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.
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pROC-package

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Description

pROC-package

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.

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.roc, 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 ROC curves (that is roc objects with the same response) can be compared with the roc.test function.

Citation

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

pROC

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

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 <Xavier.Robin@unige.ch> about any work you publish.

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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: specificitySE: 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.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
coords	Coordinates of a ROC curve
lines.roc	Add a ROC line to a ROC plot
plot.ci	Plot CIs
plot	Plot a ROC curve
print	Print a ROC curve object
roc.test	Compare the AUC of two correlated ROC curves
smooth	Smooth a ROC curve

Dataset

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

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

To load the package in S+:

pROC-package

```
library (pROC)
```

Author(s)

Xavier Robin, Natacha Turck, Jean-Charles Sanchez and Markus Müller Maintainer: Xavier Robin <Xavier.Robin@unige.ch>

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. 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: 10.1186/1471-2105-12-77

See Also

CRAN packages ROCR, verification or Bioconductor's roc.

```
data(aSAH)
# Build a ROC object and compute the AUC
roc(aSAH$outcome, aSAH$s100b)
roc(outcome ~ s100b, aSAH)
# Smooth ROC curve
roc(outcome ~ s100b, aSAH, smooth=TRUE)
# more options, CI and plotting
roc1 <- roc(aSAH$outcome,
            aSAH$s100b, percent=TRUE,
            # arguments for auc
            partial.auc=c(100, 90), partial.auc.correct=TRUE,
            partial.auc.focus="sens",
            # arguments for ci
            ci=TRUE, boot.n=100, ci.alpha=0.9, stratified=FALSE,
            # arguments for plot
            plot=TRUE, auc.polygon=TRUE, max.auc.polygon=TRUE, grid=TRUE,
            print.auc=TRUE, show.thres=TRUE)
# Add to an existing plot. Beware of 'percent' specification!
roc2 <- roc(aSAH$outcome, aSAH$wfns,
            plot=TRUE, add=TRUE, percent=roc1$percent)
## Confidence intervals ##
# CI of the AUC
ci(roc2)
```

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```
## 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=T)
## 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)
```

are.paired

Are two ROC curves paired?

Description

This function determines if two ROC curves can be paired.

Usage

```
are.paired(x, ...)
## S3 method for class 'auc'
are.paired(roc1, roc2, ...)
## S3 method for class 'smooth.roc'
are.paired(roc1, roc2, ...)
## S3 method for class 'roc'
```

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```
are.paired(roc1, roc2, return.paired.rocs=FALSE,
  reuse.auc = TRUE, reuse.ci = FALSE, reuse.smooth=TRUE, ...)
```

Arguments

a roc object from the roc function (for roc.test.roc), an auc from the auc function (for roc.test.auc) a formula (for roc.test.formula) or a response vector (for roc.test.default).

roc1, roc2 the two ROC curves to compare. Either "roc", "auc" or "smooth.roc" objects (types can be mixed).

return.paired.rocs

if TRUE and the ROC curves can be paired, the two paired ROC curves with NAs removed will be returned.

reuse.auc, reuse.ci, reuse.smooth

if return.paired.rocs=TRUE, determines if auc, ci and smooth.roc should be re-computed (with the same parameters than the original ROC curves)

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

Details

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

In practice, the paired status is granted if the response 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 \operatorname{roc1} and \operatorname{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>
```

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

# Removing the NAs manually before passing to roc() un-pairs the ROC curves
nas <- is.na(aSAH.copy$outcome) | is.na(aSAH.copy$ndka)
roc2b <- roc(aSAH.copy$outcome[!nas], aSAH.copy$ndka[!nas])
are.paired(roc1, roc2b) # FALSE

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

aSAH

Subarachnoid hemorrhage data

Description

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

Usage

aSAH

Format

A data.frame containing 113 observations of 7 variables.

Source

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

See Also

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

An example analysis with pROC is shown in:

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

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Examples

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

Arguments

x

a roc object from the roc function (for auc.roc), a smoothed roc object from the smoothed.roc function (for auc.smooth.roc) a formula (for auc.formula) or a response vector (for auc.default).

```
roc, smooth.roc
```

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

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response, predictor

arguments for the roc function.

formula, data

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

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

partial.auc.focus

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

partial.auc.correct

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

further arguments passed to or from other methods, especially arguments for roc when calling auc.default or auc.formula. 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 you can specify a partial AUC 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 accordingly 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.

partial.auc.correct is ignored if partial.auc=FALSE (default). If TRUE, the correction by McClish will be applied:

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

where min is the value of the non-discriminant AUC 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. Fully compatible with percent.

There is no difference in the computation of the area under a smoothed ROC curve.

Value

The numeric AUC value, of class "auc", in fraction of the area in percent if percent=TRUE, with the following attributes:

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References

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

Donna Katzman McClish (1989) "Analyzing a Portion of the ROC Curve". *Medical Decision Making* **9**(3), 190–195. 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: 10.1186/1471-2105-12-77

See Also

```
roc, ci.auc
```

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

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

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

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Description

ci

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

Usage

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

Arguments

```
a roc object from the roc function (for ci.roc), a formula (for ci.formula) or a
X
                  response vector (for ci.default).
roc, smooth.roc
                  a "roc" object from the roc function, or a "smooth.roc" object from the smooth.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.
                  The type of confidence interval. One of "auc", "thresholds", "sp" or "se". Note
of
                  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 or ci.se are called.

Value

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

References

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

See Also

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

```
data(aSAH)
# Syntax (response, predictor):
ci(aSAH$outcome, aSAH$s100b)
# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
# Of an AUC
ci(rocobj)
ci(rocobj, of="auc")
# this is strictly equivalent to:
ci.auc(rocobj)
# Of thresholds, sp, se...
## Not run:
ci(rocobj, of="thresholds")
ci(rocobj, of="thresholds", thresholds=0.51)
ci(rocobj, of="thresholds", thresholds="all")
ci(rocobj, of="sp", sensitivities=c(.95, .9, .85))
ci(rocobj, of="se")
## End(Not run)
# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome, aSAH$s100b, ci=TRUE, of="auc")</pre>
rocobj$ci
```

Description

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

Usage

```
ci.auc(x, ...)
## 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,
   ...)
## S3 method for class 'smooth.roc'
ci.auc(smooth.roc, conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, reuse.auc=TRUE, ...)
## 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

```
a roc object from the roc or smooth.roc functions (for ci.auc.roc or
Х
                  ci.auc.smooth.roc), a formula (for ci.auc.formula) or a response
                  vector (for ci.auc.default).
roc, smooth.roc
                  a "roc" object from the roc function, or a "smooth.roc" object from the smooth.roc
                  an "auc" object from the auc function.
auc
response, predictor
                  arguments for the roc function.
formula, data
                  a formula (and possibly a data object) of type response~predictor for the roc
                  function.
                  the width of the confidence interval as [0,1], never in percent. Default: 0.95,
conf.level
                  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.
                  the number of bootstrap replicates. Default: 2000.
boot.n
boot.stratified
                  should the bootstrap be stratified (default, same number of cases/controls in each
                  replicate than in the original sample) or not.
                  if TRUE (default) and the "roc" object contains an "auc" field, re-use these spec-
reuse.auc
                  ifications for the test. If false, use optional . . . arguments to auc. See details.
```

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 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.

Default is to use "delong" method except for comparison of partial AUC and smoothed curves, where bootstrap is used. Using "delong" for partial AUC and smoothed ROCs is not supported in pROC (with smoothed ROCs, method is ignored, otherwise for pAUC a warning is produced and "bootstrap" is employed instead).

With method="bootstrap", the function calls auc boot.n times, according to the method described by Carpenter and Bithell (2000). boot.n bootstrap replicates are drawn. Stratification of bootstrap can be controlled with boot.stratified. In stratified bootstrap, 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. Higher numbers of boot.n will give a more precise estimate of the CI, but take more time to compute. 2000 is recommanded by Carpenter and Bithell.

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) and the CI is deduced with gnorm.

Value

A numeric vector of length 3 and class "ci.auc", 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.
boot.n the number of bootstrap replicates.
boot.stratified whether or not the bootstrapping was stratified.
auc an object of class "auc" stored for reference about the compued AUC details (partial, percent, ...)
```

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

AUC specification

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

1. the "auc" field in the "roc" object if reuse.auc is set to TRUE (default). It is naturally inherited from any call to roc and fits most cases.

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

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

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

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

Warnings

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

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

Errors

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

References

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 Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164.

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

See Also

```
roc, auc, ci
```

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

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```
# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
# default values
ci.auc(rocobj)
ci(rocobj)
ci(auc(rocobj))
ci(rocobj$auc)
ci(rocobj$auc, method="delong")
# Partial AUC and customized bootstrap:
ci.auc(aSAH$outcome, aSAH$s100b,
       boot.n=100, conf.level=0.9, stratified=FALSE, partial.auc=c(1, .8),
       partial.auc.focus="se", partial.auc.correct=TRUE)
# Note that the following will NOT give a CI of the partial AUC:
ci.auc(rocobj, boot.n=500, conf.level=0.9, stratified=FALSE,
       partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE)
# This is because rocobj$auc is not a partial AUC.
## Not run:
# You can overcome this problem with reuse.auc:
ci.auc(rocobj, boot.n=500, conf.level=0.9, stratified=FALSE,
       partial.auc=c(1, .8), partial.auc.focus="se", partial.auc.correct=TRUE,
       reuse.auc=FALSE)
## End(Not run)
# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome, aSAH$s100b, ci=TRUE, of="auc")
rocobj$ci
## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth (rocobj)
# Or you can compute a new one:
ci.auc(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)
## End(Not run)
```

ci.se

Compute the confidence interval of sensitivities at given specificities

Description

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

Usage

```
ci.se(x, ...)
## S3 method for class 'roc'
```

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

Arguments

```
a roc object from the roc or smooth.roc functions (for ci.se.roc or
                 ci.se.smooth.roc), a formula (for ci.se.formula) or a response vec-
                 tor (for ci.se.default).
roc, smooth.roc
                 a "roc" object from the roc function, or a "smooth.roc" object from the smooth.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.
specificities
                 on which specificities to evaluate the CI.
                 the width of the confidence interval as [0,1], never in percent. Default: 0.95,
conf.level
                 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.
                 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.
```

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.

Stratification of bootstrap can be controlled with boot.stratified. In stratified bootstrap, 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. Higher

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numbers of boot.n will give a more precise estimate of the CI, but take more time to compute. 2000 is recommanded by Carpenter and Bithell.

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 CI for the given sensitivities. Row (names) are the specificities, the first column the lower bound, the 2nd column the median and the 3rd column the upper bound.

Additionally, the list has the following attributes:

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

boot.n the number of bootstrap replicates.

boot.stratified whether or not the bootstrapping was stratified.

specificities the specificities as given in argument.

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

Warnings

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

Errors

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

References

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

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164.

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

See Also

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

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Examples

```
data(aSAH)
## Not run:
# Syntax (response, predictor):
ci.se(aSAH$outcome, aSAH$s100b)
# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
ci.se(rocobj)
# Customized bootstrap and specific specificities:
ci.se(rocobj, c(.95, .9, .85), boot.n=500, conf.level=0.9, stratified=FALSE)
## End(Not run)
# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome,
              aSAH$s100b, ci=TRUE, of="se", boot.n=100)
rocobj$ci
# Plotting the CI
plot(rocobj)
plot(rocobj$ci)
## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth(rocobj)
# Or you can compute a new one:
ci.se(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)
## End(Not run)
```

ci.sp

Compute the confidence interval of specificities at given sensitivities

Description

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

Usage

```
ci.sp(x, ...)
## 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, ...)
## S3 method for class 'smooth.roc'
ci.sp(smooth.roc, sensitivities = seq(0, 1, .1) *
```

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```
ifelse(smooth.roc$percent, 100, 1), conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, ...)
## S3 method for class 'formula'
ci.sp(formula, data, ...)
## Default S3 method:
ci.sp(response, predictor, ...)
```

Arguments

```
a roc object from the roc or smooth.roc functions (for ci.sp.roc or
                 ci.sp.smooth.roc), a formula (for ci.sp.formula) or a response vec-
                 tor (for ci.sp.default).
roc, smooth.roc
                 a "roc" object from the roc function, or a "smooth.roc" object from the smooth.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.
sensitivities
                 on which sensitivities to evaluate the CI.
                 the width of the confidence interval as [0,1], never in percent. Default: 0.95,
conf.level
                 resulting in a 95% CI.
                 the number of bootstrap replicates. Default: 2000.
boot.n
boot.stratified
                 should the bootstrap be stratified (default, same number of cases/controls in each
                 replicate than in the original sample) or not.
                 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.
```

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.

Stratification of bootstrap can be controlled with boot.stratified. In stratified bootstrap, 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. Higher numbers of boot.n will give a more precise estimate of the CI, but take more time to compute. 2000 is recommanded by Carpenter and Bithell.

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.

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Value

A matrix of CI for the given specificities. Row (names) are the sensitivities, the first column the lower bound, the 2nd column the median and the 3rd column the upper bound.

Additionally, the list has the following attributes:

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

boot.n the number of bootstrap replicates.

boot.stratified whether or not the bootstrapping was stratified.

sensitivities the sensitivities as given in argument.

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

Warnings

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

Errors

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

References

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

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164.

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

See Also

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

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

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```
# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
ci.sp(rocobj)
# Customized bootstrap and specific specificities:
ci.sp(rocobj, c(.95, .9, .85), boot.n=500, conf.level=0.9, stratified=FALSE)
## End(Not run)
# Alternatively, you can get the CI directly from roc():
rocobj <- roc(aSAH$outcome,</pre>
              aSAH$s100b, ci=TRUE, of="sp", boot.n=100)
rocobj$ci
# Plotting the CI
plot(rocobj)
plot(rocobj$ci)
## Not run:
# On a smoothed ROC, the CI is re-computed automatically
smooth (rocobj)
# Or you can compute a new one:
ci.sp(smooth(rocobj, method="density", reuse.ci=FALSE), boot.n=100)
## End(Not run)
```

ci.thresholds

Compute the confidence interval of thresholds

Description

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

Usage

```
ci.thresholds(x, ...)
## S3 method for class 'roc'
ci.thresholds(roc, conf.level=0.95, boot.n=2000,
boot.stratified=TRUE, thresholds = "local maximas", ...)
## S3 method for class 'smooth.roc'
ci.thresholds(smooth.roc, ...)
## S3 method for class 'formula'
ci.thresholds(formula, data, ...)
## Default S3 method:
ci.thresholds(response, predictor, ...)
```

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Arguments

x a roc object from the roc function (for ci.thresholds.roc), a formula (for ci.thresholds.formula)

or a response vector (for ci.thresholds.default).

roc a "roc" object from the roc function.

smooth.roc not available for smoothed ROC curves, available only to catch the error and

provide a clear error message.

response, predictor

arguments for the roc function.

formula, data

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

function.

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

resulting in a 95% CI.

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

boot.stratified

should the bootstrap be stratified (default, same number of cases/controls in each

replicate than in the original sample) or not.

thresholds on which thresholds to evaluate the CI. Either the numeric values of the thresh-

olds, a logical vector (as index of roc\$thresholds) or a character "all",

"local maximas" or "best".

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.

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.

Stratification of bootstrap can be controlled with boot.stratified. In stratified bootstrap, 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. Higher numbers of boot.n will give a more precise estimate of the CI, but take more time to compute. 2000 is recommanded by Carpenter and Bithell.

Value

A list of length 2 and class "ci.thresholds", 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.

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```
sensitivity same than specificity.
```

Additionally, the list has the following attributes:

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

boot.n the number of bootstrap replicates.

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

thresholds the thresholds, as given in argument.

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

Warnings

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

References

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

James Carpenter and John Bithell (2000) "Bootstrap condence intervals: when, which, what? A practical guide for medical statisticians". *Statistics in Medicine* **19**, 1141–1164.

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

See Also

```
roc, ci
```

coords

Coordinates of a ROC curve

Description

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

Usage

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

Arguments

roc, smooth.roc a "roc" object from the roc function, or a "smooth.roc" object from the smooth.roc function. the coordinates to look for. Numeric (if so, their meaning is defined by the x input argument) or one of "all" (all the points of the ROC curve), "local maximas" (the local maximas of the ROC curve) or "best" (the point with the best sum of sensitivity and specificity). If x is numeric, the kind of input coordinate (x). One of "threshold", "speciinput ficity" or "sensitivity". Can be shortenend (for example to "thr", "sens" and "spec", or even to "t", "se" and "sp"). Note that "threshold" is not allowed in coords.smooth.roc, and that the argument is ignored when x is a character. The coordinates to return. One or more of "threshold", "specificity" or "sensitivret ity". Can be shortenend (for example to "thr", "sens" and "spec", or even to "t", "se" and "sp"). Note that "threshold" is not allowed in coords.smooth.roc.

as.list If the returned object must be a list. If FALSE (default), a named numeric vector is returned.

best.method if x="best", the method to determine the best threshold. See details in the 'Best thresholds' section.

best.weights if x="best", the weights to determine the best threshold. See details in the 'Best thresholds' section.

... further arguments passed to or from other methods. Ignored.

Details

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

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

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

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

Value

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

```
\begin{array}{lll} & length(x) == 1 & length(x) > 1 \\ as.list= TRUE & a list of the length of, in the order of, and named after, ret. & a list of the length of, and named after, ret. \\ as.list= FALSE & a numeric vector of the length of, in the order of, and named after, ret. & a numeric matrix with one red after, ret. \\ \end{array}
```

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

Note that if giving a character as x ("all", "local maximas" or "best"), you cannot predict the dimension of the return value, so be prepared to receive either a numeric vector or a matrix (if as.list=FALSE) or either a list of numeric or a list of lists (if as.list=TRUE). Even "best" may return more than one value (for example if the ROC curve is below the identity line, both extreme points).

coords may also return NULL when there a partial area is defined but no point of the ROC curve

falls within the region.

Best thresholds

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

"youden" The Youden index is employed. The optimal cut-off is the threshold that maximizes the distance to the identity (diagonal) line. Can be shortened to "y".

The optimality criterion is:

$$max(sensitivities + specificities)$$

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

The optimality criterion is:

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

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

- 1. the cost of of a false negative classification
- 2. the prevalence, or the proportion of cases in the total 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.

References

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

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

See Also

roc

```
data(aSAH)
# Print a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)</pre>
coords (rocobj, 0.55)
coords(rocobj, 0.9, "specificity", as.list=TRUE)
coords(rocobj, 0.5, "se", ret="se")
# fully qualified but identical:
coords(roc=rocobj, x=0.5, input="sensitivity", ret="sensitivity")
# Same in percent
rocobj <- roc(aSAH$outcome, aSAH$s100b,
              percent=TRUE)
coords (rocobj, 0.55)
coords(rocobj, 90, "specificity", as.list=TRUE)
coords(rocobj, x=50, input="sensitivity", ret=c("sen", "spec"))
# Get the sensitivities for all thresholds
sensitivities <- coords(rocobj, rocobj$thresholds, "thr", "se")
# This is equivalent to taking sensitivities from rocobj directly
stopifnot(all.equal(as.vector(rocobj$sensitivities)), as.vector(sensitivities)))
# You could also write:
sensitivities <- coords(rocobj, "all", ret="se")</pre>
stopifnot(all.equal(as.vector(rocobj$sensitivities), as.vector(sensitivities)))
# Get the best threshold
coords(rocobj, "b", ret="t")
# Get the best threshold according to different methods
rocobj <- roc(aSAH$outcome, aSAH$ndka, percent=TRUE)</pre>
coords(rocobj, "b", ret="t", best.method="youden") # default
coords(rocobj, "b", ret="t", best.method="closest.topleft")
# and with different weights
coords(rocobj, "b", ret="t", best.method="youden", best.weights=c(50, 0.2))
coords(rocobj, "b", ret="t", best.method="closest.topleft", best.weights=c(5, 0.2))
# and plot them
plot(rocobj, print.thres="best", print.thres.best.method="youden")
plot(rocobj, print.thres="best", print.thres.best.method="closest.topleft")
plot(rocobj, print.thres="best", print.thres.best.method="youden",
                                 print.thres.best.weights=c(50, 0.2))
plot(rocobj, print.thres="best", print.thres.best.method="closest.topleft",
                                  print.thres.best.weights=c(5, 0.2))
```

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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=3, ...)
## S3 method for class 'formula'
lines.roc(x, data, ...)
## Default S3 method:
lines.roc(x, predictor, ...)
## S3 method for class 'smooth.roc'
lines.roc(x, ...)
```

Arguments

Details

The lines.roc function just adds a ROC curve to an existing plot with basic styling options. To plot more details such as the AUC value or confidence interval, see the add=TRUE argument to plot.roc.

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

```
data(aSAH)

rocobj <- plot.roc(aSAH$outcome, aSAH$$100b, type="n")
lines(rocobj, type="b", pch=16, col="blue")

# Without using 'lines':
rocobj <- plot.roc(aSAH$outcome, aSAH$$100b, type="b", pch=16, col="blue")</pre>
```

plot.ci

Plot confidence intervals

Description

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

Usage

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

Arguments

```
a confidence interval object from the functions ci.thresholds, ci.se or ci.sp.

type type of plot, "bars" or "shape". Can be shortened to "b" or "s". "shape" is only available for ci.se and ci.sp, not for ci.thresholds.

length the length (as plot coordinates) of the bar ticks. Only if type="bars".

no.roc if FALSE, the ROC line is re-added over the shape. Otherwise if TRUE, only the shape is plotted. Ignored if type="bars"

col color of the bars or shape.

... further arguments for segments (if type="bars") or polygon (if type="shape").
```

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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.

Value

This function returns the confidence interval object invisibly.

Warnings

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

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

References

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

See Also

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

```
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")
```

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,
# Generic arguments for par:
xlim=if(x\$percent)\{c(100, 0)\}\ else\{c(1, 0)\},
ylim=if(x\$percent)\{c(0, 100)\} else\{c(0, 1)\},
xlab=ifelse(x$percent, "Specificity (%)", "Specificity"),
ylab=ifelse(x$percent, "Sensitivity (%)", "Sensitivity"),
width=8.5,
height=8.5,
# col, lty and lwd for the ROC line only
col=par("col"),
lty=par("lty"),
lwd=3,
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=16,
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 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.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$percent, 10, 0.1) * ifelse(x
grid.h={if (length(grid) == 1) {grid.v} else if (is.logical(grid) && grid[2]==TRUE)
grid.lty=2,
grid.lwd=1,
grid.col="#DDDDDD",
# Polygon for the AUC
auc.polygon=FALSE,
auc.polygon.col="gainsboro",
auc.polygon.lty=par("lty"),
auc.polygon.border="#000000",
auc.polygon.density=-1,
auc.polygon.angle=45,
# Polygon for the maximal AUC possible
max.auc.polygon=FALSE,
max.auc.polygon.col="#EEEEEE",
max.auc.polygon.lty=par("lty"),
max.auc.polygon.border="#000000",
max.auc.polygon.density=-1,
max.auc.polygon.angle=45,
# Confidence interval
ci=!is.null(x$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, ...)
## Default S3 method:
plot.roc(x, predictor, ...)
## S3 method for class 'smooth.roc'
plot.roc(x, ...)
```

Arguments

```
x a roc object from the roc function (for plot.roc.roc), a formula (for plot.roc.formula) or a response vector (for plot.roc.default).

predictor, data arguments for the roc function.
```

add if TRUE, the ROC curve will be added to an existing plot. If FALSE (default),

a new plot will be created.

if TRUE (default) and the "roc" object contains an "auc" field, re-use these specreuse.auc

ifications for the test. See details.

xlim, ylim, xlab, ylab

Generic arguments for the plot. See plot and plot.window for more details.

width, height

If no device is open, specify the dimensions of the plot. Further arguments can be passed to graphsheet in

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

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

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.

print.thres

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

print.thres.pch, print.thres.col, print.thres.cex

the plotting character (pch), 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.

boolean. Should the numeric value of AUC be printed on the plot? print.auc 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.cex, print.auc.col

character expansion factor and color for the printing of the AUC. See par for more details.

boolean or numeric vector of length 1 or 2. Should a background grid be added grid 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.
                 boolean. Whether or not to display the area as a polygon.
auc.polygon
auc.polygon.col, auc.polygon.lty, auc.polygon.border, auc.polygon.density, auc.poly
                 color (col), line type (lty), border, density and angle for the AdUC 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.border, max.auc.polygon.co
                 color (col), line type (lty), border, density and angle 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, points, text and plot.ci if applica-
                 ble.
```

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:

- A new plot is created if add=FALSE. If no graphical device is opened, a new graphsheet is started with margins set to make the plot square. Otherwise the plot will have the proportions defined by the device previously opened.
- 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.

Value

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

AUC specification

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

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

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

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

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

References

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

See Also

```
roc, auc, ci
```

```
data(aSAH)

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

# With a roc object:
rocobj <- roc(aSAH$outcome, aSAH$s100b)
# identical:
plot(rocobj)</pre>
```

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```
plot.roc(rocobj)
# Add a smoothed ROC:
plot.roc(smooth(rocobj), add=TRUE, col="blue")
legend(.6, .4, legend=c("Empirical", "Smoothed"),
       col=c(par("fg"), "blue"), lwd=2)
# With more options:
plot(rocobj, print.auc=TRUE, auc.polygon=TRUE, grid=c(0.1, 0.2),
     grid.col=c("green", "red"), max.auc.polygon=TRUE,
     auc.polygon.col="blue", print.thres=TRUE)
# To plot a different partial AUC, we need to ignore the existing value
# with reuse.auc=FALSE:
plot(rocobj, print.auc=TRUE, auc.polygon=TRUE, partial.auc=c(1, 0.8),
     partial.auc.focus="se", grid=c(0.1, 0.2), grid.col=c("green", "red"),
     max.auc.polygon=TRUE, auc.polygon.col="blue", print.thres=TRUE,
     reuse.auc=FALSE)
# Add a line to the previous plot:
plot.roc(aSAH$outcome, aSAH$wfns, add=TRUE)
# Alternatively, you can get the plot directly from roc():
roc(aSAH$outcome, aSAH$s100b, plot=TRUE)
```

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

Arguments

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

Value

These functions return the object they were passed invisibly.

See Also

```
roc, auc, ci, coords
```

Examples

```
data(aSAH)
# Print a roc object:
rocobj <- roc(aSAH$outcome, aSAH$$100b)
print(rocobj)
# Print a smoothed roc object
print(smooth(rocobj))
# implicit printing
roc(aSAH$outcome, aSAH$$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(x, ...)
## S3 method for class 'formula'
roc(formula, data, ...)
## Default S3 method:
roc(response, predictor,
levels=getFunction("levels")(as.factor(response)), percent=FALSE, na.rm=TRUE,
direction=c("auto", "<", ">"), smooth=FALSE, auc=TRUE, ci=FALSE,
plot=FALSE, smooth.method="binormal", ci.method=NULL, density=NULL, ...)
```

Arguments

x a formula (for roc.formula) or a response vector (for roc.default).

response a factor, numeric or character vector of responses, typically encoded with 0

(controls) and 1 (cases). The object. 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.

predictor a numeric vector, containing the value of each observation. An ordered factor is

coerced to a numeric.

formula a formula of the type response~predictor.

data a matrix or data frame containing the variables in the formula. See model.frame

for more details.

levels the value of the response for controls and cases respectively. 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 precised 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.

direction in which direction to make the comparison? "auto" (default): automatically

define in which group the median is higher and take the direction accordingly. ">": if the predictor values for the control group are higher than the values of

the case group. ">": contrary.

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 argu-

ments can be passed to auc.

ci compute the confidence interval (CI)? If TRUE (default), additional arguments

can be passed to ci.

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

```
smooth.method, ci.method
```

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

density

density argument passed to smooth.roc.

... 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
- ci.auc: reuse.auc.method
- ci.thresholds: thresholds
- ci.sp: sensitivities
- ci.se: specificities
- plot.roc: add, col and most other arguments to the plot.roc function. See plot.roc directly for more details.
- smooth: method, n, and all other arguments. See smooth for more details.

Details

This function's main job is to build a ROC object. See the "Value" section to this page for more details. Before returning, it will call (in this order) the smooth.roc, 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.

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, 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 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 converted to numeric as used to build the ROC curve. If NA

values were removed, a na.action attribute similar to na.omit stores the

row numbers.

original.predictor

the predictor vector 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.

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

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

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 bot controls and cases. Combinations such as predictor and cases are not valid and will trigger this error.

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874. 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: 10.1186/1471-2105-12-77

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$s100b)
with (aSAH, roc(outcome, s100b))
with (aSAH, roc(outcome ~ s100b))
# With a formula:
roc(outcome ~ s100b, data=aSAH)
# Inverted the levels: "Poor" are now controls and "Good" cases:
roc(aSAH$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$s100b,
    levels=c("Poor", "Good"), direction="<")</pre>
# If we prefer counting in percent:
roc(aSAH$outcome, aSAH$s100b, percent=TRUE)
# Plot and CI (see plot.roc and ci for more options):
roc(aSAH$outcome, aSAH$s100b,
    percent=TRUE, plot=TRUE, ci=TRUE)
# Smoothed ROC curve
roc(aSAH$outcome, aSAH$s100b, smooth=TRUE)
# this is not identical to
smooth(roc(aSAH$outcome, aSAH$s100b))
```

because in the latter case, the returned object contains no AUC

roc.test

Compare the AUC of two correlated ROC curves

Description

This function compares the AUC or partial AUC of two correlated (or paired) ROC curves. Several syntaxes are available: two object of class roc (which must have the same response data, but 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(x, ...)
## S3 method for class 'roc'
roc.test(roc1, roc2, method=c("delong", "bootstrap",
"venkatraman", "sensitivity", "specificity"), sensitivity = NULL,
specificity = NULL, alternative = c("two.sided", "less", "greater"),
paired=NULL, reuse.auc=TRUE, boot.n=2000, boot.stratified=TRUE,
ties.method="first", progress=getOption("pROCProgress")$name, ...)
## 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

X	a roc object from the roc function (for roc.test.roc), an auc from the auc function (for roc.test.auc) a formula (for roc.test.formula) or a response vector (for roc.test.default).
roc1, roc2	the two ROC curves to compare. Either "roc", "auc" or "smooth.roc" objects (types can be mixed as long as the original ROC curve are paired).
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.
data	a matrix or data.frame containing the variables in the formula. See $\verb model.frame $ for more details.

if TRUE, the observations with NA values will be removed. na.rm the method to use, either "delong", "bootstrap" or "venkatraman". The first method letter is sufficient. If omitted, the appropriate method is selected as explained in details. sensitivity, specificity if method="sensitivity" or method="specificity", the respective level where the test must be assessed as a numeric of length 1. alternative specifies the alternative hypothesis. Either of "two.sided", "less" or "greater". The first letter is sufficient. Default: "two.sided". Only "two.sided" is available with method="venkatraman". paired a logical indicating whether you want a paired roc.test. If NULL, the paired status will be auto-detected by are.paired. If TRUE but the paired status cannot be assessed by are.paired will produce an error. if TRUE (default) and the "roc" objects contain an "auc" field, re-use these specreuse.auc ifications for the test. See 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. for method="venkatraman" only: argument for rank specifying how ties ties.method are handled. Defaults to "first" as described in the paper. the name of progress bar to display. Typically "none", "win", "tk" or "text" (see progress the name argument to create_progress_bar for more information), but a list as returned by create_progress_bar is also accepted. See also the "Progress bars" section of this package's documentation.

further arguments passed to or from other methods, especially arguments for

roc and roc.test.roc when calling roc.test.default or roc.test.formula.

Arguments for auc, and txtProgressBar (only char and style) if ap-

plicable.

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. "delong" and "bootstrap" are available as both paired and unpaired tests, whereas "venkatraman" is only paired yet.

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 (a warning is produced and "bootstrap" is employed instead). It is spurious to use "delong" for roc with different direction (a warning is issued

but the spurious comparison is enforced). "venkatraman"s test cannot be employed to compare smoothed ROC curves. Additionally, partial AUC specifications are ignored (with a warning), and comparison of ROC curves with different direction should be used with care (a warning is produced as well).

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

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

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

Value

A list of class "htest" with following content:

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

AUC specification

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

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

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

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

The AUC specification is ignored in the Venkatraman test.

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

Computation details

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

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

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

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

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

With method="delong", the processing is done as described in DeLong *et al.* (1988) for paired ROC curves. 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 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="delong" and the AUC specification specifies a partial AUC, the warning "Using DeLong's test for partial AUC is not supported. Using bootstrap test instead." is issued. The method argument is ignored and "bootstrap" is used instead.

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

If method="venkatraman", and the AUC specification specifies a partial AUC, the AUC specification is ignored with the warning "Partial AUC is ignored in Venkatraman's test.".

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.

Errors

Both Delong and Bootstrap tests work only on paired data. This assumption is enforced by the verification that the responses of roc1 and roc2 are identical. If they are found different, and the difference cannot be explained by missing values, the error "The ROC test is defined only on paired ROC curves" is produced.

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

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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.

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

See Also

roc

Examples

```
data(aSAH)
# Basic example with 2 roc objects
roc1 <- roc(aSAH$outcome, aSAH$s100b)</pre>
roc2 <- roc(aSAH$outcome, aSAH$wfns)
roc.test(roc1, roc2)
## Not run:
# The latter used Delong's test. To use bootstrap test:
roc.test(roc1, roc2, method="bootstrap")
# Increase boot.n for a more precise p-value:
roc.test(roc1, roc2, method="bootstrap", boot.n=10000)
## End(Not run)
# Alternative syntaxes
roc.test(aSAH$outcome, aSAH$s100b, aSAH$wfns)
roc.test(aSAH$outcome, data.frame(aSAH$s100b, aSAH$wfns))
# If we had a good a priori reason to think that wfns gives a
# better classification than s100b (in other words, AUC of roc1
# should be lower than AUC of roc2):
```

```
roc.test(roc1, roc2, alternative="less")
## Not run:
# Comparison can be done on smoothed ROCs
# Smoothing is re-done at each iteration, and execution is slow
roc.test(smooth(roc1), smooth(roc2))
# or:
roc.test(aSAH$outcome, aSAH$s100b, aSAH$wfns, smooth=TRUE,
smooth.method="density", boot.n=100)
## End(Not run)
# or from an AUC (no smoothing)
roc.test(auc(roc1), roc2)
## Not run:
# Comparison of partial AUC:
roc3 <- roc(aSAH$outcome, aSAH$s100b, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc4 <- roc(aSAH$outcome, aSAH$wfns, partial.auc=c(1, 0.8), partial.auc.focus="se")
roc.test(roc3, roc4)
# This is strictly equivalent to:
roc.test(roc3, roc4, method="bootstrap")
# Alternatively, we could re-use roc1 and roc2 to get the same result:
roc.test(roc1, roc2, reuse.auc=FALSE, partial.auc=c(1, 0.8), partial.auc.focus="se")
# Comparison on specificity and sensitivity
roc.test(roc1, roc2, method="specificity", specificity=0.9)
roc.test(roc1, roc2, method="sensitivity", sensitivity=0.9)
## End(Not run)
# Spurious use of DeLong's test with different direction:
roc5 <- roc(aSAH$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$s100b)</pre>
# artificially create an roc8 unpaired with roc7
roc8 <- roc(aSAH$outcome[1:100], aSAH$s100b[1:100])</pre>
## Not run:
roc.test(roc7, roc8, paired=FALSE, method="delong")
roc.test(roc7, roc8, paired=FALSE, method="bootstrap")
roc.test(roc7, roc8, paired=FALSE, method="venkatraman")
roc.test(roc7, roc8, paired=FALSE, method="specificity", specificity=0.9)
## End(Not run)
```

smooth.roc

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(x, ...)
## Default S3 method:
smooth(x, ...)
## S3 method for class 'roc'
smooth(roc,
method=c("binormal", "density", "fitdistr"), n=512, bandwidth = "nrd",
density=NULL, density.controls=density, density.cases=density,
reuse.auc=TRUE, reuse.ci=FALSE, ...)
## S3 method for class 'smooth.roc'
smooth(smooth.roc, ...)
```

Arguments

x a roc object from the roc function (for smooth.roc), or a vector (for the regular (s+ default) smooth function).

roc, smooth.roc

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

Tunctio

"binormal", "density", "fitdistr", or a function returning a list of smoothed sen-

sitivities and specificities.

n the number of equally spaced points where the smoothed curve will be calcu-

lated.

bandwidth

method

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

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", one of "normal" (default), "exponential", "log-normal" (same as "lognormal") or "uniform", stating the shape of the underlying distribution. 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.

```
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 and window, plus kernel and adjust for compatibility with R). Also passed to to method if it is a function.

Details

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

With method="density", the density function is employed to generate a smooth kernel density of the control and case observations as described by Zhou et al. (1997), unless density.controls or density.cases are provided directly. Otherwise, bandwidth can be given to specify a bandwidth to use with density. It can be a numeric value or a character string ("nrd", "hb", "ucv", "bcv" or "sj", but any name matching a function prefixed with "bandwidth." 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. Note that the width argument to density is here called bandwidth to avoid clashes with the width argument to plot.roc. Depending on your data, it might be a good idea to specify the window argument for density. By default, "gaussian" is used, but "cosine", "3gaussian", "rectangular" and "triangular" are supported. As all the window 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, width, window, ...)
```

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 width) especially when controls and cases have a different number of observations, to avoid producing smoother or rougher densities.

If method="fitdistr", a function similar to the fitdistr function from the MASS package is employed to fit parameters for the density function density. The density function are fitted separately in control (density.controls) and case observations (density.cases).

density can be one of the character values "normal" (default), "exponential", "log-normal" or "uniform". No start parameter is supported, unlike fitdistr in the MASS package.

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

smooth.default forces the usage of the default smooth function, 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.

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.

thresholds the thresholds at which the sensitivities and specificities were computed.

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.

fit.controls, fit.cases

a list similar to a result of **MASS**'s fitdistr function for controls and cases, but with only "estimate", and an additional "densfun" item indicating the density

function, if possible as character.

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.

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

Errors

If method is a function, the return values will be checked thoroughly for validity (list with two numeric elements of the same length named "sensitivities" and "specificities" with values in the range of possible values for sensitivities and specificities).

The message "The 'density function must return a numeric vector or a list with a 'y' item." will be displayed if the density function did not return a valid output. The message "Length of 'density.controls' and 'density.cases' differ." will be displayed if the returned value differ in length.

Binormal smoothing cannot smooth ROC curve defined by only one point. Any such attempt will fail with the error "ROC curve not smoothable (not enough points).". It will also fail if the points are poorly distributed and no model can be fit. In such a case, the error from 'lm' is printed within the message.

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.

All three smoothing methods require a numeric predictor. If the ROC curve to smooth was generated with an ordered factor smoothing cannot be applied and the message "Only ROC curves of numeric predictors can be smoothed." is displayed.

References

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See Also

roc

Examples

```
data(aSAH)
## Basic example
rocobj <- roc(aSAH$outcome, aSAH$s100b)
smooth (rocobj)
# or directly with roc()
roc(aSAH$outcome, aSAH$s100b, smooth=TRUE)
# plotting
plot (rocobj)
rs <- smooth(rocobj, method="binormal")
plot(rs, add=TRUE, col="green")
rs2 <- smooth(rocobj, method="density")
plot(rs2, add=TRUE, col="blue")
rs3 <- smooth(rocobj, method="fitdistr", density="lognormal")
plot(rs3, add=TRUE, col="magenta")
legend(.6, .4, legend=c("Empirical", "Binormal", "Density", "Log-normal"),
       col=c("black", "green", "blue", "magenta"), lwd=2)
## Advanced smoothing
```

```
# different distibutions for controls and cases:
smooth(rocobj, method="fitdistr", density.controls="normal", density.cases="lognormal")
# with densities
width <- bandwidth.nrd(rocobj$predictor)</pre>
density.controls <- density(rocobj$controls, from=min(rocobj$predictor) - 3 * width,
                            to=max(rocobj$predictor) + 3*width, width=width, window="gaussia"
density.cases <- density(rocobj$cases, from=min(rocobj$predictor) - 3 * width,</pre>
                            to=max(rocobj$predictor) + 3*width, width=width, window="gaussia
smooth(rocobj, method="density", density.controls=density.controls$y,
       density.cases=density.cases$y)
# which is roughly what is done by a simple:
smooth(rocobj, method="density")
## Smoothing artificial ROC curves
# two normals
roc.norm <- roc(rep(c(0, 1), each=1000),
                c(rnorm(1000), rnorm(1000)+1), plot=TRUE)
plot(smooth(roc.norm), col="green", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="density"), col="red", lwd=1, add=TRUE)
plot(smooth(roc.norm, method="fitdistr"), col="blue", lwd=1, add=TRUE)
legend(.6, .4, legend=c("empirical", "binormal", "density",, "fitdistr"),
       col=c(par("fg"), "green", "red", "blue"), lwd=c(2, 1, 1, 1, 1))
# deviation from the normality
roc.norm.exp <- roc(rep(c(0, 1), each=1000),
                    c(rnorm(1000), rexp(1000)), plot=TRUE)
plot(smooth(roc.norm.exp), col="green", lwd=1, add=TRUE)
plot(smooth(roc.norm.exp, method="density"), col="red", lwd=1, add=TRUE)
# Wrong fitdistr: normality assumed by default
plot(smooth(roc.norm.exp, method="fitdistr"), col="blue", lwd=1, add=TRUE)
# Correct fitdistr
plot(smooth(roc.norm.exp, method="fitdistr", density.controls="normal",
            density.cases="exponential"), col="purple", lwd=1, add=TRUE)
legend(.6, .4, legend=c("empirical", "binormal", "density",
                        "wrong fitdistr", "correct fitdistr"),
       col=c(par("fg"), "green", "red", "blue", "purple"), lwd=c(2, 1, 1, 1, 1))
# large deviation from the normality
roc.unif.exp <- roc(rep(c(0, 1), each=1000),
                    c(runif(1000, -1, 1), rexp(1000)), plot=TRUE)
plot(smooth(roc.unif.exp), col="green", lwd=1, add=TRUE)
plot(smooth(roc.unif.exp, method="density"), col="red", lwd=1, add=TRUE)
# Wrong fitdistr: normality assumed by default
plot(smooth(roc.unif.exp, method="fitdistr"), col="blue", lwd=1, add=TRUE)
# Correct fitdistr
plot(smooth(roc.unif.exp, method="fitdistr", density.controls="uniform",
            density.cases="exponential"), col="purple", lwd=1, add=TRUE)
legend(.6, .4, legend=c("empirical", "binormal", "density", "density ucv",
                        "wrong fitdistr", "correct fitdistr"),
```

```
col=c(par("fg"), "green", "red", "magenta", "blue", "purple"),
lwd=c(2, 1, 1, 1, 1))
# 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(rep(c(0, 1), each=1000),
                c(runif(1000, -1, 1), runif(1000, 0, 2)), plot=TRUE)
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)
```

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