Receiver operating characteristic

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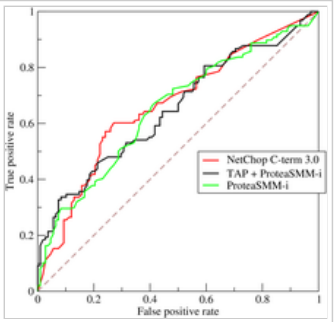
In statistics, a **receiver operating characteristic** (**ROC**), or **ROC curve**, is a graphical plot that illustrates the performance of a binary classifier system as its discrimination threshold is varied. The curve is created by plotting the true positive rate against the false positive rate at various threshold settings. The true-positive rate is also known as sensitivity or the sensitivity index *d′*, known as "d-prime" in signal detection and biomedical informatics, or recall in machine learning. The false-positive rate is also known as the fall-out and can be calculated as 1 - specificity. The ROC curve is thus the sensitivity as a function of fall-out. In general, if the probability distributions for both detection and false alarm are known, the ROC curve can be generated by plotting the cumulative distribution function (area under the probability distribution from $-\infty$ to $+\infty$) of the detection probability in the y-axis versus the cumulative distribution function of the false-alarm probability in x-axis.



ROC curve of three predictors of peptide cleaving in the proteasome.

ROC analysis provides tools to select possibly optimal models and to discard suboptimal ones independently from (and prior to specifying) the cost context or the class distribution. ROC analysis is related in a direct and natural way to cost/benefit analysis of diagnostic decision making.

The ROC curve was first developed by electrical engineers and radar engineers during World War II for detecting enemy objects in battlefields and was soon introduced to psychology to account for perceptual detection of stimuli. ROC analysis since then has been used in medicine, radiology, biometrics, and other areas for many decades and is increasingly used in machine learning and data mining research.

The ROC is also known as a relative operating characteristic curve, because it is a comparison of two operating characteristics (TPR and FPR) as the criterion changes.[1]

Contents

Basic concept

A classification model (classifier or diagnosis) is a mapping of instances between certain classes/groups. The classifier or diagnosis result can be a real value (continuous output), in which case the classifier boundary between classes must be determined by a threshold value (for instance, to determine whether a person has hypertension based on a blood pressure measure). Or it can be a discrete class label, indicating one of the classes.

Let us consider a two-class prediction problem (binary classification), in which the outcomes are labeled either as positive (*p*) or negative (*n*). There are four possible outcomes from a binary classifier. If the outcome from a prediction is *p* and the actual value is also *p*, then it is called a *true positive* (TP); however if the actual value is *n* then it is said to be a *false positive* (FP). Conversely, a *true negative* (TN) has occurred when both the prediction outcome and the actual value are *n*, and *false negative* (FN) is when the prediction outcome is *n* while the actual value is *p*.

To get an appropriate example in a real-world problem, consider a diagnostic test that seeks to determine whether a person has a certain disease. A false positive in this case occurs when the person tests positive, but actually does not have the disease. A false negative, on the other hand, occurs when the person tests negative, suggesting they are healthy, when they actually do have the disease.

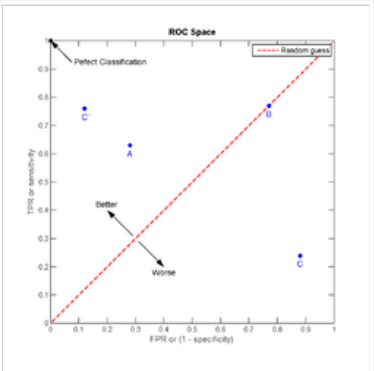
Let us define an experiment from **P** positive instances and **N** negative instances for some condition. The four outcomes can be formulated in a 2×2 *contingency table* or *confusion matrix*, as follows:

		Condition (as determined by "Gold standard")			
	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
Test outcome	Test outcome positive	**True positive**	**False positive** (Type I error)	Positive predictive value (PPV), Precision $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
	Test outcome negative	**False negative** (Type II error)	**True negative**	False omission rate (FOR) $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Test outcome negative}}$	Negative predictive value (NPV) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Test outcome negative}}$
	Accuracy (ACC) $= \frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	True positive rate (TPR), Sensitivity, Recall $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR−}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) $= \frac{\text{FNR}}{\text{TNR}}$	

ROC space

The contingency table can derive several evaluation "metrics" (see infobox). To draw a ROC curve, only the true positive rate (TPR) and false positive rate (FPR) are needed (as functions of some classifier parameter). The TPR defines how many correct positive results occur among all positive samples available during the test. FPR, on the other hand, defines how many incorrect positive results occur among all negative samples available during the test.

A ROC space is defined by FPR and TPR as *x* and *y* axes respectively, which depicts relative trade-offs between true positive (benefits) and false positive (costs). Since TPR is equivalent to sensitivity and FPR is equal to 1 − specificity, the ROC graph is sometimes called the sensitivity vs (1 − specificity) plot. Each prediction result or instance of a confusion matrix represents one point in the ROC space.



The ROC space and plots of the four prediction examples.

The best possible prediction method would yield a point in the upper left corner or coordinate (0,1) of the ROC space, representing 100% sensitivity (no false negatives) and 100% specificity (no false positives). The (0,1) point is also called a *perfect classification*. A completely random guess would give a point along a diagonal line (the so-called *line of no-discrimination*) from the left bottom to the top right corners (regardless of the positive and negative base rates). An intuitive example of random guessing is a decision by flipping coins (heads or tails). As the size of the sample increases, a random classifier's ROC point migrates towards (0.5,0.5).

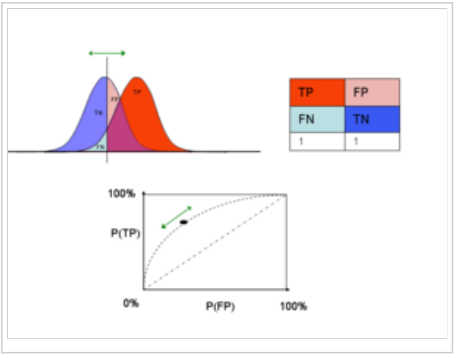
The diagonal divides the ROC space. Points above the diagonal represent good classification results (better than random), points below the line poor results (worse than random). Note that the output of a consistently poor predictor could simply be inverted to obtain a good predictor.

Let us look into four prediction results from 100 positive and 100 negative instances:

A			**B**			**C**			**C′**		
TP=63	FP=28	91	TP=77	FP=77	154	TP=24	FP=88	112	TP=76	FP=12	88
FN=37	TN=72	109	FN=23	TN=23	46	FN=76	TN=12	88	FN=24	TN=88	112
100	100	200	100	100	200	100	100	200	100	100	200
TPR = 0.63			TPR = 0.77			TPR = 0.24			TPR = 0.76		
FPR = 0.28			FPR = 0.77			FPR = 0.88			FPR = 0.12		
PPV = 0.69			PPV = 0.50			PPV = 0.21			PPV = 0.86		
F1 = 0.66			F1 = 0.61			F1 = 0.22			F1 = 0.81		
ACC = 0.68			ACC = 0.50			ACC = 0.18			ACC = 0.82		

Plots of the four results above in the ROC space are given in the figure. The result of method **A** clearly shows the best predictive power among **A**, **B**, and **C**. The result of **B** lies on the random guess line (the diagonal line), and it can be seen in the table that the accuracy of **B** is 50%. However, when **C** is mirrored across the center point (0.5,0.5), the resulting method **C′** is even better than **A**. This mirrored method simply reverses the predictions of whatever method or test produced the **C** contingency table. Although the original **C** method has negative predictive power, simply reversing its decisions leads to a new predictive method **C′** which has positive predictive power. When the **C** method predicts **p** or **n**, the **C′** method would predict **n** or **p**, respectively. In this manner, the **C′** test would perform the best. The closer a result from a contingency table is to the upper left corner, the better it predicts, but the distance from the random guess line in either direction is the best indicator of how much predictive power a method has. If the result is below the line (i.e. the method is worse than a random guess), all of the method's predictions must be reversed in order to utilize its power, thereby moving the result above the random guess line.

Curves in ROC space



Classifications are often based on a continuous random variable. Write the probability for belonging in the class as a function of a decision/threshold parameter T as $P_1(T)$ and the probability of not belonging to the class as $P_0(T)$. The false positive rate FPR is given by $\mathrm{FPR}(T) = \int_T^\infty P_0(T)\,dT$ and the true positive rate is $\mathrm{TPR}(T) = \int_T^\infty P_1(T)\,dT$. The ROC curve plots parametrically TPR(T) versus FPR(T) with T as the varying parameter.

For example, imagine that the blood protein levels in diseased people and healthy people are normally distributed with means of 2 g/dL and 1 g/dL respectively. A medical test might measure the level of a certain protein in a blood sample and classify any number above a certain threshold as indicating disease. The experimenter can adjust the threshold (black vertical line in the figure), which will in turn change the false positive rate. Increasing the threshold would result in fewer false positives (and more false negatives), corresponding to a leftward movement on the curve. The actual shape of the curve is determined by how much overlap the two distributions have.

Further interpretations

Sometimes, the ROC is used to generate a summary statistic. Common versions are:

- the intercept of the ROC curve with the line at 90 degrees to the no-discrimination line (also called Youden's J statistic)
- the area between the ROC curve and the no-discrimination line
- the area under the ROC curve, or "AUC" ("Area Under Curve"), or A' (pronounced "a-prime"),[2] or "c-statistic".[3]
- d' (pronounced "d-prime"), the distance between the mean of the distribution of activity in the system under noise-alone conditions and its distribution under signal-alone conditions, divided by their standard deviation, under the assumption that both these distributions are normal with the same standard deviation. Under these assumptions, it can be proved that the shape of the ROC depends only on d'.

However, any attempt to summarize the ROC curve into a single number loses information about the pattern of tradeoffs of the particular discriminator algorithm.

Area under the curve

When using normalized units, the area under the curve (often referred to as simply the AUC, or AUROC) is equal to the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one (assuming 'positive' ranks higher than 'negative').[4] This can be seen as follows: the area under the curve is given by (the integral boundaries are reversed as large T has a lower value on the x-axis)

$$A = \int_\infty^{-\infty} y(T)x'(T)\,dT = \int_\infty^{-\infty} \mathrm{TPR}(T)\mathrm{FPR}'(T)\,dT = \int_{-\infty}^{\infty} \mathrm{TPR}(T)P_0(T)\,dT = \langle \mathrm{TPR} \rangle.$$ The angular brackets denote average from the distribution of negative samples.

It can further be shown that the AUC is closely related to the Mann–Whitney U,[5][6] which tests whether positives are ranked higher than negatives. It is also equivalent to the Wilcoxon test of ranks.[6] The AUC is related to the Gini coefficient (G_1) by the formula $G_1 = 2\mathrm{AUC} - 1$, where:

$$G_1 = 1 - \sum_{k=1}^{n} (X_k - X_{k-1})(Y_k + Y_{k-1})$$ [7]

In this way, it is possible to calculate the AUC by using an average of a number of trapezoidal approximations.

It is also common to calculate the Area Under the ROC Convex Hull (ROC AUCH = ROCH AUC) as any point on the line segment between two prediction results can be achieved by randomly using one or other system with probabilities proportional to the relative length of the opposite component of the segment.[8] Interestingly, it is also possible to invert concavities – just as in the figure the worse solution can be reflected to become a better solution; concavities can be reflected in any line segment, but this more extreme form of fusion is much more likely to overfit the data.[9]

The machine learning community most often uses the ROC AUC statistic for model comparison.[10] However, this practice has recently been questioned based upon new machine learning research that shows that the AUC is quite noisy as a classification measure[11] and has some other significant problems in model comparison.[12][13] A reliable and valid AUC estimate can be interpreted as the probability that the classifier will assign a higher score to a randomly chosen positive example than to a randomly chosen negative example. However, the critical research[11][12] suggests frequent failures in obtaining reliable and valid AUC estimates. Thus, the practical value of the AUC measure has been called into question,[13] raising the possibility that the AUC may actually introduce more uncertainty into machine learning classification accuracy comparisons than resolution. Nonetheless, the coherence of AUC as a measure of aggregated classification performance has been vindicated, in terms of a uniform rate distribution,[14] and AUC has been linked to a number of other performance metrics such as the Brier score.[15]

One recent explanation of the problem with ROC AUC is that reducing the ROC Curve to a single number ignores the fact that it is about the tradeoffs between the different systems or performance points plotted and not the performance of an individual system, as well as ignoring the possibility of concavity repair, so that related alternative measures such as Informedness[16] or DeltaP are recommended.[17] These measures are essentially equivalent to the Gini for a single prediction point with DeltaP' = Informedness = 2AUC-1, whilst DeltaP = Markedness represents the dual (viz. predicting the prediction from the real class) and their geometric mean is the Matthews correlation coefficient.[16]

Other measures

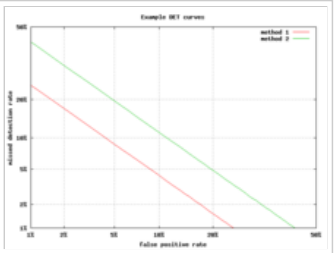
In engineering, the area between the ROC curve and the no-discrimination line is sometimes preferred (equivalent to subtracting 0.5 from the AUC), and referred to as the **discrimination'. *In psychophysics, the sensitivity index* d** (d-prime), ΔP' or DeltaP' is the most commonly used measure[18] and is equivalent to twice the discrimination, being equal also to Informedness, deskewed WRAcc and Gini Coefficient in the single point case (single parameterization or single system).[16] These measures all have the advantage that 0 represents chance performance whilst 1 represents perfect performance, and -1 represents the "perverse" case of full informedness used to always give the wrong response.[19]

These varying choices of scale are fairly arbitrary since chance performance always has a fixed value: for AUC it is 0.5, but these alternative scales bring chance performance to 0 and allow them to be interpreted as Kappa statistics. Informedness has been shown to have desirable characteristics for Machine Learning versus other common definitions of Kappa such as Cohen Kappa and Fleiss Kappa.[16][20]

Sometimes it can be more useful to look at a specific region of the ROC Curve rather than at the whole curve. It is possible to compute partial AUC.[21] For example, one could focus on the region of the curve with low false positive rate, which is often of prime interest for population screening tests.[22] Another common approach for classification problems in which P ≪ N (common in bioinformatics applications) is to use a logarithmic scale for the x-axis.[23]

Detection error tradeoff graph

An alternative to the ROC curve is the detection error tradeoff (DET) graph, which plots the false negative rate (missed detections) vs. the false positive rate (false alarms) on non-linearly transformed x- and y-axes. The transformation function is the quantile function of the normal distribution, i.e., the inverse of the cumulative normal distribution. It is, in fact, the same transformation as zROC, below, except that the complement of the hit rate, the miss rate or false negative rate, is used. This alternative spends more graph area on the region of interest. Most of the ROC area is of little interest; one primarily cares about the region tight against the y-axis and the top left corner – which, because of using miss rate instead of its complement, the hit rate, is the lower left corner in a DET plot. The DET plot is used extensively in the automatic speaker recognition community, where the name DET was first used. The analysis of the ROC performance in graphs with this warping of the axes was used by psychologists in perception studies halfway the 20th century, where this was dubbed "double probability paper".


Example DET graph

Z-score

If a standard score is applied to the ROC curve, the curve will be transformed into a straight line.[24] This z-score is based on a normal distribution with a mean of zero and a standard deviation of one. In memory strength theory, one must assume that the zROC is not only linear, but has a slope of 1.0. The normal distributions of targets (studied objects that the subjects need to recall) and lures (non studied objects that the subjects attempt to recall) is the factor causing the zROC to be linear.

The linearity of the zROC curve depends on the standard deviations of the target and lure strength distributions. If the standard deviations are equal, the slope will be 1.0. If the standard deviation of the target strength distribution is larger than the standard deviation of the lure strength distribution, then the slope will be smaller than 1.0. In most studies, it has been found that the zROC curve slopes constantly fall below 1, usually between 0.5 and 0.9.[25] Many experiments yielded a zROC slope of 0.8. A slope of 0.8 implies that the variability of the target strength distribution is 25% larger than the variability of the lure strength distribution.[26]

Another variable used is *d′* (d prime) (discussed above in "Other measures"), which can easily be expressed in terms of z-values. Although *d′* is a commonly used parameter, it must be recognized that it is only relevant when strictly adhering to the very strong assumptions of strength theory made above.[27]

The z-score of an ROC curve is always linear, as assumed, except in special situations. The Yonelinas familiarity-recollection model is a two-dimensional account of recognition memory. Instead of the subject simply answering yes or no to a specific input, the subject gives the input a feeling of familiarity, which operates like the original ROC curve. What changes, though, is a parameter for Recollection (R). Recollection is assumed to be all-or-none, and it trumps familiarity. If there were no recollection component, zROC would have a predicted slope of 1. However, when adding the recollection component, the zROC curve will be concave up, with a decreased slope. This difference in shape and slope result from an added element of variability due to some items being recollected. Patients with anterograde amnesia are unable to recollect, so their Yonelinas zROC curve would have a slope close to 1.0.[28]

History

The ROC curve was first used during World War II for the analysis of radar signals before it was employed in signal detection theory.[29] Following the attack on Pearl Harbor in 1941, the United States army began new research to increase the prediction of correctly detected Japanese aircraft from their radar signals.

In the 1950s, ROC curves were employed in psychophysics to assess human (and occasionally non-human animal) detection of weak signals.[29] In medicine, ROC analysis has been extensively used in the evaluation of diagnostic tests.[30][31] ROC curves are also used extensively in epidemiology and medical research and are frequently mentioned in conjunction with evidence-based medicine. In radiology, ROC analysis is a common technique to evaluate new radiology techniques.[32] In the social sciences, ROC analysis is often called the ROC Accuracy Ratio, a common technique for judging the accuracy of default probability models. ROC curves are widely used in laboratory medicine to assess diagnostic accuracy of a test, to choose the most optimal cut-off of a test and to compare diagnostic accuracy of several tests.

ROC curves also proved useful for the evaluation of machine learning techniques. The first application of ROC in machine learning was by Spackman who demonstrated the value of ROC curves in comparing and evaluating different classification algorithms.[33]

ROC curves beyond binary classification

The extension of ROC curves for classification problems with more than two classes has always been cumbersome, as the degrees of freedom increase quadratically with the number of classes, and the ROC space has $c(c-1)$ dimensions, where c is the number of classes.[34] Some approaches have been made for the particular case with three classes (three-way ROC).[35] The calculation of the volume under the ROC surface (VUS) has been analyzed and studied as a performance metric for multi-class problems.[36] However, because of the complexity of approximating the true VUS, some other approaches [37] based on an extension of AUC are more popular as an evaluation metric.

Given the success of ROC curves for the assessment of classification models, the extension of ROC curves for other supervised tasks has also been investigated. Notable proposals for regression problems are the so-called regression error characteristic (REC) Curves [38] and the Regression ROC (RROC) curves.[39] In the latter, RROC curves become extremely similar to ROC curves for classification, with the notions of asymmetry, dominance and convex hull. Also, the area under RROC curves is proportional to the error variance of the regression model.

ROC curve is related to the lift and uplift curves,[40][41] which are used in uplift modelling. The ROC curve itself has also been used as the optimization metric in uplift modeling.[42][43]

See also

Wikimedia Commons has media related to ***Receiver operating characteristic***.

- F1 score
- Brier score
- Coefficient of determination
- Constant false alarm rate
- Detection theory
- False alarm
- Gain (information retrieval)
- Precision and recall
- ROCCET

Terminology and derivations from a confusion matrix

true positive (TP)
eqv. with hit
true negative (TN)
eqv. with correct rejection
false positive (FP)
eqv. with false alarm, Type I error
false negative (FN)
eqv. with miss, Type II error

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sensitivity or true positive rate (TPR)
eqv. with hit rate, recall
$$TPR = TP/P = TP/(TP + FN)$$
specificity (SPC) or true negative rate (TNR)
$$SPC = TN/N = TN/(FP + TN)$$
precision or positive predictive value (PPV)
$$PPV = TP/(TP + FP)$$
negative predictive value (NPV)
$$NPV = TN/(TN + FN)$$
fall-out or false positive rate (FPR)
$$FPR = FP/N = FP/(FP + TN) = 1 - SPC$$
false discovery rate (FDR)
$$FDR = FP/(FP + TP) = 1 - PPV$$
miss rate or false negative rate (FNR)
$$FNR = FN/P = FN/(FN + TP)$$

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accuracy (ACC)
$$ACC = (TP + TN)/(P + N)$$
F1 score
is the harmonic mean of precision and sensitivity
$$F1 = 2TP/(2TP + FP + FN)$$
Matthews correlation coefficient (MCC)
$$\frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

Informedness = Sensitivity + Specificity - 1
Markedness = Precision + NPV - 1

Sources: Fawcett (2006) and Powers (2011).[44][45]

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External links

- ROC curves. Biomedical statistics (http://www.biomedicalstatistics.info/en/prognosis/roc-curves.html)

Categories: Detection theory | Data mining | Socioeconomics | Biostatistics | Statistical classification | Summary statistics for contingency tables

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