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ROC Graphs: Notes and Practical Considerations for Researchers

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Abstract. Receiver Operating Characteristics (ROC) graphs are a useful technique for organizing classifiers and visualizing their performance. ROC graphs are commonly used in medical decision making, and in recent years have been increasingly adopted in the machine learning and data mining research communities. Although ROC graphs are apparently simple, there are some common misconceptions and pitfalls when using them in practice. This article serves both as a tutorial introduction to ROC graphs and as a practical guide for using them in research.

Keywords: classification, classifier evaluation, ROC, visualization

Introduction

An ROC graph is a technique for visualizing, organizing and selecting classifiers based on their performance. ROC graphs have long been used in signal detection theory to depict the tradeoff between hit rates and false alarm rates of classifiers (Egan, 1975; Swets et al., 2000). ROC analysis has been extended for use in visualizing and analyzing the behavior of diagnostic systems (Swets, 1988). The medical decision making community has an extensive literature on the use of ROC graphs for diagnostic testing (Zou, 2002). Swets, Dawes and Monahan (2000) recently brought ROC curves to the attention of the wider public with their *Scientific American* article.

One of the earliest adopters of ROC graphs in machine learning was Spackman (1989), who demonstrated the value of ROC curves in evaluating and comparing algorithms. Recent years have seen an increase in the use of ROC graphs in the machine learning community. In addition to being a generally useful performance graphing method, they have properties that make them especially useful for domains with skewed class distribution and unequal classification error costs. These characteristics have become increasingly important as research continues into the areas of cost-sensitive learning and learning in the presence of unbalanced classes.

Most books on data mining and machine learning, if they mention ROC graphs at all, have only a brief description of the technique. ROC graphs are conceptually simple, but there are some non-obvious

complexities that arise when they are used in research. There are also common misconceptions and pitfalls when using them in practice.

This article attempts to serve as a tutorial introduction to ROC graphs and as a practical guide for using them in research. It collects some important observations that are perhaps not obvious to many in the community. Some of these points have been made in previously published articles, but they were often buried in text and were subsidiary to the main points. Other notes are the result of information passed around in email between researchers, but left unpublished. The goal of this article is to advance general knowledge about ROC graphs so as to promote better evaluation practices in the field.

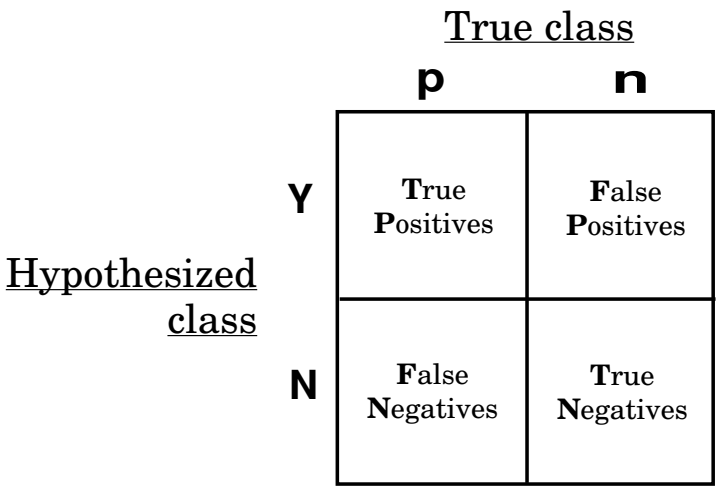
This article is divided into two parts. The first part, comprising sections 1 through 6, covers basic issues that will be encountered in most research uses of ROC graphs. Each topic has a separate section and is treated in detail, usually including algorithms. Researchers intending to use ROC curves seriously in their work should be familiar with this material. The second part, in section 7, covers some related but ancillary topics. They are more esoteric and are discussed in less detail, but pointers to further reading are included.

Note: Implementations of the algorithms in this article, in the Perl language, are collected in an archive available from: `http://www.purl.org/NET/tfawcett/software/ROC_algs.tar.gz`

1. Classifier Performance

We begin by considering classification problems using only two classes. Formally, each instance I is mapped to one element of the set $\{\mathbf{p}, \mathbf{n}\}$ of positive and negative class labels. A *classification model* (or *classifier*) is a mapping from instances to predicted classes. Some classification models produce a continuous output (e.g., an estimate of an instance's class membership probability) to which different thresholds may be applied to predict class membership. Other models produce a discrete class label indicating only the predicted class of the instance. To distinguish between the actual class and the predicted class we use the labels $\{\mathbf{Y}, \mathbf{N}\}$ for the class predictions produced by a model.

Given a classifier and an instance, there are four possible outcomes. If the instance is positive and it is classified as positive, it is counted as a *true positive*; if it is classified as negative, it is counted as a *false negative*. If the instance is negative and it is classified as negative, it is counted as a *true negative*; if it is classified as positive, it is counted as a *false positive*. Given a classifier and a set of instances (the test set), a two-by-two *confusion matrix* (also called a contingency table) can be



Column totals:	P	N

$$\text{fp rate} = \frac{FP}{N} \qquad \text{tp rate} = \frac{TP}{P}$$

$$\text{precision} = \frac{TP}{TP+FP} \qquad \text{recall} = \frac{TP}{P}$$

$$\text{accuracy} = \frac{TP+TN}{P+N} \qquad \text{F-measure} = \frac{2}{1/\text{precision}+1/\text{recall}}$$

Figure 1. Confusion matrix and common performance metrics calculated from it

constructed representing the dispositions of the set of instances. This matrix forms the basis for many common metrics.

Figure 1 shows a confusion matrix and equations of several common metrics that can be calculated from it. The numbers along the major diagonal represent the correct decisions made, and the numbers off this diagonal represent the errors—the confusion—between the various classes. The **true positive rate**[1] (also called *hit rate* and *recall*) of a classifier is estimated as:

$$tp\ rate \approx \frac{\text{Positives correctly classified}}{\text{Total positives}}$$

[1] For clarity, counts such as TP and FP will be denoted with upper-case letters and rates such as *tp rate* will be denoted with lower-case.

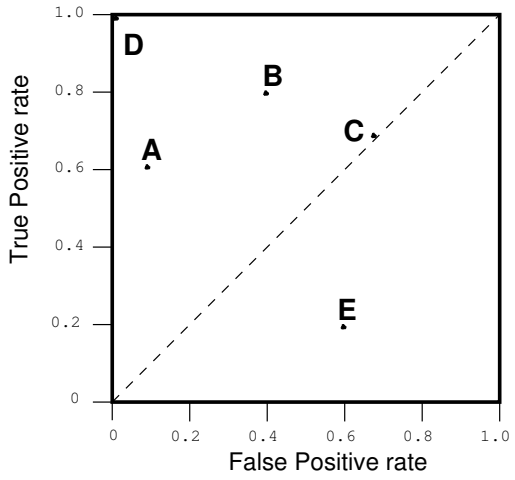


Figure 2. A basic ROC graph showing five discrete classifiers.

The **false positive rate** (also called *false alarm rate*) of the classifier is:

$$fp\ rate \approx \frac{\text{negatives incorrectly classified}}{\text{total negatives}}$$

Additional terms associated with ROC curves are:

$$\begin{aligned} \text{sensitivity} &= \text{recall} \\ \text{specificity} &= \frac{\text{True negatives}}{\text{False positives} + \text{True negatives}} \\ &= 1 - fp\ rate \\ \text{positive predictive value} &= \text{precision} \end{aligned}$$

2. ROC Space

ROC graphs are two-dimensional graphs in which *TP rate* is plotted on the Y axis and *FP rate* is plotted on the X axis. An ROC graph depicts relative trade-offs between benefits (true positives) and costs (false positives). Figure 2 shows an ROC graph with five classifiers labeled A through E.

A *discrete* classifier is one that outputs only a class label. Each discrete classifier produces an (*fp rate*, *tp rate*) pair corresponding to a single point in ROC space. The classifiers in figure 2 are all discrete classifiers.

Several points in ROC space are important to note. The lower left point $(0, 0)$ represents the strategy of never issuing a positive classification; such a classifier commits no false positive errors but also gains no true positives. The opposite strategy, of unconditionally issuing positive classifications, is represented by the upper right point $(1, 1)$.

The point $(0, 1)$ represents perfect classification. D's performance is perfect as shown.

Informally, one point in ROC space is better than another if it is to the northwest (*tp rate* is higher, *fp rate* is lower, or both) of the first. Classifiers appearing on the left hand-side of an ROC graph, near the X axis, may be thought of as "conservative": they make positive classifications only with strong evidence so they make few false positive errors, but they often have low true positive rates as well. Classifiers on the upper right-hand side of an ROC graph may be thought of as "liberal": they make positive classifications with weak evidence so they classify nearly all positives correctly, but they often have high false positive rates. In figure 2, A is more conservative than B. Many real world domains are dominated by large numbers of negative instances, so performance in the far left-hand side of the ROC graph becomes more interesting.

2.1. Random Performance

The diagonal line $y = x$ represents the strategy of randomly guessing a class. For example, if a classifier randomly guesses the positive class half the time, it can be expected to get half the positives and half the negatives correct; this yields the point $(0.5, 0.5)$ in ROC space. If it guesses the positive class 90% of the time, it can be expected to get 90% of the positives correct but its false positive rate will increase to 90% as well, yielding $(0.9, 0.9)$ in ROC space. Thus a random classifier will produce a ROC point that "slides" back and forth on the diagonal based on the frequency with which it guesses the positive class. In order to get away from this diagonal into the upper triangular region, the classifier must exploit some information in the data. In figure 2, C's performance is virtually random. At $(0.7, 0.7)$, C may be said to be guessing the positive class 70% of the time,

Any classifier that appears in the lower right triangle performs worse than random guessing. This triangle is therefore usually empty in ROC graphs. However, note that the decision space is symmetrical about the diagonal separating the two triangles. If we negate a classifier—that is, reverse its classification decisions on every instance—its true positive classifications become false negative mistakes, and its false positives become true negatives. Therefore, any classifier that produces a point

in the lower right triangle can be negated to produce a point in the upper left triangle. In figure 2, E performs much worse than random, and is in fact the negation of B. Any classifier on the diagonal may be said to have no information about the class. A classifier below the diagonal may be said to have useful information, but it is applying the information incorrectly (Flach and Wu, 2003).

Given an ROC graph in which a classifier's performance appears to be slightly better than random, it is natural to ask: "is this classifier's performance truly significant or is it only better than random by chance?" There is no conclusive test for this, but Forman (2002) has shown a methodology that addresses this question with ROC curves.

3. Curves in ROC space

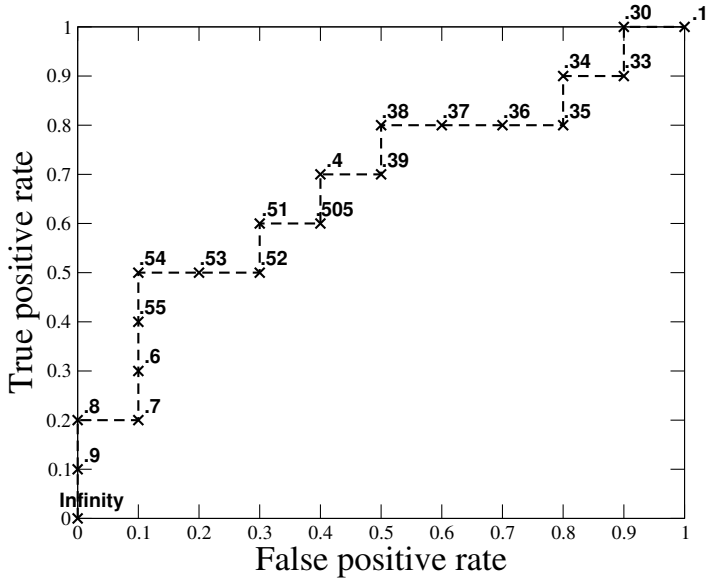
Many classifiers, such as decision trees or rule sets, are designed to produce only a class decision, i.e., a **Y** or **N** on each instance. When such a discrete classifier is applied to a test set, it yields a single confusion matrix, which in turn corresponds to one ROC point. Thus, a discrete classifier produces only a single point in ROC space.

Some classifiers, such as a Naive Bayes classifier or a neural network, naturally yield an instance *probability* or *score*, a numeric value that represents the degree to which an instance is a member of a class. These values can be strict probabilities, in which case they adhere to standard theorems of probability; or they can be general, uncalibrated scores, in which case the only property that holds is that a higher score indicates a higher probability. We shall call both a *probabilistic* classifier, in spite of the fact that the output may not be a proper probability[2].

Such a *ranking* or *scoring* classifier can be used with a threshold to produce a discrete (binary) classifier: if the classifier output is above the threshold, the classifier produces a **Y**, else a **N**. Each threshold value produces a different point in ROC space. Conceptually, we may imagine varying a threshold from $-\infty$ to $+\infty$ and tracing a curve through ROC space. Algorithm 1 describes this basic idea. Computationally, this is a poor way of generating an ROC curve, and the next section describes a more efficient and careful method.

Figure 3 shows an example of an ROC "curve" on a test set of twenty instances. The instances, ten positive and ten negative, are shown in the table beside the graph. Any ROC curve generated from a finite set of instances is actually a step function, which approaches a true curve as the number of instances approaches infinity. The step function in

[2] Techniques exist for converting an uncalibrated score into a proper probability but this conversion is unnecesary for ROC curves.



Inst#	Class	Score	Inst#	Class	Score
1	**p**	.9	11	**p**	.4
2	**p**	.8	12	**n**	.39
3	**n**	.7	13	**p**	.38
4	**p**	.6	14	**n**	.37
5	**p**	.55	15	**n**	.36
6	**p**	.54	16	**n**	.35
7	**n**	.53	17	**p**	.34
8	**n**	.52	18	**n**	.33
9	**p**	.51	19	**p**	.30
10	**n**	.505	20	**n**	.1

Figure 3. The ROC "curve" created by thresholding a test set. The table at right shows twenty data and the score assigned to each by a scoring classifier. The graph at left shows the corresponding ROC curve with each point labeled by the threshold that produces it.

figure 3 is taken from a very small instance set so that each point's derivation can be understood. In the table of figure 3, the instances are sorted by their scores, and each point in the ROC graph is labeled by the score threshold that produces it. A threshold of $+\infty$ produces the point $(0, 0)$. As we lower the threshold to 0.9 the first positive instance is classified positive, yielding $(0, 0.1)$. As the threshold is further reduced, the curve climbs up and to the right, ending up at $(1, 1)$ with a threshold

Algorithm 1 Conceptual method for calculating an ROC curve. See algorithm 2 for a practical method.

Inputs: L, the set of test instances; $f(i)$, the probabilistic classifier's estimate that instance i is positive; min and max, the smallest and largest values returned by f; $increment$, the smallest difference between any two f values.

```
1: for t = min to max by increment do
2:   FP ← 0
3:   TP ← 0
4:   for i ∈ L do
5:     if f(i) ≥ t then                    /* This example is over threshold */
6:       if i is a positive example then
7:         TP ← TP + 1
8:       else       /* i is a negative example, so this is a false positive */
9:         FP ← FP + 1
10:      end if
11:    end if
12:  end for
13:  Add point (FP/N, TP/P) to ROC curve
14: end for
15: end
```

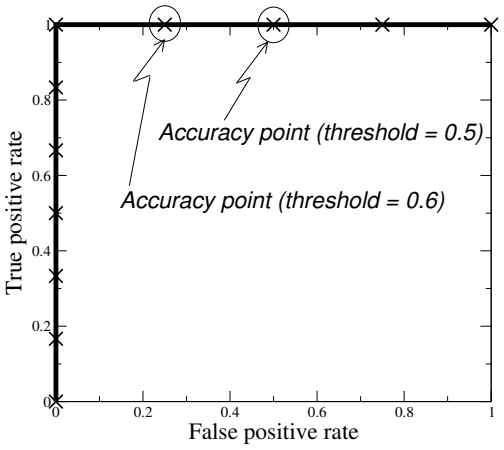
of 0.1. Note that lowering this threshold corresponds to moving from the "conservative" to the "liberal" areas of the graph.

Although the test set is very small, we can make some tentative observations about the classifier. It appears to perform better in the more conservative region of the graph; the ROC point at $(0.1, 0.5)$ produces its highest accuracy (70%). This is equivalent to saying that the classifier is better at identifying likely positives than at identifying likely negatives. Note also that the classifier's best accuracy occurs at a threshold of $\geq .54$, rather than at $\geq .5$ as we might expect with a balanced distribution. The next section discusses this phenomenon.

3.1. Relative versus absolute scores

An important point about ROC graphs is that they measure the ability of a classifier to produce good *relative* instance scores. A classifier need not produce accurate, calibrated probability estimates; it need only produce relative accurate scores that serve to discriminate positive and negative instances.

Consider the simple instance scores shown in figure 4, which came from a Naive Bayes classifier. Comparing the hypothesized class (which is **Y** if score$>$ 0.5, else **N**) against the true classes, we can see that the classifier gets instances 7 and 8 wrong, yielding 80% accuracy.



Inst no.	Class True	Class Hyp	Score
1	**p**	**Y**	0.99999
2	**p**	**Y**	0.99999
3	**p**	**Y**	0.99993
4	**p**	**Y**	0.99986
5	**p**	**Y**	0.99964
6	**p**	**Y**	0.99955
7	**n**	**Y**	0.68139
8	**n**	**Y**	0.50961
9	**n**	**N**	0.48880
10	**n**	**N**	0.44951

Figure 4. Scores and classifications of ten instances, and the resulting ROC curve.

However, consider the ROC curve on the left side of the figure. The curve rises vertically from $(0, 0)$ to $(0, 1)$, then horizontally to $(1, 1)$. This indicates perfect classification performance on this test set. Why is there a discrepancy?

The explanation lies in what each is measuring. The ROC curve shows the ability of the classifier to rank the positive instances relative to the negative instances, and it is indeed perfect in this ability. The accuracy metric imposes a threshold (score> 0.5) and measures the resulting classifications with respect to the scores. The accuracy measure would be appropriate if the scores were proper probabilities, but they are not. Another way of saying this is that the scores are not *properly calibrated*, as true probabilities are. In ROC space, the imposition of a 0.5 threshold results in the performance designated by the circled "accuracy point" in figure 4. This operating point is suboptimal. We could use the training set to estimate a prior for $p(\mathbf{p}) = 6/10 = 0.6$ and use this as a threshold, but it would still produce suboptimal performance (90% accuracy).

One way to eliminate this phenomenon is to calibrate the classifier scores. There are some methods for doing this (Zadrozny and Elkan, 2001). Another approach is to use an ROC method that chooses operating points based on their relative performance, and there are methods for doing this as well (Provost and Fawcett, 1998; Provost and Fawcett, 2001). These latter methods are discussed briefly in section 7.1.

A consequence of relative scoring is that classifier scores should not be compared across model classes. One model class may be designed

to produce scores in the range $[0, 1]$ while another produces scores in $[-1, +1]$ or $[1, 100]$. Comparing model performance at a common threshold will be meaningless.

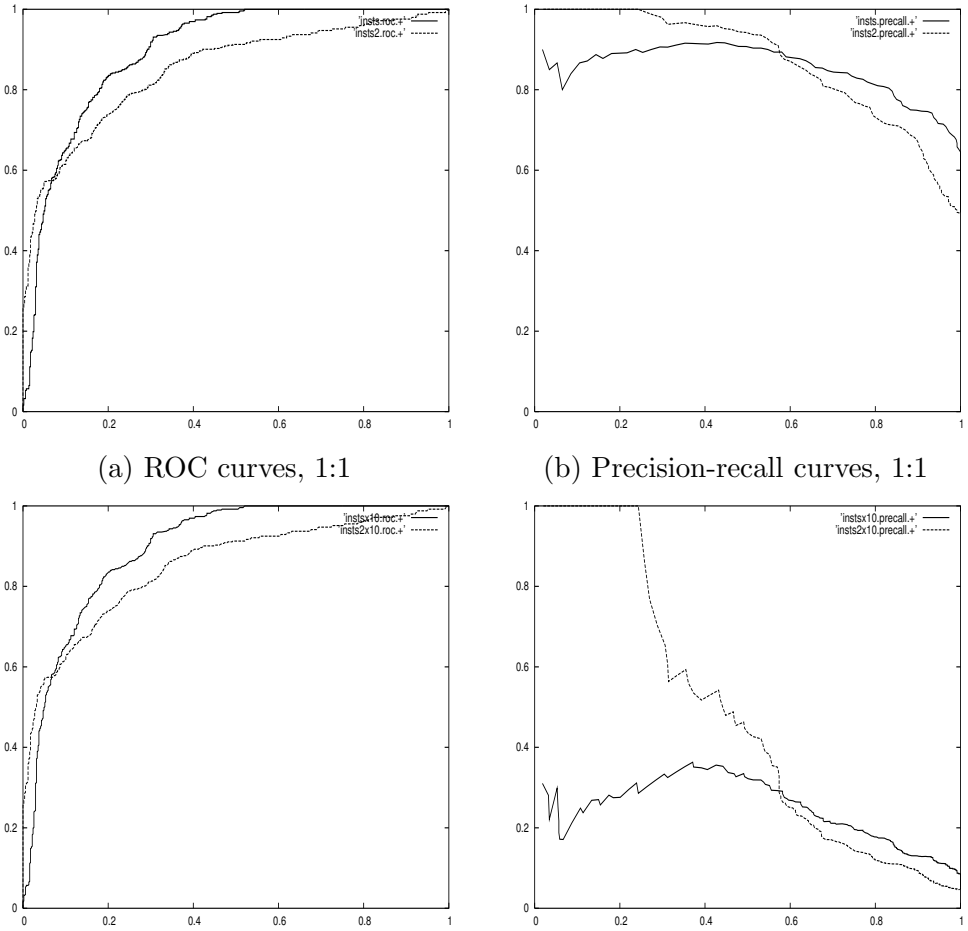
3.2. Class skew

ROC curves have an attractive property: they are insensitive to changes in class distribution. If the proportion of positive to negative instances changes in a test set, the ROC curves will not change. To see why this is so, consider the confusion matrix in figure 1. Note that the class distribution—the proportion of positive to negative instances—is the relationship of the left (+) column to the right (-) column. Any performance metric that uses values from both columns will be inherently sensitive to class skews. Metrics such as accuracy, precision, lift and F score use values from both columns of the confusion matrix. As a class distribution changes these measures will change as well, even if the fundamental classifier performance does not. ROC graphs are based upon *tp rate* and *fp rate*, in which each dimension is a strict columnar ratio, so do not depend on class distributions.

To some researchers, large class skews and large changes in class distributions may seem contrived and unrealistic. However, class skews of 10^1 and 10^2 are very common in real world domains, and skews up to 10^6 have been observed in some domains (Clearwater and Stern, 1991; Fawcett and Provost, 1996; Kubat et al., 1998; Saitta and Neri, 1998). Substantial changes in class distributions are not unrealistic either. For example, in medical decision making epidemics may cause the incidence of a disease to increase over time. In fraud detection, proportions of fraud varied significantly from month to month and place to place (Fawcett and Provost, 1997). Changes in a manufacturing practice may cause the proportion of defective units produced by a manufacturing line to increase or decrease. In each of these examples the prevalance of a class may change drastically without altering the fundamental characteristic of the class, i.e., the target concept.

Precision and recall are common in information retrieval for evaluating retrieval (classification) performance (Lewis, 1990; Lewis, 1991). Precision-recall graphs are commonly used where static document sets can sometimes be assumed; however, they are also used in dynamic environments such as web page retrieval, where the number of pages irrelevant to a query (N) is many orders of magnitude greater than P and probably increases steadily over time as web pages are created.

To see the effect of class skew, consider the curves in figure 5, which show two classifiers evaluated using ROC curves and precision-recall curves. In 5a and b, the test set has a balanced 1:1 class distribution.



(a) ROC curves, 1:1 (b) Precision-recall curves, 1:1

(c) ROC curves, 1:10 (d) Precision-recall curves, 1:10

Figure 5. ROC and precision-recall curves under class skew.

Graphs 5c and d show the same two classifiers on the same domain, but the number of negative instances has been increased ten-fold. Note that the classifiers and the underlying concept has not changed; only the class distribution is different. Observe that the ROC graphs in 5a and 5c are identical, while the precision-recall graphs in 5b and 5d differ dramatically. In some cases, the conclusion of which classifier has superior performance can change with a shifted distribution.

3.3. Creating scoring classifiers

Many classifier models are discrete: they are designed to produce only a class label from each test instance. However, we often want to generate

a full ROC curve from a classifier instead of just a single point. To this end we want to generate scores from a classifier rather than just a class label. There are several ways of producing such scores.

Many discrete classifier models may easily be converted to scoring classifiers by "looking inside" them at the instance statistics they keep. For example, a decision tree determines a class label of a leaf node from the proportion of instances at the node; the class decision is simply the most prevalent class. These class proportions may serve as a score (Provost and Domingos, 2001). Appendix A gives a basic algorithm for generating an ROC curve directly from a decision tree. A rule learner keeps similar statistics on rule confidence, and the confidence of a rule matching an instance can be used as a score (Fawcett, 2001).

Even if a classifier only produces a class label, an aggregation of them may be used to generate a score. MetaCost (Domingos, 1999) employs bagging to generate an ensemble of discrete classifiers, each of which produces a vote. The set of votes could be used to generate a score[3].

Finally, some combination of scoring and voting can be employed. For example, rules can provide basic probability estimates, which may then be used in weighted voting (Fawcett, 2001).

4. Efficient generation of ROC curves

Given a test set, we often want to generate an ROC curve efficiently from it. Although some researchers have employed methods like algorithm 1, this method is neither efficient nor practical: it requires knowing max, min and $increment$, which must be estimated from the test set and f values. It involves two nested loops; because the outer loop must increment t at least n times, the complexity is $O(n^2)$ in the number of test set instances.

A much better algorithm can be created by exploiting the monotonicity of thresholded classifications: any instance that is classified positive with respect to a given threshold will be classified positive for all lower thresholds as well. Therefore, we can simply sort the test instances decreasing by f scores and move down the list, processing one instance at a time and updating TP and FP as we go. In this way an ROC graph can be created from a linear scan.

[3] MetaCost actually works in the opposite direction because its goal is to generate a discrete classifier. It first creates a probabilistic classifier, then applies knowledge of the error costs and class skews to relabel the instances so as to "optimize" their classifications. Finally, it learns a specific discrete classifier from this new instance set. Thus, MetaCost is not a good method for creating a good scoring classifier, though its bagging method may be.

Algorithm 2 Efficient method for generating ROC points

Inputs: L, the set of test examples; $f(i)$, the probabilistic classifier's estimate that example i is positive; P and N, the number of positive and negative examples.

Outputs: R, a list of ROC points increasing by *fp rate*.

Require: $P > 0$ and $N > 0$

```
 1: L_sorted ← L sorted decreasing by f scores
 2: FP ← TP ← 0
 3: R ← ⟨⟩
 4: f_prev ← −∞
 5: i ← 1
 6: while i ≤ |L_sorted| do
 7:    if f(i) ≠ f_prev then
 8:       push (FP/N, TP/P) onto R
 9:       f_prev ← f(i)
10:    end if
11:    if L_sorted[i] is a positive example then
12:       TP ← TP + 1
13:    else                                  /* i is a negative example */
14:       FP ← FP + 1
15:    end if
16:    i ← i + 1
17: end while
18: push (FP/N, TP/P) onto R                 /* This is (1,1) */
19: end
```

The new algorithm is shown in algorithm 2. TP and FP both start at zero. For each positive instance we increment TP and for every negative instance we increment FP. We maintain a stack R of ROC points, pushing a new point onto R after each instance is processed. The final output is the stack R, which will contain points on the ROC curve.

Let n be the number of points in the test set. This algorithm requires an $O(n \log n)$ sort followed by an $O(n)$ scan down the list, resulting in $O(n \log n)$ total complexity.

4.1. Equally scored instances

Statements 7–10 need some explanation. These are necessary in order to correctly handle sequences of equally scored instances. Consider the ROC curve shown in figure 6. Assume we have a test set in which there is a sequence of instances, four negatives and six positives, all scored equally by f. The sort in line 1 of algorithm 2 does not impose any specific ordering on these instances since their f scores are equal.

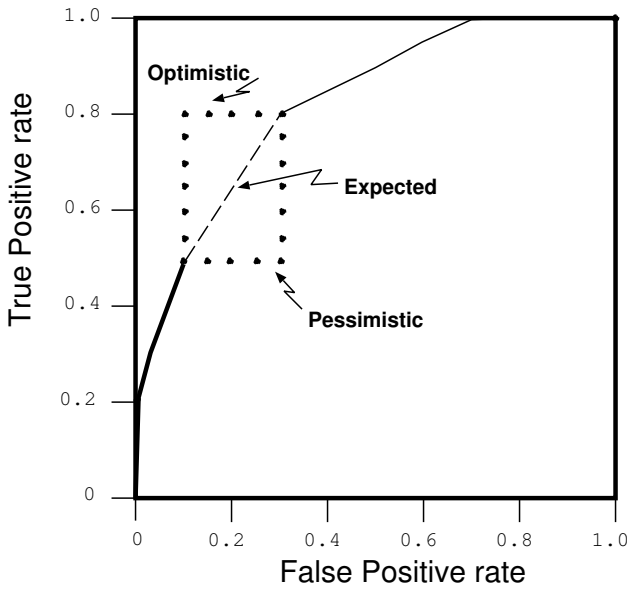


Figure 6. The optimistic, pessimistic and expected ROC segments resulting from a sequence of ten equally scored instances.

What happens when we create an ROC curve? In one extreme case, all the positives end up at the beginning of the sequence and we generate the "optimistic" upper L segment shown in figure 6. In the opposite extreme, all the negatives end up at the beginning of the sequence and we get the "pessimistic" lower L shown in figure 6. Any mixed ordering of the instances will give a different set of step segments within the rectangle formed by these two extremes. However, the ROC curve should represent the *expected* performance of the classifier, which, lacking any other information, is the average of the pessimistic and optimistic segments. This average is the diagonal of the rectangle, and can be created in the ROC curve algorithm by not emitting an ROC point until all instances of equal f values have been processed. This is what the f_{prev} variable and the **if** statement of line 7 accomplish.

Instances that are scored equally may seem unusual but with some classifier models they are common. For example, if we use instance counts at nodes in a decision tree to score instances, a large, high-entropy leaf node may produce many equally scored instances of both classes. If such instances are not averaged, the resulting ROC curves will be sensitive to the test set ordering, and different orderings can yield very misleading curves. This can be especially critical in calculating the area under an ROC curve, discussed in section 5. Consider a decision tree containing a leaf node accounting for n positives and m negatives.

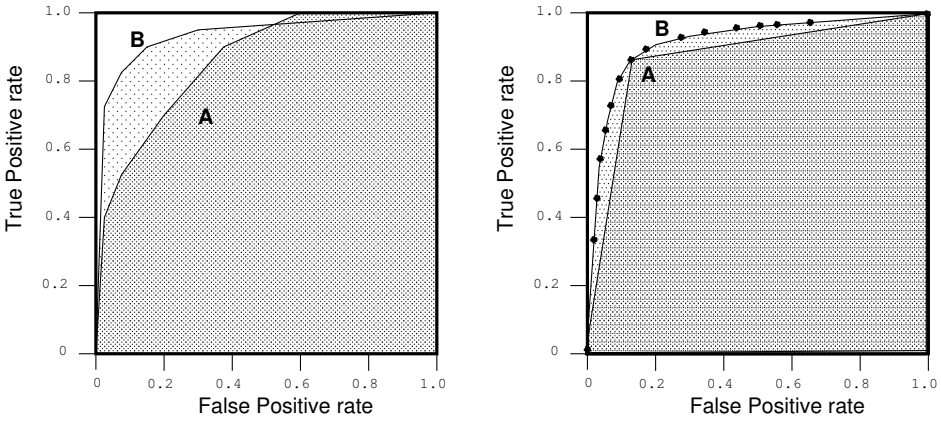


Figure 7. Two ROC graphs. The graph on the left shows the area under two ROC curves. The graph on the right shows the area under the curves of a discrete classifier (A) and a probabilistic classifier (B).

Every instance that is classified to this leaf node will be assigned the same score. The rectangle of figure 6 will be of size $\frac{nm}{PN}$, and if these instances are not averaged this one leaf may account for errors in ROC curve area as high as $\frac{nm}{2PN}$.

5. Area under an ROC Curve (AUC)

An ROC curve is a two-dimensional depiction of classifier performance. To compare classifiers we may want to reduce ROC performance to a single scalar value representing expected performance. A common method is to calculate the area under the ROC curve, abbreviated **AUC** (Bradley, 1997; Hanley and McNeil, 1982). Since the AUC is a portion of the area of the unit square, its value will always be between 0 and 1.0. However, because random guessing produces the diagonal line between $(0, 0)$ and $(1, 1)$, which has an area of 0.5, no realistic classifier should have an AUC less than 0.5.

The AUC has an important statistical property: the AUC of a classifier is equivalent to the probability that the classifier will rank a randomly chosen positive instance higher than a randomly chosen negative instance. This is equivalent to the Wilcoxon test of ranks (Hanley and McNeil, 1982). The AUC is also closely related to the Gini coefficient (Breiman et al., 1984), which is twice the area between the diagonal and the ROC curve. Hand and Till (2001) point out that $\text{Gini} + 1 = 2 \times \text{AUC}$.

Figure 7a shows the areas under two ROC curves, A and B. Classifier B has greater area and therefore better average performance. Figure 7b

Algorithm 3 Calculating the area under an ROC curve

Inputs: L, the set of test examples; $f(i)$, the probabilistic classifier's estimate that example i is positive; P and N, the number of positive and negative examples.

Outputs: A, the area under the ROC curve.

Require: $P > 0$ and $N > 0$

$L_{sorted} \leftarrow L$ sorted decreasing by f scores
$FP \leftarrow TP \leftarrow 0$
$FP_{prev} \leftarrow TP_{prev} \leftarrow 0$
$A \leftarrow 0$
$f_{prev} \leftarrow -\infty$
$i \leftarrow 1$
while $i \leq |L_{sorted}|$ **do**
  if $f(i) \neq f_{prev}$ **then**
    $A \leftarrow A +$ TRAPEZOID_AREA$(FP, FP_{prev}, TP, TP_{prev})$
    $f_{prev} \leftarrow f(i)$
    $FP_{prev} \leftarrow FP$
    $TP_{prev} \leftarrow TP$
  end if
  if i is a positive example **then**
    $TP \leftarrow TP + 1$
  else /* i is a negative example */
    $FP \leftarrow FP + 1$
  end if
end while
$A \leftarrow A +$ TRAP_AREA$(1, FP_{prev}, 1, TP_{prev})$
$A \leftarrow A/(P \times N)$ /* scale from $P \times N$ onto the unit square */
end

function TRAPEZOID_AREA$(X1, X2, Y1, Y2)$
$Base \leftarrow |X1 - X2|$
$Height_{avg} \leftarrow (Y1 + Y2)/2$
return $Base \times Height_{avg}$
end function

shows the area under the curve of a binary classifier A and a scoring classifier B. Classifier A represents the performance of B when B is used with a single, fixed threshold. Though the performance of the two is equal at the fixed point (A's threshold), A's performance becomes inferior to B further from this point.

It is possible for a high-AUC classifier to perform worse in a specific region of ROC space than a low-AUC classifier. Figure 7a shows an example of this: classifier B is generally better than A except at FPrate > 0.6 where A has a slight advantage. But in practice the

AUC performs very well and is often used when a general measure of predictiveness is desired.

The AUC may be computed easily using a small modification of algorithm 2, shown in algorithm 3. Instead of collecting ROC points, the algorithm adds successive areas of trapezoids to A. Finally, it divides A by the total possible area to scale the value to the unit square.

6. Averaging ROC curves

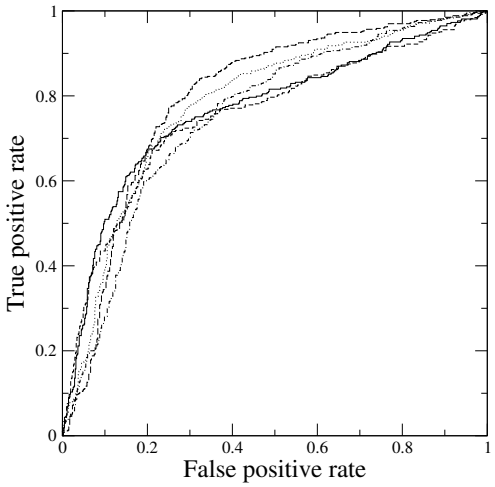
Although ROC curves may be used to evaluate classifiers, care should be taken when using them to make conclusions about classifier superiority. Some researchers have assumed that an ROC graph may be used to select the best classifiers simply by graphing them in ROC space and seeing which ones dominate. This is misleading; it is analogous to taking the maximum of a set of accuracy figures from a single test set. Without a measure of variance we cannot compare the classifiers.

Averaging ROC curves is easy if the original instances are available. Given test sets $T_1, T_2, \cdots, T_n$, generated from cross-validation or the bootstrap method, we can simply merge sort the instances together by their assigned scores[4] into one large test set T_M. We then run an ROC curve generation algorithm such as algorithm 2 on T_M and plot the result. However, the primary reason for using multiple test sets is to derive a measure of variance, which this simple merging does not provide. We need a more sophisticated method that samples individual curves at different points and averages the samples.

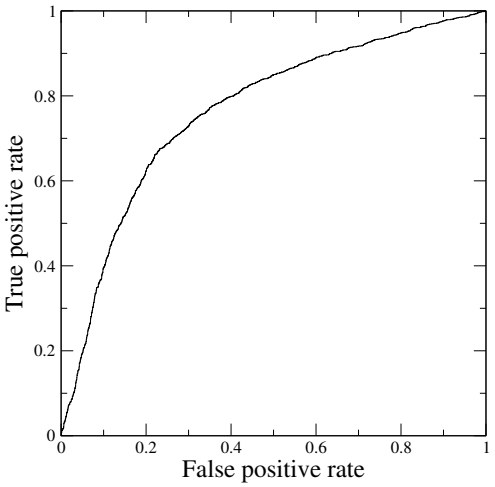
ROC space is two-dimensional, and any average is necessarily one-dimensional. ROC curves can be projected onto a single dimension and averaged conventionally, but this leads to the question of whether the projection is appropriate, or more precisely, whether it preserves characteristics of interest. The answer depends upon the reason for averaging the curves. This section presents two methods for averaging ROC curves: vertical and threshold averaging.

Figure 8a shows five ROC curves to be averaged. Each contains a thousand points and has some concavities. Figure 8b shows the curve formed by merging the five test sets and computing their combined ROC curve. Figures 8c and 8d show average curves formed by sampling the five individual ROC curves. The error bars are 95% confidence intervals.

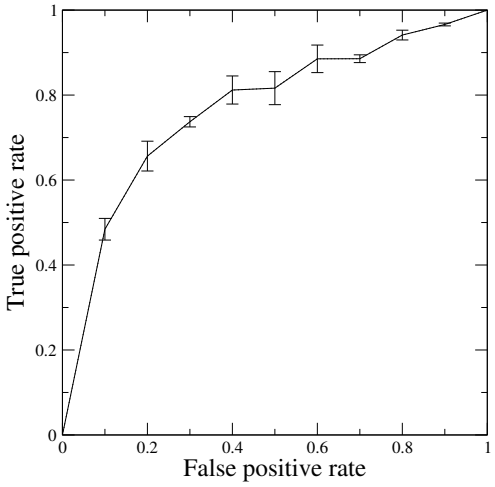
[4] This assumes that the scores generated by the models are comparable. If the same learning algorithm is being used, and the training and testing sets are representative samples of the population, the scores should be comparable.



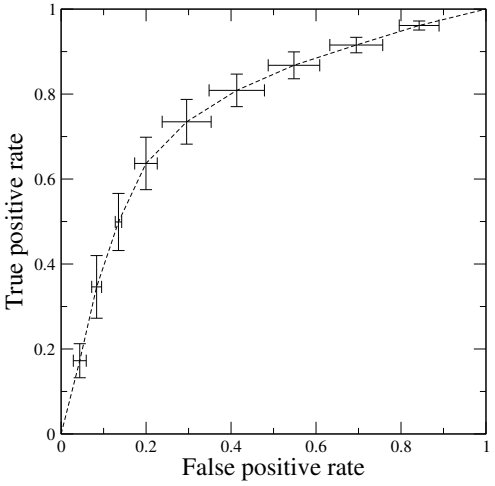
(a) ROC curves of five instance samples



(b) ROC curve formed by merging the five samples



(c) The curves of a averaged vertically



(d) The curves of a averaged by threshold

Figure 8. ROC curve averaging

6.1. Vertical averaging

Vertical averaging takes vertical samples of the ROC curves for fixed FP rates and averages the corresponding TP rates. Such averaging is appropriate when the FP rate can indeed be fixed by the researcher, or when a single-dimensional measure of variation is desired. Provost,

Algorithm 4 Vertical averaging of ROC curves.

Inputs: *samples*, the number of FP samples; *nrocs*, the number of ROC curves to be sampled, $ROCS[nrocs]$, an array of *nrocs* ROC curves; $npts[m]$, the number of points in ROC curve m. Each ROC point is a structure of two members, fpr and tpr.

Output: Array *tpravg*, containing the vertical averages.

```
1: s ← 1
2: for fpr_sample = 0 to 1 by 1/samples do
3:    tprsum ← 0
4:    for i = 1 to nrocs do
5:       tprsum ← tprsum + TPR_FOR_FPR(fpr_sample, ROCS[i], npts[i])
6:    end for
7:    tpravg[s] ← tprsum/i
8:    s ← s + 1
9: end for
10: end
```

```
1: function TPR_FOR_FPR(fpr_sample, ROC, npts)
2: i ← 1
3: while i < npts and ROC[i + 1].fpr ≤ fpr_sample do
4:    i ← i + 1
5: end while
6: if ROC[i].fpr = fpr_sample then
7:    return ROC[i].tpr
8: else
9:    return INTERPOLATE(ROC[i], ROC[i + 1], fpr_sample)
10: end if
11: end function
```

```
1: function INTERPOLATE(ROCP1, ROCP2, X)
2: slope = (ROCP2.tpr − ROCP1.tpr)/(ROCP2.fpr − ROCP1.fpr)
3: return ROCP1.tpr + slope · (X − ROCP1.fpr)
4: end function
```

Fawcett and Kohavi (1998) used this method in their work of averaging ROC curves of a classifier for k-fold cross-validation.

In this method each ROC curve is treated as a function, R_i, such that *tp rate* $= R_i$(*fp rate*). This is done by choosing the maximum *tp rate* for each *fp rate* and interpolating between points when necessary. The averaged ROC curve is the function $\hat{R}$(*fp rate*) $=$ *mean*$[R_i$(*fp rate*)$]$. To plot an average ROC curve we can sample from $\hat{R}$ at points regularly spaced along the *fp rate*-axis. Confidence intervals of the mean of *tp rate*are computed using the common assumption of a binomial distribution.

Algorithm 4 computes this vertical average of a set of ROC points. It leaves the means in the array $TPavg$.

Several extensions have been left out of this algorithm for clarity. The algorithm may easily be extended to compute standard deviations of the samples in order to draw confidence bars. Also, the function TP_FOR_FP may be optimized somwhat. Because it is only called on monotonically increasing values of FP, it need not scan each ROC array from the beginning every time; it could keep a record of the last point seen and initialize i from this array.

Figure 8c shows the vertical average of the five curves in figure 8a. The vertical bars on the curve show the 95% confidence region of the ROC mean. For this average curve, the curves were sampled at FP rates from 0 through 1 by 0.1. It is possible to sample curves much more finely but the confidence bars may become difficult to read.

6.2. Threshold averaging

Vertical averaging has the advantage that averages are made of a single dependent variable, the true positive rate, which simplifies computing confidence intervals. However, Holte (2002) has pointed out that the independent variable, false positive rate, is often not under the direct control of the researcher. It may be preferable to average ROC points using an independent variable whose value can be controlled directly, such as the threshold on the classifier scores.

Threshold averaging accomplishes this. Instead of sampling points based on their positions in ROC space, as vertical averaging does, it samples based on the thresholds that produced these points. The method must generate a set of thresholds to sample, then for each threshold it finds the corresponding point of each ROC curve and averages them.

Algorithm 5 shows the basic method for doing this. It generates an array T of classifier scores which are sorted from largest to smallest and used as the set of thresholds. These thresholds are sampled at fixed intervals determined by *samples*, the number of samples desired. For a given threshold, the algorithm selects from each ROC curve the the point of greatest score less than or equal to the threshold.[5] These points are then averaged separately along their X and Y axes, with the center point returned in the Avg array.

Figure 8d shows the result of averaging the five curves of 8a by thresholds. The resulting curve has average points and confidence bars in the X and Y directions. The bars shown are at the 95% confidence level.

[5] We assume the ROC points have been generated by an algorithm like 2 that deals correctly with equally scored instances.

Algorithm 5 Threshold averaging of ROC curves.

Inputs: *samples*, the number of threshold samples; *nrocs*, the number of ROC curves to be sampled; $ROCS[nrocs]$, an array of *nrocs* ROC curves sorted by score; $npts[m]$, the number of points in ROC curve m. Each ROC point is a structure of three members, fpr, tpr and score.

Output: *Avg*, an array of (X,Y) points constituting the average ROC curve.

Require: $samples > 1$

initialize array T to contain all scores of all ROC points
sort T in descending order
$s \leftarrow 1$
for $tidx = 1$ **to** $length(T)$ **by** $int(length(T)/samples)$ **do**
  $fprsum \leftarrow 0$
  $tprsum \leftarrow 0$
  for $i = 1$ **to** nrocs **do**
    $p \leftarrow$ ROC_POINT_AT_THRESHOLD$(ROCS[i], npts[i], T[tidx])$
    $fprsum \leftarrow fprsum + p.fpr$
    $tprsum \leftarrow tprsum + p.tpr$
  end for
  $Avg[s] \leftarrow (fprsum/i\ ,\ tprsum/i)$
  $s \leftarrow s + 1$
end for
end

function ROC_POINT_AT_THRESHOLD$(ROC, npts, thresh)$
$i \leftarrow 1$
while $i \leq npts$ **and** $ROC[i].score > thresh$ **do**
  $i \leftarrow i + 1$
end while
return $ROC[i]$
end function

There are some minor limitations of threshold averaging with respect to vertical averaging. To perform threshold averaging we need the classifier score assigned to each point. Also, section 3.1 pointed out that classifier scores should not be compared across model classes. Because of this, ROC curves averaged from different model classes may be misleading because the scores may be incommensurate.

Finally, Macskassy and Provost (2004) have investigated different techniques for generating confidence *bands* for ROC curves. They investigate confidence intervals from vertical and threshold averaging, as well as three methods from the medical field for generating bands (simultaneous join confidence regions, Working-Hotelling based bands, and fixed-width confidence bands). The reader is referred to their paper for

a much more detailed discussion of the techniques, their assumptions, and empirical studies.

7. Additional Topics

The previous sections are intended to be self-contained and to cover the basic issues that arise in using ROC curves in machine learning research. This section discusses additional, slightly more esoteric topics.

7.1. The ROC convex hull

One advantage of ROC graphs is that they enable visualizing and organizing classifier performance without regard to class distributions or error costs. This ability becomes very important when investigating learning with skewed distributions or cost-sensitive learning. A researcher can graph the performance of a set of classifiers, and that graph will remain invariant with respect to the operating conditions (class skew and error costs). As these conditions change, the region of interest may change, but the graph itself will not.

Provost and Fawcett (1998; 2001) show that a set of operating conditions may be transformed easily into a so-called *iso-performance line* in ROC space. Two points in ROC space, (FP_1,TP_1) and (FP_2,TP_2), have the same performance if

$$\frac{TP_2 - TP_1}{FP_2 - FP_1} = \frac{c(\mathbf{Y},\mathbf{n})p(\mathbf{n})}{c(\mathbf{N},\mathbf{p})p(\mathbf{p})} = m$$

This equation defines the slope of an *iso-performance line*. All classifiers corresponding to points on a line of slope m have the same expected cost. Each set of class and cost distributions defines a family of iso-performance lines. Lines "more northwest" (having a larger TP-intercept) are better because they correspond to classifiers with lower expected cost.

The details are beyond the scope of this article, but more generally a classifier is potentially optimal if and only if it lies on the convex hull (Barber et al., 1993) of the set of points in ROC space. We call the convex hull of the set of points in ROC space the *ROC convex hull* (ROCCH) of the corresponding set of classifiers.

This ROCCH formulation has a number of useful implications. Since only the classifiers on the convex hull are potentially optimal, no others need be retained. The operating conditions of the classifier may be translated into an iso-performance line, which in turn may be used to identify a portion of the ROCCH. As conditions change, the hull itself does not change; only the portion of interest will.

	fraudulent	legitimate
refuse	\$20	−\$20
approve	$-x$	$0.02x$

(a)

	fraudulent	legitimate
refuse	0	0
approve	$\$20 + x$	$0.02x + \$20$

(b)

Figure 9. Matrices for the credit approval domain. (a) original benefit matrix, (b) transformed cost-benefit matrix

7.2. Example-specific costs

In some domains the cost of a particular kind of error is not constant throughout the population, but varies by example. Consider a simple credit card transaction domain used by Elkan (2001) in which the task is to decide whether to approve or refuse a given transaction. Elkan describes a benefit matrix for the task, shown in figure 9a. This cost matrix is justified with the following explanation. A refused fraudulent transaction has a benefit of \$20 because it may prevent future fraud. Refusing a legitimate transaction has a negative benefit because it annoys a customer. Approving a fraudulent transaction has a negative benefit proporational to the transaction amount (x). Approving a legitimate transaction generates a small amount of income proportional to the transaction amount ($0.02x$).

ROC graphs have been criticized because of their inability to handle example-specific costs. In the traditional formulation this is correct because the axes graph rates that are based on simple counts of TP and FP examples, which is in turn based on the assumption that all true positives are equivalent and all false positives are equivalent.

However, with a straightforward transformation we can show how ROC graphs may be used with example-specific costs. For this domain we assume that a **Y** decision corresponds to approving a transaction, and **N** means denying it. To use the matrix for an ROC graph we transform it into a cost-benefit matrix where the costs are relative only to **Y** (approve) decisions. First we subtract the first row from both rows in the matrix. Conceptually this matrix now corresponds to a baseline situation where all transactions are refused, so all fraud is denied and all legitimate customers are annoyed. We then negate the approve-fraudulent cell to turn it into a cost. This yields the cost-benefit matrix of figure 9b which forms the definition of the cost function $c(\mathbf{Y}, \mathbf{p}, x)$ and $c(\mathbf{Y}, \mathbf{n}, x)$.

In standard ROC graphs the x axis represents the fraction of total FP mistakes possible. In the example-specific cost formulation it will represent the fraction of *total FP cost* possible, so the denominator will

Algorithm 6 Generating ROC points from an dataset with example-specific costs

Inputs: L, the set of test examples; $f(i)$, the probabilistic classifier's estimate that example i is positive; P and N, the number of positive and negative examples; $c(\mathbf{Y}, class, i)$, the cost of judging instance i of class $class$ to be $\mathbf{Y}$.
Outputs: R, a list of ROC points increasing by *fp rate*.

Require: $P > 0$ and $N > 0$

for $x \in L$ **do**
  if x is a positive example **then**
    $P\_total \leftarrow P\_total + c(\mathbf{Y}, \mathbf{p}, x)$
  else
    $N\_total \leftarrow N\_total + c(\mathbf{Y}, \mathbf{n}, x)$
  end if
end for
$L_{sorted} \leftarrow L$ sorted decreasing by f scores
$FP\_cost \leftarrow 0$
$TP\_benefit \leftarrow 0$
$R \leftarrow \langle\rangle$
$f_{prev} \leftarrow -\infty$
$i \leftarrow 1$
while $i \leq |L_{sorted}|$ **do**
  if $f(i) \neq f_{prev}$ **then**
    push $\left(\frac{FP\_cost}{N\_total}, \frac{TP\_benefit}{P\_total}\right)$ onto R
    $f_{prev} \leftarrow f(i)$
  end if
  if $L_{sorted}[i]$ is a positive example **then**
    $TP\_benefit \leftarrow TP\_benefit + c(\mathbf{Y}, \mathbf{p}, L_{sorted}[i])$
  else /* i is a negative example */
    $FP\_cost \leftarrow FP\_cost + c(\mathbf{Y}, \mathbf{n}, L\_sorted[i])$
  end if
  $i \leftarrow i + 1$
end while
push $\left(\frac{FP\_cost}{N}, \frac{TP\_benefit}{P}\right)$ onto R /* This is (1,1) */
end

now be

$$\sum_{x \in fraudulent} \$20 + x$$

Similarly the y axis will be the fraction of total TP benefits so its denominator will be

$$\sum_{x \in legitimate} 0.02x + \$20$$

Instead of incrementing TP and FP instance counts, as in algorithm 2, we increment $TP\_benefit$ and FP_cost by the cost (benefit) of each negative (positive) instance as it is processed. The ROC points are the fractions of total benefits and costs, respectively. Conceptually this transformation corresponds to replicating instances in the instance set in proportion to their cost, though this transformation has the advantage that no actual replication is performed and non-integer costs are easily accommodated. The final algorithm is shown in algorithm 6.

It is important to mention two caveats in adopting this transformation. First, while example costs may vary, ROC analysis requires that costs always be negative and benefits always be positive. For example, if we defined $c(\mathbf{Y}, \mathbf{p}, x) = x - \$20$, with example x values ranging in $[0, 40]$, this could be violated. Second, incorporating error costs into the ROC graph in this way introduces an additional assumption. Traditional ROC graphs assume that the *fp rate* and *tp rate* metrics of the test population will be similar to those of the training population; in particular that a classifier's performance on random samples will be similar. This new formulation adds the assumption that the example *costs* will be similar as well; in other words, not only will the classifier continue to score instances similarly between the training and testing sets, but the costs and benefits of those instances will be similar between the sets too.

7.3. Decision problems with more than two classes

Discussions up to this point have dealt with only two classes, and much of the ROC literature maintains this assumption. ROC analysis is commonly employed in medical decision making in which two-class diagnostic problems—presence or absence of an abnormal condition—are common. The two axes represent tradeoffs between errors (false positives) and benefits (true positives) that a classifier makes between two classes. Much of the analysis is straightforward because of the symmetry that exists in the two-class problem. The resulting performance can be graphed in two dimensions, which is easy to visualize.

7.3.1. *Multi-class ROC graphs*

With more than two classes the situation becomes much more complex if the entire space is to be managed. With n classes the confusion matrix becomes an $n \times n$ matrix containing the n correct classifications (the major diagonal entries) and $n^2 - n$ possible errors (the off-diagonal entries). Instead of managing trade-offs between TP and FP, we have n benefits and $n^2 - n$ errors. With only three classes, the surface becomes a $3^2 - 3 = 6$-dimensional polytope. Lane (2000) has written a short

paper outlining the issues involved and the prospects for addressing them. Srinivasan (1999) has shown that the analysis behind the ROC convex hull extends to multiple classes and multi-dimensional convex hulls.

One method for handling n classes is to produce n different ROC graphs, one for each class. Called this the *class reference* formulation. Specifically, if C is the set of all classes, ROC graph i plots the classification performance using class c_i as the positive class and all other classes as the negative class, i.e.,

$$P_i = c_i \tag{1}$$

$$N_i = \bigcup_{j \neq i} c_j \in C \tag{2}$$

While this is a convenient formulation, it compromises one of the attractions of ROC graphs, namely that they are insensitive to class skew (see section 3.2). Because each N_i comprises the union of $n-1$ classes, changes in prevalence within these classes may alter the c_i's ROC graph. For example, assume that some class $c_k \in N$ is particularly easy to identify. A classifier for class $c_i, i \neq k$ may exploit some characteristic of c_k in order to produce low scores for c_k instances. Increasing the prevalence of c_k might alter the performance of the classifier, and would be tantamount to changing the target concept by increasing the prevalence of one of its disjuncts. This in turn would alter the ROC curve. However, with this caveat, this method can work well in practice and provide reasonable flexibility in evaluation.

7.3.2. *Multi-class AUC*

The AUC is a measure of the discriminability of a pair of classes. In a two-class problem, the AUC is a single scalar value, but a multi-class problem introduces the issue of combining multiple pairwise discriminability values. The reader is referred to Hand and Till's (2001) article for an excellent discussion of these issues.

One approach to calculating multi-class AUCs was taken by Provost and Domingos (2001) in their work on probability estimation trees. They calculated AUCs for multi-class problems by generating each class reference ROC curve in turn, measuring the area under the curve, then summing the AUCs weighted by the reference class's prevalence in the data. More precisely, they define:

$$AUC_{total} = \sum_{c_i \in C} AUC(c_i) \cdot p(c_i)$$

where $AUC(c_i)$ is the area under the class reference ROC curve for c_i, as in equations 2. This definition requires only $|C|$ AUC calculations, so its overall complexity is $O(|C|n \log n)$.

The advantage of Provost and Domingos's AUC formulation is that AUC_{total} is generated directly from class reference ROC curves, and these curves can be generated and visualized easily. The disadvantage is that the class reference ROC is sensitive to class distributions and error costs, so this formulation of AUC_{total} is as well.

Hand and Till (2001) take a different approach in their derivation of a multi-class generalization of the AUC. They desired a measure that is insensitive to class distribution and error costs. The derivation is too detailed to summarize here, but it is based upon the fact that the AUC is equivalent to the probability that the classifier will rank a randomly chosen positive instance higher than a randomly chosen negative instance. From this probabilistic form, they derive a formulation that measures the unweighted *pairwise* discriminability of classes. Their measure, which they call M, is equivalent to:

$$AUC_{total} = \frac{2}{|C|(|C|-1)} \sum_{\{c_i,c_j\} \in C} AUC(c_i, c_j)$$

where n is the number of classes and $AUC(c_i, c_j)$ is the area under the two-class ROC curve involving classes c_i and c_j. The summation is calculated over all pairs of distinct classes, irrespective of order. There are $|C|(|C|-1)/2$ such pairs, so the time complexity of their measure is $O(|C|^2\, n \log n)$. While Hand and Till's formulation is well justified and is insensitive to changes in class distribution, there is no easy way to visualize the surface whose area is being calculated.

7.4. Combining classifiers

While ROC curves are commonly used for visualizing and evaluating individual classifiers, ROC space can also be used to estimate the performance of combinations of classifiers.

7.4.1. *Interpolating classifiers*

Sometimes the performance desired of a classifier is not exactly produced by any available classifier, but lies between two available classifiers. The desired performance can be obtained by sampling the decisions of each classifier. The sampling ratio will determine where the resulting classification performance lies.

For a concrete example, consider the decision problem of the CoIL Challenge 2000 (van der Putten and van Someren, 2000). In this challenge there is a set of 4000 clients to whom we wish to market a new

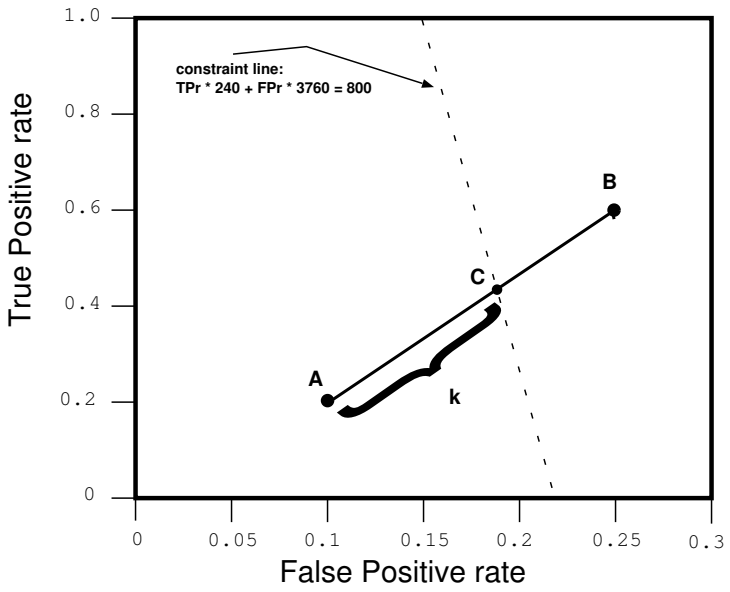


Figure 10. Interpolating classifiers

insurance policy. Our budget dictates that we can afford to market to only 800 of them, so we want to select the 800 who are most likely to respond to the offer. The expected class prior of responders is 6%, so within the population of 4000 we expect to have 240 responders (positives) and 3760 non-responders (negatives).

Assume we have generated two classifiers, A and B, which score clients by the probability they will buy the policy. In ROC space A lies at $(.1, .2)$ and B lies at $(.25, .6)$, as shown in figure 10. We want to market to exactly 800 people so our solution constraint is $fp\ rate \times 3760 + tp\ rate \times 240 = 800$. If we use A we expect $.1 \times 3760 + .2 \times 240 = 424$ candidates, which is too few. If we use B we expect $.25 \times 3760 + .6 \times 240 = 1084$ candidates, which is too many. We want a classifier between A and B.

The solution constraint is shown as a dashed line in figure 10. It intersects the line between A and B at C, approximately $(.18, .42)$. A classifier at point C would give the performance we desire and we can achieve it using linear interpolation. Calculate k as the proportional distance that C lies on the line between A and B:

$$k = \frac{0.18 - 0.1}{0.25 - 0.1} \approx 0.53$$

Therefore, if we sample B's decisions at a rate of .53 and A's decisions at a rate of $1 - .53 = .47$ we should attain C's performance. In practice this fractional sampling can be done by randomly sampling decisions

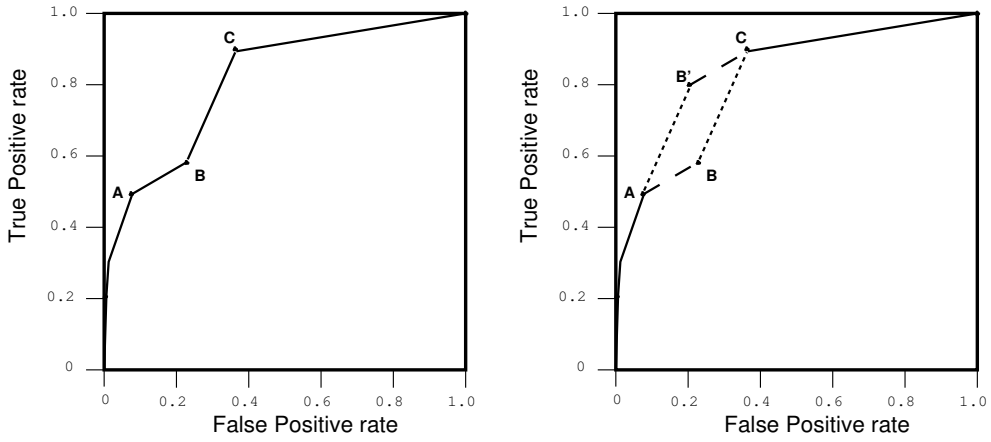


Figure 11. Removing concavities

from each: for each instance, generate a random number between zero and one. If the random number is greater than k, apply classifier A to the instance and report its decision, else pass the instance to B.

7.4.2. *Conditional combinations of classifiers to remove concavities*
A concavity in an ROC curve represents a sub-optimality in the classifier. Specifically, a concavity occurs whenever a segment of slope r is joined at the right to a segment of slope s where $s > r$. The slope of an ROC curve represents the class likelihood ratio. A concavity indicates that the group of instances producing s have a higher posterior class ratio than those accounting for r. Because s occurs to the right of r, r's instances should have been ranked more highly than s's, but were not. This is a sub-optimality of the classifier. In practice, concavities in ROC curves produced by learned classifiers may be due either to idiosyncracies in learning or to small test set effects.[6]

Section 2.1 mentioned that the diagonal $y = x$ on an ROC graph represents a zone of "no information", where a classifier is randomly guessing at classifications. Any classifier below the diagonal can have its classifications reversed to bring it above the diagonal. Flach and Wu (2003) show that in some cases this can be done locally to remove concavities in an ROC graph.

Figure 11a shows three classifiers, A, B and C. B introduces a concavity in the ROC graph. The segment BC has higher slope than AB, so ideally we would want to "swap" the position of segment BC for that

[6] Bradley's (1997) ROC curves exhibit noticeable concavities, as do the Breast cancer and RoadGrass domains of Provost *et al.* (1998).

of AB in the ROC graph. If A, B and C are related—for example, if they represent different thresholds applied to the same scoring model—then this can be done. Let $A(x)$ represent the classification assigned to instance x by classifier A. Flach and Wu's method involves creating a new classifier $\acute{B}$ defined as:

$$\acute{B}(x) = \begin{cases} \mathbf{N} & \text{if} \quad A(x) = \mathbf{N} \wedge C(x) = \mathbf{N} \\ \mathbf{Y} & \text{if} \quad A(x) = \mathbf{Y} \wedge C(x) = \mathbf{Y} \\ \neg B(x) & \text{if} \quad A(x) = \mathbf{N} \wedge C(x) = \mathbf{Y} \end{cases}$$

Figure 11b shows the new classifier $\acute{B}$. Its position is equivalent to reflecting B's about the line AC or, equivalently, transposing the decisions in AB with those in BC. Flach and Wu (2003) demonstrate this construction in greater detail and prove its performance formally.

An important caveat is that A, B and C must be dependent. Specifically, it must be the case that $TP_A \subseteq TP_B \subseteq TP_C$ and $FP_A \subseteq FP_B \subseteq FP_C$. This is commonly achieved when A, B and C are the results of imposing a threshold T on a single model and $T_A < T_B < T_C$. Because of these relationships, there need be no fourth clause covering $A(x) = \mathbf{N} \wedge C(x) = \mathbf{Y}$ in the definition of $\acute{B}$ since these conditions are contradictory.

7.4.3. *Logically combining classifiers*

As we have seen, with two classes a classifier c can be viewed as a predicate on an instance x where $c(x)$ is true iff $c(x) = \mathbf{Y}$. We can then speak of boolean combinations of classifiers, and an ROC graph can provide a way of visualizing the performance of such combinations. It can help to illustrate both the bounding region of the new classifier and its expected position.

If two classifiers c_1 and c_2 are conjoined to create $c_3 = c_1 \wedge c_2$, where will c_3 lie in ROC space? Let TPrate_3 and FPrate_3 be the ROC positions of c_3. The minimum number of instances c_3 can match is zero. The maximum is limited by the intersection of their positive sets. Since a new instance must satisfy both c_1 and c_2, we can bound c_3's position:

$$\begin{aligned} 0 \leq\ & \text{TPrate}_3 \ \leq min(\text{TPrate}_1, \text{TPrate}_2) \\ 0 \leq\ & \text{TPrate}_3 \ \leq min(\text{FPrate}_1, \text{FPrate}_2) \end{aligned}$$

Figure 12 shows this bounding rectangle for two classifiers $c_1 \wedge c_2$, the shaded rectangle in the lower left corner. Where within this rectangle do we expect c_3 to lie? Let x be an instance in the true positive set TP_3 of c_3. Then:

$$\begin{aligned} TPrate_3 \ &\approx\ p(x \in TP_3) \\ &\approx\ p(x \in TP_1 \wedge x \in TP_2) \end{aligned}$$

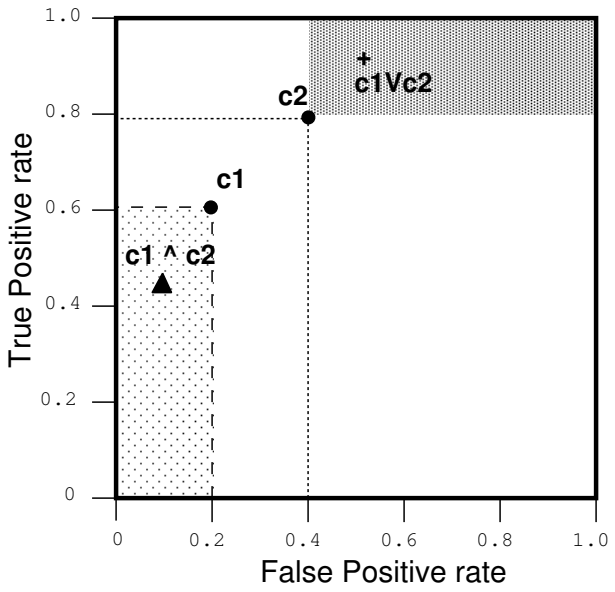


Figure 12. The expected positions of boolean combinations of c_1 and c_2.

By assuming independence of c_1 and c_2, we can continue:

$$\begin{aligned} TPrate_3 &\approx p(x \in TP_1) \cdot p(x \in TP_2) \\ &\approx \frac{\mid TP_1 \mid}{\mid P \mid} \cdot \frac{\mid TP_2 \mid}{\mid P \mid} \\ &\approx TPrate_1 \cdot TPrate2 \end{aligned}$$

A similar derivation can be done for FPrate_3, showing that $FPrate_3 \approx FPrate_1 \cdot FPrate_2$. Thus, the conjunction of two classifiers c_1 and c_2 can be expected to lie at the point

$$(\mathrm{FPrate}_1 \cdot \mathrm{FPrate}_2 \ , \ \mathrm{TPrate}_1 \cdot \mathrm{TPrate}_2)$$

in ROC space. This point is shown as the triangle in figure 12 at $(0.08, 0.42)$. This estimate assumes independence of classifiers; interactions between c_1 and c_2 may cause the position of c_3 in ROC space to vary from this estimate.

We can derive similar expressions for the disjunction $c_4 = c_1 \vee c_2$. In this case the rates are bounded by:

$$\begin{aligned} max(\mathrm{TPrate}_1, \mathrm{TPrate}_2) \leq \ \mathrm{TPrate}_4 \ &\leq min(1, \mathrm{TPrate}_1 + \mathrm{TPrate2}) \\ max(\mathrm{FPrate}_1, \mathrm{FPrate}_2) \leq \ \mathrm{FPrate}_4 \ &\leq min(1, \mathrm{FPrate}_1 + \mathrm{FPrate2}) \end{aligned}$$

This bounding region is indicated in figure 12 by the shaded rectangle in the upper right portion of the ROC graph. The expected position, assuming independence, is:

$$\begin{aligned} \text{TPrate}_4 &= 1 - [1 - \text{TPrate}_1 - \text{TPrate}_2 + \text{TPrate}_1 \cdot \text{TPrate}_2] \\ \text{FPrate}_4 &= 1 - [1 - \text{FPrate}_1 - \text{FPrate}_2 + \text{FPrate}_1 \cdot \text{FPrate}_2] \end{aligned}$$

This point is indicted by the marked + symbol within the bounding rectangle.

It is worth noting that the expected location of both $c_1 \wedge c_2$ and $c_1 \vee c_2$ are *outside* of the ROC convex hull formed by c_1 and c_2. In other words, logical combinations of classifiers can produce performance outside of the convex hull and better than what could be achieved with linear interpolation.

7.4.4. *Chaining classifiers*

Section 2 mentioned that classifiers on the left side of an ROC graph near $X = 0$ may be thought of as "conservative"; and classifiers on the upper side of an ROC graph near $Y = 1$ may be thought of as "liberal". With this interpretation it might be tempting to devise a composite scheme that applies classifiers sequentially like a rule list. Such a technique might work as follows: Given the classifiers on the ROC convex hull, an instance is first given to the most conservative (left-most) classifier. If that classifier returns **Y**, the composite classifier returns **Y**; otherwise, the second most conservative classifier is tested, and so on. The sequence terminates when some classifier issues a **Y** classification, or when the classifiers reach a maximum expected cost, such as may be specified by an iso-performance line. The resulting classifier is $c_1 \vee c_2 \vee \cdots \vee c_k$, where c_k has the highest expected cost tolerable.

Unfortunately, this chaining of classifiers may not work as desired. Classifiers' positions in ROC space are based upon their *independent* performance. When classifiers are applied in sequence this way, they are not being used independently but are instead being applied to instances which more conservative classifiers have already classified as negative. Due to classifier interactions (intersections among classifiers' TP and FP sets), the resulting classifier may have very different performance characteristics than any of the component classifiers. Although section 7.4.3 introduced an independence assumption that may be reasonable for combining two classifiers, this assumption becomes much less tenable as longer chains of classifiers are constructed.

7.4.5. *The importance of final validation*
To close this section on classifier combination, we emphasize a basic point that is easy to forget. ROC graphs are commonly used in evaluation, and are generated from a final test set. If an ROC graph is instead used to select or to combine classifiers, this use must be considered to be part of the training phase. A separate held-out validation set must be used to estimate the expected performance of the classifier(s). This is true even if the ROC curves are being used to form a convex hull.

7.5. Alternatives to ROC graphs

Recently, various alternatives to ROC graphs have been proposed. We briefly summarize them here.

7.5.1. *DET curves*
DET graphs (Martin et al., 1997) are not so much an alternative to ROC curves as an alternative way of presenting them. There are two differences. First, DET graphs plot false negatives on the Y axis instead of true positives, so they plot one kind of error against another. Second, DET graphs are log scaled on both axes so that the area of the lower left part of the curve (which corresponds to the upper left portion of an ROC graph) is expanded. Martin et al. (1997) argue that well-performing classifiers, with low false positive rates and/or low false negative rates, tend to be "bunched up" together in the lower left portion of a ROC graph. The log scaling of a DET graph gives this region greater surface area and allows these classifiers to be compared more easily.

7.5.2. *Cost curves*
Section 7.1 showed how information about class proportions and error costs could be combined to define the slope of a so-called iso-performance line. Such a line can be placed on an ROC curve and used to identify which classifier(s) perform best under the conditions of interest. In many cost minimization scenarios, this requires inspecting the curves and judging the tangent angles for which one classifier dominates.

Drummond and Holte (2000; 2002) point out that reading slope angles from an ROC curve may be difficult to do. Determining the regions of superiority, and the amount by which one classifier is superior to another, is challenging when the comparison lines are curve tangents rather than simple vertical lines. Drummond and Holte reason that if the primary use of a curve is to compare relative costs, the graphs should represent these costs explicitly. They propose *cost curves* as an alternative to ROC curves.

On a cost curve, the X axis ranges from 0 to 1 and measures the proportion of positives in the distribution. The Y axis, also from 0 to 1, is the relative expected misclassification cost. A perfect classifier is a horizontal line from $(0, 0)$ to $(0, 1)$. Cost curves are a point-line dual of ROC curves: a point (i.e., a discrete classifier) in ROC space is represented by a line in cost space, with the line designating the relative expected cost of the classifier. For any X point, the corresponding Y points represent the expected costs of the classifiers. Thus, while in ROC space the convex hull contains the set of lowest-cost classifiers, in cost space the lower envelope represents this set.

7.5.3. *Relative superiority graphs and the LC index*
Like cost curves, the LC index (Adams and Hand, 1999) is a transformation of ROC curves that facilitates comparing classifiers by cost. Adams and Hand argue that precise cost information is rare, but *some* information about costs is always available, and so the AUC is too coarse of a measure of classifier performance. An expert may not be able to specify exactly what the costs of a false positive and false negative should be, but an expert usually has some idea how much more expensive one error is than another. This can be expressed as a range of values in which the error cost ratio will lie.

Adams and Hand's method maps the ratio of error costs onto the interval (0,1). It then transforms a set of ROC curves into a set of parallel lines showing which classifier dominates at which region in the interval. An expert provides a sub-range of (0,1) within which the ratio is expected to fall, as well as a most likely value for the ratio. This serves to focus attention on the interval of interest. Upon these "relative superiority" graphs a measure of confidence—the LC index—can be defined indicating how likely it is that one classifier is superior to another within this interval.

The relative superiority graphs may be seen as a binary version of cost curves, in which we are only interested in which classifier is superior. The LC index (for loss comparison) is thus a measure of confidence of superiority rather than of cost difference.

8. Conclusion

ROC graphs are a very useful tool for visualizing and evaluating classifiers. They are able to provide a richer measure of classification performance than accuracy or error rate can, and they have advantages over other evaluation measures such as precision-recall graphs and lift curves. However, as with any evaluation metric, using them wisely

requires knowing their characteristics and limitations. It is hoped that this article advances the general knowledge about ROC graphs and helps to promote better evaluation practices in the data mining community.

Appendix

A. Generating an ROC curve from a decision tree

As a basic example of how scores can be derived from some model classes, and how a ROC curve can be generated directly from them, we present a procedure for generating a ROC curve from a decision tree. Algorithm 7 shows the basic idea. For simplicity the algorithm is written in terms of descending the tree structure, but it could just as easily extract the same information from the printed tree representation. Following C4.5 usage, each leaf node keeps a record of the number of examples matched by the condition, the number of errors (local false positives), and the class concluded by the node.

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Algorithm 7 Generating an ROC curve from a decision tree

Inputs: *pos_class* and *neg_class*, the positive and negative classes; and T, the decision tree root node. Each tree node has fields *class*, the class concluded by the node; *matched*, the number of instances matched by the condition; and *errors*, the number of non-*class* instances matched by the condition. If a node is not a leaf node it also has *children*, an array of pointers to its children, and *n_children*, the number of children.

Outputs: R, a list of ROC points.

```
1: pos_points ← (); neg_points ← ()
2: count[pos_class] ← 0; count[neg_class] ← 0
3: DESCEND(T, pos_class);
4: for pt ∈ pos_points do
5:    pt.x ← pt.x/count[neg_class]
6:    pt.y ← pt.y/count[pos_class]
7: end for
8: for pt ∈ neg_points do
9:    pt.x ← (count[neg_class] − pt.x)/count[neg_class]
10:   pt.y ← (count[pos_class] − pt.y)/count[pos_class]
11: end for
12: R ← pos_points ∪ neg_points ∪ (0, 0) ∪ (1, 1)
13: sort R increasing by x values
14: end
```

```
1: function DESCEND(node, pos_class)
2: if node is a leaf node then
3:    TP ← node.matched − node.errors
4:    FP ← node.errors
5:    count[node.class] ← count[node.class] + TP
6:    pt ← new point
7:    if node.class = pos_class then
8:       pt.x ← FP; pt.y ← TP
9:       push pt onto pos_points
10:   else
11:      pt.x ← TP; pt.y ← FP
12:      push pt onto neg_points
13:   end if
14: else                                   /* node is an internal node */
15:   for i = 1 to node.n_children do
16:      DESCEND(node.children[i], pos_class)
17:   end for
18: end if
19: end function
```