# Package 'pROC'

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### 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: doi:10.1186/147121051277

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 cproc-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 <b>ggplot2</b>

Determine if the ROC curve have a partial AUC has.partial.auc lines.roc Add a ROC line to a ROC plot plot.ci Plot CIs Plot a ROC curve plot power.roc.test Sample size and power computation Print a ROC curve object print roc.test Compare two ROC curves Smooth a ROC curve smooth Variance of the AUC var

#### **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). 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.

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

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

### **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:** Progress bars are no longer supported in pROC 1.19. The use of the progress argument is deprecated, and any value other than NULL will produce a warning. The argument will be removed in a future version.

### 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, we went to a C++ implementation (with **Rcpp**), 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.

Earlier versions of **pROC** allowed choosing the optimal algorithm. Since pROC 1.19, only a single algorithm (previously algorithm = 2) is available. This allowed us to remove legacy code and dependencies, and make **pROC** more maintainable and future proof.

**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"))</pre>
```

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:* Parallel processing is no longer supported in pROC 1.19. The use of the parallel argument is deprecated, and any value other than FALSE will produce a warning. The argument will be removed in a future version.

**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"))</pre>
```

### Author(s)

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

Maintainer: Xavier Robin 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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

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: doi: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: doi:10.1186/147121051277.

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: doi:10.1109/LSP.2014.2337313.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

### See Also

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

CRAN packages MASS and logcondens employed in this package.

```
data(aSAH)
## Build a ROC object and compute the AUC ##
roc1 <- roc(aSAH$outcome, aSAH$s100b)</pre>
print(roc1)
# With a formula
roc(outcome ~ s100b, aSAH)
# With pipes, dplyr-style:
## Not run:
library(dplyr)
aSAH %>% roc(outcome, s100b)
## End(Not run)
# Create a few more curves for the next examples
roc2 <- roc(aSAH$outcome, aSAH$wfns)</pre>
roc3 <- roc(aSAH$outcome, aSAH$ndka)</pre>
## AUC ##
auc(roc1, partial.auc = c(1, .9))
## Smooth ROC curve ##
smooth(roc1)
## Summary statistics
var(roc1)
cov(roc1, roc3)
## Plot the curve ##
plot(roc1)
# More plotting options, CI and plotting
# with all-in-one syntax:
roc4 <- roc(aSAH$outcome,</pre>
            aSAH$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!
roc5 <- roc(aSAH$outcome, aSAH$wfns,</pre>
            plot=TRUE, add=TRUE, percent=roc4$percent)
```

```
## With ggplot2 ##
if (require(ggplot2)) {
# Create multiple curves to plot
rocs <- roc(outcome ~ wfns + s100b + ndka, data = aSAH)</pre>
ggroc(rocs)
## 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))</pre>
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)
## 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)
## Power & sample size ##
```

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```
# Power
# 1 curve
power.roc.test(roc1)
# 2 curves
power.roc.test(roc3, roc2)

# Sample size
# 1 curve
power.roc.test(roc3, power = 0.9)
# 2 curves
power.roc.test(roc1, roc2, power = 0.9)

# Also without ROC objects.
# For instance what AUC would be significantly different from 0.5?
power.roc.test(ncases=41, ncontrols=72, sig.level=0.05, power=0.95)
```

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

```
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 recomputed (with the same parameters than the original ROC curves)

additionnal arguments for are.paired.roc. Ignored in are.paired.roc
```

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#### **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
```

```
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$s100b)</pre>
roc2 <- roc(aSAH.copy$outcome, aSAH.copy$ndka)</pre>
# are.paired can still find that the curves were paired
are.paired(roc1, roc2) # TRUE
# Removing the NAs manually before passing to roc() un-pairs the ROC curves
nas <- is.na(aSAH.copy$outcome) | is.na(aSAH.copy$ndka)</pre>
roc2b <- roc(aSAH.copy$outcome[!nas], aSAH.copy$ndka[!nas])</pre>
are.paired(roc1, roc2b) # FALSE
# Getting the two paired ROC curves with additional smoothing and ci options
roc2$ci <- ci(roc2)</pre>
paired <- are.paired(smooth(roc1), roc2, return.paired.rocs=TRUE, reuse.ci=TRUE)</pre>
paired.roc1 <- attr(paired, "roc1")</pre>
paired.roc2 <- attr(paired, "roc2")</pre>
```

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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: doi:10.1007/s001340091641y.

### 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: doi:10.1186/147121051277

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```
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.

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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 controlled 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 =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.

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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: doi: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: doi:10.1023/A:1010920819831.

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

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: doi:10.1186/147121051277.

### See Also

roc, ci.auc

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### **Examples**

```
# Create a ROC curve:
data(aSAH)
roc.s100b <- roc(aSAH$outcome, aSAH$s100b)

# Get the full AUC
auc(roc.s100b)

# Get the partial AUC:
auc(roc.s100b, partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE)</pre>
```

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.

### 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**

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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: doi:10.1186/147121051277.

### See Also

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

```
# Create a ROC curve:
data(aSAH)
roc1 <- roc(aSAH$outcome, aSAH$$100b)

## AUC ##
ci(roc1)
# this is equivalent to:
ci(roc1, of = "auc")
# or:
ci.auc(roc1)</pre>
```

```
## Coordinates ##
## Not run:
# Thresholds
ci(roc1, of = "thresholds")
ci(roc1, of = "thresholds", thresholds = "all")
ci(roc1, of = "thresholds", thresholds = 0.51)
# equivalent to:
ci.thresholds(roc1, thresholds = 0.51)
# SE/SP
ci(roc1, of = "sp", sensitivities = c(.95, .9, .85))
ci.sp(roc1)
ci(roc1, of = "se")
ci.se(roc1)
# Arbitrary coordinates
ci(roc1, of = "coords", "best")
ci.coords(roc1, 0.51, "threshold")
## End(Not run)
```

ci.auc

Compute the confidence interval of the AUC

### Description

This function computes the confidence interval (CI) of an area under the curve (AUC).

### 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 = NULL, 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 = NULL, 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 spec-

ifications for the test. If false, use optional . . . arguments to auc. See details.

progress DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argu-

ment will be removed in a future version.

... 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 the "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 De-Long'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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

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: doi:10.1109/LSP.2014.2337313.

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: doi:10.1186/147121051277.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

#### See Also

```
roc, auc, ci
```

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```
partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE,
       boot.n=10000, stratified=FALSE)
## End(Not run)
# Note that the following will NOT give a CI of the partial AUC:
## Not run:
ci.auc(roc1,
       partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=FALSE)
## End(Not run)
# This is because rocobj$auc is not a partial AUC and reuse.auc = TRUE by default.
# You can overcome this problem by passing an AUC instead:
auc1 <- auc(roc1, partial.auc=c(1, .8), partial.auc.focus="se",</pre>
            partial.auc.correct=FALSE)
## Not run:
ci.auc(auc1)
## End(Not run)
## On smoothed ROC curves with bootstrap ##
## Not run:
ci.auc(smooth(roc1, method="density"))
## 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.

### Usage

```
# ci.coords(...)
## S3 method for class 'roc'
ci.coords(roc, x,
input="threshold"
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 = NULL, ...)
## 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),
```

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```
best.policy = c("stop", "omit", "random"),
conf.level=0.95, boot.n=2000,
boot.stratified=TRUE,
progress = NULL, ...)
## 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

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 sam-

ple (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 DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

... 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.

When x="best", the best threshold is determined at each bootstrap iteration, effectively assessing the confidence interval of choice of the "best" threshold itself. This differs from the behavior of ci.thresholds, where the "best" threshold is assessed on the given ROC curve before resampling.

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

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#### Value

**Note:** changed in version 1.16.

A list of the same length as ret and named as ret, and of class "ci.thresholds", "ci" and "list" (in this order).

Each element of the list is a matrix of the confidence intervals with rows given by x and with 3 columns, the lower bound of the CI, the median, and the upper bound of the CI.

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.

input the input coordinate, as given in argument.

x the coordinates used to calculate the CI, as given in argument.

ret the return values, as given in argument or substituted by link{coords}.

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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

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

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

### See Also

roc, coords, ci

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### **Examples**

```
# Create a ROC curve:
data(aSAH)
roc1 <- roc(aSAH$outcome, aSAH$s100b)</pre>
## Basic example ##
## Not run:
ci.coords(roc1, x="best", input = "threshold",
          ret=c("specificity", "ppv", "tp"))
## More options ##
ci.coords(roc1, x=0.9, input = "sensitivity", ret="specificity")
ci.coords(roc1, x=0.9, input = "sensitivity", ret=c("specificity", "ppv", "tp"))
ci.coords(roc1, x=c(0.1, 0.5, 0.9), input = "sensitivity", ret="specificity")
ci.coords(roc1, x=c(0.1, 0.5, 0.9), input = "sensitivity", ret=c("specificity", "ppv", "tp"))
# Return everything we can:
rets <- c("threshold", "specificity", "sensitivity", "accuracy", "tn", "tp", "fn", "fp", "npv",
          "ppv", "1-specificity", "1-sensitivity", "1-accuracy", "1-npv", "1-ppv")
ci.coords(roc1, x="best", input = "threshold", ret=rets)
## End(Not run)
## On smoothed ROC curves with bootstrap ##
ci.coords(smooth(roc1), x=0.9, input = "sensitivity", ret=c("specificity", "ppv", "tp"))
## 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.

### Usage

```
# ci.se(...)
## S3 method for class 'roc'
ci.se(roc, specificities = seq(0, 1, .1) * ifelse(roc$percent,
100, 1), conf.level=0.95, boot.n=2000, boot.stratified=TRUE,
progress = NULL, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
ci.se(smooth.roc, specificities = seq(0, 1, .1) *
ifelse(smooth.roc$percent, 100, 1), conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, progress = NULL,
parallel=FALSE, ...)
```

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```
## 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 DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argu-

ment will be removed in a future version.

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:

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```
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.
```

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.

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

#### Errors

roc

Warnings

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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: doi: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: doi:10.1186/147121051277.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

### See Also

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

```
# Create a ROC curve:
data(aSAH)
roc1 <- roc(aSAH$outcome, aSAH$$100b)

## Basic example ##
## Not run:
ci.se(roc1)
## End(Not run)</pre>
```

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```
## More options ##
# Customized bootstrap and specificities:
## Not run:
ci.se(roc1, c(.95, .9, .85), boot.n=10000, conf.level=0.9, stratified=FALSE)
## End(Not run)

## Plotting the CI ##
ci1 <- ci.se(roc1, boot.n = 10)
plot(roc1)
plot(ci1)

## On smoothed ROC curves with bootstrap ##
## Not run:
ci.se(smooth(roc1, method="density"))
## End(Not run)</pre>
```

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.

### Usage

```
# ci.sp(...)
## S3 method for class 'roc'
ci.sp(roc, sensitivities = seq(0, 1, .1) * ifelse(roc$percent,
100, 1), conf.level=0.95, boot.n=2000, boot.stratified=TRUE,
progress = NULL, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
ci.sp(smooth.roc, sensitivities = seq(0, 1, .1) *
ifelse(smooth.roc$percent, 100, 1), conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, progress = NULL, 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.
```

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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 DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argu-

ment will be removed in a future version.

.. 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.

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### 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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: doi: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: doi:10.1186/147121051277.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

#### See Also

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

```
# Create a ROC curve:
data(aSAH)
roc1 <- roc(aSAH$outcome, aSAH$s100b)

## Basic example ##
## Not run:
ci.sp(roc1)
## End(Not run)

## More options ##
# Customized bootstrap and sensitivities:
## Not run:
ci.sp(roc1, c(.95, .9, .85), boot.n=10000, conf.level=0.9, stratified=FALSE)
## End(Not run)</pre>
```

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```
## Plotting the CI ##
ci1 <- ci.sp(roc1, boot.n = 10)
plot(roc1)
plot(ci1)

## On smoothed ROC curves with bootstrap ##
## Not run:
ci.sp(smooth(roc1, method="density"))
## End(Not run)</pre>
```

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.

### 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 = NULL, 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.

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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 thresh-

olds, 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 sup-

plied curve with coords (not on the resampled curves).

progress DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argu-

ment will be removed in a future version.

... 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. Argu-

ments 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.

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### 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: doi:10.1002/(SICI)10970258(20000515)19:9<1141::AIDSIM479>3.0.CO;2F.

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. DOI: doi: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: doi:10.1186/147121051277

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

### See Also

roc, ci

```
data(aSAH)
# Create a ROC curve:
data(aSAH)
roc1 <- roc(aSAH$outcome, aSAH$s100b)</pre>
## Basic example ##
# Compute CI of all local maxima thresholds
## Not run:
ci.thresholds(roc1)
## End(Not run)
## More options ##
# Customized bootstrap and thresholds:
## Not run:
ci.thresholds(roc1,
  thresholds=c(0.5, 1, 2),
              boot.n=10000, conf.level=0.9, stratified=FALSE)
## End(Not run)
## Plotting the CI ##
```

```
## Not run:
ci1 <- ci.thresholds(roc1)
## End(Not run)
plot(roc1)
plot(ci1)</pre>
```

coords

Coordinates of a ROC curve

### Description

This function returns the coordinates of the ROC curve at one or several specified point(s).

### Usage

### **Arguments**

auc, roc, smooth.roc

a "roc" object from the roc function, or a "smooth.roc" object from the smooth function, or an "auc" object from the auc function.

Х

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). Typically one of "threshold", "specificity" or "sensitivity", but can be any of the monotone coordinate available, see the "Valid input" column under "Available coordinates". Can be shortened like ret. Defaults to "threshold". 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 "Available coordinates" section below. Alternatively, the single value "all" can be used to return every coordinate available.

ignore.partial.auc

If the roc object contains a partial AUC specification, it will be ignored.

as.list	DEPRECATED. If the returned object must be a list. Will be removed in a future version.
drop	DEPRECATED. If TRUE the result is coerced to the lowest possible dimension, as per Extract. By default only drops if transpose = TRUE and either ret or x is of length 1.
best.method	if $x="best"$ , the method to determine the best threshold. Defaults to "youden". 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	DEPRECATED. Whether to return the thresholds in columns (TRUE) or rows (FALSE). Since pROC 1.16 the default value is FALSE. See coords_transpose for more details the change.
as.matrix	DEPRECATED. If transpose is FALSE, whether to return a matrix (TRUE) or a data.frame (FALSE, the default). A data.frame is more convenient and flexible to use, but incurs a slight speed penalty. Consider setting this argument to TRUE if you are calling the function repeatedly.
	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, and ignore.partial.auc=TRUE, 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 pROC::coords explicitly.

**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 (default). 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:

"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 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.

#### **Available coordinates:**

The following table lists the coordinates that are available in the ret and input arguments.

Value	Description	Formula	Synonyms	Va
threshold	The threshold value	-	-	Ye
tn	True negative count	-	-	Ye
tp	True positive count	-	-	Ye
fn	False negative count	-	-	Ye
fp	False positive count	-	-	Ye
specificity	Specificity	tn/(tn+fp)	tnr	Ye
sensitivity	Sensitivity	tp/(tp+fn)	recall, tpr	Ye
accuracy	Accuracy	(tp + tn) / N	-	No
npv	Negative Predictive Value	tn/(tn+fn)	-	No
ppv	Positive Predictive Value	tp / (tp + fp)	precision	No
precision	Precision	tp/(tp+fp)	ppv	No
recall	Recall	tp/(tp+fn)	sensitivity, tpr	Ye
tpr	True Positive Rate	tp/(tp+fn)	sensitivity, recall	Ye
fpr	False Positive Rate	fp / (tn + fp)	1-specificity	Ye
tnr	True Negative Rate	tn/(tn+fp)	specificity	Ye
fnr	False Negative Rate	fn/(tp+fn)	1-sensitivity	Ye
fdr	False Discovery Rate	fp/(tp+fp)	1-ppv	No
lr_pos	Positive Likelihood Ratio	se / (1 - sp)	-	No

No

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.

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.

For ret, the single value "all" can be used to return every coordinate available.

#### Value

A data. frame with ret as columns and as many rows as given by x.

In all cases where 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. Even "best" may return more than one value (for example if the ROC curve is below the identity line, both extreme points).

### 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: doi:10.1093/aje/kwj063.

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: doi:10.1186/147121051277.

W. J. Youden (1950) "Index for rating diagnostic tests". *Cancer*, **3**, 32–35. DOI: doi:10.1002/10970142(1950)3:1<32::AIDCNCR2820030106>3.0.CO;23.

### See Also

```
roc, ci.coords
```

```
# Create a ROC curve:
data(aSAH)
roc.s100b <- roc(aSAH$outcome, aSAH$s100b, percent = TRUE)
# Get the coordinates of S100B threshold 0.55
coords(roc.s100b, 0.55)</pre>
```

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```
# Get the coordinates at 50% sensitivity
coords(roc=roc.s100b, x=50, input="sensitivity")
# Can be abbreviated:
coords(roc.s100b, 50, "se")
# Works with smoothed ROC curves
coords(smooth(roc.s100b), 90, "specificity")
# Get the sensitivities for all thresholds
cc <- coords(roc.s100b, "all", ret="sensitivity")</pre>
print(cc$sensitivity)
# Get the best threshold
coords(roc.s100b, "best", ret="threshold")
# Get the best threshold according to different methods
roc.ndka <- roc(aSAH$outcome, aSAH$ndka, percent=TRUE)</pre>
coords(roc.ndka, "best", ret="threshold",
       best.method="youden") # default
coords(roc.ndka, "best", ret="threshold",
       best.method="closest.topleft")
# and with different weights
coords(roc.ndka, "best", ret="threshold",
       best.method="youden", best.weights=c(50, 0.2))
coords(roc.ndka, "best", ret="threshold",
       best.method="closest.topleft", best.weights=c(5, 0.2))
# This is available with the plot.roc function too:
plot(roc.ndka, print.thres="best", print.thres.best.method="youden",
                                 print.thres.best.weights=c(50, 0.2))
# Return more values:
coords(roc.s100b, "best", ret=c("threshold", "specificity", "sensitivity", "accuracy",
                           "precision", "recall"))
# Return all values
coords(roc.s100b, "best", ret = "all")
# You can use coords to plot for instance a sensitivity + specificity vs. cut-off diagram
plot(specificity + sensitivity ~ threshold,
     coords(roc.ndka, "all"),
     type = "1", log="x",
     subset = is.finite(threshold))
# Plot the Precision-Recall curve
plot(precision ~ recall,
     coords(roc.ndka, "all", ret = c("recall", "precision")),
     type="1", ylim = c(0, 100))
# Alternatively plot the curve with TPR and FPR instead of SE/SP
# (identical curve, only the axis change)
```

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```
plot(tpr ~ fpr,
    coords(roc.ndka, "all", ret = c("tpr", "fpr")),
    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**

Until the release of pROC 1.16, the coords function was returning a matrix with thresholds in columns, and the coordinate variables in rows.

This format didn't conform to the grammar of the tidyverse 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 pROC version 1.16, this was changed and coords now returns a data. frame with the thresholds in rows and measurement in colums by default.

```
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
```

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## 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.

# Changes in 1.16

• Change of the default transpose to TRUE.

THIS CHANGE IS BACKWARDS INCOMPATIBLE AND IS EXPECTED TO BREAK LEGACY CODE.

# Changes in 1.17

• Dropped the warning if transpose is missing.

# Changes in 1.19

- 1. Setting transpose=TRUE is deprecated and triggers a warning.
- 2. The as.list, as.matrix and drop are deprecated. Setting them to any value triggers a waring.
- 3. transpose=FALSE continues to work normally.

# Changes in future versions

- 1. Setting transpose to TRUE will stop working and result in an error.
- 2. The drop, as.list and as.matrix arguments will be removed.
- 3. transpose=FALSE will keep working indefinitely.

## Related changes in ci.coords

In version 1.16, the format of the ci.coords return value was changed from a matrix-like object with mixed x and ret in rows and 3 columns, into a list-like object which should be easier to use programatically.

### See also

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

cov.roc

Covariance of two paired ROC curves

# **Description**

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

# 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=NULL, 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: <i>TRUE</i> .	
boot.return	if <i>TRUE</i> and method="bootstrap", also return the bootstrapped values. See the "Value" section for more details.	
progress	DEPRECATED. A value other than NULL will produce a warning. The argument will be removed in a future version.	
parallel	DEPRECATED. A value other than FALSE will produce a warning. The argument will be removed in a future version.	
•••	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, ...), ...)</pre>
```

"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 De-Long 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: doi:10.1016/S10766332(97)801614.

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: doi:10.1002/(SICI)10970258(19970715)16:13<1529::AIDSIM565>3.0.CO;2H.

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: doi:10.1109/LSP.2014.2337313.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

## See Also

```
roc, var.roc
```

```
data(aSAH)

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

```
## 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)</pre>
# 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")</pre>
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="<")</pre>
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")
```

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```
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)</pre>
```

geom\_polygon\_auc

Add an AUC polygon to a ggroc plot

# **Description**

EXPERIMENTAL - Add an AUC polygon to a ggroc plot.

## Usage

```
## $3 method for class 'auc'
geom_polygon_auc(data, legacy.axes = FALSE, ...)
## $3 method for class 'roc'
geom_polygon_auc(data, ...)
## $3 method for class 'smooth.roc'
geom_polygon_auc(data, ...)
```

# **Arguments**

data a roc object from the roc function, same as the one used to build the ggroc

initially.

legacy.axes must match the value given to ggroc.

... additional aesthetics for geom\_polygon to set: alpha, colour, linetype and

linewidth.

#### **Details**

This is highly experimental and may change in the future.

#### See Also

ggroc

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## **Examples**

```
# Create a ROC curve:
data(aSAH)
roc.s100b <- roc(aSAH$outcome, aSAH$s100b)
roc.s100b.percent <- roc(aSAH$outcome, aSAH$s100b, percent = TRUE)

ggroc(roc.s100b) + geom_polygon_auc(roc.s100b$auc)

# legacy.axes must be repeated
ggroc(roc.s100b.percent, legacy.axes=TRUE) + geom_polygon_auc(roc.s100b.percent, legacy.axes=TRUE)

# Partial AUCs
auc.s100b.partial.sp <- auc(roc.s100b, partial.auc = c(0.9, 1))
auc.s100b.partial.se <- auc(roc.s100b, partial.auc = c(0.8, 0.9), partial.auc.focus="se")

ggroc(roc.s100b) + geom_polygon_auc(auc.s100b.partial.sp)
ggroc(roc.s100b) + geom_polygon_auc(auc.s100b.partial.se)</pre>
```

ggroc.roc

Plot a ROC curve with ggplot2

## Description

This function plots a ROC curve with ggplot2.

#### **Usage**

#### **Arguments**

a roc object from the roc function, or a list of roc objects.

the name(s) of the aesthetics for geom\_line to map to the different ROC curves supplied.

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, linewidth (new in ggplot2 3.4.0), and size (before ggplot2 3.4.0). The group aesthetic is always active since version 1.18.5 and is kept for backwards compatibility.

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#### **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
```

```
# Create a basic roc object
data(aSAH)
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
rocobj2 <- roc(aSAH$outcome, aSAH$wfns)</pre>
if (require(ggplot2)) {
g <- ggroc(rocobj)</pre>
# 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)</pre>
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)))</pre>
g2
# This is equivalent to using roc.formula:
roc.list <- roc(outcome ~ s100b + ndka + wfns, data = aSAH)</pre>
g.list <- ggroc(roc.list)</pre>
g.list
# You can change the aesthetics as you normally would with ggplot2:
g.list + scale_colour_brewer(palette="RdGy")
g.list + scale_colour_manual(values = c("red", "blue", "black"))
# 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"))</pre>
```

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```
g5
# OR faceting
g.list + facet_grid(.~name) + theme(legend.position="none")
}
```

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
```

```
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)</pre>
```

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```
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)
## $3 method for class 'auc'
has.partial.auc(roc)
## $3 method for class 'smooth.roc'
has.partial.auc(roc)
## $3 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

```
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))</pre>
```

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

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
```

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## **Examples**

```
# Create a few ROC curves:
data(aSAH)
roc.s100b <- roc(aSAH$outcome, aSAH$$$100b)
roc.wfns <- roc(aSAH$outcome, aSAH$wfns)

# We need a plot to be ready
plot(roc.s100b, type = "n") # but don't actually plot the curve

# Add the line
lines(roc.s100b, type="b", pch=21, col="blue", bg="grey")

# Add the line of an other ROC curve
lines(roc.wfns, type="o", pch=19, col="red")

# Without using 'lines':
rocobj <- plot.roc(aSAH$outcome, aSAH$$100b, type="b", pch=21, col="blue", bg="grey")</pre>
```

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 (true class), 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.

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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.

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

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## 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: doi:10.1023/A:1010920819831.

#### See Also

auc

```
# 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$s100b, percent=TRUE)
# Examples for multivariate decision values (e.g. class probabilities)
####
## Not run:
# Example with a multinomial log-linear model from nnet
# We use the iris dataset and split into a training and test set
requireNamespace("nnet")
data(iris)
iris.sample <- sample(1:150)</pre>
iris.train <- iris[iris.sample[1:75],]</pre>
iris.test <- iris[iris.sample[76:150],]</pre>
mn.net <- nnet::multinom(Species ~ ., iris.train)</pre>
# Use predict with type="prob" to get class probabilities
iris.predictions <- predict(mn.net, newdata=iris.test, type="prob")</pre>
head(iris.predictions)
# This can be used directly in multiclass.roc:
multiclass.roc(iris.test$Species, iris.predictions)
```

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```
## End(Not run)
# 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(</pre>
                "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)</pre>
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, ...)
```

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```
## $3 method for class 'ci.coords'
plot(x, type=c("bars", "shape"), length=NULL,
col=ifelse(type=="bars", par("fg"), "gainsboro"), ...)
```

# Arguments

x a confidence interval object from the functions ci.threshold or ci.coords.	13, C1.3C, C1.3p
type of plot, "bars" or "shape". Can be shortened to "b" or "s". available for ci.se and ci.sp, not for ci.thresholds.	. "shape" is only
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 i shape is plotted. Ignored if type="bars"	if TRUE, only the
col color of the bars or shape.	
further arguments for segments (if type="bars") or polygon (i	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: doi:10.1186/147121051277.

#### See Also

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

# **Examples**

```
data(aSAH)
## Not run:
# Start a ROC plot
rocobj <- plot.roc(aSAH$outcome, aSAH$s100b)</pre>
plot(rocobj)
# Thresholds
ci.thresolds.obj <- ci.thresholds(rocobj)</pre>
plot(ci.thresolds.obj)
# Specificities
plot(rocobj) # restart a new plot
ci.sp.obj <- ci.sp(rocobj, boot.n=500)</pre>
plot(ci.sp.obj)
# Sensitivities
plot(rocobj) # restart a new plot
ci.se.obj <- ci(rocobj, of="se", boot.n=500)</pre>
plot(ci.se.obj)
# Plotting a shape. We need more
ci.sp.obj <- ci.sp(rocobj, sensitivities=seq(0, 1, .01), boot.n=100)</pre>
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")
# CI of a PR curve
co <- coords(rocobj, x = "all", input="recall", ret=c("recall", "precision"))</pre>
ci <- ci.coords(rocobj, x = seq(0, 1, .1), input="recall", ret="precision")</pre>
plot(co, type="l", ylim = c(0, 1))
plot(ci, type="shape")
plot(ci, type="bars")
lines(co)
## 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(xpercent)\{c(100, 0)\} else\{c(1, 0)\},
ylim=if(xpercent)\{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"),
1wd=2,
type="1".
# 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**

```
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.
```

a logical indicating if the plot axes must be drawn. axes

a logical indicating if the specificity axis (x axis) must be plotted as as decreasing legacy.axes

"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 of plotting as in plot. type

identity logical: whether or not the identity line (no discrimination line) must be dis-

played. 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.

Should a selected set of thresholds be displayed on the ROC curve? FALSE, NULL print.thres

> 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.border

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.angle, max.auc.polygon.border

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: doi:10.1186/147121051277.

## See Also

```
roc, auc, ci
```

```
# Create a few ROC curves:
data(aSAH)
roc.s100b <- roc(aSAH$outcome, aSAH$s100b)
roc.wfns <- roc(aSAH$outcome, aSAH$wfns)
roc.ndka <- roc(aSAH$outcome, aSAH$wfns)</pre>
```

```
# Simple example:
plot(roc.s100b)
# Add a smoothed ROC:
plot(smooth(roc.s100b), add=TRUE, col="blue")
legend("bottomright", legend=c("Empirical", "Smoothed"),
      col=c(par("fg"), "blue"), lwd=2)
# With more options:
plot(roc.s100b, print.auc=TRUE, auc.polygon=TRUE, grid=c(0.1, 0.2),
     grid.col=c("green", "red"), max.auc.polygon=TRUE,
     auc.polygon.col="lightblue", print.thres=TRUE)
# To plot a different partial AUC, we need to ignore the existing value
# with reuse.auc=FALSE:
plot(roc.s100b, 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="lightblue",
     print.thres=TRUE, print.thres.adj = c(1, -1),
     reuse.auc=FALSE)
# Add a second ROC curve to the previous plot:
plot(roc.wfns, add=TRUE)
# Plot some thresholds, add them to the same plot
plot(roc.ndka, print.thres="best", print.thres.best.method="youden")
plot(roc.ndka, print.thres="best", print.thres.best.method="closest.topleft",
                                   add = TRUE)
plot(roc.ndka, print.thres="best", print.thres.best.method="youden",
                                   print.thres.best.weights=c(50, 0.2),
                                   print.thres.adj = c(1.1, 1.25),
                                   add = 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, kappa = 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 spec-

ifications 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, neases is computed directly from formulas 2 and 3 and neontrols is deduced with kappa (defaults to the ratio of controls to cases). 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 (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, neases is computed directly from formula 2 and neontrols is deduced with kappa (defaults to the ratio of controls to cases in roc1). 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: doi:10.1002/(SICI)10970258(19970715)16:13<1529::AIDSIM565>3.0.CO;2H.

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: doi:10.1373/clinchem.2004.031823.

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: doi:10.1109/LSP.2014.2337313.

#### See Also

```
roc, roc. test
```

```
data(aSAH)
#### One ROC curve ####

# Build a roc object:
rocobj <- roc(aSAH$outcome, aSAH$$100b)

# 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)</pre>
```

```
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)
# 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)</pre>
roc2 <- roc(aSAH$outcome, aSAH$wfns)</pre>
## 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))</pre>
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.9))</pre>
## Sample size
# With bootstrap variance (default)
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))
```

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```
## 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), ...)
```

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```
## 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
```

```
data(aSAH)
# Print a roc object:
rocobj <- roc(aSAH$outcome, aSAH$$100b)
print(rocobj)

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

# implicit printing
roc(aSAH$outcome, aSAH$$100b)

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

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 printed, plotted, 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 = 2, 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 (true class), 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 and subset, but not 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

algorithm

how are positive observations defined? "<": observations are positive when they are greater than or equal (>=) to the threshold. ">": observations are positive when they are smaller than or equal (<=) to the threshold. "auto" (default): automatically detect in which group the median is higher and take the direction accordingly. See details. 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.

DEPRECATED. A value other than 2 will produce a warning. The argument will be removed in a future version.

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.se: sensitivities

- ci.sp: 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.

Thresholds are selected as the means between any two consecutive values observed in the data. This choice is aimed to facilitate their interpretation, as any data point will be unambiguously positive or negative regardless of whether the comparison operator includes equality or not. As a corollary, thresholds do not correspond to actual values in the data.

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)</pre>
```

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)</pre>
```

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. Pa-

tients whose response is not %in% levels are discarded. If NA values were re-

moved, 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.

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. See

below for details.

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

fun.sesp DEPRECATED. The value will be removed in a future version.

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).

### **Pipelines**

The roc function can be used in pipelines, for instance with **dplyr** or **magrittr**. 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)
```

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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.

## **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".

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 both 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: doi: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: doi:10.1186/147121051277.

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## 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$s100b)
with(aSAH, roc(outcome, s100b))
with(aSAH, roc(outcome ~ s100b))
# With a formula:
roc(outcome ~ s100b, data=aSAH)
## Not run:
library(dplyr)
aSAH %>%
    filter(gender == "Female") %>%
    roc(outcome, s100b)
## End(Not run)
# Using subset (only with formula)
roc(outcome ~ s100b, data=aSAH, subset=(gender == "Male"))
roc(outcome ~ s100b, data=aSAH, subset=(gender == "Female"))
# With numeric controls/cases
roc(controls=aSAH$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$s100b,
    levels=c("Poor", "Good"), direction="<")</pre>
# If we are sure about levels and direction auto-detection,
# we can turn off the messages:
roc(aSAH$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 two ROC curves

# **Description**

This function compares two correlated (or paired) or uncorrelated (unpaired) ROC curves. Delong and bootstrap methods test for a difference in the (partial) AUC of the ROC curves. The Venkatraman method tests if the two curves are perfectly superposed. The sensitivity and specificity methods test if the sensitivity (respectively specificity) of the ROC curves are different at the given level of specificity (respectively sensitivity). 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 = NULL,
parallel=FALSE, conf.level=0.95, ...)
## 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

 $if \verb| method="sensitivity"| or \verb| method="specificity"|, the respective level where$ 

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 spec-

ifications 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 DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argu-

ment will be removed in a future version.

conf.level a numeric scalar between 0 and 1 (non-inclusive) which species the confidence

level to use for any calculated CI's.

... 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" stest 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.
conf.int	the confidence interval of the test (currently only returned for the paired De- Long's test). Has an attribute conf.level specifiying the level of the test.
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.
- 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 "(DeLonglVenkatraman)'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: doi:10.1186/147121051277.

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: doi:10.1109/LSP.2014.2337313.

- 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: doi:10.1093/biomet/83.4.835.
- E. S. Venkatraman (2000) "A Permutation Test to Compare Receiver Operating Characteristic Curves". *Biometrics* **56**, 1134–1138. DOI: doi:10.1111/j.0006341X.2000.01134.x.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

## See Also

```
roc, power.roc.test
```

# **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:</pre>
```

```
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))
roc.test(aSAH$outcome, aSAH$s100b, aSAH$wfns, smooth=TRUE, boot.n=100)
## End(Not run)
# or from an AUC (no smoothing)
roc.test(auc(roc1), roc2)
## Not run:
# Comparison of partial AUC:
roc3 <- roc(aSAH$outcome, aSAH$s100b, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.8), partial.auc.focus="se")</pre>
roc.test(roc3, roc4)
# This is strictly equivalent to:
roc.test(roc3, roc4, method="bootstrap")
# Alternatively, we could re-use roc1 and roc2 to get the same result:
roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(1, 0.8), partial.auc.focus="se")
# Comparison on specificity and sensitivity
roc.test(roc1, roc2, method="specificity", specificity=0.9)
roc.test(roc1, roc2, method="sensitivity", sensitivity=0.9)
## End(Not run)
# Spurious use of DeLong's test with different direction:
roc5 <- roc(aSAH$outcome, aSAH$s100b, direction="<")</pre>
roc6 <- roc(aSAH$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)</pre>
```

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, ...)
```

density. Defaults to "nrd0".

# **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"".

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, 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.

## **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, ...), ...)</pre>
```

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 the control and case observation with the logConROC 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 re-

sult of logcondens's logConROC function.

model with method="binormal" only: the linear model from 1m used to smooth the

ROC curve.

**Attributes:** Additionally, the original roc object is stored as a "roc" attribute.

#### **Errors**

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: doi:10.18637/jss.v039.i06.

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: doi:10.1186/147121051277.

Kaspar Rufibach (2011) "A Smooth ROC Curve Estimator Based on Log-Concave Density Estimates". *The International Journal of Biostatistics*, **8**, accepted. DOI: doi:10.1515/15574679.1378. arXiv: arXiv:1103.1787.

William N. Venables, Brian D. Ripley (2002). "Modern Applied Statistics with S". New York, Springer. Google books.

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: doi:10.1002/(SICI)10970258(19971015)16:19<2143::AIDSIM655>3.0.CO;23.

## See Also

roc

CRAN packages MASS and logcondens employed in this function.

## **Examples**

```
data(aSAH)
## Basic example
```

```
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
smooth(rocobj)
# or directly with roc()
roc(aSAH$outcome, aSAH$s100b, smooth=TRUE)
# plotting
plot(rocobj)
rs <- smooth(rocobj, method="binormal")</pre>
plot(rs, add=TRUE, col="green")
rs2 <- smooth(rocobj, method="density")</pre>
plot(rs2, add=TRUE, col="blue")
rs3 <- smooth(rocobj, method="fitdistr", density="lognormal")
plot(rs3, add=TRUE, col="magenta")
if (requireNamespace("logcondens")) {
rs4 <- smooth(rocobj, method="logcondens")</pre>
plot(rs4, add=TRUE, col="brown")
rs5 <- smooth(rocobj, method="logcondens.smooth")</pre>
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$predictor)</pre>
density.controls <- density(rocobj$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)</pre>
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)
if (requireNamespace("logcondens")) {
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)</pre>
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)
if (requireNamespace("logcondens")) {
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, 1, 1))
# large deviation from the normality
roc.unif.exp <- roc(controls=runif(1000, 2, 3), cases=rexp(1000)+2, plot=TRUE)</pre>
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)
if (requireNamespace("logcondens")) {
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, 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)</pre>
 smooth.y <- dunif(smooth.x, min=min(x), max=max(x))</pre>
 return(smooth.y)
}
roc.unif <- roc(controls=runif(1000, -1, 1), cases=runif(1000, 0, 2), plot=TRUE)</pre>
s <- smooth(roc.unif, method="density", density=unif.density)</pre>
```

```
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 = NULL, parallel=FALSE, ...)
## S3 method for class 'smooth.roc'
var(smooth.roc, ...)
```

## **Arguments**

roc, smooth.roc, auc

a "roc" object from the  ${\hbox{roc}}$  function, a "smooth.roc" object from the  ${\hbox{smooth}}$ 

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 spec-

ifications for the test. See details.

boot.n for method="bootstrap" only: the number of bootstrap replicates or permuta-

tions. 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 DEPRECATED. A value other than NULL will produce a warning. The argument

will be removed in a future version.

parallel DEPRECATED. A value other than FALSE will produce a warning. The argument will be removed in a future version.

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 applica-

ble.

#### **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, ...), ...)</pre>
```

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

### Warnings

If method="delong" and the AUC specification specifies a partial AUC, the warning "Using De-Long 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: doi:10.1016/S10766332(97)801614.

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: doi:10.1002/(SICI)10970258(19970715)16:13<1529::AIDSIM565>3.0.CO;2H.

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: doi:10.1109/LSP.2014.2337313.

Hadley Wickham (2011) "The Split-Apply-Combine Strategy for Data Analysis". *Journal of Statistical Software*, **40**, 1–29. URL: doi:10.18637/jss.v040.i01.

## See Also

```
roc, cov.roc
```

# **Examples**

```
data(aSAH)
## Basic example
roc1 <- roc(aSAH$outcome, aSAH$s100b)</pre>
roc2 <- roc(aSAH$outcome, aSAH$wfns)</pre>
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))
## Test data from Hanley and Hajian-Tilaki, 1997
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)</pre>
roc4 <- roc(disease.present, field.strength.2)</pre>
# Assess the variance:
var(roc3)
var(roc4)
## Not run:
# With bootstrap:
var(roc3, method="bootstrap")
var(roc4, method="bootstrap")
## End(Not run)
```

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