

# On Averaging ROC Curves

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## Abstract

Receiver operating characteristic (ROC) curves are a popular method of summarising the performance of classifiers. The ROC curve describes the separability of the distributions of predictions from a two-class classifier. There are a variety of situations in which an analyst seeks to aggregate multiple ROC curves into a single representative example. A number of methods of doing so are available; however, there is a degree of subtlety that is often overlooked when selecting the appropriate one. An important component of this relates to the interpretation of the decision process for which the classifier will be used. This paper summarises a number of methods of aggregation and carefully delineates the interpretations of each in order to inform their correct usage. A toy example is provided that highlights how an injudicious choice of aggregation method can lead to erroneous conclusions.

## 1 Introduction

ROC curves are widely used to present performance assessment results in classification studies. Their usage spans many disciplines, including pattern recognition (Webb, 2003), medical diagnostics (Swets et al., 2000), consumer credit scoring (Hand & Henley, 1997), and biometrics (Ross & Jain, 2003). Typically, the design and construction of a classifier is an iterative process: at each stage, choices are made regarding feature selection, distributional assumptions etc., and the classifier must be re-evaluated to assess the impact of these choices on performance. As described in Section 2.3, a scalar performance measure is often not sufficient for comparing classifier performance. ROC curves offer a useful visual evaluation of the trade-off between misclassification rates, from which operating points of interest—motivated by the specific application of the researcher—can be compared.

There are many situations in which there is a requirement to produce a *single* summary ROC curve from a collection of individual curves. For example, in credit card fraud detection, a bank may be running classifiers based on the same features for each customer (Juszczak et al., 2008); in biometric face verification, separate classifiers are trained for each individual subject (Marcialis & Roli, 2002); in radiology, multi-reader multi-case (MRMC) studies involve multiple radiologists producing scores for a collection of image cases (Skaron et al., 2012). It is perhaps natural in these settings to seek to report a single ROC curve summarising the performance of all the individual classifiers. Such a curve will be useful for classifier development and selection. Another situation involves the use of  $k$ -fold cross-validation procedures, which attempt to provide some sense of the average and the uncertainty in the ROC curve. Note that a related problem is that of constructing a *covariate-adjusted* ROC curve (Janes & Pepe, 2009), which aims to account for factors or characteristics that influence the predictions made by a classifier on certain instances within a single dataset. The focus of this paper is on constructing a single ROC curve from *multiple* datasets.

Reasoning about a summary or “average” ROC curve calls for fundamental considerations relating to the operational use of the classifier. Crucially, an aggregate ROC curve should represent performance in accordance with how the individual classifiers are to be deployed. As described in Section 2, a threshold  $T$  is required to produce a decision from most classifiers. In this context featuring multiple classifiers, the question is whether every classifier is to employ the same threshold  $T$  or if classifier  $i$  operates using threshold  $T_i$ . Next, it is important that the method of aggregating individual ROC curves is compatible with the application-specific operating points or characteristics of interest, upon which performance assessments will be made.

The literature contains a number of methods for aggregating ROC curves (Swets & Pickett, 1982; Fawcett, 2006). However, this paper will show that care must be taken when choosing the appropriate method, in particular with respect to the fundamental considerations described above. We argue that existing guidance is often unclear and, in some cases, misleading. We will provide an example that demonstrates that incorrectly combining curves can lead to misrepresentation of results. The purpose of this paper is not to provide a deeply novel result but rather to clearly delineate the characteristics of different aggregation procedures and provide clear guidance for their correct usage.

The remainder of the paper proceeds as follows: Section 2 introduces the background and notation for individual ROC graphs. In Section 3 we describe and illustrate the construction of average ROC curves under the three proposed combination methods. In Section 4, a discussion of the interpretations of different aggregating methods motivates guidelines for selecting the appropriate method. One of the existing methods is extended to further reduce misinterpretations of results. Finally, Section 5 provides a simple illustration to demonstrate that the choice of combination method is crucial in the context of comparing classifiers.

## 2 ROC graphs

Here we follow closely the framework presented by Krzanowski & Hand (2009). Suppose that there exists two populations—a ‘positive’ population  $P$  and a ‘negative’ population  $N$ —together with a classification rule for allocating unlabelled instances to one or other of these populations. A classification rule (*classifier*) is a function  $S(\mathbf{X})$  of the random vector  $\mathbf{X}$  of variables measured on each instance, used to predict class membership of a given instance. Some classifiers produce as output a discrete class label indicating only the predicted class of the instance; others produce a continuous output or *score*. The focus of this paper is the latter set of classifiers, as it is only for these that ROC curves can be produced. Suppose  $\mathbf{x}$  is the observed value of  $\mathbf{X}$  for a particular instance. The score  $s(\mathbf{x})$  can be used to predict class membership according to whether  $s(\mathbf{x})$  exceeds or does not exceed some threshold  $T$ . As  $S$  is a continuous variable, we can consider the distribution of scores pertaining to instances from populations  $P$  and  $N$ . Let  $f_{S|P}(s) = p(s | P)$  and  $f_{S|N}(s) = p(s | N)$  be the probability density functions of scores in  $P$  and  $N$ , respectively, with corresponding distribution functions  $F_{S|P}$  and  $F_{S|N}$ . A ROC graph is essentially a visual description of the degree of separability of these score distributions generated by a particular classifier.

We do not discuss how a classifier should be chosen or indeed calibrated for a particular task. These are well studied problems (Wolpert, 1996; Vapnik, 2013). Rather, we discuss how ROC curves are used to assess the performance of classifiers, in particular when applied to multiple datasets.

### 2.1 Definition

The score produced by a classifier can be a probability, representing the likelihood that an instance is a member of a particular class (the positive class, by convention), or simply a general, uncalibrated score, in which case it is conventional that higher scores are more indicative of positive class membership and lower scores indicative of negative class membership. In either case, the choice of threshold  $T$  will dictate the class assignments made by the classifier. Suppose that  $t$  is the value of the threshold  $T$  chosen for a particular classifier; an instance is assigned to  $P$  if its score  $s$  exceeds  $t$ , otherwise  $N$ . In order to assess the efficacy of this choice of  $T$ , we must consider four possible outcomes and the *rate* at which these occur:

1. an instance from  $P$  is correctly classified, i.e. the true positive rate  $tp = p(s > t | P)$ ;
2. an instance from  $N$  is misclassified, i.e. the false positive rate  $fp = p(s > t | N)$ ;
3. an instance from  $N$  is correctly classified, i.e. the true negative rate  $tn = p(s \leq t | N)$ ;
4. an instance from  $P$  is misclassified, i.e. the false negative rate  $fn = p(s \leq t | P)$ .

The choice of operating threshold  $t$  is application-specific and often complicated. By varying  $t$  and evaluating the four quantities above, we can inform a decision regarding which value to choose. In fact, as  $tp + fn = 1$  and  $fp + tn = 1$ , we need only consider two of the above quantities, typically  $fp$  and  $tp$ . A ROC curve is

obtained by varying  $t$  from  $-\infty$  to  $\infty$  and tracing a curve of  $(fp, tp)$ . We can write down the equation of this curve in terms of the distribution functions defined above:

$$\begin{aligned} tp &= p(s > t \mid P), \quad -\infty < t < \infty \\ &= 1 - F_{S|P}(t), \quad -\infty < t < \infty \\ &= 1 - F_{S|P} \left[ F_{S|N}^{-1}(1 - fp) \right], \quad 0 \leq fp \leq 1. \end{aligned}$$

## 2.2 Estimation

The role of the ROC curve is to present an assessment of the performance of a classifier over the whole range of potential thresholds. This performance will be determined by the degree of overlap of the scores assigned by the classifier to instances from  $P$  and  $N$ . In practice, we hardly ever know anything about the true underlying distributions of these scores. One typically only has available the values of  $\mathbf{X}$  for a set of instances whose class labels are known. The data is commonly split into two portions: a *training set* is used to estimate any parameters required by the chosen classifier, and this classifier can then be applied to a *test set* in order to estimate the score distributions, and hence  $fp$  and  $tp$ .

Standard methods of statistical inference are available to the researcher for this task. One may wish to assume parametric models for  $F_{S|P}$  and  $F_{S|N}$  and estimate parameters using maximum likelihood on the sample data. However, in this case, caution must be taken as the accuracy of the resulting ROC curve and any derived quantities strongly depends on the validity of the assumptions made (Krzanowski & Hand, 2009; Zhou et al., 2009). If a large number of test instances are available, then empirical estimation is preferred.

Let  $n_P$  and  $n_N$  be the number of instances in the samples from populations  $P$  and  $N$ , respectively. We write  $n_{P(t)}$  and  $n_{N(t)}$  for the number of those instances whose classification scores are greater than  $t$ . Then the empirical estimators of  $tp$  and  $fp$  at the classifier threshold  $t$  are given by

$$\hat{tp} = \frac{n_{P(t)}}{n_P} \quad \text{and} \quad \hat{fp} = \frac{n_{N(t)}}{n_N}.$$

The empirical ROC curve is then constructed by plotting the points  $(\hat{fp}, \hat{tp})$  for varying  $t$ .

## 2.3 Area under the ROC curve

A quantity widely used to summarise an important element of the information portrayed by a ROC curve is the area under the curve (AUC). The AUC can be interpreted as an average true positive rate, or as the probability that the classifier will allocate a higher score to a randomly chosen instance from  $P$  than it will to a randomly and independently chosen instance from  $N$ . Clearly, a higher AUC is desirable; however, classifiers should not be compared solely on their AUCs, as a higher AUC does not imply an everywhere dominating ROC curve. As a scalar measure of performance, a lot of valuable information contained in the ROC curve is lost, such as performance in specific regions of ROC space that may be of interest to the researcher. Moreover, there exists a fundamental incoherence in the use of AUC to compare *different* classifiers—see Hand (2009) for details, and Ferri et al. (2011) for an alternative interpretation of AUC.

## 3 Averaging ROC curves

The ROC graph described in the preceding section relates to a single dataset comprising instances belonging to either of two classes. Often we have multiple independent datasets of this type and a set of classification scores for each. In these settings, a separate ROC curve can be constructed from each set of scores. One approach for comparing different classifiers, or different iterations during classifier design and development, would be to compare average AUCs. However, for the reasons given in Section 2.3, it may be preferable to construct a single ROC curve that serves as a summary or average of the collection of individual ROC curves. In this way, the average performance at specific operating points can be assessed.

Methods for combining or averaging ROC curves have been proposed; however the properties of the resulting curves have not been properly explored nor compared in this context. Moreover, there is very little guidance

in the literature regarding which of the methods is most appropriate for a given task; in fact, existing guidance can even be misleading. As we will see, the interpretation of a summary ROC curve differs according to the averaging technique used, and so care should be taken both in choosing the appropriate method and in presenting results. Note that methods for averaging parametric ROC curves have also been proposed, based on averaging the estimated parameters of each curve (Metz, 1989). However, the focus of this discussion is on empirical ROC curves.

In this section we adapt the notation slightly to allow for the case where there is a collection of datasets, each consisting of instances to be classified. Say that there are  $M$  datasets, and dataset  $i$  comprises a positive population  $P_i$  and a negative population  $N_i$ . A classifier produces scores for each instance, so the ROC curve for dataset  $i$  describes the separability of the score distributions  $p(s | P_i)$  and  $p(s | N_i)$ .

For a simple illustration of the proposed averaging methods, we simulate scores arising from a probabilistic classifier employed on *two* datasets: the first ‘well separable’, the second ‘poorly separable’. We assume equally balanced classes for both datasets but allow the total number of instances to differ between datasets. The number of scores simulated for the negative and positive classes of the well separable dataset was  $n_{N_1} = n_{P_1} = 150$ ; for the poorly separable dataset  $n_{N_2} = n_{P_2} = 75$ . Density estimates of the simulated positive and negative scores for the two datasets are shown in the top two panels of Figure 1a.

### 3.1 Pooling

Swets & Pickett (1982) propose simply merging or *pooling* all the scores assigned to all instances from all datasets. A ROC curve is then constructed in the usual way as if every instance came from the one dataset:

$$\begin{aligned} \tilde{tp} &= \frac{\sum_{i=1}^M n_{P_i}(t)}{\sum_{i=1}^M n_{P_i}} & \tilde{fp} &= \frac{\sum_{i=1}^M n_{N_i}(t)}{\sum_{i=1}^M n_{N_i}} \\ &= \frac{n_{P(t)}}{n_P} & &= \frac{n_{N(t)}}{n_N}, \end{aligned}$$

where  $P$  and  $N$  are the total number of positive and negative instances among all  $M$  datasets, respectively.

The pooled ROC curve is a representation of the degree of separability of the mixture distributions that result from pooling scores between the two datasets. Density estimates of these mixture distributions can be seen in the bottom panel of Figure 1a. A fixed threshold is shown in all three plots of Figure 1a and the corresponding points in ROC space can be seen on the ROC curves in Figure 1b.

### 3.2 Vertical Averaging

In Provost et al. (1998), *vertical averaging* is proposed, whereby points are sampled uniformly along the  $fp$  axis and the corresponding  $tp$  values from each individual ROC curve are averaged. Each ROC curve is treated as a function  $R_i$  such that  $tp = R_i(fp)$ . This is done by choosing the maximum  $tp$  for each  $fp$  sampled between 0 and 1, interpolating between points where necessary. The vertical average ROC curve is

$$\bar{R}(fp) = \frac{1}{M} \sum_{i=1}^M R_i(fp), \quad 0 \leq fp \leq 1.$$

Standard errors can also be calculated and used to construct confidence intervals for the average curve (a related but different problem is that of constructing confidence *bands* for a ROC curve estimated from a single dataset—see Macskassy & Provost (2004)).

Note that the threshold that yields a given value of  $fp$  on each ROC curve will usually be different. The fixed threshold in Figure 1a yields a false positive rate of 0.12 for the well-separable dataset; the threshold yielding the same false positive rate for the poorly-separable dataset is shown in green. The corresponding true positive values for each dataset are shown on the ROC curves in Figure 1c, along with the vertical average curve.

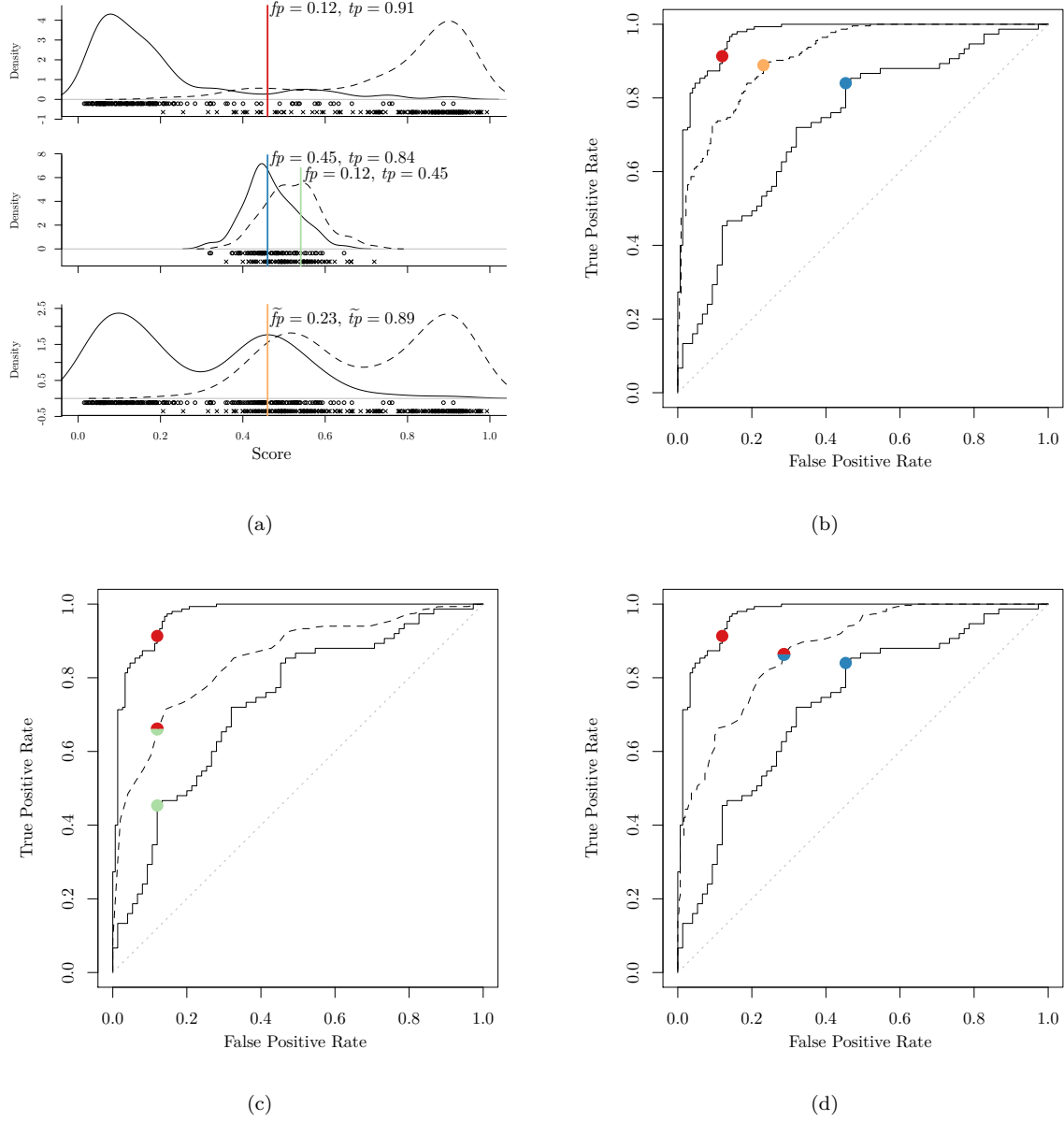


Figure 1: Illustration of three methods of averaging ROC curves. (a) Simulated classification scores for two datasets (top and middle) with density estimates of the negative and positive score distributions. The bottom plot shows density estimates of the pooled score distributions. (b) ROC curve pooling. (c) Vertical averaging. (d) Threshold averaging. In (b)–(d), coloured markers correspond to the fixed thresholds in (a); a split-colour marker indicates an average of the rates at the corresponding thresholds.

### 3.3 Threshold Averaging

Instead of sampling points based on their positions in ROC space, *threshold averaging* (Fawcett, 2006) samples uniformly from the threshold values  $t$  and averages separately the  $fp$  and  $tp$  rates achieved by each

ROC curve for that value of  $t$ .

$$\begin{aligned}\overline{tp} &= \frac{1}{M} \sum_{i=1}^M tp_i & \overline{fp} &= \frac{1}{M} \sum_{i=1}^M fp_i \\ &= \frac{1}{M} \sum_{i=1}^M \frac{n_{P_i(t)}}{n_{P_i}} & &= \frac{1}{M} \sum_{i=1}^M \frac{n_{N_i(t)}}{n_{N_i}}.\end{aligned}$$

The threshold average ROC curve is shown in Figure 1d. Note that for the fixed threshold shown in Figure 1a, the average  $fp$  and  $tp$  values do not equal  $\tilde{fp}$  and  $\tilde{tp}$  (the pooled rates). As  $n_{N_1} > n_{N_2}$  and  $n_{P_1} > n_{P_2}$ , the well separable scores dominate in the calculation of  $\tilde{fp}$  and  $\tilde{tp}$ , so the pooled ROC curve is drawn closer to the well separable ROC curve. If instead  $n_{N_1} = n_{N_2}$  and  $n_{P_1} = n_{P_2}$ , then the threshold average curve and the pooled curve would in fact be identical.

## 4 Interpreting Average ROC Curves

In most cases, the methods described each result in different average ROC curves. This can be seen clearly in the simple illustration provided in Figure 1. Furthermore, the interpretation of each is subtly different. It is important therefore to consider which method is most appropriate for a given study.

*Pooling* classification scores disregards datasets. The pooled ROC curve can be considered as a weighted average of the individual ROC curves, weighted by the number of instances scored in each. If one dataset contains a substantially larger number of instances than the other datasets, the pooled ROC curve will be biased towards the ROC curve for that dataset. Pooling also assumes that the score distributions between datasets are commensurate. Often this may not be the case, e.g. when different classification algorithms are being used, or if the training and testing sets are not representative samples of the population. Pooling is unsuitable in such situations. Furthermore, pooling produces only a single curve and so provides no information regarding uncertainty.

*Vertical averaging* offers a way of obtaining such a measure of variance. In Fawcett (2006, p. 869), it is claimed that this method of averaging “is appropriate when the [false positive] rate can indeed be fixed by the researcher, or when a single-dimensional measure of variation is desired.” *Threshold averaging* is presented as an alternative approach for situations when the false positive rate is not under the direct control of the researcher. The proposed solution is to average ROC points with respect to fixed thresholds, as these can be controlled by the researcher. We argue that this guidance is highly misleading, and the choice of averaging technique should instead be made under careful consideration of the *interpretation* of the resulting ROC curve. The vertical average ROC curve should be interpreted as the average true positive rate achieved amongst datasets for each fixed false positive rate, *allowing the threshold yielding that false positive rate to vary between datasets*. The threshold average ROC curve’s interpretation is the average performance achieved amongst datasets *if the threshold is fixed across all datasets*.

The way in which the classifier is to be deployed should therefore be the first consideration to guide whether ROC curves should be averaged by threshold or averaged in ROC space. If a fixed threshold is used in practice, then threshold averaging is appropriate. Otherwise, averaging should take place in ROC space and the researcher must next consider the characteristics of the curve upon which evaluation or comparisons will be made.

### 4.1 ROC Space Averaging

In situations where we do not assume a fixed threshold, vertical averaging is preferable to threshold averaging to provide a representation of the average performance achieved. Indeed, in many operational settings, the researcher is concerned with the average true positive rate achieved for small false positive rates. However, in other settings it may be more relevant to assess the average false positive rate suffered in order to achieve a high true positive rate, say. This information will not be conveyed by the vertical average curve. Similarly, it is common in biometrics studies (Wayman, 1999) to consider a ROC curve in terms of the ratio of the false acceptance rate ( $fp$ ) and the false rejection rate ( $1 - tp$ ). The equal error rate (EER), the point at

which these rates are equal, is then often used to assess and compare classifier performance. The vertical average ROC curve will again be a misleading description of the average performance when considered from this point of reference.

When averaging ROC curves in ROC space, the researcher must consider how the curve will be read, i.e. the axis of reference from which characteristics of interest are compared. To compare performance with respect to fixed false positive rates, averaging should take place *vertically*; for performance with respect to fixed true positive rates, averaging should take place *horizontally*; for performance with respect to fixed error rate ratios, averaging should take place *diagonally*. We therefore generalise the vertical averaging method in Fawcett (2006).

Under this approach, the  $fp$  and  $tp$  axes are first rotated clockwise by an angle  $\theta$  by applying a rotation matrix

$$\begin{bmatrix} fp' \\ tp' \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} fp \\ tp \end{bmatrix}.$$

The procedure is then the same as vertical averaging: values of  $fp'$  are sampled uniformly and the corresponding  $tp'$  values are averaged, yielding  $\overline{tp'}$ . The  $(fp', \overline{tp'})$  pairs are then rotated anti-clockwise to the original ROC space:

$$\begin{bmatrix} fp \\ tp \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} fp' \\ \overline{tp'} \end{bmatrix}.$$

Vertical, horizontal and diagonal averaging can then be achieved using  $\theta = 0, \pi/2, \pi/4$  respectively.

Averages along other directions may also be of interest. For example, denote the *cost* of misclassifying an instance from P and N by  $c_P$  and  $c_N$ , respectively. If the ratio of these costs is known or estimated, the threshold that minimises cost corresponds to the point of intersection of the ROC curve and a line originating from the point (0,1) with slope  $-\pi_P c_P / \pi_N c_N$ , where  $\pi_P$  and  $\pi_N$  are the probability that an instance comes from P and N, respectively (Adams & Hand, 1999). Hence, ROC curves can also be averaged with respect to fixed costs using  $\theta = \arctan(\pi_N c_N / \pi_P c_P)$ . However, Adams & Hand (1999) point out that it is rare in practice for these costs to be known precisely, hence the pre-eminence of ROC curves in practical applications.

## 5 Simulated Example

We now present an example of a realistic use-case of ROC curve averaging in which the resulting conclusion depends on the method of averaging used. Suppose a researcher wishes to compare the performance of two different classifiers on data arising from a collection of  $M$  datasets. Classification rules are learnt and scores generated by both classifiers using data from each dataset separately. The aim is to choose the classifier that has the better overall or average performance. We illustrate two scenarios.

**Scenario 1.** The output classification scores for two arbitrary classifiers were simulated as follows: For classifier 1 (C-1), negative and positive class scores for dataset  $i$  are simulated from Gaussian distributions  $N(\mu_{i0}, \sigma_{i0})$  and  $N(\mu_{i1}, \sigma_{i1})$  respectively. For classifier 2a (C-2a), the scores for dataset  $i$  are simulated from  $N(\mu_{i0} + \varepsilon_i, \sigma_{i0})$  and  $N(\mu_{i1} + \varepsilon_i, \sigma_{i1})$ , where  $\varepsilon_i \sim N(0, 1)$  is some random noise that differs between datasets but is the same for positive and negative populations within a dataset. As such, the locations of the modes of the score distributions of the two classifiers will be shifted but the class separability will be the same.

The first two panels of Figure 2 show ROC curves for both classifiers constructed using scores for  $M = 100$  datasets simulated in this way. The vertical and threshold average ROC curves are shown for both classifiers. 95% confidence intervals for the averages were constructed at each point using the assumption of normality. Note that the vertical average curves remain approximately equal for both classifiers but the threshold average curves differ. This highlights the importance of considering the interpretations of average ROC curves in order to avoid erroneous comparisons. Here, if the operational intention is to fix a threshold across all datasets, but vertical averaging is used, no difference between the classifiers is evident and the researcher will choose either.

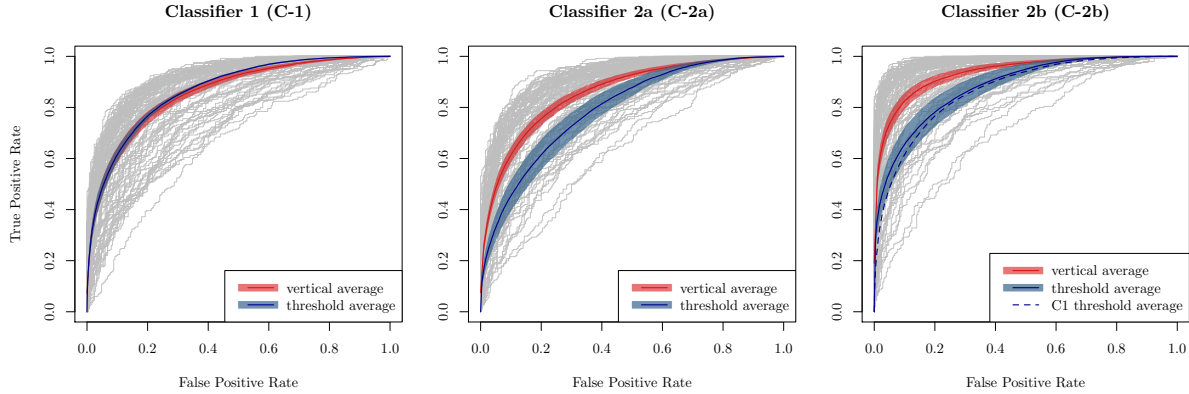


Figure 2: Simulated ROC curves for three classifiers and their averages under vertical and threshold averaging. The locations of the distributions used to simulate classification scores for C-1 are perturbed such that, for C-2a, the ROC curves—and hence the vertical average curves—are comparable but the threshold average curves differ, and for C-2b, the threshold average curves are comparable but the vertical average curves differ.

**Scenario 2.** The opposite scenario is also possible. We simulate scores for an alternative classifier (C-2b), this time shifting the modes of C-1’s score distributions unequally in order to increase the class separability. We do this by simulating negative class scores for dataset  $i$  from  $N(\mu_{i0} + \varepsilon_i, \sigma_{i0})$  as we did for C-2a but simulating positive class scores from  $N(\mu_{i1} + |\varepsilon_i|, \sigma_{i1})$ . For datasets where  $\varepsilon_i < 0$ , the score distributions become more separable. In Figure 2, the vertical average ROC curve for C-2b dominates both average curves for C-1; however the threshold average ROC curve remains approximately equal. Again, an averaging method unsuitable for the operational intentions can result in a misguided choice of classifier.

## 6 Conclusion

The naïve use of ROC curve combination methods is fraught with risk. We have summarised the common methods and pointed towards their interpretation in the operational context. Fundamentally, the appropriate choice of combination method *must* correspond to the operational approach for the classifier. To drive the message home, we provide a very simple illustration to show that incorrect decisions can result from ill-considered choice of combination method. We hope to have highlighted that in the context of classifier design and development, valuable information may be lost if due care and consideration is not paid when presenting and assessing results.

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