Package 'pROC'

July 22, 2019

Type Package

Title Display and Analyze ROC Curves

Version 1.15.3

Date 2019-07-21

Encoding UTF-8

Depends R (>= 2.14)

Imports methods, plyr, Rcpp (>= 0.11.1)

Suggests microbenchmark, tcltk, MASS, logcondens, doParallel, testthat, vdiffr, ggplot2

LinkingTo Rcpp

Description Tools for visualizing, smoothing and comparing receiver operating characteristic (ROC curves). (Partial) area under the curve (AUC) can be compared with statistical tests based on U-statistics or bootstrap. Confidence intervals can be computed for (p)AUC or ROC curves.

License GPL (>= 3)

URL `http://expasy.org/tools/pROC/`

BugReports `https://github.com/xrobin/pROC/issues`

LazyData yes

NeedsCompilation yes

Author Xavier Robin [cre, aut] (<https://orcid.org/0000-0002-6813-3200>),
Natacha Turck [aut],
Alexandre Hainard [aut],
Natalia Tiberti [aut],
Frédérique Lisacek [aut],
Jean-Charles Sanchez [aut],
Markus Müller [aut],
Stefan Siegert [ctb] (Fast DeLong code),
Matthias Doering [ctb] (Hand & Till Multiclass)

Maintainer Xavier Robin <pROC-cran@xavier.robin.name>

Repository CRAN

Date/Publication 2019-07-21 22:40:02 UTC

R topics documented:

`pROC-package` *pROC*

Description

Tools for visualizing, smoothing and comparing receiver operating characteristic (ROC curves). (Partial) area under the curve (AUC) can be compared with statistical tests based on U-statistics or bootstrap. Confidence intervals can be computed for (p)AUC or ROC curves. Sample size / power computation for one or two ROC curves are available.

Details

The basic unit of the pROC package is the `roc` function. It will build a ROC curve, smooth it if requested (if `smooth=TRUE`), compute the AUC (if `auc=TRUE`), the confidence interval (CI) if requested (if `ci=TRUE`) and plot the curve if requested (if `plot=TRUE`).

The `roc` function will call `smooth`, `auc`, `ci` and `plot` as necessary. See these individual functions for the arguments that can be passed to them through `roc`. These function can be called separately.

Two paired (that is `roc` objects with the same `response`) or unpaired (with different `response`) ROC curves can be compared with the `roc.test` function.

Citation

If you use pROC in published research, please cite the following paper:

Xavier Robin, Natacha Turck, Alexandre Hainard, Natalia Tiberti, Frédérique Lisacek, Jean-Charles Sanchez and Markus Müller (2011). "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **12**, p. 77. DOI: 10.1186/1471-2105-12-77[1]

Type `citation("pROC")` for a BibTeX entry.

The authors would be glad to hear how pROC is employed. You are kindly encouraged to notify Xavier Robin <pROC-cran@xavier.robin.name> about any work you publish.

Abbreviations

The following abbreviations are employed extensively in this package:

- ROC: receiver operating characteristic
- AUC: area under the ROC curve
- pAUC: partial area under the ROC curve
- CI: confidence interval
- SP: specificity
- SE: sensitivity

Functions

`roc`	Build a ROC curve
`are.paired`	Dertermine if two ROC curves are paired
`auc`	Compute the area under the ROC curve
`ci`	Compute confidence intervals of a ROC curve
`ci.auc`	Compute the CI of the AUC
`ci.coords`	Compute the CI of arbitrary coordinates
`ci.se`	Compute the CI of sensitivities at given specificities
`ci.sp`	Compute the CI of specificities at given sensitivities
`ci.thresholds`	Compute the CI of specificity and sensitivity of thresholds
`ci.coords`	Compute the CI of arbitrary coordinates
`coords`	Coordinates of the ROC curve
`cov`	Covariance between two AUCs
`ggroc`	Plot a ROC curve with **ggplot2**
`has.partial.auc`	Determine if the ROC curve have a partial AUC
`lines.roc`	Add a ROC line to a ROC plot
`plot.ci`	Plot CIs
`plot`	Plot a ROC curve
`print`	Print a ROC curve object
`roc.test`	Compare the AUC of two ROC curves
`smooth`	Smooth a ROC curve
`var`	Variance of the AUC

[1] `http://dx.doi.org/10.1186/1471-2105-12-77`

Dataset

This package comes with a dataset of 141 patients with aneurysmal subarachnoid hemorrhage: `aSAH`.

Installing and using

To install this package, make sure you are connected to the internet and issue the following command in the R prompt:

```
install.packages("pROC")
```

To load the package in R:

```
library(pROC)
```

Experimental: pipelines

Since version 1.15.0, the `roc` function can be used in pipelines, for instance with **dplyr** or **magrittr**. This is still a highly experimental feature and will change significantly in future versions (see issue 54[2]). The `roc.data.frame` method supports both standard and non-standard evaluation (NSE), and the `roc_` function supports standard evaluation only.

```
library(dplyr)
aSAH %>%
    filter(gender == "Female") %>%
    roc(outcome, s100b)
```

By default it returns the `roc` object, which can then be piped to the `coords` function to extract coordinates that can be used in further pipelines.

```
library(dplyr)
aSAH %>%
    filter(gender == "Female") %>%
    roc(outcome, s100b) %>%
    coords(transpose=FALSE) %>%
    filter(sensitivity > 0.6,
           specificity > 0.6)
```

More details and use cases are available in the `roc` help page.

[2] https://github.com/xrobin/pROC/issues/54

Bootstrap

All the bootstrap operations for significance testing, confidence interval, variance and covariance computation are performed with non-parametric stratified or non-stratified resampling (according to the `stratified` argument) and with the percentile method, as described in Carpenter and Bithell (2000) sections 2.1 and 3.3.

Stratification of bootstrap can be controlled with `boot.stratified`. In stratified bootstrap (the default), each replicate contains the same number of cases and controls than the original sample. Stratification is especially useful if one group has only little observations, or if groups are not balanced.

The number of bootstrap replicates is controlled by `boot.n`. Higher numbers will give a more precise estimate of the significance tests and confidence intervals but take more time to compute. 2000 is recommanded by Carpenter and Bithell (2000) for confidence intervals. In our experience this is sufficient for a good estimation of the first significant digit only, so we recommend the use of 10000 bootstrap replicates to obtain a good estimate of the second significant digit whenever possible.

Progress bars: A progressbar shows the progress of bootstrap operations. It is handled by the **plyr** package (Wickham, 2011), and is created by the `progress_*` family of functions. Sensible defaults are guessed during the package loading:

- In non-interactive mode, no progressbar is displayed.
- In embedded GNU Emacs "ESS", a `txtProgressBar`
- In Windows, a `winProgressBar` bar.
- In other systems with or without a graphical display, a `txtProgressBar`.

The default can be changed with the option "pROCProgress". The option must be a list with a `name` item setting the type of progress bar ("none", "win", "tk" or "text"). Optional items of the list are "width", "char" and "style", corresponding to the arguments to the underlying progressbar functions. For example, to force a text progress bar:

```
options(pROCProgress = list(name = "text", width = NA, char = "=", style = 3)
```

To inhibit the progress bars completely:

```
options(pROCProgress = list(name = "none"))
```

Handling large datasets

Algorithms: Over the years, a significant amount of time has been invested in making pROC run faster and faster. From the naive algorithm iterating over all thresholds implemented in the first version (`algorithm = 1`), we went to a C++ implementation (with **Rcpp**, `algorithm = 3`), and a different algorithm using cummulative sum of responses sorted by the predictor, which scales only with the number of data points, independently on the number of thresholds (`algorithm = 2`). The curves themselves are identical, but computation time has been decreased massively.

Since version 1.12, pROC was able to automatically select the fastest algorithm for your dataset based on the number of thresholds of the ROC curve. Initially this number was around 1500 thresholds, above which algorithm 3 was selected. But with pROC 1.15 additional code profiling enabled us implement additional speedups that brought this number down to less than 100 thresholds. As the detection of the number of thresholds itself can have a large impact comparatively (up

to 10% now), a new `algorithm = 6` was implemented, which assumes that `ordered` datasets should have relatively few levels, and hence thresholds. These predictors are processed with `algorithm = 3`. Any numeric dataset is now assumed to have a sufficient number of thresholds to be processed with `algorithm = 2` efficiently. In the off-chance that you have a very large numeric dataset with very few thresholds, `algorithm = 3` can be selected manually (in the call to `roc`). For instance with 5 thresholds you can expect a speedup of around to 3 times. This effect disappears altogether as soon as the curve gets to 50-100 thresholds.

This simple selection should work in most cases. However if you are unsure or want to test it for yourself, use `algorithm=0` to run a quick benchmark between 2 and 3. Make sure **microbenchmark** is installed. Beware, this is very slow as it will repeat the computation 10 times to obtain a decent estimate of each algorithm speed.

```
if (!requireNamespace("microbenchmark")) install.packages("microbenchmark")

# First a ROC curve with many thresholds. Algorithm 2 is much faster.
response <- rbinom(5E3, 1, .5)
predictor <- rnorm(5E3)
rocobj <- roc(response, predictor, algorithm = 0)


# Next a ROC curve with few thresholds but more data points
response <- rbinom(1E6, 1, .5)
predictor <- rpois(1E6, 1)
rocobj <- roc(response, predictor, algorithm = 0)
```

Other functions have been optimized too, and bottlenecks removed. In particular, the `coords` function is orders of magnitude faster in pROC 1.15. The DeLong algorithm has been improved in versions 1.6, 1.7 and 1.9.1, and currently uses a much more efficient algorithm, both in computation time and memory footprint. We will keep working on improvements to make pROC more suited to large datasets in the future.

Boostrap: Bootstrap is typically slow because it involves repeatedly computing the ROC curve (or a part of it).

Some bootstrap functions are faster than others. Typically, `ci.thresholds` is the fastest, and `ci.coords` the slowest. Use `ci.coords` only if the CI you need cannot be computed by the specialized CI functions `ci.thresholds`, `ci.se` and `ci.sp`. Note that `ci.auc` cannot be replaced anyway.

A naive way to speed-up the boostrap is by removing the progress bar:

```
rocobj <- roc(response, round(predictor))
system.time(ci(rocobj))
system.time(ci(rocobj, progress = "none"))
```

It is of course possible to reduce the number of boostrap iterations. See the `boot.n` argument to `ci`. This will reduce the precision of the bootstrap estimate.

Parallel processing: Bootstrap operations can be performed in parallel. The backend provided by the **plyr** package is used, which in turn relies on the **foreach** package.

To enable parallell processing, you first need to load an adaptor for the **foreach** package (**doMC**, **doMPI**, **doParallel**, **doRedis**, **doRNG** or **doSNOW**)), register the backend, and set `parallel=TRUE`.

```
library(doParallel)
registerDoParallel(cl <- makeCluster(getOption("mc.cores", 2)))
ci(rocobj, method="bootstrap", parallel=TRUE)
stopCluster(cl)
```

Progress bars are not available when parallel processing is enabled.

Using DeLong instead of boostrap: DeLong is an asymptotically exact method to evaluate the uncertainty of an AUC (DeLong *et al.* (1988)). Since version 1.9, pROC uses the algorithm proposed by Sun and Xu (2014) which has an O(N log N) complexity and is always faster than bootstrapping. By default, pROC will choose the DeLong method whenever possible.

```
rocobj <- roc(response, round(predictor), algorithm=3)
system.time(ci(rocobj, method="delong"))
system.time(ci(rocobj, method="bootstrap", parallel = TRUE))
```

Author(s)

Xavier Robin, Natacha Turck, Jean-Charles Sanchez and Markus Müller

Maintainer: Xavier Robin <pROC-cran@xavier.robin.name>

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[3].

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[4].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[5].

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[6].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[7].

[3] http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F

[4] http://dx.doi.org/10.1016/j.patrec.2005.10.010

[5] http://dx.doi.org/10.1186/1471-2105-12-77

[6] http://dx.doi.org/10.1109/LSP.2014.2337313

[7] http://www.jstatsoft.org/v40/i01

See Also

CRAN packages **ROCR**, **verification** or Bioconductor's **roc** for ROC curves.

CRAN packages **plyr**, **MASS** and **logcondens** employed in this package.

Examples

```
data(aSAH)

# Build a ROC object and compute the AUC
roc(aSAH$outcome, aSAH$s100b)
roc(outcome ~ s100b, aSAH)

# Smooth ROC curve
roc(outcome ~ s100b, aSAH, smooth=TRUE)

# more options, CI and plotting
roc1 <- roc(aSAH$outcome,
            aSAH$s100b, percent=TRUE,
            # arguments for auc
            partial.auc=c(100, 90), partial.auc.correct=TRUE,
            partial.auc.focus="sens",
            # arguments for ci
            ci=TRUE, boot.n=100, ci.alpha=0.9, stratified=FALSE,
            # arguments for plot
            plot=TRUE, auc.polygon=TRUE, max.auc.polygon=TRUE, grid=TRUE,
            print.auc=TRUE, show.thres=TRUE)

# Add to an existing plot. Beware of 'percent' specification!
roc2 <- roc(aSAH$outcome, aSAH$wfns,
            plot=TRUE, add=TRUE, percent=roc1$percent)

## Coordinates of the curve ##
coords(roc1, "best", ret=c("threshold", "specificity", "1-npv"))
coords(roc2, "local maximas", ret=c("threshold", "sens", "spec", "ppv", "npv"))

## Confidence intervals ##

# CI of the AUC
ci(roc2)

## Not run:
# CI of the curve
sens.ci <- ci.se(roc1, specificities=seq(0, 100, 5))
plot(sens.ci, type="shape", col="lightblue")
plot(sens.ci, type="bars")

## End(Not run)

# need to re-add roc2 over the shape
plot(roc2, add=TRUE)

## Not run:
```

```
# CI of thresholds
plot(ci.thresholds(roc2))

## End(Not run)

# In parallel
if (require(doParallel)) {
    registerDoParallel(cl <- makeCluster(getOption("mc.cores", 2L)))
    ## Not run: ci(roc2, method="bootstrap", parallel=TRUE)

    stopCluster(cl)
}

## Comparisons ##

# Test on the whole AUC
roc.test(roc1, roc2, reuse.auc=FALSE)

## Not run:
# Test on a portion of the whole AUC
roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(100, 90),
         partial.auc.focus="se", partial.auc.correct=TRUE)

# With modified bootstrap parameters
roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(100, 90),
         partial.auc.correct=TRUE, boot.n=1000, boot.stratified=FALSE)

## End(Not run)
```

`are.paired` *Are two ROC curves paired?*

Description

This function determines if two ROC curves can be paired.

Usage

```
are.paired(...)
## S3 method for class 'auc'
are.paired(roc1, roc2, ...)
## S3 method for class 'smooth.roc'
are.paired(roc1, roc2, ...)
## S3 method for class 'roc'
are.paired(roc1, roc2, return.paired.rocs=FALSE,
  reuse.auc = TRUE, reuse.ci = FALSE, reuse.smooth=TRUE, ...)
```

Arguments

roc1, roc2	the two ROC curves to compare. Either "roc", "auc" or "smooth.roc" objects (types can be mixed).
return.paired.rocs	if TRUE and the ROC curves can be paired, the two paired ROC curves with NAs removed will be returned.
reuse.auc, reuse.ci, reuse.smooth	if return.paired.rocs=TRUE, determines if auc, ci and smooth should be re-computed (with the same parameters than the original ROC curves)
...	additionnal arguments for are.paired.roc. Ignored in are.paired.roc

Details

Two ROC curves are paired if they are built on two variables observed on the same sample.

In practice, the paired status is granted if the response and levels vector of both ROC curves are identical. If the responses are different, this can be due to missing values differing between the curves. In this case, the function will strip all NAs in both curves and check for identity again.

It can raise false positives if the responses are identical but correspond to different patients.

Value

TRUE if roc1 and roc2 are paired, FALSE otherwise.

In addition, if TRUE and return.paired.rocs=TRUE, the following atributes are defined:

roc1, roc2	the two ROC curve with all NAs values removed in both curves.

See Also

roc, roc.test

Examples

```
data(aSAH)
aSAH.copy <- aSAH

# artificially insert NAs for demonstration purposes
aSAH.copy$outcome[42] <- NA
aSAH.copy$s100b[24] <- NA
aSAH.copy$ndka[1:10] <- NA

# Call roc() on the whole data
roc1 <- roc(aSAH.copy$outcome, aSAH.copy$s100b)
roc2 <- roc(aSAH.copy$outcome, aSAH.copy$ndka)
# are.paired can still find that the curves were paired
are.paired(roc1, roc2) # TRUE

# Removing the NAs manually before passing to roc() un-pairs the ROC curves
nas <- is.na(aSAH.copy$outcome) | is.na(aSAH.copy$ndka)
roc2b <- roc(aSAH.copy$outcome[!nas], aSAH.copy$ndka[!nas])
```

```
are.paired(roc1, roc2b) # FALSE

# Getting the two paired ROC curves with additional smoothing and ci options
roc2$ci <- ci(roc2)
paired <- are.paired(smooth(roc1), roc2, return.paired.rocs=TRUE, reuse.ci=TRUE)
paired.roc1 <- attr(paired, "roc1")
paired.roc2 <- attr(paired, "roc2")
```

---

aSAH *Subarachnoid hemorrhage data*

Description

This dataset summarizes several clinical and one laboratory variable of 113 patients with an aneurysmal subarachnoid hemorrhage.

Usage

```
aSAH
```

Format

A data.frame containing 113 observations of 7 variables.

Source

Natacha Turck, Laszlo Vutskits, Paola Sanchez-Pena, Xavier Robin, Alexandre Hainard, Marianne Gex-Fabry, Catherine Fouda, Hadiji Bassem, Markus Mueller, Frédérique Lisacek, Louis Puybasset and Jean-Charles Sanchez (2010) "A multiparameter panel method for outcome prediction following aneurysmal subarachnoid hemorrhage". *Intensive Care Medicine* **36**(1), 107–115. DOI: 10.1007/s00134-009-1641-y[8].

See Also

Other examples can be found in all the documentation pages of this package: `roc`, `auc`, `ci`, `ci.auc`, `ci.se`, `ci.sp`, `ci.thresholds`, `coords`, `plot.ci`, `plot.roc`, `print.roc`, `roc.test` and `smooth`.

An example analysis with pROC is shown in:

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[9]

[8] http://dx.doi.org/10.1007/s00134-009-1641-y
[9] http://dx.doi.org/10.1186/1471-2105-12-77

Examples

```
# load the dataset
data(aSAH)

# Gender, outcome and set
with(aSAH, table(gender, outcome))

# Age
with(aSAH, by(age, outcome, mean))
with(aSAH, by(age, outcome,
     function(x) sprintf("mean: %.1f (+/- %.1f), median: %.1f (%i-%i)",
                         mean(x), sd(x), median(x), min(x), max(x))))

# WFNS score
with(aSAH, table(wfns=ifelse(wfns<=2, "1-2", "3-4-5"), outcome))
```

`auc` *Compute the area under the ROC curve*

Description

This function computes the numeric value of area under the ROC curve (AUC) with the trapezoidal rule. Two syntaxes are possible: one object of class "roc", or either two vectors (response, predictor) or a formula (response~predictor) as in the `roc` function. By default, the total AUC is computed, but a portion of the ROC curve can be specified with `partial.auc`.

Usage

```
auc(...)
## S3 method for class 'roc'
auc(roc, partial.auc=FALSE, partial.auc.focus=c("specificity",
"sensitivity"), partial.auc.correct=FALSE,
allow.invalid.partial.auc.correct = FALSE, ...)
## S3 method for class 'smooth.roc'
auc(smooth.roc, ...)
## S3 method for class 'multiclass.roc'
auc(multiclass.roc, ...)
## S3 method for class 'formula'
auc(formula, data, ...)
## Default S3 method:
auc(response, predictor, ...)
```

Arguments

`roc, smooth.roc, multiclass.roc`
: a "roc" object from the `roc` function, a "smooth.roc" object from the `smooth` function, or a "multiclass.roc" or "mv.multiclass.roc" from the `multiclass.roc` function.

`response, predictor`
: arguments for the `roc` function.

`formula, data`
: a formula (and possibly a data object) of type response~predictor for the `roc` function.

`partial.auc`
: either `FALSE` (default: consider total area) or a numeric vector of length 2: boundaries of the AUC to consider in [0,1] (or [0,100] if percent is `TRUE`).

`partial.auc.focus`
: if `partial.auc` is not `FALSE` and a partial AUC is computed, specifies if `partial.auc` specifies the bounds in terms of specificity (default) or sensitivity. Can be shortened to spec/sens or even sp/se. Ignored if `partial.auc=FALSE`.

`partial.auc.correct`
: logical indicating if the correction of AUC must be applied in order to have a maximal AUC of 1.0 and a non-discriminant AUC of 0.5 whatever the `partial.auc` defined. Ignored if `partial.auc=FALSE`. Default: `FALSE`.

`allow.invalid.partial.auc.correct`
: logical indicating if the correction must return `NA` (with a `warning`) when attempting to correct a pAUC below the diagonal. Set to `TRUE` to return a (probably invalid) corrected AUC. This is useful especially to avoid introducing a bias against low pAUCs in bootstrap operations.

`...`
: further arguments passed to or from other methods, especially arguments for `roc` when calling `auc.default`, `auc.formula`, `auc.smooth.roc`. Note that the `auc` argument of `roc` is not allowed. Unused in `auc.roc`.

Details

This function is typically called from `roc` when `auc=TRUE` (default). It is also used by `ci`. When it is called with two vectors (response, predictor) or a formula (response~predictor) arguments, the `roc` function is called and only the AUC is returned.

By default the total area under the curve is computed, but a partial AUC (pAUC) can be specified with the `partial.auc` argument. It specifies the bounds of specificity or sensitivity (depending on `partial.auc.focus`) between which the AUC will be computed. As it specifies specificities or sensitivities, you must adapt it in relation to the 'percent' specification (see details in `roc`).

`partial.auc.focus` is ignored if `partial.auc=FALSE` (default). If a partial AUC is computed, `partial.auc.focus` specifies if the bounds specified in `partial.auc` must be interpreted as sensitivity or specificity. Any other value will produce an error. It is recommended to `plot` the ROC curve with `auc.polygon=TRUE` in order to make sure the specification is correct.

If a pAUC is defined, it can be standardized (corrected). This correction is controled by the `partial.auc.correct` argument. If `partial.auc.correct=TRUE`, the correction by McClish will be applied:

$$\frac{1 + \frac{auc - min}{max - min}}{2}$$

where auc is the uncorrected pAUC computed in the region defined by `partial.auc`, min is the value of the non-discriminant AUC (with an AUC of 0.5 or 50 in the region and max is the maximum

possible AUC in the region. With this correction, the AUC will be 0.5 if non discriminant and 1.0 if maximal, whatever the region defined. This correction is fully compatible with `percent`.

Note that this correction is undefined for curves below the diagonal (auc < min). Attempting to correct such an AUC will return `NA` with a warning.

Value

The numeric AUC value, of class `c("auc","numeric")` (or `c("multiclass.auc","numeric")` or `c("mv.multiclass.auc","numeric")` if a "multiclass.roc" was supplied), in fraction of the area or in percent if `percent=TRUE`, with the following attributes:

- `partial.auc` if the AUC is full (FALSE) or partial (and in this case the bounds), as defined in argument.
- `partial.auc.focus` only for a partial AUC, if the bound specifies the sensitivity or specificity, as defined in argument.
- `partial.auc.correct` only for a partial AUC, was it corrected? As defined in argument.
- `percent` whether the AUC is given in percent or fraction.
- `roc` the original ROC curve, as a "roc", "smooth.roc" or "multiclass.roc" object.

Smoothed ROC curves

There is no difference in the computation of the area under a smoothed ROC curve, except for curves smoothed with `method="binomial"`. In this case and only if a full AUC is requested, the classical binormal AUC formula is applied:

$$auc = \phi \frac{a}{\sqrt{1+b^2}}.$$

If the ROC curve is smoothed with any other `method` or if a partial AUC is requested, the empirical AUC described in the previous section is applied.

Multi-class AUCs

With an object of class "multiclass.roc", a multi-class AUC is computed as an average AUC as defined by Hand and Till (equation 7).

$$auc = \frac{2}{c(c-1)} \sum aucs$$

with aucs all the pairwise roc curves.

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[10].

[10] `http://dx.doi.org/10.1016/j.patrec.2005.10.010`

David J. Hand and Robert J. Till (2001). A Simple Generalisation of the Area Under the ROC Curve for Multiple Class Classification Problems. *Machine Learning* **45**(2), p. 171–186. DOI: 10.1023/A:1010920819831[11].

Donna Katzman McClish (1989) "Analyzing a Portion of the ROC Curve". *Medical Decision Making* **9**(3), 190–195. DOI: 10.1177/0272989X8900900307[12].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[13].

See Also

`roc`, `ci.auc`

Examples

```
data(aSAH)

# Syntax (response, predictor):
auc(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
# Full AUC:
auc(rocobj)
# Partial AUC:
auc(rocobj, partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE)

# Alternatively, you can get the AUC directly from roc():
roc(aSAH$outcome, aSAH$s100b)$auc
roc(aSAH$outcome, aSAH$s100b,
    partial.auc=c(1, .8), partial.auc.focus="se",
    partial.auc.correct=TRUE)$auc
```

---

ci *Compute the confidence interval of a ROC curve*

Description

This function computes the confidence interval (CI) of a ROC curve. The `of` argument controls the type of CI that will be computed. By default, the 95% CI are computed with 2000 stratified bootstrap replicates.

[11] http://dx.doi.org/10.1023/A:1010920819831
[12] http://dx.doi.org/10.1177/0272989X8900900307
[13] http://dx.doi.org/10.1186/1471-2105-12-77

Usage

```
ci(...)
## S3 method for class 'roc'
ci(roc, of = c("auc", "thresholds", "sp", "se", "coords"), ...)
## S3 method for class 'smooth.roc'
ci(smooth.roc, of = c("auc", "sp", "se", "coords"), ...)
## S3 method for class 'multiclass.roc'
ci(multiclass.roc, of = "auc", ...)
## S3 method for class 'multiclass.auc'
ci(multiclass.auc, of = "auc", ...)
## S3 method for class 'formula'
ci(formula, data, ...)
## Default S3 method:
ci(response, predictor, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`multiclass.roc, multiclass.auc`
: not implemented.

`response, predictor`
: arguments for the `roc` function.

`formula, data`
: a formula (and possibly a data object) of type response~predictor for the `roc` function.

`of`
: The type of confidence interval. One of "auc", "thresholds", "sp", "se" or "coords". Note that confidence interval on "thresholds" are not available for smoothed ROC curves.

`...`
: further arguments passed to or from other methods, especially `auc`, `roc`, and the specific `ci` functions `ci.auc`, `ci.se`, `ci.sp` and `ci.thresholds`.

Details

`ci.formula` and `ci.default` are convenience methods that build the ROC curve (with the `roc` function) before calling `ci.roc`. You can pass them arguments for both `roc` and `ci.roc`. Simply use `ci` that will dispatch to the correct method.

This function is typically called from `roc` when `ci=TRUE` (not by default). Depending on the `of` argument, the specific `ci` functions `ci.auc`, `ci.thresholds`, `ci.sp`, `ci.se` or `ci.coords` are called.

When the ROC curve has an `auc` of 1 (or 100%), the confidence interval will always be null (there is no interval). This is true for both "delong" and "bootstrap" methods that can not properly assess the variance in this case. This result is misleading, as the variance is of course not null. A `warning` will be displayed to inform of this condition, and of the misleading output.

CI of multiclass ROC curves and AUC is not implemented yet. Attempting to call these methods returns an error.

Value

The return value of the specific `ci` functions `ci.auc`, `ci.thresholds`, `ci.sp`, `ci.se` or `ci.coords`, depending on the `of` argument.

References

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[14].

See Also

`roc`, `auc`, `ci.auc`, `ci.thresholds`, `ci.sp`, `ci.se`, `ci.coords`

Examples

```
data(aSAH)

# Syntax (response, predictor):
ci(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)

# Of an AUC
ci(rocobj)
ci(rocobj, of="auc")
# this is strictly equivalent to:
ci.auc(rocobj)

# Of thresholds, sp, se...
## Not run:
ci(rocobj, of="thresholds")
ci(rocobj, of="thresholds", thresholds=0.51)
ci(rocobj, of="thresholds", thresholds="all")
ci(rocobj, of="sp", sensitivities=c(.95, .9, .85))
ci(rocobj, of="se")

## End(Not run)

# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome, aSAH$s100b, ci=TRUE, of="auc")
rocobj$ci
```

[14] http://dx.doi.org/10.1186/1471-2105-12-77

`ci.auc` *Compute the confidence interval of the AUC*

Description

This function computes the confidence interval (CI) of an area under the curve (AUC). By default, the 95% CI is computed with 2000 stratified bootstrap replicates.

Usage

```
# ci.auc(...)
## S3 method for class 'roc'
ci.auc(roc, conf.level=0.95, method=c("delong",
"bootstrap"), boot.n = 2000, boot.stratified = TRUE, reuse.auc=TRUE,
progress = getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
ci.auc(smooth.roc, conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, reuse.auc=TRUE,
progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'auc'
ci.auc(auc, ...)
## S3 method for class 'multiclass.roc'
ci.auc(multiclass.roc, ...)
## S3 method for class 'multiclass.auc'
ci.auc(multiclass.auc, ...)
## S3 method for class 'auc'
ci.auc(auc, ...)
## S3 method for class 'formula'
ci.auc(formula, data, ...)
## Default S3 method:
ci.auc(response, predictor, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`auc`
: an "auc" object from the `auc` function.

`multiclass.roc, multiclass.auc`
: not implemented.

`response, predictor`
: arguments for the `roc` function.

`formula, data`
: a formula (and possibly a data object) of type response~predictor for the `roc` function.

`conf.level` the width of the confidence interval as [0,1], never in percent. Default: 0.95, resulting in a 95% CI.

`method` the method to use, either "delong" or "bootstrap". The first letter is sufficient. If omitted, the appropriate method is selected as explained in details.

`boot.n` the number of bootstrap replicates. Default: 2000.

`boot.stratified` should the bootstrap be stratified (default, same number of cases/controls in each replicate than in the original sample) or not.

`reuse.auc` if `TRUE` (default) and the "roc" object contains an "auc" field, re-use these specifications for the test. If false, use optional `...` arguments to `auc`. See details.

`progress` the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.

`parallel` if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).

`...` further arguments passed to or from other methods, especially arguments for `roc` and `roc.test.roc` when calling `roc.test.default` or `roc.test.formula`. Arguments for `auc` and `txtProgressBar` (only `char` and `style`) if applicable.

Details

This function computes the CI of an AUC. Two methods are available: "delong" and "bootstrap" with the parameters defined in "roc$auc" to compute a CI. When it is called with two vectors (response, predictor) or a formula (response~predictor) arguments, the `roc` function is called to build the ROC curve first.

The default is to use "delong" method except for comparison of partial AUC and smoothed curves, where `bootstrap` is used. Using "delong" for partial AUC and smoothed ROCs is not supported.

With `method="bootstrap"`, the function calls `auc` `boot.n` times. For more details about the bootstrap, see the Bootstrap section in this package's documentation.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided `density.cases` or `density.controls` the bootstrap cannot be performed and an error is issued.

With `method="delong"`, the variance of the AUC is computed as defined by DeLong *et al.* (1988) using the algorithm by Sun and Xu (2014) and the CI is deduced with `qnorm`.

CI of multiclass ROC curves and AUC is not implemented yet. Attempting to call these methods returns an error.

Value

A numeric vector of length 3 and class "ci.auc", "ci" and "numeric" (in this order), with the lower bound, the median and the upper bound of the CI, and the following attributes:

`conf.level` the width of the CI, in fraction.

`method` the method employed.

`boot.n` the number of bootstrap replicates.

`boot.stratified` whether or not the bootstrapping was stratified.

`auc` an object of class "auc" stored for reference about the compued AUC details (partial, percent, ...)

The `aucs` item is not included in this list since version 1.2 for consistency reasons.

AUC specification

The comparison of the CI needs a specification of the AUC. This allows to compute the CI for full or partial AUCs. The specification is defined by:

1. the "auc" field in the "roc" object if `reuse.auc` is set to `TRUE` (default). It is naturally inherited from any call to `roc` and fits most cases.
2. passing the specification to `auc` with ... (arguments `partial.auc`, `partial.auc.correct` and `partial.auc.focus`). In this case, you must ensure either that the `roc` object do not contain an `auc` field (if you called `roc` with `auc=FALSE`), or set `reuse.auc=FALSE`.

If `reuse.auc=FALSE` the `auc` function will always be called with `...` to determine the specification, even if the "roc" object do contain an `auc` field.

As well if the "roc" object do not contain an `auc` field, the `auc` function will always be called with `...` to determine the specification.

Warning: if the roc object passed to ci contains an `auc` field and `reuse.auc=TRUE`, auc is not called and arguments such as `partial.auc` are silently ignored.

Warnings

If `method="delong"` and the AUC specification specifies a partial AUC, the warning "Using DeLong's test for partial AUC is not supported. Using bootstrap test instead." is issued. The `method` argument is ignored and "bootstrap" is used instead.

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that there are not enough points for smoothing, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

Errors

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the statistic on ROC curves smoothed with density.controls and density.cases." is issued.

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[15].

[15] `http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F`

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[16].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[17].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[18].

See Also

`roc`, `auc`, `ci`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

# Syntax (response, predictor):
ci.auc(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
# default values
ci.auc(rocobj)
ci(rocobj)
ci(auc(rocobj))
ci(rocobj$auc)
ci(rocobj$auc, method="delong")

# Partial AUC and customized bootstrap:
ci.auc(aSAH$outcome, aSAH$s100b,
       boot.n=100, conf.level=0.9, stratified=FALSE, partial.auc=c(1, .8),
       partial.auc.focus="se", partial.auc.correct=TRUE)

# Note that the following will NOT give a CI of the partial AUC:
ci.auc(rocobj, boot.n=500, conf.level=0.9, stratified=FALSE,
       partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE)
# This is because rocobj$auc is not a partial AUC.
## Not run:
# You can overcome this problem with reuse.auc:
ci.auc(rocobj, boot.n=500, conf.level=0.9, stratified=FALSE,
       partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE,
       reuse.auc=FALSE)
```

[16] http://dx.doi.org/10.1109/LSP.2014.2337313
[17] http://dx.doi.org/10.1186/1471-2105-12-77
[18] http://www.jstatsoft.org/v40/i01

```
## End(Not run)

# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome, aSAH$s100b, ci=TRUE, of="auc")
rocobj$ci

## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth(rocobj)
# Or you can compute a new one:
ci.auc(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)

## End(Not run)
```

`ci.coords` *Compute the confidence interval of arbitrary coordinates*

Description

This function computes the confidence interval (CI) of the coordinates of a ROC curves with the `coords` function. By default, the 95% CI are computed with 2000 stratified bootstrap replicates.

Usage

```
# ci.coords(...)
## S3 method for class 'roc'
ci.coords(roc, x,
input=c("threshold", "specificity", "sensitivity"),
ret=c("threshold", "specificity", "sensitivity"),
best.method=c("youden", "closest.topleft"), best.weights=c(1, 0.5),
best.policy = c("stop", "omit", "random"),
conf.level=0.95, boot.n=2000,
boot.stratified=TRUE,
progress=getOption("pROCProgress")$name, ...)
## S3 method for class 'formula'
ci.coords(formula, data, ...)
## S3 method for class 'smooth.roc'
ci.coords(smooth.roc, x,
input=c("specificity", "sensitivity"), ret=c("specificity", "sensitivity"),
best.method=c("youden", "closest.topleft"), best.weights=c(1, 0.5),
best.policy = c("stop", "omit", "random"),
conf.level=0.95, boot.n=2000,
boot.stratified=TRUE,
progress=getOption("pROCProgress")$name, ...)
## Default S3 method:
ci.coords(response, predictor, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`response, predictor`
: arguments for the `roc` function.

`formula, data`
: a formula (and possibly a data object) of type response~predictor for the `roc` function.

`x, input, ret, best.method, best.weights`
: Arguments passed to `coords`. See there for more details. The only difference is on the `x` argument which cannot be "all" or "local maximas".

`best.policy`
: The policy follow when multiple "best" thresholds are returned by `coords`. "stop" will abort the processing with `stop` (default), "omit" will ignore the sample (as in `NA`) and "random" will select one of the threshold randomly.

`conf.level`
: the width of the confidence interval as [0,1], never in percent. Default: 0.95, resulting in a 95% CI.

`boot.n`
: the number of bootstrap replicates. Default: 2000.

`boot.stratified`
: should the bootstrap be stratified (default, same number of cases/controls in each replicate than in the original sample) or not.

`progress`
: the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.

`...`
: further arguments passed to or from other methods, especially arguments for `roc` and `ci.coords.roc` when calling `ci.coords.default` or `ci.coords.formula`. Arguments for `txtProgressBar` (only `char` and `style`) if applicable.

Details

`ci.coords.formula` and `ci.coords.default` are convenience methods that build the ROC curve (with the `roc` function) before calling `ci.coords.roc`. You can pass them arguments for both `roc` and `ci.coords.roc`. Simply use `ci.coords` that will dispatch to the correct method.

This function creates `boot.n` bootstrap replicate of the ROC curve, and evaluates the coordinates specified by the `x`, `input`, `ret`, `best.method` and `best.weights` arguments. Then it computes the confidence interval as the percentiles given by `conf.level`.

For more details about the bootstrap, see the Bootstrap section in this package's documentation.

Value

A matrix of class "ci.coords", "ci" and "matrix" (in this order), with the confidence intervals of the CI. The matrix has 3 columns (lower bound, median and upper bound) and as many rows as `x` * `ret` were requested. Rows are sorted by `x` and then by `ret` and named as "input x: return".

Additionally, the list has the following attributes:

`conf.level` the width of the CI, in fraction.

`boot.n` the number of bootstrap replicates.

`boot.stratified` whether or not the bootstrapping was stratified.

`roc` the object of class "roc" that was used to compute the CI.

Warnings

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

This warning will also be displayed if you chose `best.policy = "omit"` and a ROC curve with multiple "best" threshold was generated during at least one of the replicates.

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[19].

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[20].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[21].

See Also

`roc`, `coords`, `ci`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

## Not run:
# Syntax (response, predictor):
ci.coords(aSAH$outcome, aSAH$s100b, x="best", input = "threshold",
          ret=c("specificity", "ppv", "tp"))

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.coords(rocobj, x=0.9, input = "sensitivity", ret="specificity")
ci.coords(rocobj, x=0.9, input = "sensitivity", ret=c("specificity", "ppv", "tp"))
```

[19] http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F

[20] http://dx.doi.org/10.1016/j.patrec.2005.10.010

[21] http://www.jstatsoft.org/v40/i01

```
ci.coords(rocobj, x=c(0.1, 0.5, 0.9), input = "sensitivity", ret="specificity")
ci.coords(rocobj, x=c(0.1, 0.5, 0.9), input = "sensitivity", ret=c("specificity", "ppv", "tp

# With a smoothed roc:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.coords(smooth(rocobj), x=0.9, input = "sensitivity", ret=c("specificity", "ppv", "tp"))

# Return everything we can:
rets <- c("threshold", "specificity", "sensitivity", "accuracy", "tn", "tp", "fn", "fp", "np
          "ppv", "1-specificity", "1-sensitivity", "1-accuracy", "1-npv", "1-ppv")
ci.coords(rocobj, x="best", input = "threshold", ret=rets)

## End(Not run)
```

`ci.se` *Compute the confidence interval of sensitivities at given specificities*

Description

This function computes the confidence interval (CI) of the sensitivity at the given specificity points. By default, the 95% CI are computed with 2000 stratified bootstrap replicates.

Usage

```
# ci.se(...)
## S3 method for class 'roc'
ci.se(roc, specificities = seq(0, 1, .1) * ifelse(roc$percent,
100, 1), conf.level=0.95, boot.n=2000, boot.stratified=TRUE,
progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
ci.se(smooth.roc, specificities = seq(0, 1, .1) *
ifelse(smooth.roc$percent, 100, 1), conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, progress=getOption("pROCProgress")$name,
parallel=FALSE, ...)
## S3 method for class 'formula'
ci.se(formula, data, ...)
## Default S3 method:
ci.se(response, predictor, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`response, predictor`
: arguments for the `roc` function.

formula, data
: a formula (and possibly a data object) of type response~predictor for the roc function.

specificities
: on which specificities to evaluate the CI.

conf.level
: the width of the confidence interval as [0,1], never in percent. Default: 0.95, resulting in a 95% CI.

boot.n
: the number of bootstrap replicates. Default: 2000.

boot.stratified
: should the bootstrap be stratified (default, same number of cases/controls in each replicate than in the original sample) or not.

progress
: the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the name argument to create_progress_bar for more information), but a list as returned by create_progress_bar is also accepted. See also the "Progress bars" section of this package's documentation.

parallel
: if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).

...
: further arguments passed to or from other methods, especially arguments for roc and ci.se.roc when calling ci.se.default or ci.se.formula. Arguments for txtProgressBar (only char and style) if applicable.

Details

ci.se.formula and ci.se.default are convenience methods that build the ROC curve (with the roc function) before calling ci.se.roc. You can pass them arguments for both roc and ci.se.roc. Simply use ci.se that will dispatch to the correct method.

The ci.se.roc function creates boot.n bootstrap replicate of the ROC curve, and evaluates the sensitivity at specificities given by the specificities argument. Then it computes the confidence interval as the percentiles given by conf.level.

For more details about the bootstrap, see the Bootstrap section in this package's documentation.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided density.cases or density.controls the bootstrap cannot be performed and an error is issued.

Value

A matrix of class "ci.se", "ci" and "matrix" (in this order) containing the given sensitivities. Row (names) are the specificities, the first column the lower bound, the 2nd column the median and the 3rd column the upper bound.

Additionally, the list has the following attributes:

conf.level
: the width of the CI, in fraction.

boot.n
: the number of bootstrap replicates.

boot.stratified
: whether or not the bootstrapping was stratified.

`specificities`
: the specificities as given in argument.

`roc`
: the object of class "roc" that was used to compute the CI.

Warnings

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that there are not enough points for smoothing, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

Errors

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the statistic on ROC curves smoothed with density.controls and density.cases." is issued.

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[22].

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[23].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[24].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[25].

See Also

`roc`, `ci`, `ci.sp`, `plot.ci`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

## Not run:
# Syntax (response, predictor):
ci.se(aSAH$outcome, aSAH$s100b)

# With a roc object and less bootstrap:
```

[22] http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F

[23] http://dx.doi.org/10.1016/j.patrec.2005.10.010

[24] http://dx.doi.org/10.1186/1471-2105-12-77

[25] http://www.jstatsoft.org/v40/i01

```
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.se(rocobj, boot.n=100)

# Customized bootstrap and specific specificities:
ci.se(rocobj, c(.95, .9, .85), boot.n=500, conf.level=0.9, stratified=FALSE)

## End(Not run)

# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome,
              aSAH$s100b, ci=TRUE, of="se", boot.n=100)
rocobj$ci

# Plotting the CI
plot(rocobj)
plot(rocobj$ci)

## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth(rocobj)
# Or you can compute a new one:
ci.se(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)

## End(Not run)
```

`ci.sp` *Compute the confidence interval of specificities at given sensitivities*

Description

This function computes the confidence interval (CI) of the specificity at the given sensitivity points. By default, the 95% CI are computed with 2000 stratified bootstrap replicates.

Usage

```
# ci.sp(...)
## S3 method for class 'roc'
ci.sp(roc, sensitivities = seq(0, 1, .1) * ifelse(roc$percent,
100, 1), conf.level=0.95, boot.n=2000, boot.stratified=TRUE,
progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
ci.sp(smooth.roc, sensitivities = seq(0, 1, .1) *
ifelse(smooth.roc$percent, 100, 1), conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'formula'
ci.sp(formula, data, ...)
## Default S3 method:
ci.sp(response, predictor, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`response, predictor`
: arguments for the `roc` function.

`formula, data`
: a formula (and possibly a data object) of type response~predictor for the `roc` function.

`sensitivities`
: on which sensitivities to evaluate the CI.

`conf.level`
: the width of the confidence interval as [0,1], never in percent. Default: 0.95, resulting in a 95% CI.

`boot.n`
: the number of bootstrap replicates. Default: 2000.

`boot.stratified`
: should the bootstrap be stratified (default, same number of cases/controls in each replicate than in the original sample) or not.

`progress`
: the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.

`parallel`
: if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).

`...`
: further arguments passed to or from other methods, especially arguments for `roc` and `ci.sp.roc` when calling `ci.sp.default` or `ci.sp.formula`. Arguments for `txtProgressBar` (only `char` and `style`) if applicable.

Details

`ci.sp.formula` and `ci.sp.default` are convenience methods that build the ROC curve (with the `roc` function) before calling `ci.sp.roc`. You can pass them arguments for both `roc` and `ci.sp.roc`. Simply use `ci.sp` that will dispatch to the correct method.

The `ci.sp.roc` function creates `boot.n` bootstrap replicate of the ROC curve, and evaluates the specificity at sensitivities given by the `sensitivities` argument. Then it computes the confidence interval as the percentiles given by `conf.level`.

For more details about the bootstrap, see the Bootstrap section in this package's documentation.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided `density.cases` or `density.controls` the bootstrap cannot be performed and an error is issued.

Value

A matrix of class "ci.sp", "ci" and "matrix" (in this order) containing the given specificities. Row (names) are the sensitivities, the first column the lower bound, the 2nd column the median and the 3rd column the upper bound.

Additionally, the list has the following attributes:

`conf.level` the width of the CI, in fraction.

`boot.n` the number of bootstrap replicates.

`boot.stratified`
whether or not the bootstrapping was stratified.

`sensitivities`
the sensitivities as given in argument.

`roc` the object of class "roc" that was used to compute the CI.

Warnings

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that there are not enough points for smoothing, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

Errors

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the statistic on ROC curves smoothed with density.controls and density.cases." is issued.

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[26].

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[27].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[28].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[29].

See Also

`roc`, `ci`, `ci.se`, `plot.ci`

CRAN package **plyr**, employed in this function.

[26] http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F

[27] http://dx.doi.org/10.1016/j.patrec.2005.10.010

[28] http://dx.doi.org/10.1186/1471-2105-12-77

[29] http://www.jstatsoft.org/v40/i01

Examples

```
data(aSAH)

## Not run:
# Syntax (response, predictor):
ci.sp(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.sp(rocobj)

# Customized bootstrap and specific specificities:
ci.sp(rocobj, c(.95, .9, .85), boot.n=500, conf.level=0.9, stratified=FALSE)

## End(Not run)

# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome,
              aSAH$s100b, ci=TRUE, of="sp", boot.n=100)
rocobj$ci

# Plotting the CI
plot(rocobj)
plot(rocobj$ci)

## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth(rocobj)
# Or you can compute a new one:
ci.sp(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)

## End(Not run)
```

---

ci.thresholds *Compute the confidence interval of thresholds*

Description

This function computes the confidence interval (CI) of the sensitivity and specificity of the thresholds given in argument. By default, the 95% CI are computed with 2000 stratified bootstrap replicates.

Usage

```
# ci.thresholds(...)
## S3 method for class 'roc'
ci.thresholds(roc, conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, thresholds = "local maximas",
progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
```

```
## S3 method for class 'formula'
ci.thresholds(formula, data, ...)
## S3 method for class 'smooth.roc'
ci.thresholds(smooth.roc, ...)
## Default S3 method:
ci.thresholds(response, predictor, ...)
```

Arguments

`roc`	a "roc" object from the `roc` function.
`smooth.roc`	not available for smoothed ROC curves, available only to catch the error and provide a clear error message.
`response, predictor`	arguments for the `roc` function.
`formula, data`	a formula (and possibly a data object) of type response~predictor for the `roc` function.
`conf.level`	the width of the confidence interval as [0,1], never in percent. Default: 0.95, resulting in a 95% CI.
`boot.n`	the number of bootstrap replicates. Default: 2000.
`boot.stratified`	should the bootstrap be stratified (default, same number of cases/controls in each replicate than in the original sample) or not.
`thresholds`	on which thresholds to evaluate the CI. Either the numeric values of the thresholds, a logical vector (as index of `roc$thresholds`) or a character "all", "local maximas" or "best" that will be used to determine the threshold(s) on the supplied curve with `coords` (not on the resampled curves).
`progress`	the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.
`parallel`	if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).
`...`	further arguments passed to or from other methods, especially arguments for `roc` and `ci.thresholds.roc` when calling `ci.thresholds.default` or `ci.thresholds.formula`. Arguments for `txtProgressBar` (only `char` and `style`) if applicable. Arguments `best.method` and `best.weights` to `coords`.

Details

`ci.thresholds.formula` and `ci.thresholds.default` are convenience methods that build the ROC curve (with the `roc` function) before calling `ci.thresholds.roc`. You can pass them arguments for both `roc` and `ci.thresholds.roc`. Simply use `ci.thresholds` that will dispatch to the correct method.

This function creates `boot.n` bootstrap replicate of the ROC curve, and evaluates the sensitivity and specificity at thresholds given by the `thresholds` argument. Then it computes the confidence interval as the percentiles given by `conf.level`.

A threshold given as a `logical` vector or `character` is converted to the corresponding numeric vector once *using the supplied ROC curve*, and not at each bootstrap iteration. See `ci.coords` for the latter behaviour.

For more details about the bootstrap, see the Bootstrap section in this package's documentation.

Value

A list of length 2 and class "ci.thresholds", "ci" and "list" (in this order), with the confidence intervals of the CI and the following items:

`specificity` a matrix of CI for the specificity. Row (names) are the thresholds, the first column the lower bound, the 2nd column the median and the 3rd column the upper bound.

`sensitivity` same than specificity.

Additionally, the list has the following attributes:

`conf.level` the width of the CI, in fraction.

`boot.n` the number of bootstrap replicates.

`boot.stratified` whether or not the bootstrapping was stratified.

`thresholds` the thresholds, as given in argument.

`roc` the object of class "roc" that was used to compute the CI.

Warnings

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

References

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164. DOI: 10.1002/(SICI)1097-0258(20000515)19:9<1141::AID-SIM479>3.0.CO;2-F[30].

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[31].

[30] `http://dx.doi.org/10.1002/(SICI)1097-0258(20000515)19\%3A9\%3C1141\%3A\%3AAID-SIM479\%3E3.0.CO\%3B2-F`

[31] `http://dx.doi.org/10.1016/j.patrec.2005.10.010`

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[32].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[33].

See Also

`roc`, `ci`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

## Not run:
# Syntax (response, predictor):
ci.thresholds(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.thresholds(rocobj)

# Customized bootstrap and specific thresholds:
ci.thresholds(aSAH$outcome, aSAH$s100b,
              boot.n=500, conf.level=0.9, stratified=FALSE,
              thresholds=c(0.5, 1, 2))

## End(Not run)

# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome,
              aSAH$s100b, ci=TRUE, of="thresholds")
rocobj$ci

# Plotting the CI
plot(rocobj)
plot(rocobj$ci)
```

`coords` *Coordinates of a ROC curve*

Description

This function returns the coordinates of the ROC curve at the specified point.

[32] http://dx.doi.org/10.1186/1471-2105-12-77
[33] http://www.jstatsoft.org/v40/i01

Usage

```
coords(...)
## S3 method for class 'roc'
coords(roc, x, input=c("threshold", "specificity",
"sensitivity"), ret=c("threshold", "specificity", "sensitivity"),
as.list=FALSE, drop=TRUE, best.method=c("youden", "closest.topleft"),
best.weights=c(1, 0.5), transpose = TRUE, ...)
## S3 method for class 'smooth.roc'
coords(smooth.roc, x, input=c("specificity",
"sensitivity"), ret=c("specificity", "sensitivity"), as.list=FALSE,
drop=TRUE, best.method=c("youden", "closest.topleft"),
best.weights=c(1, 0.5), transpose = TRUE, ...)
```

Arguments

`roc, smooth.roc`	a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.
`x`	the coordinates to look for. Numeric (if so, their meaning is defined by the `input` argument) or one of "all" (all the points of the ROC curve), "local maximas" (the local maximas of the ROC curve) or "best" (see `best.method` argument). If missing or `NULL`, defaults to "all".
`input`	If `x` is numeric, the kind of input coordinate (x). One of "threshold", "specificity" or "sensitivity". Can be shortenend (for example to "thr", "sens" and "spec", or even to "t", "se" and "sp"). Note that "threshold" is not allowed in `coords.smooth.roc`, and that the argument is ignored when `x` is a character.
`ret`	The coordinates to return. See "Valid `ret` arguments" section below. Alternatively, the single value "all" can be used to return every coordinate available.
`as.list`	DEPRECATED. If the returned object must be a list. Will be removed in a future version.
`drop`	If `TRUE` the result is coerced to the lowest possible dimension, as per Extract. With `FALSE` if either `ret` or `x` is of length 1, the object returned will have the same format than if `x` was of length > 1.
`best.method`	if `x="best"`, the method to determine the best threshold. See details in the 'Best thresholds' section.
`best.weights`	if `x="best"`, the weights to determine the best threshold. See details in the 'Best thresholds' section.
`transpose`	when returning a matrix (`as.list=FALSE`), whether to return of thresholds in columns (`TRUE`) or rows (`FALSE`). The current default is `TRUE` and has been so since the initial version. However an upcoming version will change the default to `FALSE`, and a warning is printed if the argument is not passed explicitly. See coords_transpose for more details about upcoming changes.
`...`	further arguments passed from other methods. Ignored.

Details

This function takes a "roc" or "smooth.roc" object as first argument, on which the coordinates will be determined. The coordinates are defined by the `x` and `input` arguments. "threshold" coordinates cannot be determined in a smoothed ROC.

If `input="threshold"`, the coordinates for the threshold are reported, even if the exact threshold do not define the ROC curve. The following convenience characters are allowed: "all", "local maximas" and "best". They will return all the thresholds, only the thresholds defining local maximas (upper angles of the ROC curve), or only the threshold(s) corresponding to the best sum of sensitivity + specificity respectively. Note that "best" can return more than one threshold. If `x` is a character, the coordinates are limited to the thresholds within the partial AUC if it has been defined, and not necessarily to the whole curve.

For `input="specificity"` and `input="sensitivity"`, the function checks if the specificity or sensitivity is one of the points of the ROC curve (in `roc$sensitivities` or `roc$specificities`). More than one point may match (in *step* curves), then only the upper-left-most point coordinates are returned. Otherwise, the specificity and specificity of the point is interpolated and `NA` is returned as threshold.

The coords function in this package is a generic, but it might be superseded by functions in other packages such as **colorspace** or **spatstat** if they are loaded after **pROC**. In this case, call the `coords.roc` or `coords.smooth.roc` functions directly.

Best thresholds: If `x="best"`, the `best.method` argument controls how the optimal threshold is determined.

"youden" Youden's J statistic (Youden, 1950) is employed. The optimal cut-off is the threshold that maximizes the distance to the identity (diagonal) line. Can be shortened to "y".
The optimality criterion is:

$$max(sensitivities + specificities)$$

"closest.topleft" The optimal threshold is the point closest to the top-left part of the plot with perfect sensitivity or specificity. Can be shortened to "c" or "t".
The optimality criterion is:

$$min((1 - sensitivities)^2 + (1 - specificities)^2)$$

In addition, weights can be supplied if false positive and false negative predictions are not equivalent: a numeric vector of length 2 to the `best.weights` argument. The elements define

1. the relative cost of of a false negative classification (as compared with a false positive classification)
2. the prevalence, or the proportion of cases in the population ($\frac{n_{cases}}{n_{controls}+n_{cases}}$).

The optimality criteria are modified as proposed by Perkins and Schisterman:

"youden"

$$max(sensitivities + r * specificities)$$

"closest.topleft"

$$min((1 - sensitivities)^2 + r * (1 - specificities)^2)$$

with

$$r = \frac{1 - prevalence}{cost * prevalence}$$

By default, prevalence is 0.5 and cost is 1 so that no weight is applied in effect.
Note that several thresholds might be equally optimal.

Valid `ret` arguments:

The following table lists valid `ret` arguments.

Value	Description	Formula	Synonyms
`threshold`	The threshold value	-	-
`tn`	True negative count	-	-
`tp`	True positive count	-	-
`fn`	False negative count	-	-
`fp`	False positive count	-	-
`specificity`	Specificity	tn / (tn + fp)	tnr
`sensitivity`	Sensitivity	tp / (tp + fn)	recall, tpr
`accuracy`	Accuracy	(tp + tn) / N	-
`npv`	Negative Predictive Value	tn / (tn + fn)	-
`ppv`	Positive Predictive Value	tp / (tp + fp)	precision
`precision`	Precision	tp / (tp + fp)	ppv
`recall`	Recall	tp / (tp + fn)	sensitivity, tpr
`tpr`	True Positive Rate	tp / (tp + fn)	sensitivity, recall
`fpr`	False Positive Rate	fp / (tn + fp)	1-specificity
`tnr`	True Negative Rate	tn / (tn + fp)	specificity
`fnr`	False Negative Rate	fn / (tp + fn)	1-sensitivity
`fdr`	False Discovery Rate	fp / (tp + fp)	1-ppv
`youden`	Youden Index	se + r * sp	-
`closest.topleft`	Distance to the top left corner of the ROC space	- ((1 - se)^2 + r * (1 - sp)^2)	-

The value "threshold" is not allowed in `coords.smooth.roc`.

Values can be shortenend (for example to "thr", "sens" and "spec", or even to "se", "sp" or "1-np"). In addition, some values can be prefixed with `1-` to get their complement: `1-specificity`, `1-sensitivity`, `1-accuracy`, `1-npv`, `1-ppv` (but they cannot be shortened).

The values `npe` and `ppe` are automatically replaced with `1-npv` and `1-ppv`, respectively (and will therefore not appear as is in the output, but as `1-npv` and `1-ppv` instead). These must be used verbatim in ROC curves with `percent=TRUE` (ie. "100-ppv" is never accepted).

The "youden" and "closest.topleft" are weighted with `r`, according to the value of the `best.weights` argument. See the "Best thresholds" section above for more details.

The single value "all" can be used to return every coordinate available.

Value

Depending on the length of `x` and `as.list` argument.

length(x) == 1 or length(ret) == 1

`as.list=TRUE` a list of the length of, in the order of, and named after, `ret`.
`as.list=FALSE` a numeric vector of the length of, in the order of, and named after, `ret` (if `length(x) == 1`) or a num

In all cases if `input="specificity"` or `input="sensitivity"` and interpolation was required, threshold is returned as `NA`.

Note that if giving a character as `x` ("all", "local maximas" or "best"), you cannot predict the dimension of the return value unless `drop=FALSE`. Even "best" may return more than one value (for example if the ROC curve is below the identity line, both extreme points).

`coords` may also return `NULL` when there a partial area is defined but no point of the ROC curve falls within the region.

References

Neil J. Perkins, Enrique F. Schisterman (2006) "The Inconsistency of "Optimal" Cutpoints Obtained using Two Criteria based on the Receiver Operating Characteristic Curve". *American Journal of Epidemiology* **163**(7), 670–675. DOI: 10.1093/aje/kwj063[34].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[35].

W. J. Youden (1950) "Index for rating diagnostic tests". *Cancer*, **3**, 32–35. DOI: 10.1002/1097-0142(1950)3:1<32::AID-CNCR2820030106>3.0.CO;2-3[36].

See Also

`roc`, `ci.coords`

Examples

```
data(aSAH)

# Print a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b, percent = TRUE)

# Get the coordinates of S100B threshold 0.55
coords(rocobj, 0.55, transpose = FALSE)

# Get the coordinates at 50% sensitivity
coords(roc=rocobj, x=50, input="sensitivity", transpose = FALSE)
# Can be abbreviated:
coords(rocobj, 50, "se", transpose = FALSE)

# Works with smoothed ROC curves
coords(smooth(rocobj), 90, "specificity", transpose = FALSE)
```

[34] http://dx.doi.org/10.1093/aje/kwj063
[35] http://dx.doi.org/10.1186/1471-2105-12-77
[36] http://dx.doi.org/10.1002/1097-0142(1950)3\%3A1\%3C32\%3A\%3AAID-CNCR2820030106\%3E3.0.CO\%3B2-3

```
# Get the sensitivities for all thresholds
sensitivities <- coords(rocobj, rocobj$thresholds, "thr", "se", transpose = FALSE)
print(sensitivities)

# This is equivalent to taking sensitivities from rocobj directly
stopifnot(all.equal(as.vector(rocobj$sensitivities), as.vector(sensitivities)))
# You could also write:
sensitivities <- coords(rocobj, "all", ret="se", transpose = FALSE)
stopifnot(all.equal(as.vector(rocobj$sensitivities), as.vector(sensitivities)))

# Get the best threshold
coords(rocobj, "b", ret="t", transpose = FALSE)

# Get the best threshold according to different methods
rocobj <- roc(aSAH$outcome, aSAH$ndka, percent=TRUE)
coords(rocobj, "best", ret="threshold", transpose = FALSE,
       best.method="youden") # default
coords(rocobj, "best", ret="threshold", transpose = FALSE,
       best.method="closest.topleft")

# and with different weights
coords(rocobj, "best", ret="threshold", transpose = FALSE,
       best.method="youden", best.weights=c(50, 0.2))
coords(rocobj, "best", ret="threshold", transpose = FALSE,
       best.method="closest.topleft", best.weights=c(5, 0.2))

# and plot them
plot(rocobj, print.thres="best", print.thres.best.method="youden")
plot(rocobj, print.thres="best", print.thres.best.method="closest.topleft")
plot(rocobj, print.thres="best", print.thres.best.method="youden",
                                 print.thres.best.weights=c(50, 0.2))
plot(rocobj, print.thres="best", print.thres.best.method="closest.topleft",
                                 print.thres.best.weights=c(5, 0.2))

# Return more values:
coords(rocobj, "best", ret=c("threshold", "specificity", "sensitivity", "accuracy",
                             "precision", "recall"), transpose = FALSE)

# Return all values
coords(rocobj, "best", ret = "all", transpose = FALSE)

# You can use coords to plot for instance a sensitivity + specificity vs. cut-off diagram

plot(specificity + sensitivity ~ threshold,
     coords(rocobj, "all", transpose = FALSE),
     type = "l", log="x",
     subset = is.finite(threshold))

# Plot the Precision-Recall curve
plot(precision ~ recall,
     coords(rocobj, "all", ret = c("recall", "precision"), transpose = FALSE),
     type="l", ylim = c(0, 100))
```

```
# Alternatively plot the curve with TPR and FPR instead of SE/SP
# (identical curve, only the axis change)
plot(tpr ~ fpr,
     coords(rocobj, "all", ret = c("tpr", "fpr"), transpose = FALSE),
     type="l")
```

`coords_transpose` *Transposing the output of* `coords`

Description

This help page desribes recent and upcoming changes in the return values of the `coords` function.

Background information

Since the initial release of pROC, the `coords` has been returning a matrix with thresholds in columns, and the coordinate variables in rows.

```
data(aSAH)
rocobj <- roc(aSAH$outcome, aSAH$s100b)
coords(rocobj, c(0.05, 0.2, 0.5))
#                    0.05       0.2       0.5
# threshold   0.05000000 0.2000000 0.5000000
# specificity 0.06944444 0.8055556 0.9722222
# sensitivity 0.97560976 0.6341463 0.2926829
```

This format doesn't conform to the grammar of the tidyverse[37] which has become prevalent in modern R language.

In addition, the dropping of dimensions by default makes it difficult to guess what type of data `coords` is going to return.

```
coords(rocobj, "best")
#   threshold specificity sensitivity
#   0.2050000   0.8055556   0.6341463
# A numeric vector
```

Although it is possible to pass `drop = FALSE`, the fact that it is not the default makes the behaviour unintuitive.

In an upcoming version of pROC, this will be changed and `coords` will return a `data.frame` with the thresholds in rows and measurement in colums by default.

[37] `https://www.tidyverse.org/`

Changes in 1.15

1. Addition of the `transpose` argument.
2. Display a warning if `transpose` is missing. Pass `transpose` explicitly to silence the warning.
3. Deprecation of `as.list`.

With `transpose = FALSE`, the output is a `data.frame` looking like this:

```
 coords(rocobj, c(0.05, 0.2, 0.5), transpose = FALSE)
#      threshold specificity sensitivity
# 0.05      0.05  0.06944444   0.9756098
# 0.2       0.20  0.80555556   0.6341463
# 0.5       0.50  0.97222222   0.2926829
```

It is recommended that new developments set `transpose = FALSE` explicitly.

These changes are neutral to the API and do not affect functionality outside of a warning.

Upcoming backward incompatible changes in future versions

The next version of pROC will change the default `transpose` to `FALSE`. This is a backward incompatible change that will break any script that did not previously set `transpose` and will initially come with a warning to make debugging easier. The warning will eventually be removed. Scripts that set `transpose` explicitly will be unaffected.

Recommendations

If you are writing a script calling the `coords` function, set `transpose = FALSE` to silence the warning and make sure your script keeps running smoothly once the default `transpose` is changed to `FALSE`.

See also

The GitHub issue tracking the changes described in this manual page[38].

`cov.roc` *Covariance of two paired ROC curves*

Description

This function computes the covariance between the AUC of two correlated (or paired) ROC curves.

[38] `https://github.com/xrobin/pROC/issues/54`

Usage

```
cov(...)
## Default S3 method:
cov(...)
## S3 method for class 'auc'
cov(roc1, roc2, ...)
## S3 method for class 'smooth.roc'
cov(roc1, roc2, ...)
## S3 method for class 'roc'
cov(roc1, roc2, method=c("delong", "bootstrap", "obuchowski"),
  reuse.auc=TRUE, boot.n=2000, boot.stratified=TRUE, boot.return=FALSE,
  progress=getOption("pROCProgress")$name, parallel=FALSE, ...)
```

Arguments

`roc1, roc2`	the two ROC curves on which to compute the covariance. Either "roc", "auc" or "smooth.roc" objects (types can be mixed as long as the original ROC curve are paired).
`method`	the method to use, either "delong" or "bootstrap". The first letter is sufficient. If omitted, the appropriate method is selected as explained in details.
`reuse.auc`	if `TRUE` (default) and the "roc" objects contain an "auc" field, re-use these specifications for the test. See details.
`boot.n`	for `method="bootstrap"` only: the number of bootstrap replicates or permutations. Default: *2000*.
`boot.stratified`	for `method="bootstrap"` only: should the bootstrap be stratified (same number of cases/controls in each replicate than in the original sample) or not. Default: *TRUE*.
`boot.return`	if *TRUE* and `method="bootstrap"`, also return the bootstrapped values. See the "Value" section for more details.
`progress`	the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.
`parallel`	if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).
`...`	further arguments passed to or from other methods, especially arguments for `cov.roc` when calling `cov`, `cov.auc` or `cov.smooth.roc`. Arguments for `auc` (if `reuse.auc=FALSE`) and `txtProgressBar` (only `char` and `style`) if applicable.

Details

This function computes the covariance between the AUC of two correlated (or paired, according to the detection of `are.paired`) ROC curves. It is typically called with the two roc objects of interest. Two methods are available: "delong" and "bootstrap" (see "Computational details" section below).

The default is to use "delong" method except with partial AUC and smoothed curves where "bootstrap" is employed. Using "delong" for partial AUC and smoothed ROCs is not supported.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided `density.cases` or `density.controls` the bootstrap cannot be performed and an error is issued.

`cov.default` forces the usage of the `cov` function in the **stats** package, so that other code relying on `cov` should continue to function normally.

Value

The numeric value of the covariance.

If `boot.return=TRUE` and `method="bootstrap"`, an attribute `resampled.values` is set with the resampled (bootstrapped) values. It contains a matrix with the columns representing the two ROC curves, and the rows the `boot.n` bootstrap replicates.

AUC specification

To compute the covariance of the AUC of the ROC curves, `cov` needs a specification of the AUC. The specification is defined by:

1. the "auc" field in the "roc" objects if `reuse.auc` is set to `TRUE` (default)
2. passing the specification to `auc` with ... (arguments `partial.auc`, `partial.auc.correct` and `partial.auc.focus`). In this case, you must ensure either that the `roc` object do not contain an `auc` field (if you called `roc` with `auc=FALSE`), or set `reuse.auc=FALSE`.

If `reuse.auc=FALSE` the `auc` function will always be called with `...` to determine the specification, even if the "roc" objects do contain an `auc` field.

As well if the "roc" objects do not contain an `auc` field, the `auc` function will always be called with `...` to determine the specification.

Warning: if the roc object passed to roc.test contains an `auc` field and `reuse.auc=TRUE`, auc is not called and arguments such as `partial.auc` are silently ignored.

Computation details

With `method="bootstrap"`, the processing is done as follow:

1. `boot.n` bootstrap replicates are drawn from the data. If `boot.stratified` is *TRUE*, each replicate contains exactly the same number of controls and cases than the original sample, otherwise if *FALSE* the numbers can vary.
2. for each bootstrap replicate, the AUC of the two ROC curves are computed and stored.
3. the variance (as per `var.roc`) of the resampled AUCs and their covariance are assessed in a single bootstrap pass.
4. The following formula is used to compute the final covariance: $Var[AUC1] + Var[AUC2] - 2cov[AUC1, AUC2]$

With `method="delong"`, the processing is done as described in Hanley and Hajian-Tilaki (1997) using the algorithm by Sun and Xu (2014).

With `method="obuchowski"`, the processing is done as described in Obuchowski and McClish (1997), Table 1 and Equation 5, p. 1531. The computation of g for partial area under the ROC curve is modified as:

$$expr1 * (2 * pi * expr2)^{(-1)} * (-expr4) - A * B * expr1 * (2 * pi * expr2^3)^{(-1/2)} * expr3$$

.

Binormality assumption

The "obuchowski" method makes the assumption that the data is binormal. If the data shows a deviation from this assumption, it might help to normalize the data first (that is, before calling `roc`), for example with quantile normalization:

```
norm.x <- qnorm(rank(x)/(length(x)+1))
cov(roc(response, norm.x, ...), ...)
```

"delong" and "bootstrap" methods make no such assumption.

Errors

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the covariance on ROC curves smoothed with density.controls and density.cases." is issued.

Warnings

If "auc" specifications are different in both roc objects, the warning "Different AUC specifications in the ROC curves. Enforcing the inconsistency, but unexpected results may be produced." is issued. Unexpected results may be produced.

If one or both ROC curves are "smooth.roc" objects with different smoothing specifications, the warning "Different smoothing parameters in the ROC curves. Enforcing the inconsistency, but unexpected results may be produced." is issued. This warning can be benign, especially if ROC curves were generated with `roc(...,smooth=TRUE)` with different arguments to other functions (such as plot), or if you really want to compare two ROC curves smoothed differently.

If `method="delong"` and the AUC specification specifies a partial AUC, the warning "Using DeLong for partial AUC is not supported. Using bootstrap test instead." is issued. The `method` argument is ignored and "bootstrap" is used instead.

If `method="delong"` and the ROC curve is smoothed, the warning "Using DeLong for smoothed ROCs is not supported. Using bootstrap instead." is issued. The `method` argument is ignored and "bootstrap" is used instead.

DeLong ignores the direction of the ROC curve so that if two ROC curves have a different `direction`, the warning ""DeLong should not be applied to ROC curves with a different direction."" is printed. However, the spurious computation is enforced.

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that

there are not enough points for smoothing, producing a NA area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep boot.stratified=TRUE.

When both ROC curves have an auc of 1 (or 100%), their covariance will always be null. This is true for both "delong" and "bootstrap" and methods. This result is misleading, as the covariance is of course not null. A warning will be displayed to inform of this condition, and of the misleading output.

Messages

The covariance can only be computed on paired data. This assumption is enforced by are.paired. If the ROC curves are not paired, the covariance is 0 and the message "ROC curves are unpaired." is printed. If your ROC curves are paired, make sure they fit are.paired criteria.

References

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

James A. Hanley and Karim O. Hajian-Tilaki (1997) "Sampling variability of nonparametric estimates of the areas under receiver operating characteristic curves: An update". *Academic Radiology* **4**, 49–58. DOI: 10.1016/S1076-6332(97)80161-4[39].

Nancy A. Obuchowski, Donna K. McClish (1997). "Sample size determination for diagnostic accurary studies involving binormal ROC curve indices". *Statistics in Medicine*, **16**(13), 1529–1542. DOI: (SICI)1097-0258(19970715)16:13<1529::AID-SIM565>3.0.CO;2-H[40].

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[41].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[42].

See Also

roc, var.roc

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

# Basic example with 2 roc objects
roc1 <- roc(aSAH$outcome, aSAH$s100b)
roc2 <- roc(aSAH$outcome, aSAH$wfns)
```

[39] http://dx.doi.org/10.1016/S1076-6332(97)80161-4

[40] http://dx.doi.org/10.1002/(SICI)1097-0258(19970715)16\%3A13\%3C1529\%3A\%3AAID-SIM565\%3E3.0.CO\%3B2-H

[41] http://dx.doi.org/10.1109/LSP.2014.2337313

[42] http://www.jstatsoft.org/v40/i01

```
cov(roc1, roc2)

## Not run:
# The latter used Delong. To use bootstrap:
cov(roc1, roc2, method="bootstrap")
# Decrease boot.n for a faster execution:
cov(roc1, roc2, method="bootstrap", boot.n=1000)

## End(Not run)

# To use Obuchowski:
cov(roc1, roc2, method="obuchowski")

## Not run:
# Comparison can be done on smoothed ROCs
# Smoothing is re-done at each iteration, and execution is slow
cov(smooth(roc1), smooth(roc2))

## End(Not run)
# or from an AUC (no smoothing)
cov(auc(roc1), roc2)

## Not run:
# With bootstrap and return.values, one can compute the variances of the
# ROC curves in one single bootstrap run:
cov.rocs <- cov(roc1, roc2, method="bootstrap", boot.return=TRUE)
# var(roc1):
var(attr(cov.rocs, "resampled.values")[,1])
# var(roc2):
var(attr(cov.rocs, "resampled.values")[,2])

## End(Not run)

## Not run:
# Covariance of partial AUC:
roc3 <- roc(aSAH$outcome, aSAH$s100b, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.8), partial.auc.focus="se")
cov(roc3, roc4)
# This is strictly equivalent to:
cov(roc3, roc4, method="bootstrap")

# Alternatively, we could re-use roc1 and roc2 to get the same result:
cov(roc1, roc2, reuse.auc=FALSE, partial.auc=c(1, 0.8), partial.auc.focus="se")

## End(Not run)

# Spurious use of DeLong's test with different direction:
roc5 <- roc(aSAH$outcome, aSAH$s100b, direction="<")
roc6 <- roc(aSAH$outcome, aSAH$s100b, direction=">")
cov(roc5, roc6, method="delong")

## Test data from Hanley and Hajian-Tilaki, 1997
disease.present <- c("Yes", "No", "Yes", "No", "No", "Yes", "Yes", "No",
```

```
                      "No", "Yes", "No", "No", "Yes", "No", "No")
field.strength.1 <- c(1, 2, 5, 1, 1, 1, 2, 1, 2, 2, 1, 1, 5, 1, 1)
field.strength.2 <- c(1, 1, 5, 1, 1, 1, 4, 1, 2, 2, 1, 1, 5, 1, 1)
roc7 <- roc(disease.present, field.strength.1)
roc8 <- roc(disease.present, field.strength.2)
# Assess the covariance:
cov(roc7, roc8)

## Not run:
# With bootstrap:
cov(roc7, roc8, method="bootstrap")

## End(Not run)
```

`ggroc.roc` *Plot a ROC curve with ggplot2*

Description

This function plots a ROC curve with ggplot2.

Usage

```
## S3 method for class 'roc'
ggroc(data, legacy.axes = FALSE, ...)
## S3 method for class 'list'
ggroc(data, aes = c("colour", "alpha", "linetype", "size", "group"),
      legacy.axes = FALSE, ...)
```

Arguments

`data`	a roc object from the roc function, or a list of roc objects.
`aes`	the name(s) of the aesthetics for `geom_line` to map to the different ROC curves supplied. Use "group" if you want the curves to appear with the same aestetic, for instance if you are faceting instead.
`legacy.axes`	a logical indicating if the specificity axis (x axis) must be plotted as as decreasing "specificity" (`FALSE`, the default) or increasing "1 - specificity" (`TRUE`) as in most legacy software.
`...`	additional aesthetics for `geom_line` to set: `alpha`, `colour`, `linetype` and `size`.

Details

This function initializes a ggplot object from a ROC curve (or multiple if a list is passed). It returns the ggplot with a line layer on it. You can print it directly or add your own layers and theme elements.

See Also

roc, plot.roc, **ggplot2**

Examples

```
# Create a basic roc object
data(aSAH)
rocobj <- roc(aSAH$outcome, aSAH$s100b)
rocobj2 <- roc(aSAH$outcome, aSAH$wfns)

library(ggplot2)
g <- ggroc(rocobj)
g
# with additional aesthetics:
ggroc(rocobj, alpha = 0.5, colour = "red", linetype = 2, size = 2)

# You can then your own theme, etc.
g + theme_minimal() + ggtitle("My ROC curve") +
    geom_segment(aes(x = 1, xend = 0, y = 0, yend = 1), color="grey", linetype="dashed")

# And change axis labels to FPR/FPR
gl <- ggroc(rocobj, legacy.axes = TRUE)
gl
gl + xlab("FPR") + ylab("TPR") +
    geom_segment(aes(x = 0, xend = 1, y = 0, yend = 1), color="darkgrey", linetype="dashed")

# Multiple curves:
g2 <- ggroc(list(s100b=rocobj, wfns=rocobj2, ndka=roc(aSAH$outcome, aSAH$ndka)))
g2

# This is equivalent to using roc.formula:
roc.list <- roc(outcome ~ s100b + ndka + wfns, data = aSAH)
g.list <- ggroc(roc.list)
g.list

# with additional aesthetics:
g3 <- ggroc(roc.list, linetype=2)
g3
g4 <- ggroc(roc.list, aes="linetype", color="red")
g4
# changing multiple aesthetics:
g5 <- ggroc(roc.list, aes=c("linetype", "color"))
g5

# OR faceting
g.list + facet_grid(.~name) + theme(legend.position="none")
# To have all the curves of the same color, use aes="group":
g.group <- ggroc(roc.list, aes="group")
g.group
g.group + facet_grid(.~name)
```

`groupGeneric` *pROC Group Generic Functions*

Description

Redefine **base** groupGeneric functions to handle `auc` and `ci` objects properly on operations and mathematical operations. Attributes are dropped so that the AUC/CI behaves as a numeric value/matrix, respectively. In the case of AUC, all attributes are dropped, while in CI only the CI-specific attributes are, keeping those necessary for the matrices.

Usage

```
Math(x, ...)
Ops(e1, e2)
```

Arguments

`x, e1, e2`	`auc` objects, or mixed numerics and `auc` objects.
`...`	further arguments passed to other Math methods.

See Also

`groupGeneric`, `auc`

Examples

```
data(aSAH)

# Create a roc object:
aucobj1 <- auc(roc(aSAH$outcome, aSAH$s100b))
aucobj2 <- auc(roc(aSAH$outcome, aSAH$wfns))

# Math
sqrt(aucobj1)
round(aucobj2, digits=1)

# Ops
aucobj1 * 2
2 * aucobj2
aucobj1 + aucobj2

# With CI
ciaucobj <- ci(aucobj1)
ciaucobj * 2
sqrt(ciaucobj)
```

`has.partial.auc` *Does the ROC curve have a partial AUC?*

Description

This function determines if the ROC curve has a partial AUC.

Usage

```
has.partial.auc(roc)
## S3 method for class 'auc'
has.partial.auc(roc)
## S3 method for class 'smooth.roc'
has.partial.auc(roc)
## S3 method for class 'roc'
has.partial.auc(roc)
```

Arguments

`roc`	the ROC curve to check.

Value

`TRUE` if the AUC is a partial AUC, `FALSE` otherwise.

If the AUC is not defined (i. e. if roc was called with `AUC=FALSE`), returns `NULL`.

See Also

`auc`

Examples

```
data(aSAH)

# Full AUC
roc1 <- roc(aSAH$outcome, aSAH$s100b)
has.partial.auc(roc1)
has.partial.auc(auc(roc1))
has.partial.auc(smooth(roc1))

# Partial AUC
roc2 <- roc(aSAH$outcome, aSAH$s100b, partial.auc = c(1, 0.9))
has.partial.auc(roc2)
has.partial.auc(smooth(roc2))

# No AUC
roc3 <- roc(aSAH$outcome, aSAH$s100b, auc = FALSE)
has.partial.auc(roc3)
```

lines.roc *Add a ROC line to a ROC plot*

Description

This convenience function adds a ROC line to a ROC curve.

Usage

```
## S3 method for class 'roc'
lines(x, ...)
## S3 method for class 'smooth.roc'
lines(x, ...)
## S3 method for class 'roc'
lines.roc(x, lwd=2, ...)
## S3 method for class 'formula'
lines.roc(x, data, subset, na.action, ...)
## Default S3 method:
lines.roc(x, predictor, ...)
## S3 method for class 'smooth.roc'
lines.roc(x, ...)
```

Arguments

x	a roc object from the roc function (for plot.roc.roc), a formula (for plot.roc.formula) or a response vector (for plot.roc.default).
predictor, data	arguments for the roc function.
subset,na.action	arguments for model.frame
lwd	line width (see par).
...	graphical parameters for lines, and especially type (see plot.default) and arguments for par such as col (color), lty (line type) or line characteristics lend, ljoin and lmitre.

Value

This function returns a list of class "roc" invisibly. See roc for more details.

See Also

roc, plot.roc

Examples

```
data(aSAH)

rocobj <- plot.roc(aSAH$outcome, aSAH$s100b, type="n")
lines(rocobj, type="b", pch=21, col="blue", bg="grey")

# Without using 'lines':
rocobj <- plot.roc(aSAH$outcome, aSAH$s100b, type="b", pch=21, col="blue", bg="grey")
```

---

multiclass.roc *Multi-class AUC*

Description

This function builds builds multiple ROC curve to compute the multi-class AUC as defined by Hand and Till.

Usage

```
multiclass.roc(...)
## S3 method for class 'formula'
multiclass.roc(formula, data, ...)
## Default S3 method:
multiclass.roc(response, predictor,
levels=base::levels(as.factor(response)),
percent=FALSE, direction = c("auto", "<", ">"), ...)
```

Arguments

response	a factor, numeric or character vector of responses, typically encoded with 0 (controls) and 1 (cases), as in roc.
predictor	either a numeric vector, containing the value of each observation, as in roc, or, a matrix giving the decision value (e.g. probability) for each class.
formula	a formula of the type response~predictor.
data	a matrix or data.frame containing the variables in the formula. See model.frame for more details.
levels	the value of the response for controls and cases respectively. In contrast with levels argument to roc, all the levels are used and combined to compute the multiclass AUC.
percent	if the sensitivities, specificities and AUC must be given in percent (TRUE) or in fraction (FALSE, default).

direction — in which direction to make the comparison? "auto" (default for univariate curves): automatically define in which group the median is higher and take the direction accordingly. Not available for multivariate curves. ">" (default for multivariate curves): if the predictor values for the control group are higher than the values of the case group (controls > t >= cases). "<": if the predictor values for the control group are lower or equal than the values of the case group (controls < t <= cases).

... — further arguments passed to roc.

Details

This function performs multiclass AUC as defined by Hand and Till (2001). A multiclass AUC is a mean of several auc and cannot be plotted. Only AUCs can be computed for such curves. Confidence intervals, standard deviation, smoothing and comparison tests are not implemented.

The multiclass.roc function can handle two types of datasets: uni- and multi-variate. In the univariate case, a single predictor vector is passed and all the combinations of responses are assessed. I the multivariate case, a matrix or data.frame is passed as predictor. The columns must be named according to the levels of the response.

This function has been much less tested than the rest of the package and is more subject to bugs. Please report them if you find one.

Value

If predictor is a vector, a list of class "multiclass.roc" (univariate) or "mv.multiclass.roc" (multivariate), with the following fields:

auc — if called with auc=TRUE, a numeric of class "auc" as defined in auc. Note that this is not the standard AUC but the multi-class AUC as defined by Hand and Till.

ci — if called with ci=TRUE, a numeric of class "ci" as defined in ci.

response — the response vector as passed in argument. If NA values were removed, a na.action attribute similar to na.omit stores the row numbers.

predictor — the predictor vector as passed in argument. If NA values were removed, a na.action attribute similar to na.omit stores the row numbers.

levels — the levels of the response as defined in argument.

percent — if the sensitivities, specificities and AUC are reported in percent, as defined in argument.

call — how the function was called. See match.call for more details.

Warnings

If response is an ordered factor and one of the levels specified in levels is missing, a warning is issued and the level is ignored.

References

David J. Hand and Robert J. Till (2001). A Simple Generalisation of the Area Under the ROC Curve for Multiple Class Classification Problems. *Machine Learning* **45**(2), p. 171–186. DOI: 10.1023/A:1010920819831[43].

See Also

auc

Examples

```
####
# Examples for a univariate decision value
####
data(aSAH)

# Basic example
multiclass.roc(aSAH$gos6, aSAH$s100b)
# Produces an innocuous warning because one level has no observation

# Select only 3 of the aSAH$gos6 levels:
multiclass.roc(aSAH$gos6, aSAH$s100b, levels=c(3, 4, 5))

# Give the result in percent
multiclass.roc(aSAH$gos6, aSAH$s100b, percent=TRUE)

####
# Examples for multivariate decision values (e.g. class probabilities)
####

## Not run:
# Example with a multinomial log-linear model from nnet
# We use the iris dataset and split into a training and test set
requireNamespace("nnet")
data(iris)
iris.sample <- sample(1:150)
iris.train <- iris[iris.sample[1:75],]
iris.test <- iris[iris.sample[76:150],]
mn.net <- nnet::multinom(Species ~ ., iris.train)

# Use predict with type="prob" to get class probabilities
iris.predictions <- predict(mn.net, newdata=iris.test, type="prob")
head(iris.predictions)

# This can be used directly in multiclass.roc:
multiclass.roc(iris.test$Species, iris.predictions)

## End(Not run)
```

[43] http://dx.doi.org/10.1023/A:1010920819831

```
# Let's see an other example with an artificial dataset
n <- c(100, 80, 150)
responses <- factor(c(rep("X1", n[1]), rep("X2", n[2]), rep("X3", n[3])))
# construct prediction matrix: one column per class

preds <- lapply(n, function(x) runif(x, 0.4, 0.6))
predictor <- as.matrix(data.frame(
                "X1" = c(preds[[1]], runif(n[2] + n[3], 0, 0.7)),
                "X2" = c(runif(n[1], 0.1, 0.4), preds[[2]], runif(n[3], 0.2, 0.8)),
                "X3" = c(runif(n[1] + n[2], 0.3, 0.7), preds[[3]])
            ))
multiclass.roc(responses, predictor)

# One can change direction , partial.auc, percent, etc:
multiclass.roc(responses, predictor, direction = ">")
multiclass.roc(responses, predictor, percent = TRUE,
partial.auc = c(100, 90), partial.auc.focus = "se")


# Limit set of levels
multiclass.roc(responses, predictor, levels = c("X1", "X2"))
# Use with formula. Here we need a data.frame to store the responses as characters
data <- cbind(as.data.frame(predictor), "response" = responses)
multiclass.roc(response ~ X1+X3, data)
```

`plot.ci` *Plot confidence intervals*

Description

This function adds confidence intervals to a ROC curve plot, either as bars or as a confidence shape.

Usage

```
## S3 method for class 'ci.thresholds'
plot(x, length=.01*ifelse(attr(x,
  "roc")$percent, 100, 1), col=par("fg"), ...)
## S3 method for class 'ci.sp'
plot(x, type=c("bars", "shape"), length=.01*ifelse(attr(x,
"roc")$percent, 100, 1), col=ifelse(type=="bars", par("fg"),
"gainsboro"), no.roc=FALSE, ...)
## S3 method for class 'ci.se'
plot(x, type=c("bars", "shape"), length=.01*ifelse(attr(x,
"roc")$percent, 100, 1), col=ifelse(type=="bars", par("fg"),
"gainsboro"), no.roc=FALSE, ...)
```

Arguments

x	a confidence interval object from the functions ci.thresholds, ci.se or ci.sp.
type	type of plot, "bars" or "shape". Can be shortened to "b" or "s". "shape" is only available for ci.se and ci.sp, not for ci.thresholds.
length	the length (as plot coordinates) of the bar ticks. Only if type="bars".
no.roc	if FALSE, the ROC line is re-added over the shape. Otherwise if TRUE, only the shape is plotted. Ignored if type="bars"
col	color of the bars or shape.
...	further arguments for segments (if type="bars") or polygon (if type="shape").

Details

This function adds confidence intervals to a ROC curve plot, either as bars or as a confidence shape, depending on the state of the type argument. The shape is plotted over the ROC curve, so that the curve is re-plotted unless no.roc=TRUE.

Graphical functions are called with suppressWarnings.

Value

This function returns the confidence interval object invisibly.

Warnings

With type="shape", the warning "Low definition shape" is issued when the shape is defined by less than 15 confidence intervals. In such a case, the shape is not well defined and the ROC curve could pass outside the shape. To get a better shape, increase the number of intervals, for example with:

```
plot(ci.sp(rocobj, sensitivities=seq(0, 1, .01)), type="shape")
```

References

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[44].

See Also

plot.roc, ci.thresholds, ci.sp, ci.se

[44] http://dx.doi.org/10.1186/1471-2105-12-77

Examples

```
data(aSAH)
## Not run:
# Start a ROC plot
rocobj <- plot.roc(aSAH$outcome, aSAH$s100b)
plot(rocobj)
# Thresholds
ci.thresolds.obj <- ci.thresholds(rocobj)
plot(ci.thresolds.obj)
# Specificities
plot(rocobj) # restart a new plot
ci.sp.obj <- ci.sp(rocobj, boot.n=500)
plot(ci.sp.obj)
# Sensitivities
plot(rocobj) # restart a new plot
ci.se.obj <- ci(rocobj, of="se", boot.n=500)
plot(ci.se.obj)

# Plotting a shape. We need more
ci.sp.obj <- ci.sp(rocobj, sensitivities=seq(0, 1, .01), boot.n=100)
plot(rocobj) # restart a new plot
plot(ci.sp.obj, type="shape", col="blue")

# Direct syntax (response, predictor):
plot.roc(aSAH$outcome, aSAH$s100b,
         ci=TRUE, of="thresholds")

## End(Not run)
```

---

plot.roc *Plot a ROC curve*

Description

This function plots a ROC curve. It can accept many arguments to tweak the appearance of the plot. Two syntaxes are possible: one object of class "roc", or either two vectors (response, predictor) or a formula (response~predictor) as in the `roc` function.

Usage

```
## S3 method for class 'roc'
plot(x, ...)
## S3 method for class 'smooth.roc'
plot(x, ...)
## S3 method for class 'roc'
plot.roc(x, add=FALSE, reuse.auc=TRUE,
axes=TRUE, legacy.axes=FALSE,
# Generic arguments for par:
xlim=if(x$percent){c(100, 0)} else{c(1, 0)},
```

```
ylim=if(x$percent){c(0, 100)} else{c(0, 1)},
xlab=ifelse(x$percent, ifelse(legacy.axes, "100 - Specificity (%)", "Specificity (%
           ifelse(legacy.axes, "1 - Specificity", "Specificity")),
ylab=ifelse(x$percent, "Sensitivity (%)", "Sensitivity"),
asp=1,
mar=c(4, 4, 2, 2)+.1,
mgp=c(2.5, 1, 0),
# col, lty and lwd for the ROC line only
col=par("col"),
lty=par("lty"),
lwd=2,
type="l",
# Identity line
identity=!add,
identity.col="darkgrey",
identity.lty=1,
identity.lwd=1,
# Print the thresholds on the plot
print.thres=FALSE,
print.thres.pch=20,
print.thres.adj=c(-.05,1.25),
print.thres.col="black",
print.thres.pattern=ifelse(x$percent, "%.1f (%.1f%%, %.1f%%)", "%.3f (%.3f, %.3f)")
print.thres.cex=par("cex"),
print.thres.pattern.cex=print.thres.cex,
print.thres.best.method=NULL,
print.thres.best.weights=c(1, 0.5),
# Print the AUC on the plot
print.auc=FALSE,
print.auc.pattern=NULL,
print.auc.x=ifelse(x$percent, 50, .5),
print.auc.y=ifelse(x$percent, 50, .5),
print.auc.adj=c(0,1),
print.auc.col=col,
print.auc.cex=par("cex"),
# Grid
grid=FALSE,
grid.v={if(is.logical(grid) && grid[1]==TRUE)
          {seq(0, 1, 0.1) * ifelse(x$percent, 100, 1)}
        else if(is.numeric(grid))
          {seq(0, ifelse(x$percent, 100, 1), grid[1])} else {NULL}},
grid.h={if (length(grid) == 1) {grid.v}
        else if (is.logical(grid) && grid[2]==TRUE)
          {seq(0, 1, 0.1) * ifelse(x$percent, 100, 1)}
        else if(is.numeric(grid))
          {seq(0, ifelse(x$percent, 100, 1), grid[2])} else {NULL}},
grid.lty=3,
grid.lwd=1,
```

```
grid.col="#DDDDDD",
# Polygon for the AUC
auc.polygon=FALSE,
auc.polygon.col="gainsboro",
auc.polygon.lty=par("lty"),
auc.polygon.density=NULL,
auc.polygon.angle=45,
auc.polygon.border=NULL,
# Polygon for the maximal AUC possible
max.auc.polygon=FALSE,
max.auc.polygon.col="#EEEEEE",
max.auc.polygon.lty=par("lty"),
max.auc.polygon.density=NULL,
max.auc.polygon.angle=45,
max.auc.polygon.border=NULL,
# Confidence interval
ci=!is.null(x$ci),
ci.type=c("bars", "shape", "no"),
ci.col=ifelse(ci.type=="bars", par("fg"), "gainsboro"),
...)
## S3 method for class 'formula'
plot.roc(x, data, subset, na.action, ...)
## Default S3 method:
plot.roc(x, predictor, ...)
## S3 method for class 'smooth.roc'
plot.roc(x, ...)
```

Arguments

`x`	a roc object from the roc function (for plot.roc.roc), a formula (for plot.roc.formula) or a response vector (for plot.roc.default).
`predictor, data`	arguments for the roc function.
`subset,na.action`	arguments for `model.frame`
`add`	if TRUE, the ROC curve will be added to an existing plot. If FALSE (default), a new plot will be created.
`reuse.auc`	if `TRUE` (default) and the "roc" object contains an "auc" field, re-use these specifications for the plot (specifically `print.auc`, `auc.polygon` and `max.auc.polygon` arguments). See details.
`axes`	a logical indicating if the plot axes must be drawn.
`legacy.axes`	a logical indicating if the specificity axis (x axis) must be plotted as as decreasing "specificity" (`FALSE`, the default) or increasing "1 - specificity" (`TRUE`) as in most legacy software. This affects only the axis, not the plot coordinates.
`xlim, ylim, xlab, ylab, asp, mar, mgp`	Generic arguments for the plot. See plot and plot.window for more details. Only used if `add=FALSE`.

`col, lty, lwd` color, line type and line width for the ROC curve. See par for more details.

`type` type of plotting as in `plot`.

`identity` logical: whether or not the identity line (no discrimination line) must be displayed. Default: only on new plots.

`identity.col, identity.lty, identity.lwd`
color, line type and line width for the identity line. Used only if identity=TRUE. See par for more details.

`print.thres` Should a selected set of thresholds be displayed on the ROC curve? `FALSE`, `NULL` or "no": no threshold is displayed. `TRUE` or "best": the threshold with the highest sum sensitivity + specificity is plotted (this might be more than one threshold). "all": all the points of the ROC curve. "local maximas": all the local maximas. Numeric vector: direct definition of the thresholds to display. Note that on a smoothed ROC curve, only "best" is supported.

`print.thres.pch, print.thres.adj, print.thres.col, print.thres.cex`
the plotting character (pch), text string adjustment (adj), color (col) and character expansion factor (cex) parameters for the printing of the thresholds. See points and par for more details.

`print.thres.pattern`
the text pattern for the thresholds, as a sprintf format. Three numerics are passed to sprintf: threshold, specificity, sensitivity.

`print.thres.pattern.cex`
the character expansion factor (cex) for the threshold text pattern. See par for more details.

`print.thres.best.method, print.thres.best.weights`
if `print.thres="best"` or `print.thres=TRUE`, what method must be used to determine which threshold is the best. See argument `best.method` and `best.weights` to `coords` for more details.

`print.auc` boolean. Should the numeric value of AUC be printed on the plot?

`print.auc.pattern`
the text pattern for the AUC, as a sprintf format. If NULL, a reasonable value is computed that takes partial AUC, CI and percent into account. If the CI of the AUC was computed, three numerics are passed to sprintf: AUC, lower CI bound, higher CI bound. Otherwise, only AUC is passed.

`print.auc.x, print.auc.y`
x and y position for the printing of the AUC.

`print.auc.adj, print.auc.cex, print.auc.col`
the text adjustment, character expansion factor and color for the printing of the AUC. See par for more details.

`grid` boolean or numeric vector of length 1 or 2. Should a background grid be added to the plot? Numeric: show a grid with the specified interval between each line; Logical: show the grid or not. Length 1: same values are taken for horizontal and vertical lines. Length 2: grid value for vertical (grid[1]) and horizontal (grid[2]). Note that these values are used to compute grid.v and grid.h. Therefore if you specify a grid.h and grid.v, it will be ignored.

`grid.v, grid.h`
numeric. The x and y values at which a vertical or horizontal line (respectively) must be drawn. NULL if no line must be added.

`grid.lty, grid.lwd, grid.col`
: the line type (lty), line width (lwd) and color (col) of the lines of the grid. See par for more details. Note that you can pass vectors of length 2, in which case it specifies the vertical (1) and horizontal (2) lines.

`auc.polygon`
: boolean. Whether or not to display the area as a polygon.

`auc.polygon.col, auc.polygon.lty, auc.polygon.density, auc.polygon.angle, auc.polygon`
: color (col), line type (lty), density, angle and border for the AUC polygon. See `polygon` and `par` for more details.

`max.auc.polygon`
: boolean. Whether or not to display the maximal possible area as a polygon.

`max.auc.polygon.col, max.auc.polygon.lty, max.auc.polygon.density, max.auc.polygon.a`
: color (col), line type (lty), density, angle and border for the maximum AUC polygon. See `polygon` and `par` for more details.

`ci`
: boolean. Should we plot the confidence intervals?

`ci.type, ci.col`
: `type` and `col` arguments for `plot.ci`. The special value "no" disables the plotting of confidence intervals.

`...`
: further arguments passed to or from other methods, especially arguments for `roc` and `plot.roc.roc` when calling `plot.roc.default` or `plot.roc.formula`. Note that the `plot` argument for `roc` is not allowed. Arguments for `auc` and graphical functions `plot`, `abline`, `polygon`, `points`, `text` and `plot.ci` if applicable.

Details

This function is typically called from `roc` when plot=TRUE (not by default). `plot.roc.formula` and `plot.roc.default` are convenience methods that build the ROC curve (with the `roc` function) before calling `plot.roc.roc`. You can pass them arguments for both `roc` and `plot.roc.roc`. Simply use `plot.roc` that will dispatch to the correct method.

The plotting is done in the following order:

1. A new plot is created if `add=FALSE`.
2. The grid is added if `grid.v` and `grid.h` are not NULL.
3. The maximal AUC polygon is added if `max.auc.polygon=TRUE`.
4. The CI shape is added if `ci=TRUE`, `ci.type="shape"` and `x$ci` isn't a "ci.auc".
5. The AUC polygon is added if `auc.polygon=TRUE`.
6. The identity line if `identity=TRUE`.
7. The actual ROC line is added.
8. The CI bars are added if `ci=TRUE`, `ci.type="bars"` and `x$ci` isn't a "ci.auc".
9. The selected thresholds are printed if `print.thres` is `TRUE` or numeric.
10. The AUC is printed if `print.auc=TRUE`.

Graphical functions are called with suppressWarnings.

Value

This function returns a list of class "roc" invisibly. See roc for more details.

AUC specification

For `print.auc`, `auc.polygon` and `max.auc.polygon` arguments, an AUC specification is required. By default, the total AUC is plotted, but you may want a partial AUCs. The specification is defined by:

1. the "auc" field in the "roc" object if `reuse.auc` is set to `TRUE` (default). It is naturally inherited from any call to `roc` and fits most cases.
2. passing the specification to `auc` with ... (arguments `partial.auc`, `partial.auc.correct` and `partial.auc.focus`). In this case, you must ensure either that the `roc` object do not contain an `auc` field (if you called `roc` with `auc=FALSE`), or set `reuse.auc=FALSE`.

If `reuse.auc=FALSE` the `auc` function will always be called with `...` to determine the specification, even if the "roc" object do contain an `auc` field.

As well if the "roc" object do not contain an `auc` field, the `auc` function will always be called with `...` to determine the specification.

Warning: if the roc object passed to plot.roc contains an `auc` field and `reuse.auc=TRUE`, auc is not called and arguments such as `partial.auc` are silently ignored.

References

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[45].

See Also

`roc`, `auc`, `ci`

Examples

```
data(aSAH)

# Syntax (response, predictor):
plot.roc(aSAH$outcome, aSAH$s100b)

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
# identical:
plot(rocobj)
plot.roc(rocobj)

# Add a smoothed ROC:
plot.roc(smooth(rocobj), add=TRUE, col="blue")
legend("bottomright", legend=c("Empirical", "Smoothed"),
```

[45] http://dx.doi.org/10.1186/1471-2105-12-77

```
       col=c(par("fg"), "blue"), lwd=2)

# With more options:
plot(rocobj, print.auc=TRUE, auc.polygon=TRUE, grid=c(0.1, 0.2),
     grid.col=c("green", "red"), max.auc.polygon=TRUE,
     auc.polygon.col="blue", print.thres=TRUE)

# To plot a different partial AUC, we need to ignore the existing value
# with reuse.auc=FALSE:
plot(rocobj, print.auc=TRUE, auc.polygon=TRUE, partial.auc=c(1, 0.8),
     partial.auc.focus="se", grid=c(0.1, 0.2), grid.col=c("green", "red"),
     max.auc.polygon=TRUE, auc.polygon.col="blue", print.thres=TRUE,
     reuse.auc=FALSE)

# Add a line to the previous plot:
plot.roc(aSAH$outcome, aSAH$wfns, add=TRUE)

# Alternatively, you can get the plot directly from roc():
roc(aSAH$outcome, aSAH$s100b, plot=TRUE)
```

`power.roc.test` *Sample size and power computation for ROC curves*

Description

Computes sample size, power, significance level or minimum AUC for ROC curves.

Usage

```
power.roc.test(...)
# One or Two ROC curves test with roc objects:
## S3 method for class 'roc'
power.roc.test(roc1, roc2, sig.level = 0.05,
power = NULL, alternative = c("two.sided", "one.sided"),
reuse.auc=TRUE, method = c("delong", "bootstrap", "obuchowski"), ...)
# One ROC curve with a given AUC:
## S3 method for class 'numeric'
power.roc.test(auc = NULL, ncontrols = NULL,
ncases = NULL, sig.level = 0.05, power = NULL, kappa = 1,
alternative = c("two.sided", "one.sided"), ...)
# Two ROC curves with the given parameters:
## S3 method for class 'list'
power.roc.test(parslist, ncontrols = NULL,
ncases = NULL, sig.level = 0.05, power = NULL,  kappa = 1,
alternative = c("two.sided", "one.sided"), ...)
```

Arguments

roc1, roc2	one or two "roc" object from the roc function.
auc	expected AUC.
parslist	a list of parameters for the two ROC curves test with Obuchowski variance when no empirical ROC curve is known: **A1** binormal A parameter for ROC curve 1 **B1** binormal B parameter for ROC curve 1 **A2** binormal A parameter for ROC curve 2 **B2** binormal B parameter for ROC curve 2 **rn** correlation between the variables in control patients **ra** correlation between the variables in case patients **delta** the difference of AUC between the two ROC curves For a partial AUC, the following additional parameters must be set: **FPR11** Upper bound of FPR (1 - specificity) of ROC curve 1 **FPR12** Lower bound of FPR (1 - specificity) of ROC curve 1 **FPR21** Upper bound of FPR (1 - specificity) of ROC curve 2 **FPR22** Lower bound of FPR (1 - specificity) of ROC curve 2
ncontrols, ncases	number of controls and case observations available.
sig.level	expected significance level (probability of type I error).
power	expected power of the test (1 - probability of type II error).
kappa	expected balance between control and case observations. Must be positive. Only for sample size determination, that is to determine ncontrols and ncases.
alternative	whether a one or two-sided test is performed.
reuse.auc	if TRUE (default) and the "roc" objects contain an "auc" field, re-use these specifications for the test. See the *AUC specification* section for more details.
method	the method to compute variance and covariance, either "delong", "bootstrap" or "obuchowski". The first letter is sufficient. Only for Two ROC curves power calculation. See var and cov documentations for more details.
...	further arguments passed to or from other methods, especially auc (with reuse.auc=FALSE or no AUC in the ROC curve), cov and var (especially arguments method, boot.n and boot.stratified). Ignored (with a warning) with a parslist.

Value

An object of class power.htest (such as that given by power.t.test) with the supplied and computed values.

One ROC curve power calculation

If one or no ROC curves are passed to power.roc.test, a one ROC curve power calculation is performed. The function expects either power, sig.level or auc, or both ncontrols and

ncases to be missing, so that the parameter is determined from the others with the formula by Obuchowski *et al.*, 2004 (formulas 2 and 3, p. 1123).

For the sample size, ncases is computed directly from formulas 2 and 3 and ncontrols is deduced with kappa. AUC is optimized by uniroot while sig.level and power are solved as quadratic equations.

power.roc.test can also be passed a roc object from the roc function, but the empirical ROC will not be used, only the number of patients and the AUC.

Two paired ROC curves power calculation

If two ROC curves are passed to power.roc.test, the function will compute either the required sample size (if power is supplied), the significance level (if sig.level=NULL and power is supplied) or the power of a test of a difference between to AUCs according to the formula by Obuchowski and McClish, 1997*et al.* (formulas 2 and 3, p. 1530–1531). The null hypothesis is that the AUC of roc1 is the same than the AUC of roc2, with roc1 taken as the reference ROC curve.

For the sample size, ncases is computed directly from formula 2 and ncontrols is deduced from the ratio observed in roc1 and roc2. sig.level and power are solved as quadratic equations.

The variance and covariance of the ROC curve are computed with the var and cov functions. By default, DeLong method using the algorithm by Sun and Xu (2014) is used for full AUCs and the bootstrap for partial AUCs. It is possible to force the use of Obuchowski's variance by specifying method="obuchowski".

Alternatively when no empirical ROC curve is known, or if only one is available, a list can be passed to power.roc.test, with the contents defined in the "Arguments" section. The variance and covariance are computed from Table 1 and Equation 4 and 5 of Obuchowski and McClish (1997), p. 1530–1531.

Power calculation for unpaired ROC curves is not implemented.

AUC specification

The comparison of the AUC of the ROC curves needs a specification of the AUC. The specification is defined by:

1. the "auc" field in the "roc" objects if reuse.auc is set to TRUE (default)
2. passing the specification to auc with ... (arguments partial.auc, partial.auc.correct and partial.auc.focus). In this case, you must ensure either that the roc object do not contain an auc field (if you called roc with auc=FALSE), or set reuse.auc=FALSE.

If reuse.auc=FALSE the auc function will always be called with ... to determine the specification, even if the "roc" objects do contain an auc field.

As well if the "roc" objects do not contain an auc field, the auc function will always be called with ... to determine the specification.

Warning: if the roc object passed to roc.test contains an auc field and reuse.auc=TRUE, auc is not called and arguments such as partial.auc are silently ignored.

Acknowledgements

The authors would like to thank Christophe Combescure and Anne-Sophie Jannot for their help with the implementation of this section of the package.

References

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

Nancy A. Obuchowski, Donna K. McClish (1997). "Sample size determination for diagnostic accurary studies involving binormal ROC curve indices". *Statistics in Medicine*, **16**, 1529–1542. DOI: 10.1002/(SICI)1097-0258(19970715)16:13<1529::AID-SIM565>3.0.CO;2-H[46].

Nancy A. Obuchowski, Micharl L. Lieber, Frank H. Wians Jr. (2004). "ROC Curves in Clinical Chemistry: Uses, Misuses, and Possible Solutions". *Clinical Chemistry*, **50**, 1118–1125. DOI: 10.1373/clinchem.2004.031823[47].

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[48].

See Also

`roc`, `roc.test`

Examples

```
data(aSAH)

#### One ROC curve ####

# Build a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)

# Determine power of one ROC curve:
power.roc.test(rocobj)
# Same as:
power.roc.test(ncases=41, ncontrols=72, auc=0.73, sig.level=0.05)
# sig.level=0.05 is implicit and can be omitted:
power.roc.test(ncases=41, ncontrols=72, auc=0.73)

# Determine ncases & ncontrols:
power.roc.test(auc=rocobj$auc, sig.level=0.05, power=0.95, kappa=1.7)
power.roc.test(auc=0.73, sig.level=0.05, power=0.95, kappa=1.7)

# Determine sig.level:
power.roc.test(ncases=41, ncontrols=72, auc=0.73, power=0.95, sig.level=NULL)
```

[46] http://dx.doi.org/10.1002/(SICI)1097-0258(19970715)16\%3A13\%3C1529\%3A\%3AAID-SIM565\%3E3.0.CO\%3B2-H

[47] http://dx.doi.org/10.1373/clinchem.2004.031823

[48] http://dx.doi.org/10.1109/LSP.2014.2337313

```
# Derermine detectable AUC:
power.roc.test(ncases=41, ncontrols=72, sig.level=0.05, power=0.95)


#### Two ROC curves ####

###  Full AUC
roc1 <- roc(aSAH$outcome, aSAH$ndka)
roc2 <- roc(aSAH$outcome, aSAH$wfns)

## Sample size
# With DeLong variance (default)
power.roc.test(roc1, roc2, power=0.9)
# With Obuchowski variance
power.roc.test(roc1, roc2, power=0.9, method="obuchowski")

## Power test
# With DeLong variance (default)
power.roc.test(roc1, roc2)
# With Obuchowski variance
power.roc.test(roc1, roc2, method="obuchowski")

## Significance level
# With DeLong variance (default)
power.roc.test(roc1, roc2, power=0.9, sig.level=NULL)
# With Obuchowski variance
power.roc.test(roc1, roc2, power=0.9, sig.level=NULL, method="obuchowski")

### Partial AUC
roc3 <- roc(aSAH$outcome, aSAH$ndka, partial.auc=c(1, 0.9))
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.9))

## Sample size
# With bootstrap variance (default)
## Not run:
power.roc.test(roc3, roc4, power=0.9)

## End(Not run)
# With Obuchowski variance
power.roc.test(roc3, roc4, power=0.9, method="obuchowski")

## Power test
# With bootstrap variance (default)
## Not run:
power.roc.test(roc3, roc4)
# This is exactly equivalent:
power.roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(1, 0.9))

## End(Not run)
# With Obuchowski variance
power.roc.test(roc3, roc4, method="obuchowski")
```

```
## Significance level
# With bootstrap variance (default)
## Not run:
power.roc.test(roc3, roc4, power=0.9, sig.level=NULL)

## End(Not run)
# With Obuchowski variance
power.roc.test(roc3, roc4, power=0.9, sig.level=NULL, method="obuchowski")

## With only binormal parameters given
# From example 2 of Obuchowski and McClish, 1997.
ob.params <- list(A1=2.6, B1=1, A2=1.9, B2=1, rn=0.6, ra=0.6, FPR11=0,
FPR12=0.2, FPR21=0, FPR22=0.2, delta=0.037)

power.roc.test(ob.params, power=0.8, sig.level=0.05)
power.roc.test(ob.params, power=0.8, sig.level=NULL, ncases=107)
power.roc.test(ob.params, power=NULL, sig.level=0.05, ncases=107)
```

`print` *Print a ROC curve object*

Description

This function prints a ROC curve, AUC or CI object and return it invisibly.

Usage

```
## S3 method for class 'roc'
print(x, digits=max(3, getOption("digits") - 3), call=TRUE, ...)
## S3 method for class 'multiclass.roc'
print(x, digits=max(3, getOption("digits") -
  3), call=TRUE, ...)
## S3 method for class 'mv.multiclass.roc'
print(x, digits=max(3, getOption("digits") -
  3), call=TRUE, ...)
## S3 method for class 'smooth.roc'
print(x, digits=max(3, getOption("digits") - 3),
call=TRUE, ...)
## S3 method for class 'auc'
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'multiclass.auc'
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'ci.auc'
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'ci.thresholds'
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'ci.se'
```

```
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'ci.sp'
print(x, digits=max(3, getOption("digits") - 3), ...)
## S3 method for class 'ci.coords'
print(x, digits=max(3, getOption("digits") - 3), ...)
```

Arguments

x	a roc, auc or ci object, from the roc, auc or ci functions respectively.
call	if the call is printed.
digits	the number of significant figures to print. See signif for more details.
...	further arguments passed to or from other methods. In particular, print.roc calls print.auc and the print.ci variants internally, and a digits argument is propagated. Not used in print.auc and print.ci variants.

Value

These functions return the object they were passed invisibly.

See Also

roc, auc, ci, coords

Examples

```
data(aSAH)

# Print a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
print(rocobj)

# Print a smoothed roc object
print(smooth(rocobj))

# implicit printing
 roc(aSAH$outcome, aSAH$s100b)

# Print an auc and a ci object, from the ROC object or calling
# the dedicated function:
print(rocobj$auc)
print(ci(rocobj))
```

`roc` *Build a ROC curve*

Description

This is the main function of the pROC package. It builds a ROC curve and returns a "roc" object, a list of class "roc". This object can be `print`ed, `plot`ted, or passed to the functions `auc`, `ci`, `smooth.roc` and `coords`. Additionally, two `roc` objects can be compared with `roc.test`.

Usage

```
roc(...)
## S3 method for class 'formula'
roc(formula, data, ...)
## S3 method for class 'data.frame'
roc(data, response, predictor,
ret = c("roc", "coords", "all_coords"), ...)
## Default S3 method:
roc(response, predictor, controls, cases,
density.controls, density.cases,
levels=base::levels(as.factor(response)), percent=FALSE, na.rm=TRUE,
direction=c("auto", "<", ">"), algorithm = 6, quiet = FALSE,
smooth=FALSE, auc=TRUE, ci=FALSE, plot=FALSE, smooth.method="binormal",
smooth.n=512, ci.method=NULL, density=NULL, ...)
roc_(data, response, predictor, ret = c("roc", "coords", "all_coords"), ...)
```

Arguments

`response` a factor, numeric or character vector of responses, typically encoded with 0 (controls) and 1 (cases). Only two classes can be used in a ROC curve. If the vector contains more than two unique values, or if their order could be ambiguous, use `levels` to specify which values must be used as control and case value. If the first argument was a `data.frame`, `response` should be the name of the column in `data` containing the response, quoted for `roc_`, and optionally quoted for `roc.data.frame` (non-standard evaluation or NSE).

`predictor` a `numeric` or `ordered` vector of the same length than `response`, containing the predicted value of each observation. If the first argument was a `data.frame`, `predictor` should be the name of the column in `data` containing the predictor, quoted for `roc_`, and optionally quoted for `roc.data.frame` (non-standard evaluation or NSE).

`controls, cases` instead of `response`, `predictor`, the data can be supplied as two `numeric` or `ordered` vectors containing the predictor values for control and case observations.

`density.controls, density.cases` a smoothed ROC curve can be built directly from two densities on identical `x` points, as in `smooth`.

formula, data
: a formula of the type response~predictor. If mulitple predictors are passed, a named list of roc objects will be returned. Additional arguments data, subset and na.action are supported, see model.frame for more details.

levels
: the value of the response for controls and cases respectively. By default, the first two values of levels(as.factor(response)) are taken, and the remaining levels are ignored. It usually captures two-class factor data correctly, but will frequently fail for other data types (response factor with more than 2 levels, or for example if your response is coded "controls" and "cases", the levels will be inverted) and must then be specified here. If your data is coded as 0 and 1 with 0 being the controls, you can safely omit this argument.

percent
: if the sensitivities, specificities and AUC must be given in percent (TRUE) or in fraction (FALSE, default).

na.rm
: if TRUE, the NA values will be removed (ignored by roc.formula).

direction
: in which direction to make the comparison? "auto" (default): automatically define in which group the median is higher and take the direction accordingly. ">": if the predictor values for the control group are higher than the values of the case group (controls > t >= cases). "<": if the predictor values for the control group are lower or equal than the values of the case group (controls < t <= cases). You should set this explicity to ">" or "<" whenever you are resampling or randomizing the data, otherwise the curves will be biased towards higher AUC values.

algorithm
: the method used to compute sensitivity and specificity, an integer of length 1 between 0 and 6. 1: a safe, well-tested, pure-R code that is efficient when the number of thresholds is low. It goes with O(T*N). 2: an alternative pure-R algorithm that goes in O(N). Typically faster than 1 when the number of thresholds of the ROC curve is above 1000. Less tested than 1. 3: a C++ implementation of 1, about 3-5x faster. Typically the fastest with ROC curves with less than 50-100 thresholds, but has a very bad worst-case when that number increases. 4 (debug only, slow): runs algorithms 1 to 3 and makes sure they return the same values. 5: select 2 or 3 based on the number of thresholds. 6 (default): quickly select the algorithm on the class of the data: 2 for numeric and 3 for ordered. 0: use **microbenchmark** to choose between 2 and 3.

ret
: for roc.data.frame only, whether to return the threshold sensitivity and specificity at all thresholds ("coords"), all the coordinates at all thresholds ("all_coords") or the roc object ("roc").

quiet
: set to TRUE to turn off messages when direction and levels are auto-detected.

smooth
: if TRUE, the ROC curve is passed to smooth to be smoothed.

auc
: compute the area under the curve (AUC)? If TRUE (default), additional arguments can be passed to auc.

ci
: compute the confidence interval (CI)? If set to TRUE, additional arguments can be passed to ci.

plot
: plot the ROC curve? If TRUE, additional arguments can be passed to plot.roc.

`smooth.method, smooth.n, ci.method`
: in `roc.formula` and `roc.default`, the `method` and `n` arguments to `smooth` (if `smooth=TRUE`) and `of="auc"`) must be passed as `smooth.method`, `smooth.n` and `ci.method` to avoid confusions.

`density`
: `density` argument passed to `smooth`.

`...`
: further arguments passed to or from other methods, and especially:

- `auc`: `partial.auc`, `partial.auc.focus`, `partial.auc.correct`.
- `ci`: `of`, `conf.level`, `boot.n`, `boot.stratified`, `progress`
- `ci.auc`:, `reuse.auc`, `method`
- `ci.thresholds`: `thresholds`
- `ci.sp`: `sensitivities`
- `ci.se`: `specificities`
- `plot.roc`: `add`, `col` and most other arguments to the `plot.roc` function. See `plot.roc` directly for more details.
- `smooth`: `method`, `n`, and all other arguments. See `smooth` for more details.

Details

This function's main job is to build a ROC object. See the "Value" section to this page for more details. Before returning, it will call (in this order) the `smooth`, `auc`, `ci` and `plot.roc` functions if `smooth` `auc`, `ci` and `plot.roc` (respectively) arguments are set to TRUE. By default, only `auc` is called.

Data can be provided as `response,predictor`, where the predictor is the numeric (or ordered) level of the evaluated signal, and the response encodes the observation class (control or case). The `level` argument specifies which response level must be taken as controls (first value of `level`) or cases (second). It can safely be ignored when the response is encoded as `0` and `1`, but it will frequently fail otherwise. By default, the first two values of `levels(as.factor(response))` are taken, and the remaining levels are ignored. This means that if your response is coded "control" and "case", the levels will be inverted.

In some cases, it is more convenient to pass the data as `controls,cases`, but both arguments are ignored if `response,predictor` was specified to non-`NULL` values. It is also possible to pass density data with `density.controls,density.cases`, which will result in a smoothed ROC curve even if `smooth=FALSE`, but are ignored if `response,predictor` or `controls,cases` are provided.

Specifications for `auc`, `ci` and `plot.roc` are not kept if `auc`, `ci` or `plot` are set to `FALSE`. Especially, in the following case:

```
myRoc <- roc(..., auc.polygon=TRUE, grid=TRUE, plot=FALSE)
plot(myRoc)
```

the plot will not have the AUC polygon nor the grid. Similarly, when comparing "roc" objects, the following is not possible:

```
roc1 <- roc(..., partial.auc=c(1, 0.8), auc=FALSE)
roc2 <- roc(..., partial.auc=c(1, 0.8), auc=FALSE)
roc.test(roc1, roc2)
```

This will produce a test on the full AUC, not the partial AUC. To make a comparison on the partial AUC, you must repeat the specifications when calling `roc.test`:

```
roc.test(roc1, roc2, partial.auc=c(1, 0.8))
```

Note that if `roc` was called with `auc=TRUE`, the latter syntax will not allow redefining the AUC specifications. You must use `reuse.auc=FALSE` for that.

Value

If the data contained any `NA` value and `na.rm=FALSE`, `NA` is returned. Otherwise, if `smooth=FALSE`, a list of class "roc" with the following fields:

`auc`	if called with `auc=TRUE`, a numeric of class "auc" as defined in `auc`.
`ci`	if called with `ci=TRUE`, a numeric of class "ci" as defined in `ci`.
`response`	the response vector. Patients whose response is not `%in% levels` are discarded. If `NA` values were removed, a `na.action` attribute similar to `na.omit` stores the row numbers.
`predictor`	the predictor vector converted to numeric as used to build the ROC curve. Patients whose response is not `%in% levels` are discarded. If `NA` values were removed, a `na.action` attribute similar to `na.omit` stores the row numbers.
`original.predictor, original.response`	the response and predictor vectors as passed in argument.
`levels`	the levels of the response as defined in argument.
`controls`	the predictor values for the control observations.
`cases`	the predictor values for the cases.
`percent`	if the sensitivities, specificities and AUC are reported in percent, as defined in argument.
`direction`	the direction of the comparison, as defined in argument.
`fun.sesp`	the function used to compute sensitivities and specificities. Will be re-used in bootstrap operations.
`sensitivities`	the sensitivities defining the ROC curve.
`specificities`	the specificities defining the ROC curve.
`thresholds`	the thresholds at which the sensitivities and specificities were computed.
`call`	how the function was called. See `match.call` for more details.

If `smooth=TRUE` a list of class "smooth.roc" as returned by `smooth`, with or without additional elements `auc` and `ci` (according to the call).

Experimental: pipelines

Since version 1.15.0, the `roc` function can be used in pipelines, for instance with **dplyr** or **magrittr**. This is still a highly experimental feature and will change significantly in future versions (see issue 54[49]). The `roc.data.frame` method supports both standard and non-standard evaluation (NSE):

```
library(dplyr)
# Standard evaluation:
aSAH %>%
    filter(gender == "Female") %>%
    roc("outcome", "s100b")
# Non-Standard Evaluation:
aSAH %>%
    filter(gender == "Female") %>%
    roc(outcome, s100b)
```

For tasks involving programming and variable column names, the `roc_` function provides standard evaluation:

```
# Standard evaluation:
aSAH %>%
    filter(gender == "Female") %>%
    roc_("outcome", "s100b")
```

By default it returns the `roc` object, which can then be piped to the `coords` function to extract coordinates that can be used in further pipelines.

```
# Returns thresholds, sensitivities and specificities:
aSAH  %>%
    roc(outcome, s100b) %>%
    coords(transpose = FALSE) %>%
    filter(sensitivity > 0.6,
           specificity > 0.6)

# Returns all existing coordinates, then select precision and recall:
aSAH  %>%
    roc(outcome, s100b) %>%
    coords(ret = "all", transpose = FALSE) %>%
    select(precision, recall)
```

Errors

If no control or case observation exist for the given levels of response, no ROC curve can be built and an error is triggered with message “No control observation” or “No case observation”.

[49] https://github.com/xrobin/pROC/issues/54

If the predictor is not a numeric or ordered, as defined by `as.numeric` or `as.ordered`, the message "Predictor must be numeric or ordered" is returned.

The message "No valid data provided" is issued when the data wasn't properly passed. Remember you need both `response` and `predictor` of the same (not null) length, or bot `controls` and `cases`. Combinations such as `predictor` and `cases` are not valid and will trigger this error.

Infinite values of the predictor cannot always be thresholded by infinity and can cause ROC curves to not reach 0 or 100% specificity or sensitivity. Since version 1.13.0, pROC returns `NaN` with a warning message "Infinite value(s) in predictor" if `predictor` contains any infinite values.

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: 10.1016/j.patrec.2005.10.010[50].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[51].

See Also

`auc`, `ci`, `plot.roc`, `print.roc`, `roc.test`

Examples

```
data(aSAH)

# Basic example
roc(aSAH$outcome, aSAH$s100b,
    levels=c("Good", "Poor"))
# As levels aSAH$outcome == c("Good", "Poor"),
# this is equivalent to:
roc(aSAH$outcome, aSAH$s100b)
# In some cases, ignoring levels could lead to unexpected results
# Equivalent syntaxes:
roc(outcome ~ s100b, aSAH)
roc(aSAH$outcome ~ aSAH$s100b)
with(aSAH, roc(outcome, s100b))
with(aSAH, roc(outcome ~ s100b))

# With a formula:
roc(outcome ~ s100b, data=aSAH)

## Not run:
library(dplyr)
aSAH %>%
    filter(gender == "Female") %>%
    roc(outcome, s100b)

## End(Not run)
```

[50] http://dx.doi.org/10.1016/j.patrec.2005.10.010
[51] http://dx.doi.org/10.1186/1471-2105-12-77

```
# Using subset (only with formula)
roc(outcome ~ s100b, data=aSAH, subset=(gender == "Male"))
roc(outcome ~ s100b, data=aSAH, subset=(gender == "Female"))

# With numeric controls/cases
roc(controls=aSAH$s100b[aSAH$outcome=="Good"], cases=aSAH$s100b[aSAH$outcome=="Poor"])
# With ordered controls/cases
roc(controls=aSAH$wfns[aSAH$outcome=="Good"], cases=aSAH$wfns[aSAH$outcome=="Poor"])

# Inverted the levels: "Poor" are now controls and "Good" cases:
roc(aSAH$outcome, aSAH$s100b,
    levels=c("Poor", "Good"))

# The result was exactly the same because of direction="auto".
# The following will give an AUC < 0.5:
roc(aSAH$outcome, aSAH$s100b,
    levels=c("Poor", "Good"), direction="<")

# If we are sure about levels and direction auto-detection,
# we can turn off the messages:
roc(aSAH$outcome, aSAH$s100b, quiet = TRUE)

# If we prefer counting in percent:
roc(aSAH$outcome, aSAH$s100b, percent=TRUE)

# Plot and CI (see plot.roc and ci for more options):
roc(aSAH$outcome, aSAH$s100b,
    percent=TRUE, plot=TRUE, ci=TRUE)

# Smoothed ROC curve
roc(aSAH$outcome, aSAH$s100b, smooth=TRUE)
# this is not identical to
smooth(roc(aSAH$outcome, aSAH$s100b))
# because in the latter case, the returned object contains no AUC
```

`roc.test` *Compare the AUC of two ROC curves*

Description

This function compares the AUC or partial AUC of two correlated (or paired) or uncorrelated (unpaired) ROC curves. Several syntaxes are available: two object of class roc (which can be AUC or smoothed ROC), or either three vectors (response, predictor1, predictor2) or a response vector and a matrix or data.frame with two columns (predictors).

Usage

```
# roc.test(...)
## S3 method for class 'roc'
```

```
roc.test(roc1, roc2, method=c("delong", "bootstrap",
"venkatraman", "sensitivity", "specificity"), sensitivity = NULL,
specificity = NULL, alternative = c("two.sided", "less", "greater"),
paired=NULL, reuse.auc=TRUE, boot.n=2000, boot.stratified=TRUE,
ties.method="first", progress=getOption("pROCProgress")$name,
parallel=FALSE, ...)
## S3 method for class 'auc'
roc.test(roc1, roc2, ...)
## S3 method for class 'smooth.roc'
roc.test(roc1, roc2, ...)
## S3 method for class 'formula'
roc.test(formula, data, ...)
## Default S3 method:
roc.test(response, predictor1, predictor2=NULL,
na.rm=TRUE, method=NULL, ...)
```

Arguments

roc1, roc2	the two ROC curves to compare. Either "roc", "auc" or "smooth.roc" objects (types can be mixed).
response	a vector or factor, as for the roc function.
predictor1	a numeric or ordered vector as for the roc function, or a matrix or data.frame with predictors two colums.
predictor2	only if predictor1 was a vector, the second predictor as a numeric vector.
formula	a formula of the type response~predictor1+predictor2. Additional arguments `data`, `subset` and `na.action` are supported, see `model.frame` for more details.
data	a matrix or data.frame containing the variables in the formula. See `model.frame` for more details.
na.rm	if `TRUE`, the observations with `NA` values will be removed.
method	the method to use, either "delong", "bootstrap" or "venkatraman". The first letter is sufficient. If omitted, the appropriate method is selected as explained in details.
sensitivity, specificity	if `method="sensitivity"` or `method="specificity"`, the respective level where the test must be assessed as a numeric of length 1.
alternative	specifies the alternative hypothesis. Either of "two.sided", "less" or "greater". The first letter is sufficient. Default: "two.sided". Only "two.sided" is available with `method="venkatraman"`.
paired	a logical indicating whether you want a paired roc.test. If `NULL`, the paired status will be auto-detected by `are.paired`. If `TRUE` but the paired status cannot be assessed by `are.paired` will produce an error.
reuse.auc	if `TRUE` (default) and the "roc" objects contain an "auc" field, re-use these specifications for the test. See the *AUC specification* section for more details.
boot.n	for `method="bootstrap"` and `method="venkatraman"` only: the number of bootstrap replicates or permutations. Default: *2000*.

`boot.stratified`
: for `method="bootstrap"` only: should the bootstrap be stratified (same number of cases/controls in each replicate than in the original sample) or not. Ignored with `method="venkatraman"`. Default: *TRUE*.

`ties.method`
: for `method="venkatraman"` only: argument for `rank` specifying how ties are handled. Defaults to "first" as described in the paper.

`progress`
: the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.

`parallel`
: if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).

`...`
: further arguments passed to or from other methods, especially arguments for `roc` and `roc.test.roc` when calling `roc.test.default` or `roc.test.formula`. Arguments for `auc`, and `txtProgressBar` (only `char` and `style`) if applicable.

Details

This function compares two ROC curves. It is typically called with the two roc objects to compare. `roc.test.default` is provided as a convenience method and creates two roc objects before calling `roc.test.roc`.

Three methods are available: "delong", "bootstrap" and "venkatraman" (see "Computational details" section below). "delong" and "bootstrap" are tests over the AUC whereas "venkatraman" compares the the ROC curves themselves.

Default is to use "delong" method except for comparison of partial AUC, smoothed curves and curves with different `direction`, where `bootstrap` is used. Using "delong" for partial AUC and smoothed ROCs is not supported in pROC and result in an error. It is spurious to use "delong" for `roc` with different `direction` (a warning is issued but the spurious comparison is enforced). "venkatraman"'s test cannot be employed to compare smoothed ROC curves, or curves with partial AUC specifications. In addition, and comparison of ROC curves with different `direction` should be used with care (a warning is produced as well).

If `alternative="two.sided"`, a two-sided test for difference in AUC is performed. If `alternative="less"`, the alternative is that the AUC of roc1 is smaller than the AUC of roc2. For `method="venkatraman"`, only "two.sided" test is available.

If the `paired` argument is not provided, the `are.paired` function is employed to detect the paired status of the ROC curves. It will test if the original `response` is identical between the two ROC curves (this is always the case if the call is made with `roc.test.default`). This detection is unlikely to raise false positives, but this possibility cannot be excluded entierly. It would require equal sample sizes and `response` values and order in both ROC curves. If it happens to you, use `paired=FALSE`. If you know the ROC curves are paired you can pass `paired=TRUE`. However this is useless as it will be tested anyway.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided `density.cases` or `density.controls` the bootstrap cannot be performed and an error is issued.

Value

A list of class "htest" with following content:

`p.value`	the p-value of the test.
`statistic`	the value of the Z (`method="delong"`) or D (`method="bootstrap"`) statistics.
`alternative`	the alternative hypothesis.
`method`	the character string "DeLong's test for two correlated ROC curves" (if `method="delong"`) or "Bootstrap test for two correlated ROC curves" (if `method="bootstrap"`).
`null.value`	the expected value of the statistic under the null hypothesis, that is 0.
`estimate`	the AUC in the two ROC curves.
`data.name`	the names of the data that was used.
`parameter`	for `method="bootstrap"` only: the values of the `boot.n` and `boot.stratified` arguments.

AUC specification

The comparison of the AUC of the ROC curves needs a specification of the AUC. The specification is defined by:

1. the "auc" field in the "roc" objects if `reuse.auc` is set to `TRUE` (default)
2. passing the specification to `auc` with ... (arguments `partial.auc`, `partial.auc.correct` and `partial.auc.focus`). In this case, you must ensure either that the `roc` object do not contain an `auc` field (if you called `roc` with `auc=FALSE`), or set `reuse.auc=FALSE`.

If `reuse.auc=FALSE` the `auc` function will always be called with `...` to determine the specification, even if the "roc" objects do contain an `auc` field.

As well if the "roc" objects do not contain an `auc` field, the `auc` function will always be called with `...` to determine the specification.

The AUC specification is ignored in the Venkatraman test.

Warning: if the roc object passed to roc.test contains an `auc` field and `reuse.auc=TRUE`, auc is not called and arguments such as `partial.auc` are silently ignored.

Computation details

With `method="bootstrap"`, the processing is done as follow:

1. `boot.n` bootstrap replicates are drawn from the data. If `boot.stratified` is *TRUE*, each replicate contains exactly the same number of controls and cases than the original sample, otherwise if *FALSE* the numbers can vary.
2. for each bootstrap replicate, the AUC of the two ROC curves are computed and the difference is stored.
3. The following formula is used:

$$D = \frac{AUC1 - AUC2}{s}$$

where s is the standard deviation of the bootstrap differences and AUC1 and AUC2 the AUC of the two (original) ROC curves.

4. D is then compared to the normal distribution, according to the value of `alternative`.

See also the Bootstrap section in this package's documentation.

With `method="delong"`, the processing is done as described in DeLong *et al.* (1988) for paired ROC curves, using the algorithm of Sun and Xu (2014). Only comparison of two ROC curves is implemented. The method has been extended for unpaired ROC curves where the p-value is computed with an unpaired t-test with unequal sample size and unequal variance, with

$$D = \frac{V^r(\theta^r) - V^s(\theta^s)}{\sqrt{S^r + S^s}}$$

With `method="venkatraman"`, the processing is done as described in Venkatraman and Begg (1996) (for paired ROC curves) and Venkatraman (2000) (for unpaired ROC curves) with `boot.n` permutation of sample ranks (with ties breaking). For consistency reasons, the same argument `boot.n` as in bootstrap defines the number of permutations to execute, even though no bootstrap is performed.

For `method="specificity"`, the test assesses if the sensitivity of the ROC curves are different at the level of specificity given by the `specificity` argument, which must be a numeric of length 1. Bootstrap is employed as with `method="bootstrap"` and `boot.n` and `boot.stratified` are available. This is identical to the test proposed by Pepe *et al.* (2009). The `method="sensitivity"` is very similar, but assesses if the specificity of the ROC curves are different at the level of sensitivity given by the `sensitivity` argument.

Warnings

If "auc" specifications are different in both roc objects, the warning "Different AUC specifications in the ROC curves. Enforcing the inconsistency, but unexpected results may be produced." is issued. Unexpected results may be produced.

If one or both ROC curves are "smooth.roc" objects with different smoothing specifications, the warning "Different smoothing parameters in the ROC curves. Enforcing the inconsistency, but unexpected results may be produced." is issued. This warning can be benign, especially if ROC curves were generated with `roc(...,smooth=TRUE)` with different arguments to other functions (such as plot), or if you really want to compare two ROC curves smoothed differently.

If `method="venkatraman"`, and `alternative` is "less" or "greater", the warning "Only two-sided tests are available for Venkatraman. Performing two-sided test instead." is produced and a two tailed test is performed.

Both DeLong and Venkatraman's test ignores the direction of the ROC curve so that if two ROC curves have a different differ in the value of `direction`, the warning "(DeLong|Venkatraman)'s test should not be applied to ROC curves with different directions." is printed. However, the spurious test is enforced.

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that there are not enough points for smoothing, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

When both ROC curves have an `auc` of 1 (or 100%), their variances and covariance will always be null, and therefore the p-value will always be 1. This is true for both "delong", "bootstrap" and

"venkatraman" methods. This result is misleading, as the variances and covariance are of course not null. A `warning` will be displayed to inform of this condition, and of the misleading output.

Errors

An error will also occur if you give a `predictor2` when `predictor1` is a `matrix` or a `data.frame`, if `predictor1` has more than two columns, or if you do not give a `predictor2` when `predictor1` is a vector.

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the statistic on ROC curves smoothed with density.controls and density.cases." is issued.

If `method="venkatraman"` and one of the ROC curves is smoothed, the error "Using Venkatraman's test for smoothed ROCs is not supported." is produced.

With `method="specificity"`, the error "Argument 'specificity' must be numeric of length 1 for a specificity test." is given unless the specificity argument is specified as a numeric of length 1. The "Argument 'sensitivity' must be numeric of length 1 for a sensitivity test." message is given for `method="sensitivity"` under similar conditions.

Acknowledgements

We would like to thank E. S. Venkatraman and Colin B. Begg for their support in the implementation of their test.

References

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

James A. Hanley and Barbara J. McNeil (1982) "The meaning and use of the area under a receiver operating characteristic (ROC) curve". *Radiology* **143**, 29–36.

Margaret Pepe, Gary Longton and Holly Janes (2009) "Estimation and Comparison of Receiver Operating Characteristic Curves". *The Stata journal* **9**, 1.

Xavier Robin, Natacha Turck, Jean-Charles Sanchez and Markus Müller (2009) "Combination of protein biomarkers". *useR! 2009*, Rennes. `https://www.r-project.org/nosvn/conferences/useR-2009/abstracts/user_author.html`

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[52].

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[53].

E. S. Venkatraman and Colin B. Begg (1996) "A distribution-free procedure for comparing receiver operating characteristic curves from a paired experiment". *Biometrika* **83**, 835–848. DOI: 10.1093/biomet/83.4.835[54].

[52] `http://dx.doi.org/10.1186/1471-2105-12-77`
[53] `http://dx.doi.org/10.1109/LSP.2014.2337313`
[54] `http://dx.doi.org/10.1093/biomet/83.4.835`

E. S. Venkatraman (2000) "A Permutation Test to Compare Receiver Operating Characteristic Curves". *Biometrics* **56**, 1134–1138. DOI: 10.1111/j.0006-341X.2000.01134.x[55].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[56].

See Also

`roc`, `power.roc.test`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

# Basic example with 2 roc objects
roc1 <- roc(aSAH$outcome, aSAH$s100b)
roc2 <- roc(aSAH$outcome, aSAH$wfns)
roc.test(roc1, roc2)

## Not run:
# The latter used Delong's test. To use bootstrap test:
roc.test(roc1, roc2, method="bootstrap")
# Increase boot.n for a more precise p-value:
roc.test(roc1, roc2, method="bootstrap", boot.n=10000)

## End(Not run)

# Alternative syntaxes
roc.test(aSAH$outcome, aSAH$s100b, aSAH$wfns)
roc.test(aSAH$outcome, data.frame(aSAH$s100b, aSAH$wfns))

# If we had a good a priori reason to think that wfns gives a
# better classification than s100b (in other words, AUC of roc1
# should be lower than AUC of roc2):
roc.test(roc1, roc2, alternative="less")

## Not run:
# Comparison can be done on smoothed ROCs
# Smoothing is re-done at each iteration, and execution is slow
roc.test(smooth(roc1), smooth(roc2))
# or:
roc.test(aSAH$outcome, aSAH$s100b, aSAH$wfns, smooth=TRUE, boot.n=100)

## End(Not run)
# or from an AUC (no smoothing)
roc.test(auc(roc1), roc2)

## Not run:
# Comparison of partial AUC:
```

[55] http://dx.doi.org/10.1111/j.0006-341X.2000.01134.x
[56] http://www.jstatsoft.org/v40/i01

```
roc3 <- roc(aSAH$outcome, aSAH$s100b, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc.test(roc3, roc4)
# This is strictly equivalent to:
roc.test(roc3, roc4, method="bootstrap")

# Alternatively, we could re-use roc1 and roc2 to get the same result:
roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(1, 0.8), partial.auc.focus="se")

# Comparison on specificity and sensitivity
roc.test(roc1, roc2, method="specificity", specificity=0.9)
roc.test(roc1, roc2, method="sensitivity", sensitivity=0.9)

## End(Not run)

# Spurious use of DeLong's test with different direction:
roc5 <- roc(aSAH$outcome, aSAH$s100b, direction="<")
roc6 <- roc(aSAH$outcome, aSAH$s100b, direction=">")
roc.test(roc5, roc6, method="delong")

## Not run:
# Comparisons of the ROC curves
roc.test(roc1, roc2, method="venkatraman")

## End(Not run)

# Unpaired tests
roc7 <- roc(aSAH$outcome, aSAH$s100b)
# artificially create an roc8 unpaired with roc7
roc8 <- roc(aSAH$outcome[1:100], aSAH$s100b[1:100])
## Not run:
roc.test(roc7, roc8, paired=FALSE, method="delong")
roc.test(roc7, roc8, paired=FALSE, method="bootstrap")
roc.test(roc7, roc8, paired=FALSE, method="venkatraman")
roc.test(roc7, roc8, paired=FALSE, method="specificity", specificity=0.9)

## End(Not run)
```

`smooth` *Smooth a ROC curve*

Description

This function smoothes a ROC curve of numeric predictor. By default, a binormal smoothing is performed, but density or custom smoothings are supported.

Usage

```
smooth(...)
## Default S3 method:
```

```
smooth(...)
## S3 method for class 'roc'
smooth(roc,
method=c("binormal", "density", "fitdistr", "logcondens",
"logcondens.smooth"), n=512, bw = "nrd0", density=NULL,
density.controls=density, density.cases=density,
start=NULL, start.controls=start, start.cases=start,
reuse.auc=TRUE, reuse.ci=FALSE, ...)
## S3 method for class 'smooth.roc'
smooth(smooth.roc, ...)
```

Arguments

`roc, smooth.roc`
: a "roc" object from the `roc` function, or a "smooth.roc" object from the `smooth` function.

`method`
: "binormal", "density", "fitdistr", "logcondens", ""logcondens.smooth"", or a function returning a list of smoothed sensitivities and specificities.

`n`
: the number of equally spaced points where the smoothed curve will be calculated.

`bw`
: if `method="density"` and `density.controls` and `density.cases` are not provided, `bw` is passed to `density` to determine the bandwidth of the density Can be a character string ("nrd0", "nrd", "ucv", "bcv" or "SJ", but any name matching a function prefixed with "bw." is supported) or a numeric value, as described in `density`. Defaults to "nrd0".

`density, density.controls, density.cases`
: if `method="density"`, a numeric value of density (over the y axis) or a function returning a density (such as `density`. If `method="fitdistr"`, a `densfun` argument for `fitdistr`. If the value is different for control and case observations, `density.controls` and `density.cases` can be employed instead, otherwise `density` will be propagated to both `density.controls` and `density.cases`.

`start, start.controls, start.cases`
: if `method="fitdistr"`, optionnal `start` arguments for . `start.controls` and `start.cases` allows to specify different distributions for controls and cases.

`reuse.auc, reuse.ci`
: if `TRUE` (default for reuse.auc) and the "roc" objects contain "auc" or "ci" fields, re-use these specifications to regenerate `auc` or `ci` on the smoothed ROC curve with the original parameters. If `FALSE`, the object returned will not contain "auc" or "ci" fields. It is currently not possible to redefine `auc` and `ci` options directly: you need to call `auc` or `ci` later for that.

`...`
: further arguments passed to or from other methods, and especially to `density` (only `cut`, `adjust`, and `kernel`, plus `window` for compatibility with S+) and `fitdistr`. Also passed to to `method` if it is a function.

Details

If `method="binormal"`, a linear model is fitted to the quantiles of the sensitivities and specificities. Smoothed sensitivities and specificities are then generated from this model on `n` points. This simple approach was found to work well for most ROC curves, but it may produce hooked smooths in some situations (see in Hanley (1988)).

With `method="density"`, the `density` function is employed to generate a smooth kernel density of the control and case observations as described by Zhou *et al.* (1997), unless `density.controls` or `density.cases` are provided directly. `bw` can be given to specify a bandwidth to use with `density`. It can be a numeric value or a character string ("nrd0", "nrd", "ucv", "bcv" or "SJ", but any name matching a function prefixed with "bw." is supported). In the case of a character string, the whole predictor data is employed to determine the numeric value to use on both controls and cases. Depending on your data, it might be a good idea to specify the `kernel` argument for `density`. By default, "gaussian" is used, but "epanechnikov", "rectangular", "triangular", "biweight", "cosine" and "optcosine" are supported. As all the kernels are symetrical, it might help to normalize the data first (that is, before calling `roc`), for example with quantile normalization:

```
norm.x <- qnorm(rank(x)/(length(x)+1))
smooth(roc(response, norm.x, ...), ...)
```

Additionally, `density` can be a function which must return either a numeric vector of densities over the y axis or a list with a "y" item like the `density` function. It must accept the following input:

```
density.fun(x, n, from, to, bw, kernel, ...)
```

It is important to honour `n`, `from` and `to` in order to have the densities evaluated on the same points for controls and cases. Failing to do so and returning densities of different length will produce an error. It is also a good idea to use a constant smoothing parameter (such as `bw`) especially when controls and cases have a different number of observations, to avoid producing smoother or rougher densities.

If `method="fitdistr"`, the `fitdistr` function from the **MASS** package is employed to fit parameters for the density function `density` with optionnal start parameters `start`. The density function are fitted separately in control (`density.controls`, `start.controls`) and case observations (`density.cases`, `start.cases`). `density` can be one of the character values allowed by `fitdistr` or a density function (such as `dnorm`, `dweibull`, ...).

The `method="logcondens"` and `method="logcondens.smooth"` use the **logcondens** package to generate a non smoothed or smoothed (respectively) log-concave density estimate of of the control and case observation with the logConROC function.

Finally, `method` can also be a function. It must return a list with exactly 2 elements named "sensitivities" and "specificities", which must be numeric vectors between 0 and 1 or 100 (depending on the `percent` argument to `roc`). It is passed all the arguments to the `smooth` function.

`smooth.default` forces the usage of the `smooth` function in the **stats** package, so that other code relying on `smooth` should continue to function normally.

Smoothed ROC curves can be passed to smooth again. In this case, the smoothing is not re-applied on the smoothed ROC curve but the original "roc" object will be re-used.

Note that a `smooth.roc` curve has no threshold.

Value

A list of class "smooth.roc" with the following fields:

`sensitivities`
: the smoothed sensitivities defining the ROC curve.

`specificities`
: the smoothed specificities defining the ROC curve.

`percent`
: if the sensitivities, specificities and AUC are reported in percent, as defined in argument.

`direction`
: the direction of the comparison, as defined in argument.

`call`
: how the function was called. See `match.call` for more details.

`smoothing.args`
: a list of the arguments used for the smoothing. Will serve to apply the smoothing again in further bootstrap operations.

`auc`
: if the original ROC curve contained an AUC, it is computed again on the smoothed ROC.

`ci`
: if the original ROC curve contained a CI, it is computed again on the smoothed ROC.

`fit.controls, fit.cases`
: with `method="fitdistr"` only: the result of **MASS**'s `fitdistr` function for controls and cases, with an additional "densfun" item indicating the density function, if possible as character.

`logcondens`
: with `method="logcondens"` and `method="logcondens.smooth"` only: the result of **logcondens**'s logConROC function.

`model`
: with `method="binormal"` only: the linear model from `lm` used to smooth the ROC curve.

Attributes: Additionally, the original `roc` object is stored as a "roc" attribute.

Errors

If `method` is a function, the return values will be checked thoroughly for validity (list with two numeric elements of the same length named "sensitivities" and "specificities" with values in the range of possible values for sensitivities and specificities).

The message "The 'density' function must return a numeric vector or a list with a 'y' item." will be displayed if the `density` function did not return a valid output. The message "Length of 'density.controls' and 'density.cases' differ." will be displayed if the returned value differ in length.

Binormal smoothing cannot smooth ROC curve defined by only one point. Any such attempt will fail with the error "ROC curve not smoothable (not enough points).".

If the smooth ROC curve was generated by `roc` with `density.controls` and `density.cases` numeric arguments, it cannot be smoothed and the error "Cannot smooth a ROC curve generated directly with numeric 'density.controls' and 'density.cases'." is produced.

`fitdistr` and `density` smoothing methods require a numeric `predictor`. If the ROC curve to smooth was generated with an ordered factor only binormal smoothing can be applied and the

message "ROC curves of ordered predictors can be smoothed only with binormal smoothing." is displayed otherwise.

`fitdistr`, `logcondens` and `logcondens.smooth` methods require additional packages. If not available, the following message will be displayed with the required command to install the package: "Package ? not available, required with method='?'. Please install it with 'install.packages("?")'. "

References

James E. Hanley (1988) "The robustness of the "binormal" assumptions used in fitting ROC curves". *Medical Decision Making* **8**, 197–203.

Lutz Duembgen, Kaspar Rufibach (2011) "logcondens: Computations Related to Univariate Log-Concave Density Estimation". *Journal of Statistical Software*, **39**, 1–28. URL: jstatsoft.org/v39/i06[57].

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77. DOI: 10.1186/1471-2105-12-77[58].

Kaspar Rufibach (2011) "A Smooth ROC Curve Estimator Based on Log-Concave Density Estimates". *The International Journal of Biostatistics*, **8**, accepted. DOI: 10.1515/1557-4679.1378[59]. arXiv: 1103.1787[60].

William N. Venables, Brian D. Ripley (2002). "Modern Applied Statistics with S". New York, Springer. Google books[61].

Kelly H. Zou, W. J. Hall and David E. Shapiro (1997) "Smooth non-parametric receiver operating characteristic (ROC) curves for continuous diagnostic tests". *Statistics in Medicine* **18**, 2143–2156. DOI: 10.1002/(SICI)1097-0258(19971015)16:19<2143::AID-SIM655>3.0.CO;2-3[62].

See Also

`roc`

CRAN packages **MASS** and **logcondens** employed in this function.

Examples

```
data(aSAH)

##  Basic example
rocobj <- roc(aSAH$outcome, aSAH$s100b)
smooth(rocobj)
# or directly with roc()
roc(aSAH$outcome, aSAH$s100b, smooth=TRUE)

# plotting
```

[57] http://www.jstatsoft.org/v39/i06/
[58] http://dx.doi.org/10.1186/1471-2105-12-77
[59] http://dx.doi.org/10.1515/1557-4679.1378
[60] http://arxiv.org/abs/1103.1787
[61] http://books.google.ch/books?id=974c4vKurNkC
[62] http://dx.doi.org/10.1002/(SICI)1097-0258(19971015)16\%3A19\%3C2143\%3A\%3AAID-SIM655\%3E3.0.CO\%3B2-3

```
plot(rocobj)
rs <- smooth(rocobj, method="binormal")
plot(rs, add=TRUE, col="green")
rs2 <- smooth(rocobj, method="density")
plot(rs2, add=TRUE, col="blue")
rs3 <- smooth(rocobj, method="fitdistr", density="lognormal")
plot(rs3, add=TRUE, col="magenta")
rs4 <- smooth(rocobj, method="logcondens")
plot(rs4, add=TRUE, col="brown")
rs5 <- smooth(rocobj, method="logcondens.smooth")
plot(rs5, add=TRUE, col="orange")
legend("bottomright", legend=c("Empirical", "Binormal", "Density", "Log-normal",
                               "Log-concave density", "Smoothed log-concave density"),
       col=c("black", "green", "blue", "magenta", "brown", "orange"), lwd=2)

## Advanced smoothing

# if we know the distributions are normal with sd=0.1 and an unknown mean:
smooth(rocobj, method="fitdistr", density=dnorm, start=list(mean=1), sd=.1)
# different distibutions for controls and cases:
smooth(rocobj, method="fitdistr", density.controls="normal", density.cases="lognormal")

# with densities
bw <- bw.nrd0(rocobj$predictor)
density.controls <- density(rocobj$controls, from=min(rocobj$predictor) - 3 * bw,
                            to=max(rocobj$predictor) + 3*bw, bw=bw, kernel="gaussian")
density.cases <- density(rocobj$cases, from=min(rocobj$predictor) - 3 * bw,
                            to=max(rocobj$predictor) + 3*bw, bw=bw, kernel="gaussian")
smooth(rocobj, method="density", density.controls=density.controls$y,
       density.cases=density.cases$y)
# which is roughly what is done by a simple:
smooth(rocobj, method="density")

## Not run:
## Smoothing artificial ROC curves

rand.unif <- runif(1000, -1, 1)
rand.exp <- rexp(1000)
rand.norm <-
rnorm(1000)

# two normals
roc.norm <- roc(controls=rnorm(1000), cases=rnorm(1000)+1, plot=TRUE)
plot(smooth(roc.norm), col="green", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="density"), col="red", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="fitdistr"), col="blue", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="logcondens"), col="brown", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="logcondens.smooth"), col="orange", lwd=1, add=TRUE)
legend("bottomright", legend=c("empirical", "binormal", "density", "fitdistr",
                               "logcondens", "logcondens.smooth"),
       col=c(par("fg"), "green", "red", "blue", "brown", "orange"), lwd=c(2, 1, 1, 1))

# deviation from the normality
```

```
roc.norm.exp <- roc(controls=rnorm(1000), cases=rexp(1000), plot=TRUE)
plot(smooth(roc.norm.exp), col="green", lwd=1, add=TRUE)
plot(smooth(roc.norm.exp, method="density"), col="red", lwd=1, add=TRUE)
# Wrong fitdistr: normality assumed by default
plot(smooth(roc.norm.exp, method="fitdistr"), col="blue", lwd=1, add=TRUE)
# Correct fitdistr
plot(smooth(roc.norm.exp, method="fitdistr", density.controls="normal",
            density.cases="exponential"), col="purple", lwd=1, add=TRUE)
plot(smooth(roc.norm.exp, method="logcondens"), col="brown", lwd=1, add=TRUE)
plot(smooth(roc.norm.exp, method="logcondens.smooth"), col="orange", lwd=1, add=TRUE)
legend("bottomright", legend=c("empirical", "binormal", "density",
                               "wrong fitdistr", "correct fitdistr",
                               "logcondens", "logcondens.smooth"),
       col=c(par("fg"), "green", "red", "blue", "purple", "brown", "orange"), lwd=c(2, 1, 1,

# large deviation from the normality
roc.unif.exp <- roc(controls=runif(1000, 2, 3), cases=rexp(1000)+2, plot=TRUE)
plot(smooth(roc.unif.exp), col="green", lwd=1, add=TRUE)
plot(smooth(roc.unif.exp, method="density"), col="red", lwd=1, add=TRUE)
plot(smooth(roc.unif.exp, method="density", bw="ucv"), col="magenta", lwd=1, add=TRUE)
# Wrong fitdistr: normality assumed by default (uniform distributions not handled)
plot(smooth(roc.unif.exp, method="fitdistr"), col="blue", lwd=1, add=TRUE)
plot(smooth(roc.unif.exp, method="logcondens"), col="brown", lwd=1, add=TRUE)
plot(smooth(roc.unif.exp, method="logcondens.smooth"), col="orange", lwd=1, add=TRUE)
legend("bottomright", legend=c("empirical", "binormal", "density",
                               "density ucv", "wrong fitdistr",
                               "logcondens", "logcondens.smooth"),
       col=c(par("fg"), "green", "red", "magenta", "blue", "brown", "orange"), lwd=c(2, 1, 1

## End(Not run)

# 2 uniform distributions with a custom density function
unif.density <- function(x, n, from, to, bw, kernel, ...) {
  smooth.x <- seq(from=from, to=to, length.out=n)
  smooth.y <- dunif(smooth.x, min=min(x), max=max(x))
  return(smooth.y)
}
roc.unif <- roc(controls=runif(1000, -1, 1), cases=runif(1000, 0, 2), plot=TRUE)
s <- smooth(roc.unif, method="density", density=unif.density)
plot(roc.unif)
plot(s, add=TRUE, col="grey")

## Not run:
# you can bootstrap a ROC curve smoothed with a density function:
ci(s, boot.n=100)

## End(Not run)
```

`var.roc` *Variance of a ROC curve*

Description

These functions compute the variance of the AUC of a ROC curve.

Usage

```
var(...)
## Default S3 method:
var(...)
## S3 method for class 'auc'
var(auc, ...)
## S3 method for class 'roc'
var(roc, method=c("delong", "bootstrap", "obuchowski"),
boot.n = 2000, boot.stratified = TRUE, reuse.auc=TRUE,
progress = getOption("pROCProgress")$name, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
var(smooth.roc, ...)
```

Arguments

`roc, smooth.roc, auc`
: a "roc" object from the `roc` function, a "smooth.roc" object from the `smooth` function or an "auc" object from the `auc` function.

`method`
: the method to use, either "delong" or "bootstrap". The first letter is sufficient. If omitted, the appropriate method is selected as explained in details.

`reuse.auc`
: if `TRUE` (default) and the "roc" objects contain an "auc" field, re-use these specifications for the test. See details.

`boot.n`
: for `method="bootstrap"` only: the number of bootstrap replicates or permutations. Default: *2000*.

`boot.stratified`
: for `method="bootstrap"` only: should the bootstrap be stratified (same number of cases/controls in each replicate than in the original sample) or not. Default: *TRUE*.

`progress`
: the name of progress bar to display. Typically "none", "win", "tk" or "text" (see the `name` argument to `create_progress_bar` for more information), but a list as returned by `create_progress_bar` is also accepted. See also the "Progress bars" section of this package's documentation.

`parallel`
: if TRUE, the bootstrap is processed in parallel, using parallel backend provided by plyr (foreach).

`...`
: further arguments passed to or from other methods, especially arguments for `var.roc` when calling `var`, `var.auc` and `var.smooth.roc`. Arguments for `auc` (if `reuse.auc=FALSE`) and `txtProgressBar` (only `char` and `style`) if applicable.

Details

The `var` function computes the variance of the AUC of a ROC curve. It is typically called with the roc object of interest. Two methods are available: "delong" and "bootstrap" (see "Computational details" section below).

The default is to use "delong" method except for with partial AUC and smoothed curves where "bootstrap" is employed. Using "delong" for partial AUC and smoothed ROCs is not supported.

For smoothed ROC curves, smoothing is performed again at each bootstrap replicate with the parameters originally provided. If a density smoothing was performed with user-provided `density.cases` or `density.controls` the bootstrap cannot be performed and an error is issued.

`var.default` forces the usage of the `var` function in the **stats** package, so that other code relying on `var` should continue to function normally.

Value

The numeric value of the variance.

AUC specification

`var` needs a specification of the AUC to compute the variance of the AUC of the ROC curve. The specification is defined by:

1. the "auc" field in the "roc" objects if `reuse.auc` is set to `TRUE` (default)
2. passing the specification to `auc` with ... (arguments `partial.auc`, `partial.auc.correct` and `partial.auc.focus`). In this case, you must ensure either that the `roc` object do not contain an `auc` field (if you called `roc` with `auc=FALSE`), or set `reuse.auc=FALSE`.

If `reuse.auc=FALSE` the `auc` function will always be called with `...` to determine the specification, even if the "roc" objects do contain an `auc` field.

As well if the "roc" objects do not contain an `auc` field, the `auc` function will always be called with `...` to determine the specification.

Warning: if the roc object passed to roc.test contains an `auc` field and `reuse.auc=TRUE`, auc is not called and arguments such as `partial.auc` are silently ignored.

Computation details

With `method="bootstrap"`, the processing is done as follow:

1. `boot.n` bootstrap replicates are drawn from the data. If `boot.stratified` is *TRUE*, each replicate contains exactly the same number of controls and cases than the original sample, otherwise if *FALSE* the numbers can vary.
2. for each bootstrap replicate, the AUC of the ROC curve is computed and stored.
3. the variance of the resampled AUCs are computed and returned.

With `method="delong"`, the processing is done as described in Hanley and Hajian-Tilaki (1997) using the algorithm by Sun and Xu (2014).

With `method="obuchowski"`, the processing is done as described in Obuchowski and McClish (1997), Table 1 and Equation 4, p. 1530–1531. The computation of g for partial area under the ROC curve is modified as:

$$expr1 * (2 * pi * expr2)^{(-1)} * (-expr4) - A * B * expr1 * (2 * pi * expr2^3)^{(-1/2)} * expr3$$

.

Binormality assumption

The "obuchowski" method makes the assumption that the data is binormal. If the data shows a deviation from this assumption, it might help to normalize the data first (that is, before calling `roc`), for example with quantile normalization:

```
norm.x <- qnorm(rank(x)/(length(x)+1))
var(roc(response, norm.x, ...), ...)
```

"delong" and "bootstrap" methods make no such assumption.

Warnings

If `method="delong"` and the AUC specification specifies a partial AUC, the warning "Using DeLong for partial AUC is not supported. Using bootstrap test instead." is issued. The `method` argument is ignored and "bootstrap" is used instead.

If `method="delong"` and the ROC curve is smoothed, the warning "Using DeLong for smoothed ROCs is not supported. Using bootstrap test instead." is issued. The `method` argument is ignored and "bootstrap" is used instead.

If `boot.stratified=FALSE` and the sample has a large imbalance between cases and controls, it could happen that one or more of the replicates contains no case or control observation, or that there are not enough points for smoothing, producing a `NA` area. The warning "NA value(s) produced during bootstrap were ignored." will be issued and the observation will be ignored. If you have a large imbalance in your sample, it could be safer to keep `boot.stratified=TRUE`.

When the ROC curve has an `auc` of 1 (or 100%), the variance will always be null. This is true for both "delong" and "bootstrap" methods that can not properly assess the variance in this case. This result is misleading, as the variance is of course not null. A `warning` will be displayed to inform of this condition, and of the misleading output.

Errors

If `density.cases` and `density.controls` were provided for smoothing, the error "Cannot compute the covariance on ROC curves smoothed with density.controls and density.cases." is issued.

References

Elisabeth R. DeLong, David M. DeLong and Daniel L. Clarke-Pearson (1988) "Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach". *Biometrics* **44**, 837–845.

James A. Hanley and Karim O. Hajian-Tilaki (1997) "Sampling variability of nonparametric estimates of the areas under receiver operating characteristic curves: An update". *Academic Radiology* **4**, 49–58. DOI: 10.1016/S1076-6332(97)80161-4[63].

[63] `http://dx.doi.org/10.1016/S1076-6332(97)80161-4`

Nancy A. Obuchowski, Donna K. McClish (1997). "Sample size determination for diagnostic accurary studies involving binormal ROC curve indices". *Statistics in Medicine*, **16**(13), 1529–1542. DOI: (SICI)1097-0258(19970715)16:13<1529::AID-SIM565>3.0.CO;2-H[64].

Xu Sun and Weichao Xu (2014) "Fast Implementation of DeLongs Algorithm for Comparing the Areas Under Correlated Receiver Operating Characteristic Curves". *IEEE Signal Processing Letters*, **21**, 1389–1393. DOI: 10.1109/LSP.2014.2337313[65].

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: www.jstatsoft.org/v40/i01[66].

See Also

`roc`, `cov.roc`

CRAN package **plyr**, employed in this function.

Examples

```
data(aSAH)

##  Basic example
roc1 <- roc(aSAH$outcome, aSAH$s100b)
roc2 <- roc(aSAH$outcome, aSAH$wfns)
var(roc1)
var(roc2)

# We could also write it in one line:
var(roc(aSAH$outcome, aSAH$s100b))

## Not run:
# The latter used Delong. To use bootstrap:
var(roc1, method="bootstrap")
# Decrease boot.n for a faster execution
var(roc1,method="bootstrap", boot.n=1000)

## End(Not run)

# To use obuchowski:
var(roc1, method="obuchowski")

## Not run:
# Variance of smoothed ROCs:
# Smoothing is re-done at each iteration, and execution is slow
var(smooth(roc1))

## End(Not run)

# or from an AUC (no smoothing)
var(auc(roc1))
```

[64] http://dx.doi.org/10.1002/(SICI)1097-0258(19970715)16\%3A13\%3C1529\%3A\%3AAID-SIM565\%3E3.0.CO\%3B2-H

[65] http://dx.doi.org/10.1109/LSP.2014.2337313

[66] http://www.jstatsoft.org/v40/i01

```
## Test data from Hanley and Hajian-Tilaki, 1997
disease.present <- c("Yes", "No", "Yes", "No", "No", "Yes", "Yes", "No",
                     "No", "Yes", "No", "No", "Yes", "No", "No")
field.strength.1 <- c(1, 2, 5, 1, 1, 1, 2, 1, 2, 2, 1, 1, 5, 1, 1)
field.strength.2 <- c(1, 1, 5, 1, 1, 1, 4, 1, 2, 2, 1, 1, 5, 1, 1)
roc3 <- roc(disease.present, field.strength.1)
roc4 <- roc(disease.present, field.strength.2)
# Assess the variance:
var(roc3)
var(roc4)

## Not run:
# With bootstrap:
var(roc3, method="bootstrap")
var(roc4, method="bootstrap")

## End(Not run)
```