Partial AUC Maximization via 
Nonlinear Scoring Functions

Naonori Ueda  Akinori Fujino
NTT Communication Science Laboratories
2-4 Hikaradai, Seika-cho, “Keihanna Science City”, Kyoto 619-0237 Japan

Abstract

We propose a method for maximizing a partial area under a receiver operating characteristic
(ROC) curve (pAUC) for binary classification tasks. In binary classification tasks, accuracy
is the most commonly used as a measure of classifier performance. In some applications
such as anomaly detection and diagnostic testing, accuracy is not an appropriate measure
since prior probabilities are often greatly biased. Although in such cases the pAUC has been
utilized as a performance measure, few methods have been proposed for directly maximizing the
pAUC. This optimization is achieved by using a scoring function. The conventional approach
utilizes a linear function as the scoring function. In contrast we newly introduce nonlinear
scoring functions for this purpose. Specifically, we present two types of nonlinear scoring
functions based on generative models and deep neural networks. We show experimentally that
nonlinear scoring functions improve the conventional methods through the application of a
binary classification of real and bogus objects obtained with the Hyper Suprime-Cam on the
Subaru telescope.

1 Introduction

The binary classification task, in which the outcomes are labeled either positive or negative, is one
of the most basic problems in machine learning. Accuracy is the most commonly used performance
measure for the binary classifiers, and it is defined as the proportion of a given set of data that are
correctly classified by a classifier. In some applications such as anomaly detection and diagnostic
test, prior probabilities are often severely biased. Accuracy is not a suitable measure when there
is an imbalance between the numbers of positive and negative samples on training samples due to
the bias of the priors. Instead, we may want to evaluate classifiers not with a simple error measure
with the two types of errors, the false positive rate (FPR) and the false negative rate (FNR). The
former (latter) is also called a type I error (type II error). In anomaly detection, for example,
anomaly data is very rare compared with normal data and so usually pay more attention to FNR
than to FPR.

The area under the receiver operating characteristic (ROC) curve (AUC) can capture the
relationship between the two types of errors. The ROC curve is defined by the true positive
rate (TPR=1−FNR) and FPR as x and y axes, respectively, which depicts the relative trade-offs
between the true positive and the false positive when the classifier’s threshold is varied. For that
reason, AUC has been used as a performance measure for binary classifiers, especially under the
condition where the prior probabilities of two classes are biased. Several methods for learning a
binary classifier by directly maximizing AUC have already been reported [1][2][3].

Recently, however, the partial AUC (pAUC) has attracted more attention than the AUC because
it can focus on a suitable range of the false positive rate. For example, in sample imbalanced
applications where there are many fewer positive samples than negative samples, false positives
are intolerable. Therefore, we want to increase TPR while keeping FPR in a range from 0 to
a small value. In such a case, pAUC is more appropriate than AUC as a performance measure. However, few methods have yet been reported for directly maximizing pAUC [4] [5]. The pAUC is defined by using a scoring function, which maps an input sample to a score (a rank value), and so it is important to design better scoring function for maximizing pAUC. Previous studies [4] [5] proposed a linear function as a scoring function.

In this paper, we present two new types of nonlinear scoring functions based on generative models and deep neural networks. We show the effectiveness of the proposed methods through an application involving the binary classification of real and bogus objects obtained with the Hyper Suprime-Cam (HSC) [6] on the Subaru telescope.

2 Partial AUC

2.1 AUC

Let $X$ be a sample space. Let $D^+$ and $D^-$ be probability distributions on $X$. Let $S = (S^+, S^-)$ be a given training sample. Here, $S^+ = \{x^+_1, \ldots, x^+_n\}$ represents $n^+$ positive samples drawn iid according to $D^+$, and $S^- = \{x^-_1, \ldots, x^-_n\}$ represents $n^-$ negative samples drawn iid according to $D^-$. Let $f$ be a scoring function:

$$f : X \rightarrow \mathbb{R}. \quad (1)$$

We can obtain a binary classifier by using $f$ and a threshold $t \in \mathbb{R}$. That is, a sample $x$ is classified as positive (negative) when $f(x) > t$ ($f(x) < t$), assuming there is no tie. Therefore, if $f(x) > f(x')$, then $x$ should be classified as more positive than $x'$. The true positive rate is defined as the probability that the classifier correctly classifies a sample from $D^+$ as positive.

$$TPR_f(t) = P[f(x^+) > t]. \quad (2)$$

In a similar manner, the false positive rate is defined as the probability that the classifier misclassifies a sample from $D^-$ as positive.

$$FPR_f(t) = P[f(x^-) > t]. \quad (3)$$

The receiver operating characteristic curve (ROC curve) is then drawn by using the values of TPR as a function of FPR by changing the threshold $t$. Then the area under the curve (AUC) is formulated [8] as

$$AUC = P[f(x^+) > f(x^-)] = \int_0^1 TPR_f(FPR_f^{-1}(u))du. \quad (4)$$

Here,

$$FPR_f^{-1}(u) = \inf\{t \in \mathbb{R} | FPR_f(t) \leq u\}. \quad (5)$$

Given a sample set $S = (S^+, S^-)$, assuming there are no ties, the empirical AUC is given by

$$A\hat{U}C_f = \frac{1}{n^+ n^-} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} I(f(x^+_i) > f(x^-_j)). \quad (6)$$
2.2 Partial AUC

The partial AUC (pAUC) is different from AUC in the sense that the FPR range is limited when \( \alpha \leq \text{FPR}(t) \leq \beta \) \((0 \leq \alpha < \beta \leq 1)\). Therefore, when \( \beta \) is small, pAUC is maximized by increasing TPR while keeping small FPR. The pAUC is formulated as

\[
pAUC(\alpha, \beta) = \frac{1}{\beta - \alpha} \int_{\alpha}^{\beta} \text{TPR}_f(\text{FPR}_f^{-1}(u)) du.
\] (7)

Similarly to AUC, given \( S = (S^+, S^-) \), the empirical partial AUC of \( f \) in the FPR range \((\alpha, \beta)\) can be estimated as [4][5]

\[
\hat{pAUC}_f = \frac{1}{n^+ n^- (\beta - \alpha)} \sum_{i=1}^{n^+} [(j_\alpha - an^-) I(f(x_{i,1}^+) > f(x_{i,1}^-)) + \sum_{j=j_\alpha+1}^{j_\beta} I(f(x_{i,j}^+) > f(x_{i,j}^-))]
+ (\beta n^- - j_\beta) I(f(x_{i,j}^+) > f(x_{i,j+1}^-)),
\] (8)

where \( j_\alpha = \lfloor an^- \rfloor, j_\beta = \lfloor \beta n^- \rfloor \), and \( x_{i,j}^- \) denotes the negative instance ranked in \( j \)th position among \( S^- \) in descending order of scores by \( f \). \([a]\) is the smallest integer greater than or equal to \( a \), and \([a]\) is the largest integer less than or equal to \( a \). \( I(z) \) is a Heaviside step function where \( I(z) = 1 \) if \( z \) is true, \( I(z) = 0 \) otherwise. The derivation of Eq. (8) is detailed in [4][5]. Therefore, the remaining problem is to develop a better scoring function so that Eq. (8) can be larger.

3 Scoring Functions

In this section, we discuss the scoring function which plays an important role in maximizing the pAUC. The scoring function is modeled with a set of parameters \( \theta \) and is therefore denoted by \( f(x; \theta) \). Ideally, the scoring function should satisfy

\[
f(x_+; \theta) > f(x_-; \theta)
\] (9)

for any \( x_+ \sim D^+ \) and \( x_- \sim D^- \). This enables us to maximize the empirical pAUC given by Eq. (8) with respect to \( \theta \). However, such ideal scoring function is difficult to construct, and therefore in practice we try to find a better scoring function that provides the largest possible empirical pAUC. Note that since the Heaviside function in Eq. (8) is undifferentiable, it is often approximated by using a logistic sigmoid function [7],

\[
s(x_+, x_-; \theta) = \frac{1}{1 + \exp[-\{f(x_+; \theta) - f(x_-; \theta)\}]}. \] (10)

Here \( f(x; \theta) \) is also assumed to be differentiable w.r.t. \( \theta \). When the logistic sigmoid function is used, Eq. (8) is replaced by

\[
\hat{pAUC}(\theta) = \frac{1}{n^+ n^- (\beta - \alpha)} \sum_{i=1}^{n^+} [(j_\alpha - an^-) s(x_{i,j_\alpha}^+, x_{i,j_\alpha}^-; \theta) + \sum_{j=j_\alpha+1}^{j_\beta} s(x_{i,j}^+, x_{i,j}^-; \theta)]
+ (\beta n^- - j_\beta) s(x_{i,j}^+, x_{i,j+1}^-; \theta)].
\] (11)

So, all that remains is to specify the scoring function \( f \).
3.1 Linear scoring function

A linear scoring function has been presented in previous studies [4][5];

\[ f(x; \theta) = \theta^T x. \] (12)

Here \( \theta^T \) denotes a transpose of a vector \( \theta \). Although the linear function is easy to optimize, it is clear that a nonlinear function is more flexible than the linear function and therefore the former is much more effective than the latter in the sense of Eq. (9).

3.2 Nonlinear scoring function

Deep Neural Networks

In recent years, deep neural networks (DNNs) have been widely utilized in various fields. The most straightforward way is to construct a DNN as the nonlinear scoring function \( f \). In this setting, the parameter \( \theta \) of a DNN is trained so as to maximize the objective given by Eq. (11). In other words, as shown in the experiment, when training a set of parameters of a DNN by using \( S \), we simply set the objective function as Eq. (11).

Probabilistic Generative Models

In another approach, which we newly present in this paper, we employ generative models. In the machine learning literature, many researchers have developed and utilized probabilistic generative models in various applications. For example, the Gaussian mixture model has been utilized for real-valued data. A mixture of multinominals has been utilized for count data such as bag-of-words for text data. Therefore, it is reasonable that the probabilistic generative model will be suitable for a given application namely designing a scoring function. This motivated us to consider a scoring function based on the probabilistic generative models.

Let \( p(x; \theta^+) \) (\( p(x; \theta^-) \)) be the probability distribution of positive (negative) samples\(^1\). Here, \( \theta^+ (\theta^-) \) is the parameter of a probabilistic generative model for positive (negative) samples. Then, we consider the following ratio of the probability distribution of positive and negative samples;

\[ r(x; \theta) = \frac{p(x; \theta^+)}{p(x; \theta^-)}, \] (13)

where \( \theta = (\theta^+, \theta^-) \). Moreover, let \( P(\omega^+) \) (\( P(\omega^-) \)) denote the class prior of positive (negative) samples. Then the ratio can be rewritten with the Bayes rule as

\[
\begin{align*}
\log r(x; \theta) &= \log \frac{p(x; \theta^+)}{p(x; \theta^-)} \\
&= \log \frac{P(\omega^+) p(x; \theta^+)}{P(\omega^-) p(x; \theta^-)} - \log \frac{P(\omega^-) p(x; \theta^-)}{P(\omega^+) p(x; \theta^+)} + \text{const}.
\end{align*}
\] (15)

Here, the last term of Eq. (15) is a constant independent of \( x \).

If \( x \) is a positive class sample, then \( \log P(\omega^+|x, \theta^+) > \log P(\omega^-|x, \theta^-) \) should hold. Likewise, if \( x \) is a negative class sample, then \( \log P(\omega^-|x, \theta^-) < \log P(\omega^-|x, \theta^-) \) should hold. This means\(^1\)

\(^1\)Note that if \( x \) is continuous (discrete), \( p \) is a probability density (mass) function.
that the ratio given by Eq. (15) is appropriate as a scoring function. Therefore, we define the scoring function as

\[ f(x; \theta) = \log \frac{p(x; \theta^+)}{p(x; \theta^-)} \]  

(16)

Using Eq. (16), we can employ various kinds of generative models, depending on application. Typically, a mixture of Gaussian model is useful for continuous data, while a mixture multinomial model is useful for discrete data. In a conventional generative model approach to classification tasks, each positive and negative model is independently trained by using positive or negative samples. In contrast, the parameters of positive and negative models are simultaneously optimized so that Eq. (11) is maximized. Moreover, in a related matter, in the context of statistical hypothesis testing, the Neyman-Pearson lemma states that the likelihood ratio test, in which the likelihood ratio of the two classes is used as the test statistic, is optimal in the sense that it is the most powerful \[9\].

4 Experiments

4.1 Test Collection

We used the Hyper Suprime-Cam (HSC) dataset reported in \[6\] for an empirical evaluation of our proposed method. The HSC dataset includes the image data of 487 real and 267074 bogus optical transient objects collected with the HSC using the Subaru telescope. The image data are represented by using thirteen features as shown in \[10\], and each image is assigned with either real (positive class) or bogus (negative class) labels.

We examined the performance of the proposed method in an imbalanced binary classification task whose aim was to predict the true label of each image from the feature vectors of the image. In our experiments, we used 70 percent of the image data to train classifiers designed with the proposed method and the remaining 30 percent to test classifier performance. We formed five different evaluation sets by randomly dividing the image data into training and test data.

4.2 Experimental Setting

We compared the performance of the proposed method with that of conventional methods, namely DNN-CE, GMM, SVM-pAUC, SVM-AUC, SVM, and RF.

The DNN-CE classifier is a neural network classifier constructed by using TensorFlow\(^2\), where a cross-entropy objective function is employed to train the neural networks. The number of hidden layers was selected from candidate values of \(\{1, 2, 3, 4\}\), and the unit number of each layer was selected from candidate values of \(\{50n|1 \leq n \leq 20, n \in I\}\). We used either “tanh” or “selu” activation functions, and tuned the weight of L1-regularizer between \(10^{-3}\) and 10. The dropout ratio was selected from candidate values of \(\{0, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8\}\).

The GMM classifier is a generative classifier based on Gaussian mixture models (GMMs) designed for each class. We trained the classifier by the maximum likelihood estimation of the GMM parameters. The number of Gaussian models used for each class was selected from candidate values of \(\{n|1 \leq n \leq 19, n \in I\}\).

The SVM-pAUC classifier was trained by using SVM\(_{pAUC\text{-tight}}\)^3, which is a pAUC-optimized SVM implementation introduced in \[4\][5]. We examined the performance of SVM-pAUC classifiers.

\(^2\)https://www.tensorflow.org/

\(^3\)http://clweb.csa.iisc.ernet.in/harikrishna/Papers/SVMpAUC-tight/
whose $\beta$ values were set at 0.01, 0.05, and 0.1. We also examined the performance of an SVM-AUC classifier trained to maximize the AUC performance for training data. The SVM-AUC classifiers were obtained by setting $\beta = 1$ in the objective function of the SVM-pAUC classifier. Moreover, we examined the performance of an SVM classifier trained by using `sklearn.svm.SVC`\(^4\). For the SVM-pAUC, SVM-AUC, and SVM classifiers, we used a linear kernel and tuned their cost parameter values $C$ between $10^{-3}$ and $10^3$. The RF classifier is a random forest classifier constructed by using `sklearn.ensemble.RandomForestClassifier`\(^5\).

We set 100 for the `n_estimators` option, either “gini” or “entropy” for the `criterion` option, an integer between 1 to 13 for the `max_features` option. We used our proposed method to train the scoring functions of binary classifiers designed with a neural network (DNN) and a Gaussian mixture model (GMM). In this paper, we call the DNN-based classifier DNN-pAUC and the GMM-based classifier GMM-pAUC. By using the Adam optimizer included in `TensorFlow`, we estimated the parameter values of the DNN-based and GMM-based scoring functions that maximize the objective function shown in Eq. (8). The hyperparameter values of the neural network used for the DNN-pAUC classifier were selected from the same candidate values as for the DNN-CE classifier. The number of Gaussian models for the GMM-pAUC classifier was selected from the same candidate values as for the GMM classifier. We set $\alpha = 0$ for both the DNN-pAUC and GMM-pAUC classifiers. We examined the performance of the DNN-pAUC and GMM-pAUC classifiers whose $\beta$ values were set at 0.01, 0.05, and 0.1. We also examined the performance of the DNN-based and GMM-based classifiers, called DNN-AUC and GMM-AUC, respectively, that were trained to maximize the AUC performance for training data. The DNN-AUC and GMM-AUC classifiers were obtained by setting $\beta = 1$ in the objective functions of the DNN-pAUC and GMM-pAUC classifiers, respectively.

We tuned the hyperparameter values of the classifiers with a five-fold cross-validation of the training data. We selected the best combination of hyperparameter values from all the candidate values for the GMM-pAUC, GMM-AUC, GMM, and RF classifiers with a grid search. We tuned the hyperparameter values of the DNN-pAUC, DNN-AUC, DNN-CE, SVM-pAUC, SVM-AUC, and SVM classifiers with a tree-structured Parzen estimator, `hyperopt`\(^6\), which is a Bayesian optimization method.

### 4.3 Results

Table 1 shows the average pAUC values at three fixed FPR values, 0.01, 0.05, and 0.1, over the five evaluation sets obtained with the proposed and compared classifiers. Each number in parentheses in the table denotes the standard deviation of the pAUC values. Table 2 shows the average TPR values at the three fixed FPR values over the five evaluation sets obtained with the proposed and compared classifiers. Each number in parentheses in the table denotes the standard deviation of the TPR values.

As shown in Table 1, the GMM-pAUC classifiers trained with $\beta = 0.05$ and 0.1 provided better average pAUC values than the GMM-AUC classifier. The DNN-pAUC classifiers trained with $\beta = 0.05$ and 0.1 also provided better average pAUC values than the DNN-AUC classifier. These results show that training the GMM- and DNN-based scoring functions with the proposed method was effective in improving their pAUC performance.

The performance of the GMM-pAUC classifier trained with $\beta = 0.01$ was worse than that when $\beta = 0.05$ and 0.1. The performance of the DNN-pAUC classifier trained with $\beta = 0.01$ was also worse than that with $\beta = 0.05$ and 0.1. When the $\beta$ value is small, the number of negative

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\(^4\)http://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.htm

\(^5\)http://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

\(^6\)http://hyperopt.github.io/hyperopt/
### Table 1: Average pAUC value (%)

| Method               | $FPR = 0.01$ | $FPR = 0.05$ | $FPR = 0.1$ |
|----------------------|--------------|--------------|-------------|
| GMM-pAUC ($\beta = 0.01$) | 31.4 (2.7)   | 63.5 (5.1)   | 76.0 (3.9)  |
| GMM-pAUC ($\beta = 0.05$) | 31.6 (0.8)   | 67.8 (1.6)   | 79.9 (1.7)  |
| GMM-pAUC ($\beta = 0.1$)  | 31.7 (2.0)   | 67.1 (2.7)   | 79.8 (2.3)  |
| DNN-pAUC ($\beta = 0.01$) | 16.1 (5.3)   | 43.9 (10.0)  | 60.4 (10.4) |
| DNN-pAUC ($\beta = 0.05$) | 25.1 (5.3)   | 57.6 (9.1)   | 71.4 (7.8)  |
| DNN-pAUC ($\beta = 0.1$)  | 24.0 (2.8)   | 57.9 (2.9)   | 73.0 (2.5)  |
| SVM-pAUC ($\beta = 0.01$) | 12.4 (6.5)   | 40.6 (10.1)  | 55.9 (8.8)  |
| SVM-pAUC ($\beta = 0.05$) | 13.8 (4.6)   | 45.2 (6.0)   | 60.9 (4.9)  |
| SVM-pAUC ($\beta = 0.1$)  | 18.9 (1.5)   | 48.9 (2.8)   | 63.6 (2.3)  |
| GMM-AUC               | 29.3 (6.6)   | 66.3 (3.5)   | 79.6 (1.5)  |
| DNN-AUC               | 23.0 (4.1)   | 56.9 (2.3)   | 72.1 (1.7)  |
| SVM-AUC               | 16.0 (2.1)   | 42.9 (3.5)   | 58.0 (2.7)  |
| GMM                   | 22.6 (1.5)   | 61.5 (2.3)   | 75.5 (1.7)  |
| DNN-CE                | 13.9 (7.7)   | 38.6 (15.7)  | 53.4 (17.2) |
| SVM                   | 4.4 (3.7)    | 17.9 (8.9)   | 30.4 (13.2) |
| RF                    | 27.5 (2.7)   | 56.4 (4.0)   | 67.3 (4.6)  |

### Table 2: Average TPR values (%)

| Method               | $FPR = 0.01$ | $FPR = 0.05$ | $FPR = 0.1$ |
|----------------------|--------------|--------------|-------------|
| GMM-pAUC ($\beta = 0.01$) | 47.4 (3.4)   | 83.6 (4.6)   | 91.8 (2.8)  |
| GMM-pAUC ($\beta = 0.05$) | 49.7 (1.0)   | 88.4 (2.6)   | 94.0 (2.9)  |
| GMM-pAUC ($\beta = 0.1$)  | 50.5 (2.5)   | 88.1 (3.0)   | 94.7 (1.8)  |
| DNN-pAUC ($\beta = 0.01$) | 29.0 (9.3)   | 66.8 (14.2)  | 84.7 (9.0)  |
| DNN-pAUC ($\beta = 0.05$) | 43.2 (8.1)   | 79.3 (9.0)   | 88.9 (4.8)  |
| DNN-pAUC ($\beta = 0.1$)  | 41.9 (4.4)   | 81.6 (2.5)   | 92.3 (3.0)  |
| SVM-pAUC ($\beta = 0.01$) | 23.7 (10.2)  | 62.7 (10.5)  | 78.8 (5.1)  |
| SVM-pAUC ($\beta = 0.05$) | 27.1 (8.1)   | 68.2 (5.1)   | 83.6 (3.6)  |
| SVM-pAUC ($\beta = 0.1$)  | 33.8 (2.8)   | 69.2 (2.1)   | 85.5 (1.9)  |
| GMM-AUC               | 47.1 (7.0)   | 89.0 (1.4)   | 95.1 (1.9)  |
| DNN-AUC               | 41.9 (4.7)   | 80.3 (1.2)   | 92.2 (1.6)  |
| SVM-AUC               | 28.5 (4.3)   | 63.3 (3.8)   | 79.9 (1.6)  |
| GMM                   | 41.4 (3.1)   | 85.1 (2.8)   | 93.2 (1.4)  |
| DNN-CE                | 24.5 (13.2)  | 58.8 (20.0)  | 75.5 (18.5) |
| SVM                   | 8.6 (6.5)    | 32.6 (15.6)  | 54.1 (17.0) |
| RF                    | 44.4 (5.6)   | 70.3 (4.5)   | 82.6 (5.5)  |
training samples used to estimate the parameter values of the GMM-pAUC and DNN-pAUC classifiers is small. Setting too small a $\beta$ value may overfit the classifiers into a small number of negative training samples.

The GMM-pAUC and DNN-pAUC classifiers outperformed the SVM-pAUC classifier as shown in Tables 1 and 2. The GMM-pAUC and DNN-pAUC classifiers were designed with non-linear scoring functions, while a linear kernel was employed for the SVM-pAUC classifier. These experimental results show that optimizing the non-linear scoring functions with the proposed method is effective in obtaining better classifiers for the image classification of real and bogus optical transient objects.

The GMM-pAUC classifier outperformed the DNN-pAUC classifier, although neural networks often provide better classifiers. The GMM classifier provided similar or better performance than the DNN- and SVM-based classifiers. We assume that the distribution of image data used in our experiments was better fitted to a GMM-based scoring function, and thus the GMM-pAUC classifier provided better performance.

5 Conclusion

We have proposed a pAUC maximization method based on nonlinear scoring functions for binary classification tasks. Specifically, we have presented two types of scoring functions; a deep neural network based scoring function and a probabilistic generative model based scoring function. Through the application of the binary classification of real and bogus objects obtained with the Hyper Suprime-Cam on the Subaru telescope, we have experimentally confirmed that nonlinear scoring functions outperform the conventional linear scoring function for pAUC maximization. It is worth mentioning that the results of the probabilistic generative model based scoring function, which is proposed in this paper, were better than those of a deep neural network.

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