems, weather forecasting, stock market prediction, to image super resolution, feature learning via auto-encoders, and image compression.

Models such as linear regression, random forest, XGboost, convolutional neural network, recurrent neural network are some of the most popular regression models.

Metrics used to evaluate these models should be able to work on a set of continuous values (with infinite cardinality), and are therefore slightly different from classification metrics.

9- MSE

"Mean squared error" is perhaps the most popular metric used for regression problems. It essentially finds the average squared error between the predicted and actual values.

Let's assume we have a regression model which predicts the price of houses in Seattle area (show them with $\hat{y}_i$), and let's say for each house we also have the actual price the house was sold for (denoted with y_i). Then the MSE can be calculated as:

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Sometimes people use RMSE to have a metric with scale as the target values, which is essentially the square root of MSE.

Looking at house pricing prediction, RMSE essentially shows what is the average deviation in your model predicted house prices from the target values (the prices the houses are sold for).

10- MAE

Mean absolute error (or mean absolute deviation) is another metric which finds the average absolute distance between the predicted and target values. MAE is define as below:

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

MAE is known to be more robust to the outliers than MSE. The main reason being that in MSE by squaring the errors, the outliers (which usually have higher errors than other samples) get more attention and dominance in the final error and impacting the model parameters.

It is also worth mentioning that there is a nice maximum likelihood (MLE) interpretation behind MSE and MAE metrics. If we assume a linear dependence between features and targets, then MSE and MAE correspond to the MLE on the model parameters by assuming Gaussian and Laplace priors on the model errors respectively.