Area under ROC curve – review and efficient computation in R

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Abstract The AUC (Area Under the Curve) measure is widely used in statistical classification and machine learning, including credit scoring, where it is employed to assess the quality of predictive models. The goal of this paper is to review methods for calculating the AUC measure, followed by an analysis of the efficiency of computing this measure in R.

1 Introduction

Assessing the quality of predictive models is a critical stage in machine learning and statistical inference processes. Among the many available metrics, the Area Under the Receiver Operating Characteristic curve (AUC) has established itself as a standard measure of discrimination, particularly in binary classification problems. The popularity of this metric stems from its independence from the chosen cut-off point and its robustness to class imbalance, making it useful in diverse fields such as medical diagnostics, psychology, and credit risk assessment.

Modern statistical applications require not only methodological correctness but also high computational efficiency. In the era of Big Data and increasing complexity of validation procedures, a single calculation of the AUC is often insufficient. Similar challenges are posed by simulation market models in banking, where generating ROC curves without historical data serves to estimate the impact of scoring models on portfolio profitability. In such scenarios, classical algorithm implementations can become a computational bottleneck, rendering procedures like the bootstrap impractical.

The goal of this paper is to review methods for calculating the AUC measure and to analyze the efficiency of available implementations within the R environment. In the first part of the work, we organize definitions and highlight the mathematical links between AUC and other measures, such as the Gini coefficient. Next, we discuss the main classes of algorithms used for AUC estimation: trapezoidal integration, optimized pairwise comparisons, and rank-based approaches. Finally, we present the results of performance benchmarks for popular R packages and propose our alternatives, identifying optimal solutions for different sizes of large datasets.

2 ROC curve

The ROC curve is one of the most important tools for assessing the effectiveness of binary classifiers. It was introduced in the 1940s in the context of radar signal analysis, which is the origin of its name – *Receiver Operating Characteristic* (Junge and Dettori, 2018). Today, the ROC curve is used in fields such as medicine, biotechnology, computer science, and banking, where it is used to evaluate scoring models.

Definition

The ROC curve is a graph created by "plotting the qualitative characteristics of binary classifiers generated from a model using many different cut-off points" (Gromada, 2016), illustrating the model's predictive effectiveness. Each point on the curve corresponds to TPR (sensitivity) and FPR (1 – specificity) values as a function of the classifier's varying cut-off point (Fawcett, 2006).

Construction of the ROC Curve

To construct an ROC curve, the threshold that determines whether the classifier assigns an observation to the positive class is modified. For each threshold, TPR and FPR are calculated. The results are presented on a graph where the X-axis represents FPR and the Y-axis represents TPR.

Point (0,1) represents an ideal classifier: no false positives and full detection of positive cases. A curve closer to this point is more desirable (Hanley and McNeil, 1982) – this is equivalent to a larger Area Under the Curve, or AUC. The diagonal line from (0,0) to (1,1) represents a random classifier (AUC = 0.5).

3 AUC – alternative names and related measures

The Area Under the Receiver Operating Characteristic (ROC) curve, commonly abbreviated as AUC, is a fundamental metric for evaluating the performance of classification models. However, due to its

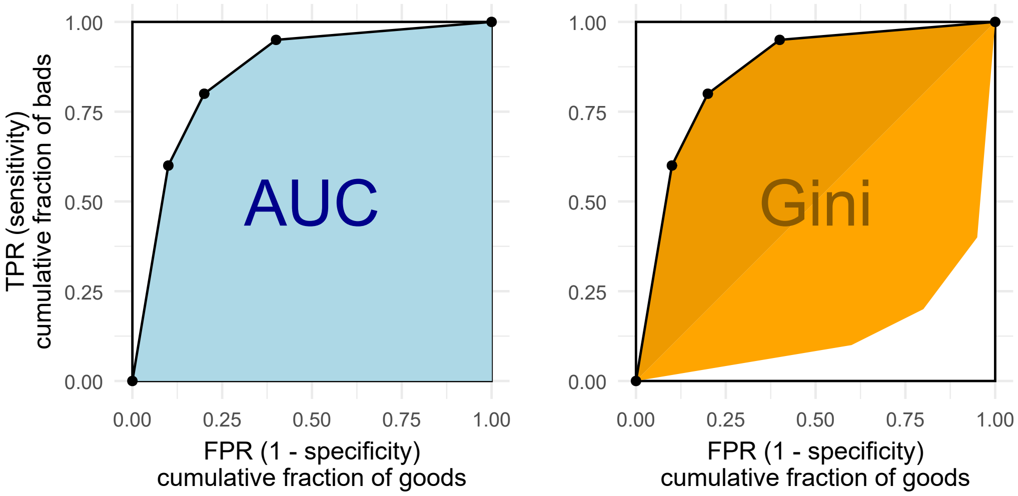


Figure 1: Geometric interpretation: AUC (AUROC) is the area under the ROC curve, Gini is twice the area between the diagonal y=x and the ROC curve.

independent adoption and development across diverse fields, ranging from biomedical statistics and psychology to econometrics and credit scoring, this measure appears in the literature under numerous aliases and mathematical formulations. Recognizing these equivalences is essential for researchers to leverage efficient computational algorithms developed in different domains.

Alternative names and interpretations of AUC

In medical statistics and epidemiology, particularly when evaluating logistic regression models with binary outcomes, the AUC is frequently referred to as the *c-statistic* (or concordance statistic). This term defined by Harrell et al. (Harrell et al., 1982) and further elaborated by, for example Austin and Steyerberg (Austin and Steyerberg, 2012), represents the probability of concordance between predicted probabilities and observed outcomes. It quantifies the predictive accuracy of a model by estimating the probability that a randomly selected subject who experienced the outcome has a higher predicted probability than a randomly selected subject who did not.

This probabilistic interpretation serves as the bridge to non-parametric statistics. Area under the ROC curve is statistically equivalent to the Mann-Whitney U statistic divided by the product of the sample sizes of the two groups, where in this context, the metric is often interpreted as the *probability of superiority* indicating the likelihood that a randomly chosen positive case ranks higher than a randomly chosen negative case (Hanley and McNeil, 1982).

In the behavioral sciences and psychology, similar concepts have been developed to measure effect sizes. There the AUC corresponds to the *Common Language Effect Size* (CL/CLES) (McGraw and Wong, 1992), which converts an effect size into a probability, specifically defined as the probability that a score sampled at random from one distribution will be greater than a score sampled from another. This metric was developed to provide an index of effect size that is intuitively interpretable by audiences without statistical training. While the original formulation by McGraw and Wong focused on normal distributions, the later proposed *measure of stochastic superiority* (denoted as A) (Vargha and Delaney, 2000) generalized CLES concept so that it could be applicable to any variable that is at least ordinally scaled, regardless of the distribution form, and is identical to the CL statistic in the continuous case. Furthermore, in the context of non-parametric analysis for longitudinal data the *relative treatment effect* was defined (Brunner et al., 2002). This metric estimates the probability that an observation from one group is smaller than an observation from another, effectively serving as a probabilistic analog to the AUC (Brunner et al., 2002), (Engelmann et al., 2003).

The Gini coefficient and other AUC related measures

While the AUC scales from 0.5 (random classification) to 1.0 (perfect classification), many disciplines prefer a measure scaled between 0 and 1 (or -1 and 1) to represent the strength of association or discriminatory power. This leads to the Gini coefficient (or Gini index). The Gini coefficient used in classification contexts is simply a linear transformation of the AUC, defined by the relationship (Hand and Till, 2001):

$$\text{Gini} = 2 \cdot \text{AUC} - 1$$

Cliff [1993] discusses an ordinal statistic, d, which compares the number of times a score from one group is higher than one from another versus the reverse. This statistic of ordinal dominance, later named *Cliff's Delta* (Bais and Van Der Neut, 2022) was described as a non-parametric effect size based on data observations, which quantifies the difference between the probability that a value from one group is higher than a value from the other and the reverse probability.

Relation to the U statistic in the Mann-Whitney

There is a direct relationship between AUC and the Mann-Whitney U statistic.

AUC is equivalent to the probability that a randomly selected positive case will have a higher score than a randomly selected negative case (Hanley and McNeil, 1982; Bamber, 1975).

$$\text{AUC} = \frac{U}{n_1 \times n_0}$$

where U is the number of pairs in which the “bad” score is < the “good” score, n_1 is the number of “bad” scores, and n_0 is the number of “good” scores.

This relationship provides the statistical basis for treating AUC as a measure of discrimination and allows confidence intervals to be constructed using Mann-Whitney statistics theory (Hanley and McNeil, 1982).

Relation to the Somers' D

Somers' D coefficient is a measure of association between ordinal variables, which also shows a direct relationship with AUC. It can be considered a generalization of AUC for ordinal variables (Newson, 2002).

Somers' D is defined based on concordant and discordant pairs. A pair of observations (i,j) is concordant if the ranking of the independent variable X and the ranking of the dependent variable Y are in the same order, i.e., if $(X_i - X_j)$ and $(Y_i - Y_j)$ have the same sign. A pair is discordant if the signs are opposite. Somers' D is calculated as the difference between the number of concordant and discordant pairs, divided by the number of unrelated pairs on the independent variable X (Somers, 1962).

In binary classification:

$$\text{Somers' D} = 2 \cdot \text{AUC} - 1$$

which links it directly to AUC (Newson, 2002).

Cumulative accuracy profile

The CAP curve is a graphical tool used to evaluate the performance of classification models, primarily in the area of creditworthiness assessment. It shows the cumulative percentage of positive cases relative to the cumulative percentage of the entire population, sorted by predicted probability of default (Engelmann et al., 2003).

Accuracy Ratio (AR):

$$\text{AR} = \frac{A}{B}$$

where A is the area between the model CAP and the random CAP, and B is the area between the ideal CAP and the random CAP. Areas A and B are calculated using the trapezoidal method (Engelmann et al., 2003).

Within the credit scoring literature, the AR metric is sometimes referred to as the *pseudo Gini* index to differentiate it from the classical Gini index used in economics to measure inequality. It was established that the pseudo Gini index is based on the concentration curve (CAP) and that its value is always equal to the Accuracy Ratio (referred to as Accuracy Rate) for any scoring model (Idczak, 2019).

The relationship between AUC and the CAP curve can be described by the following formula (Engelmann et al., 2003):

$$\text{AUC} = \frac{\text{AR} + 1}{2}$$

4 The need for computational efficiency in AUC estimation

In the context of modern statistical modeling and machine learning, a single calculation of the AUC metric is often insufficient for a comprehensive assessment of model quality. Complex validation, optimization, and simulation procedures require the AUC statistic to be computed repeatedly, imposing high demands on the computational efficiency of the underlying algorithms. The following sections outline key areas where the performance of AUC estimation is critical.

Uncertainty estimation and permutation tests

The estimation of confidence intervals and the verification of statistical hypotheses for the AUC often rely on resampling methods, such as bootstrapping or permutation tests. While necessary when simple parametric assumptions cannot be met, these methods generate significant computational loads.

In the case of massive datasets, the process of generating a single performance estimate can be computationally expensive (LeDell et al., 2015). The authors point out that when using complex prediction methods, even with relatively small datasets, cross-validation can consume a large amount of time, making the bootstrap a computationally intractable approach to variance estimation in many practical settings.

Similarly, in the context of meta-analysis of diagnostic accuracy studies, there are instances of bootstrap algorithms usage to determine confidence intervals for the AUC of the Summary ROC (SROC) curve (Noma et al., 2021). Their approach involves computing AUC estimates from a large number of bootstrap samples (e.g., $B = 1000$), which necessitates efficient calculation routines.

Permutation-based inference also demands repeated calculation. Bandos, Rockette, and Gur (2006) developed a permutation test for comparing ROC curves in multireader studies. An exact permutation test in this setting is formed by determining the frequency of the statistic—estimating the average difference in AUCs across all possible exchanges of reader ratings. For larger samples, this requires an asymptotic approach due to the computational intensity of calculating differences for every permutation (Bandos et al., 2006). Furthermore, Pauly, Asendorf, and Konietschke (2016) proposed rank-based studentized permutation methods for the nonparametric Behrens-Fisher problem, which corresponds to inference for the AUC. They demonstrated that the studentized permutation distribution ofthe Brunner-Munzel rank statistic is asymptotically standard normal, providing a theoretical foundation for consistent confidence intervals and tests, which rely on these intensive permutation procedures (Pauly et al., 2016).

Variable importance measures

Efficient AUC computation is a prerequisite for specific Variable Importance Measures (VIM). Therefore an AUC-based permutation variable importance measure for Random Forests was introduced, designed to be more robust to unbalanced classes than standard error-rate-based measures. This procedure requires the AUC to be computed for each tree in the forest, both before and after permuting the values of a given predictor. Given the number of trees in a forest and the number of predictors, this approach results in a vast number of AUC calculations, far exceeding the computational cost of standard single-pass metrics (Janitza et al., 2013).

Beyond model-specific methods, model-agnostic interpretability frameworks also rely heavily on repeated metric estimation. The DALEX package (Biecek, 2018) implements a permutation-based variable importance method applicable to any predictive model. This approach measures the change in model performance, such as the drop in AUC (represented as the loss function $L(y, \hat{y}) = 1 - AUC$), after permuting the values of a single predictor. To ensure stability of the importance estimates, this permutation process is typically repeated B times (e.g., $B = 10$) for every feature in the dataset. Consequently, for a model with p features, assessing global feature importance requires $p \times B$ independent AUC calculations, creating a linear dependency between the number of features and the computational cost.

AUC maximization algorithms

In the era of Big Data, learning algorithms that directly maximize AUC, rather than accuracy, are gaining importance but algorithms maximizing model accuracy do not necessarily maximize the AUC score. However, direct AUC maximization presents a computational challenge because the function is non-decomposable over individual examples. This has led to the development of stochastic AUC maximization methods for big data and "Deep AUC Maximization" (DAM) for deep learning, where optimization must be performed efficiently on large-scale datasets (Yang and Ying, 2023).

Simulation and curve modeling in credit risk

In credit risk management, theoretical ROC curve models are employed to simulate and assess the impact of scoring models when actual data is unavailable or limited. Kochański (2022) notes that fitting models such as the binormal or bigamma curves is helpful for "generating ROC curves without underlying data". This capability is essential for assessing the impact of a credit scorecard that is "yet to be built" (Kochański, 2022). Such simulation analyses often involve generating numerous curves and estimating their parameters to forecast portfolio quality, further justifying the need for computationally efficient AUC estimation methods.

Beyond single-curve fitting, Kochański (2021) extends the analysis to a dynamic market environment, proposing a simulation model for risk and pricing competition. This framework explores how the discrimination power of credit scoring models influences key business metrics, illustrating the "trade-off between profitability, market share, and credit loss rates" (Kochański, 2021). The study demonstrates that even marginal improvements in discrimination power can yield substantial benefits, a conclusion derived from simulation scenarios that model the interactions between lenders and borrowers. Such comprehensive market analyses require processing numerous scenarios to identify profit-maximizing strategies, further highlighting the role of performance metrics as fundamental parameters in complex economic models.

5 R packages

Table 1: Functions computing AUC.

Package	Function	Usage	Method	Language
bigstatsr	AUC	`AUC(-pred, target)`	Pairwise comparison (optimized)	C++, R
caTools	colAUC	`colAUC(-pred, target)[1, 1]`	Rank sum	R
cvAUC	AUC	`AUC(-pred, target)`	Trapezoidal rule	R
DescTools	Cstat	`Cstat(-pred, target)`	Pairwise comparison (optimized)	C++, R
effsize	VD.A	`VD.A(pred ~ factor(target))$estimate`	Rank sum	R
fbroc	boot.roc	`boot.roc(-pred, as.logical(target))$auc`	Trapezoidal rule	C++, R
Hmisc	somers2	`somers2(-pred, target)["C"]`	Rank sum	R
MLmetrics	AUC	`AUC(-pred, target)`	Rank sum	R
mltools	auc_roc	`auc_roc(-pred, target)`	Trapezoidal rule	R
ModelMetrics	auc	`auc(target, -pred)`	Rank sum	C++, R
precrec	evalmod	`evalmod(mmdata(scores = -pred, labels = target), mode="aucroc")$uaucs$aucs`	Rank sum	C++, R
pROC	auc	`auc(target, pred, lev=c('0', '1'), dir=">")`	Trapezoidal rule	R
rcompanion	vda	`vda(x = pred[target == 0], y = pred[target == 1], digits=100)`	Rank sum	R
ROCR	performance	`performance(prediction(-pred, target), "auc")@y.values[[1]]`	Trapezoidal rule	R
scikit-learn	roc_auc_score	`import("sklearn.metrics")$roc_auc_score(target, -pred)`	Trapezoidal rule	Python, C
scorecard	perf_eva	`perf_eva(-pred, target, binomial_metric = "auc", show_plot=FALSE)$binomial_metric$dat$AUC`	Trapezoidal rule	R
yardstick	roc_auc_vec	`roc_auc_vec(as.factor(target), pred)`	Trapezoidal rule	R
DescTools	SomersDelta	`SomersDelta(-pred, target)/2 + 1/2`	Pairwise comparison (unoptimized)	C++, R

We identified three main types of algorithms for AUC computation: (1) trapezoidal integration over the ROC Curve, (2) (optimized) pairwise comparison, (3) and rank-based (Mann–Whitney U statistic formulation).

Let (s_i, y_i) for $i = 1, \dots, n$ denote the score assigned to an account and its corresponding true label. In line with standard practice in credit scoring, we assume that $y_i = 1$ indicates a "bad" account (e.g., one that defaults, doesn't repay the loan), while $y_i = 0$ represents a good account. A properly functioning scoring should assign lower scores to accounts with a higher predicted probability of being bad, and higher scores to those likely to be good.

Let $n_1 = \sum_{i=1}^{n} \mathbb{I}(y_i = 1)$ denote the number of bad accounts, and $n_0 = \sum_{i=1}^{n} \mathbb{I}(y_i = 0)$ – number of good accounts.

Trapezoidal integration over the ROC curve

$$\text{AUC} = \sum_{k=1}^{m-1} (\text{FPR}_{k+1} - \text{FPR}_k) \cdot \frac{\text{TPR}_{k+1} + \text{TPR}_k}{2}$$

where m is the number of distinct score thresholds from lowest to the highest score, TPR_k is the True Positive Rate, FPR_k is the False Positive Rate. $TPR_k = TP_k / n_1$ and $FPR_k = FP_k / n_0$, where TP_k is the number of true positives, FP_k is the number of false positives, n_1 is the number of positive cases, n_0 is the number of negative cases.

Optimized pairwise comparison

AUC as the probability that a randomly chosen positive instance receives a higher score than a randomly chosen negative instance:

$$\text{AUC} = \frac{1}{n_1 n_0} \sum_{i:y_i=1} \sum_{j:y_j=0} \left[\mathbb{I}(s_i < s_j) + \frac{1}{2} \mathbb{I}(s_i = s_j) \right]$$

Rank-based (Mann–Whitney U statistic formulation)

$$\text{AUC} = \frac{\bar{R}_1 - n_1(n_1+1)/2}{n_0}$$

where $\bar{R}_1$ is the mean rank for s_i where $y_i = 1$:

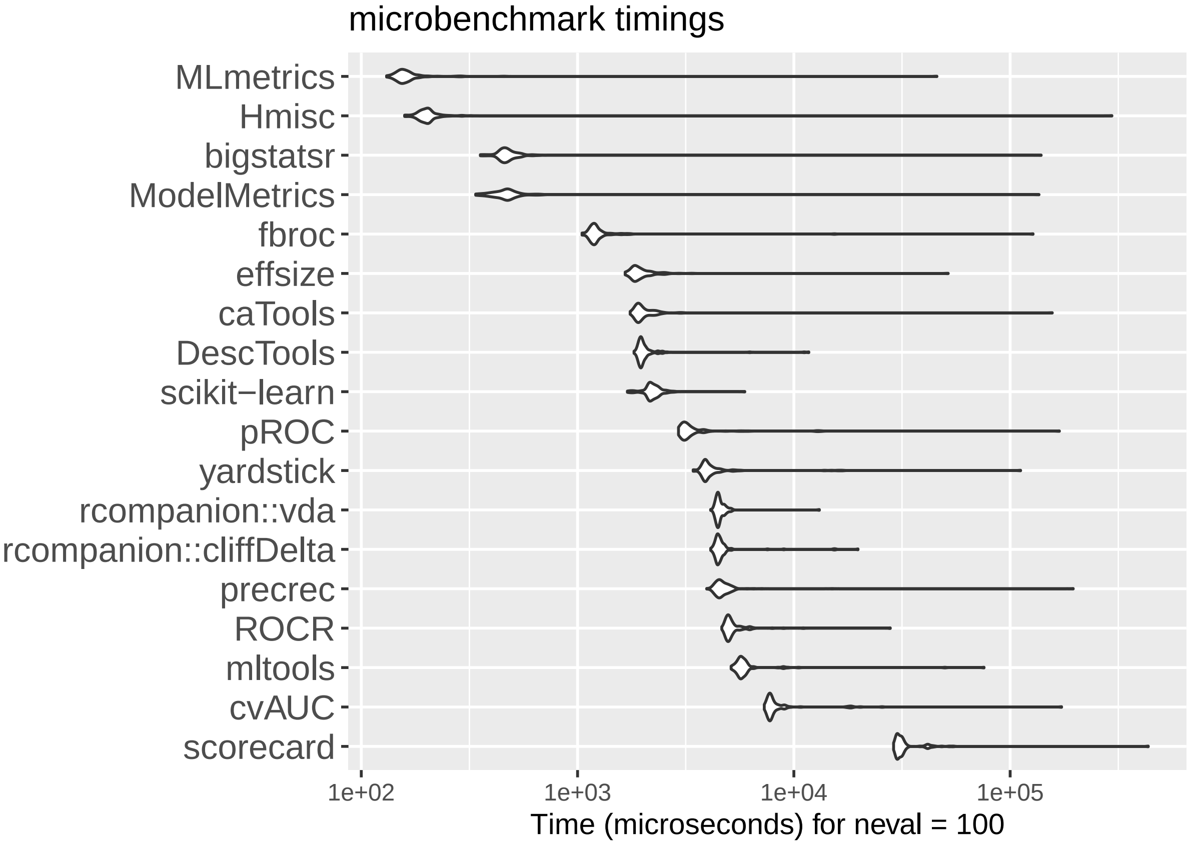
$$\bar{R}_1 = \frac{1}{n_1} \sum_{i:y_i=1} \text{Rank}(s_i)$$

6 Efficiency study

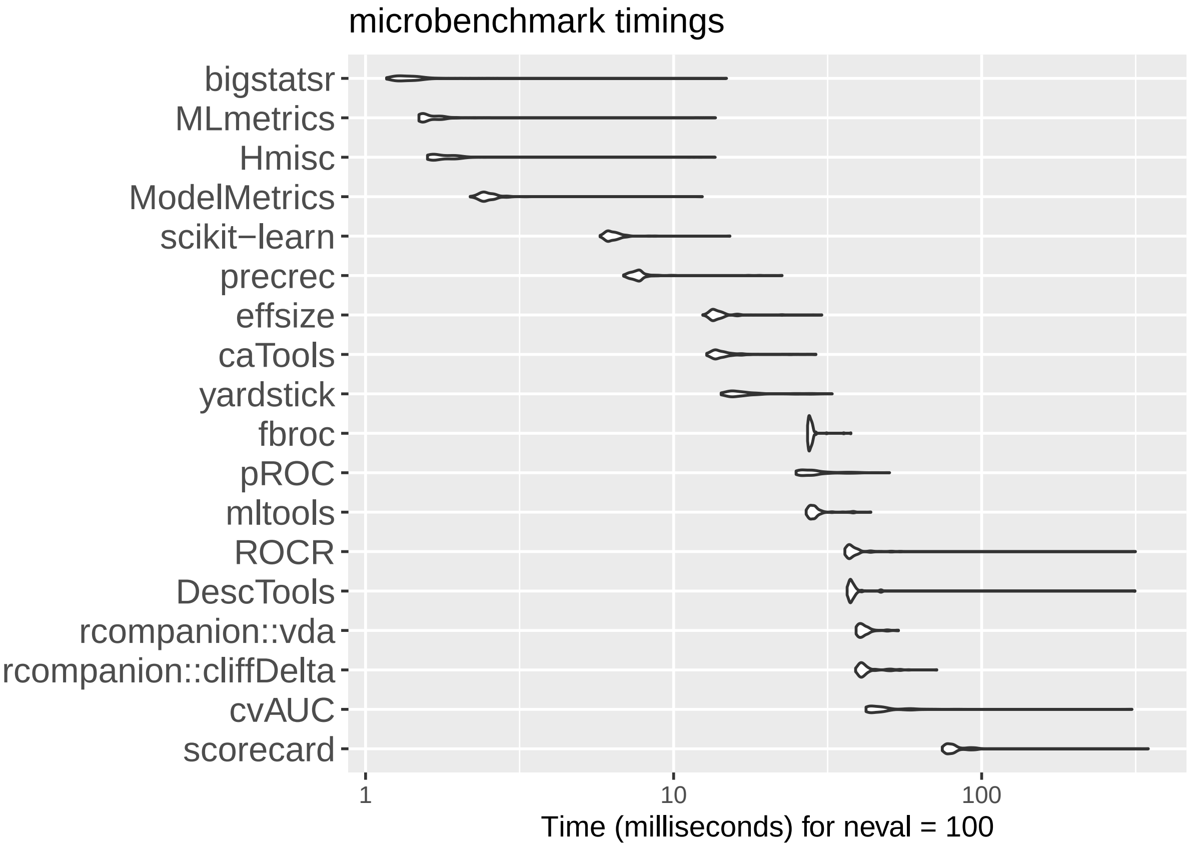
Benchmarking packages

All of the R packages that can be used to calculate the AUC measure have had their performance speed tested. In every benchmark, each function was called 100 times, and there are a total of three benchmarks, each with a different number of observations. The predictor *pred* has been generated from the normal distribution, with the first half of the observations using $N(0,1)$, and the second half being $N(1,1)$. The *target* variable is a vector, where the first half of values are all equal to 1 and the second half of values are all equal to 0.

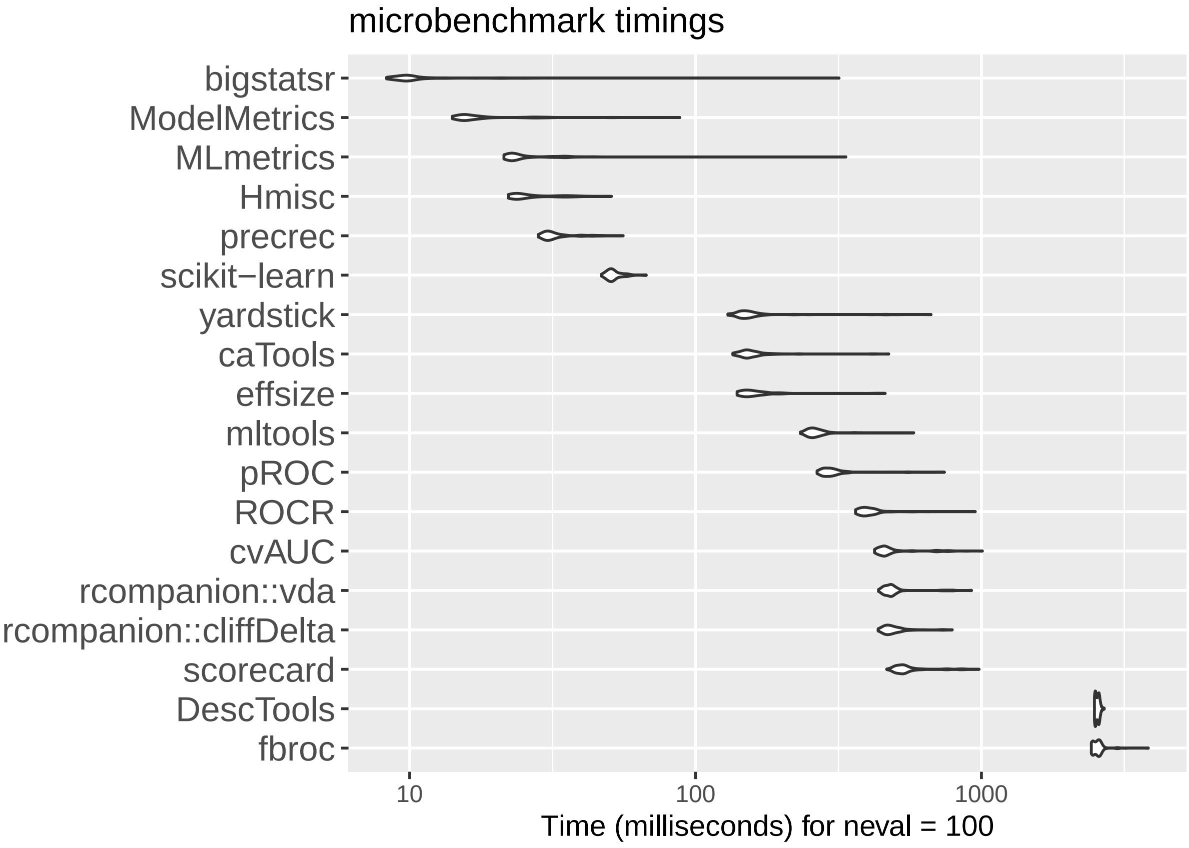
First benchmark - 1000 observations



Second benchmark - 10000 observations



Third benchmark - 100000 observations



The time needed to complete the calculations varies greatly and spans multiple orders of magnitude. For example, using *bigstatsr* to calculate the AUC metrics is almost 100 times faster than by using the *scorecard* package. There may be different causes to this, for example a function might additionally perform other calculations, like generating confidence intervals or also calculating other metrics, or otherwise due to the algorithms used being inefficient, or perhaps even both of these issues at once.

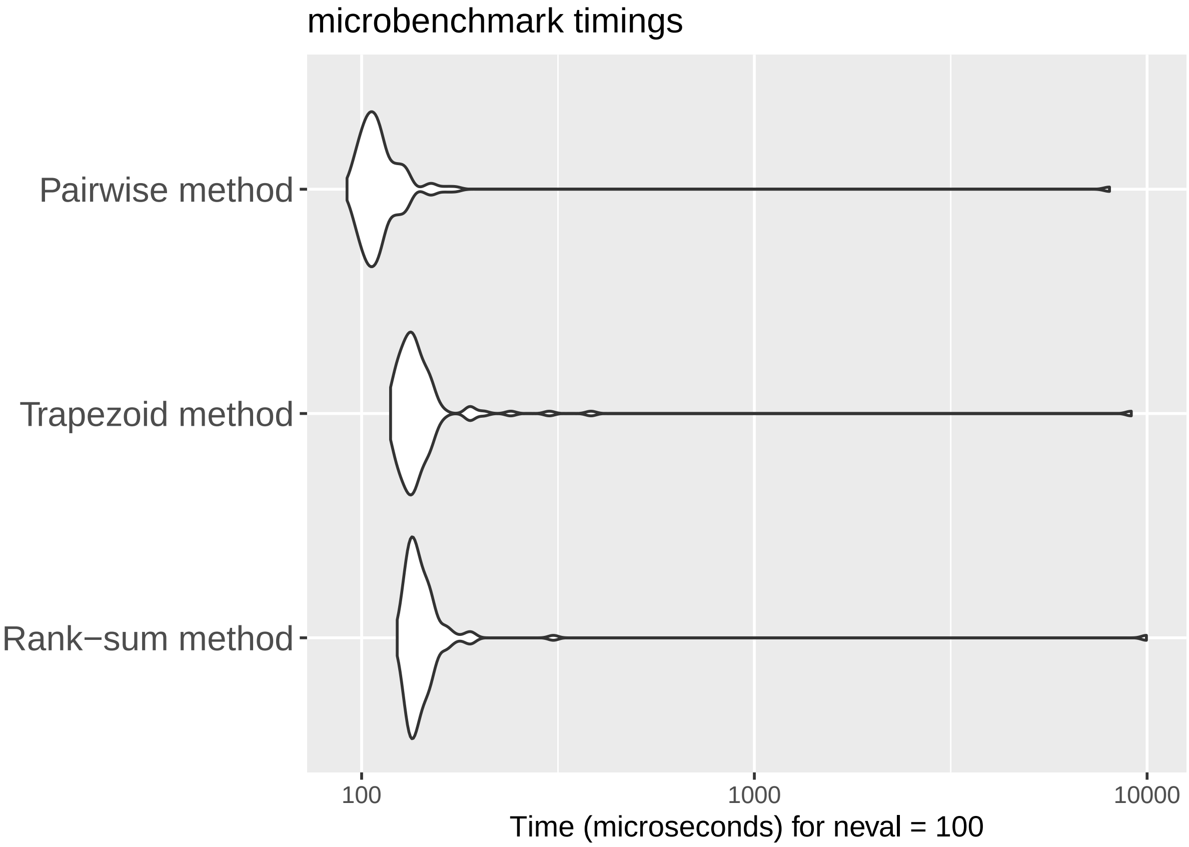
In general, *bigstatsr* offers the fastest way of computation overall. While *MLMetrics* and *Hmisc* are slightly faster on the smallest data set, *bigstatsr* noticeably outperforms them as the number of observations increases.

It is therefore recommended to use the *AUC* function from the *bigstatsr* package whenever calculating the AUC metric in R, whenever an already existing function is desired.

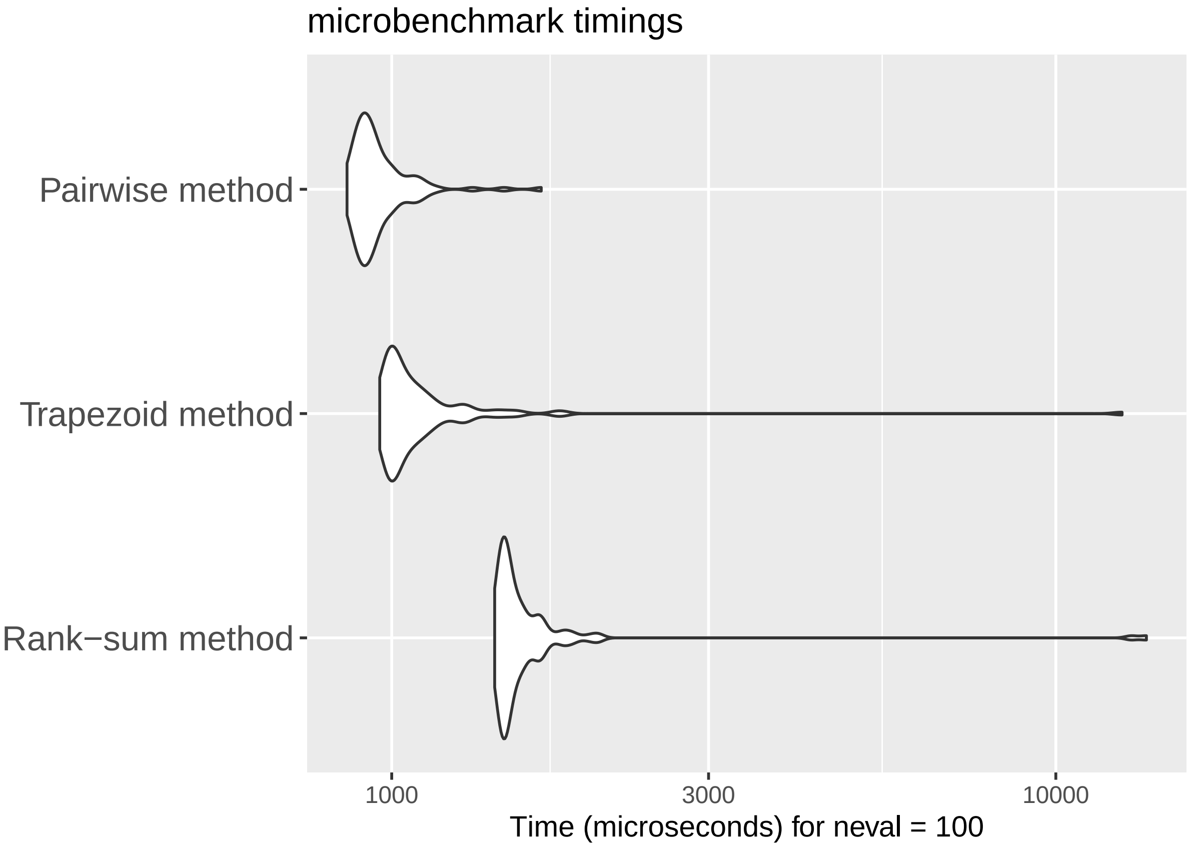
Benchmarking the algorithms

The three identified algorithms have been tested against each other, by creating as optimised functions implementing them as possible. They only contain the calculation, with no checks whether the inputs are correct, to minimise potential interference and isolate the algorithms. They have been performed on the same observations as the package benchmarks.

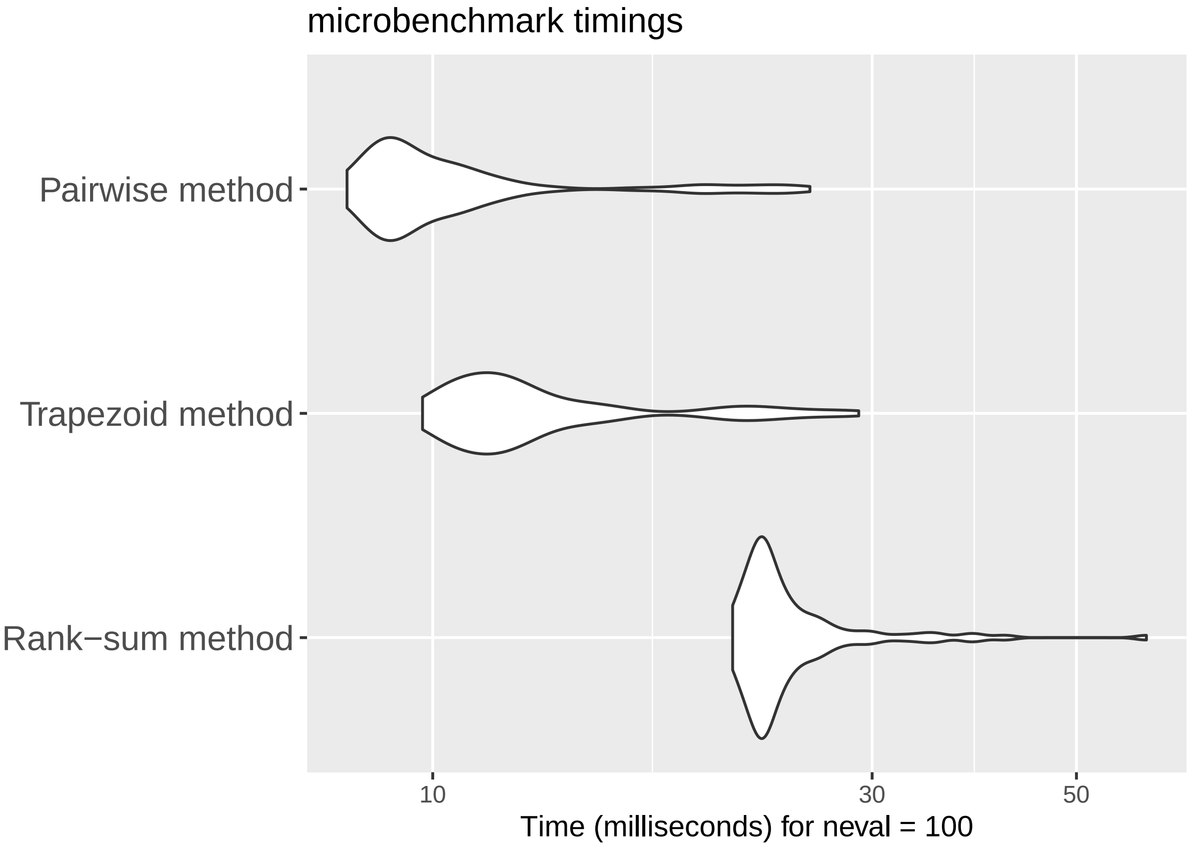
First benchmark - 1000 observations



Second benchmark - 10000 observations



Third benchmark - 100000 observations



In all the benchmarks, the optimised pairwise comparison method is the fastest, with the trapezoid method being only slightly slower. The rank-sum method becomes noticeably slower as the number of observations increases. As a result, whenever developing a new function to calculate the AUC metric, it is recommended to implement it using the pairwise comparison method.

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