

Package ‘ROCS’

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Type Package

Title Receiver Operating Characteristics Surface

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Description Plots the Receiver Operating Characteristics Surface for high-throughput class-skewed data, calculates the Volume under the Surface (VUS) and the FDR-Controlled Area Under the Curve (FCAUC), and conducts tests to compare two ROC surfaces. Computes eROC curve and the corresponding AUC for imperfect reference standard.

License GPL-2

Depends rgl, poibin

NeedsCompilation no

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ROCS-package

Receiver Operating Characteristics Surface for class-skewed data

Description

The package constructs Receiver Operating Characteristics Surface (ROCS) using the false positive rate (FPR), true positive rate (TPR) and the false discovery rate (FDR). It computes the volume under the surface (VUS) and FDR-controlled area under the curve (FCAUC) to gauge the separability between two classes while taking into account the proportion of false discoveries.

Details

Package: ROCS
Type: Package
Version: 1.0
Date: 2012-02-12
License: GPL 2.0 or later

Major functions are `rocs.x` and `fcauc.x`.

Author(s)

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e.roc

Calculating expected Receiver Operating Characteristics Curve in the presence of imperfect reference standards.

Description

This function builds an eROC curve and returns the expected values of TPR, FPR, and TDR. It also calculates the AUC of the eROC curve. The 95% bootstrap percentile confidence interval for the AUC is provided.

Usage

```
e.roc(x, mu, method='RNA', bt.ci=TRUE, bt.nreps=100, do.plot=TRUE)
```

Arguments

x	Vector; the scores yielded by the classifier.
mu	Vector; the probabilistic confidence assigned by the imperfect reference standard.
method	The method used to compute the cumulative distribution function for the Poisson binomial distribution. “DFT-CF” for the DFT-CF method, “RF” for the recursive formula, “RNA” for the refined normal approximation, “NA” for the normal approximation.
bt.ci	Whether to compute the bootstrap confidence interval.
bt.nreps	The number of bootstrap replicates.
do.plot	Whether to plot the eROC curve.

Details

The eROC curve is a generalization of ROC curve given the class membership uncertainties. See the reference for the definition of the eROC curve.

Value

Returns the area under the eROC curve, the expected values of TPR, FPR, and TDR.

Author(s)

Peizhou Liao. Email: pliao3@emory.edu.

References

Liao P, Wu H, and Yu T (2016). ROC Curve Analysis in the Presence of Imperfect Reference Standards. Stat Biosci doi:10.1007/s12561-016-9159-7.

Examples

```
## normal scores
sample.p <- rnorm(100, mean=1, sd=sqrt(2))
sample.n <- rnorm(100, mean=-1, sd=sqrt(2))

## probabilistic confidence
mu.p <- rbeta(100, shape1=5, shape2=1)
mu.n <- rbeta(100, shape1=1, shape2=5)

## combine the sample
x.sample <- c(sample.p, sample.n)
mu.sample <- c(mu.p, mu.n)

## build eROC curve
e.roc.fit <- e.roc(x=x.sample, mu=mu.sample)
```

fcauc.comp.fntp *Plotting two ROC curves, highlighting the segments of the curves corresponding to acceptable FDR levels.*

Description

The function draws two colored ROC curves in one plot. For each curve, the segment that corresponds to acceptable FDR (e.g. ≤ 0.2) is colored differently than the rest of the curve.

Usage

```
fcauc.comp.fntp(roc.1, roc.2, FDR.cut = 0.2, lwd = 3,
  colors = c("blue", "green", "cyan", "red"),
  exp.labels = c("experiment 1", "experiment 2"))
```

Arguments

roc.1	A list object with three components: TP, FP and TDR, each being a vector.
roc.2	A list object with three components: TP, FP and TDR, each being a vector.
FDR.cut	The cutoff value of FDR.
lwd	The line width parameter to be passed on to the function lines().
colors	A vector of at least four colors. It is used for the coloring of the two ROC curves.
exp.labels	Experiment labels in the plot.

Value

No value is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598.

See Also

fcauc.fntp()

fcauc.fptp	<i>Generating ROC plot with shading based on FDR using user-provided FPR, TPR, FDR values</i>
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Description

The function plots the ROC curve using user-provided FPR, TPR, FDR values. It shades the area corresponding to acceptable FDR level. The FDR-controlled area under the curve (FCAUC) is calculated for the shaded area.

Usage

```
fcauc.fptp(FP, TP, TDR, FDR.cut = 0.2, do.plot=TRUE)
```

Arguments

FP	Vector of false positive rate.
TP	Vector of true positive rate.
TDR	Vector of true discovery rate.
FDR.cut	The cutoff value of FDR, for the purpose of FCAUC calculation.
do.plot	Whether to generate the plot.

Value

The FCAUC value is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598.

See Also

fcauc.x

`fcauc.x`*Generating ROC plot with shading based on FDR*

Description

The function plots the ROC curve. It shades the area corresponding to acceptable FDR level. The FDR-controlled area under the curve (FCAUC) is calculated for the shaded area.

Usage

```
fcauc.x(x0, x1, FDR.cut = 0.2)
```

Arguments

<code>x0</code>	Vector; the raw data of the null class.
<code>x1</code>	Vector; the raw data of the non-null class.
<code>FDR.cut</code>	The FDR level at which to shade the AUC and calculate the FCAUC.

Value

The FCAUC value is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598.

See Also

`fcauc.fptp`

Examples

```
#perfect separation
x0<-runif(1000)
x1<-runif(100)+2

fcauc.x(x0, x1)

#partial separation
x0<-rnorm(1000, mean=0, sd=1.5)
x1<-rnorm(100, mean=3, sd=1)

fcauc.x(x0, x1)
```

rocs.fptp *Plotting Receiver Operating Characteristics Surface with user-provided FPR, TPR & TDR*

Description

The function plots the colored ROCS in 3 dimensions using the rgl utilities. It shades the FDR-controlled AUC in the FPR-TPR plain. The VUS of the surface and the FCAUC area are calculated.

Usage

```
rocs.fptp(FP, TP, TDR, FDR.cut = 0.2)
```

Arguments

FP	Vector of false positive rate.
TP	Vector of true positive rate.
TDR	Vector of true discovery rate.
FDR.cut	The cutoff value of FDR, for the purpose of FCAUC calculation.

Details

The ROCS is the surface spanned by the TPR-FPR-TDR and its projection to the TPR-TDR plain. The volume is between the surface and its projection on the TPR-FDR plain (i.e. the AUC of ROC).

Value

The volume under the surface (VUS) is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598.

See Also

rocs.x

rocs.x *Calculating Receiver Operating Characteristics Surface from one-dimensional data.*

Description

The function plots the colored ROCS in 3 dimensions using the rgl utilities. It shades the FDR-controlled AUC in the FPR-TPR plain. The VUS of the surface and the FCAUC area are calculated. The significance of the VUX is assessed by one-sided permutation test.

Usage

```
rocs.x(x0, x1, s0=NULL, s1=NULL, n.perm = 1000, do.plot = TRUE, FDR.cut=0.2)
```

Arguments

x0	Vector; the raw data of the null class.
x1	Vector; the raw data of the non-null class.
s0	Vector; the confidence level of the class assignment of the null class observations. The length should be the same as x0. The default is NULL, in which case all observations are considered to be assigned without uncertainty.
s1	Vector; the confidence level of the class assignment of the non-null class observations. The length should be the same as x0. The default is NULL, in which case all observations are considered to be assigned without uncertainty.
n.perm	The number of permutations to assess the significance of the VUX.
do.plot	Whether to plot the 3D surface, or just return the VUX.
FDR.cut	The FDR level at which to shade the AUC and calculate the FCAUC.

Details

The ROCS is the surface spanned by the TPR-FPR-TDR and its projection to the TPR-TDR plain. The volume is between the surface and its projection on the TPR-FDR plain (i.e. the AUC of ROC).

Value

The volume under the surface (VUS) is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598. Yu T, Jones DP. (2014) Improving peak detection in high-resolution LC/MS metabolomics data using preexisting knowledge and machine learning approach. Bioinformatics. 30(20): 2941-2948.

See Also

rocs.fptp

Examples

```
x0<-rnorm(500, mean=0, sd=1.5)
x1<-rnorm(50, mean=4, sd=1)

rocs.x(x0, x1)$vus
```

test.rocs

Testing for significant difference between two ROCS

Description

The null hypothesis being tested is that the two ROCS are generated from populations with equal class-separating power. This function uses a bootstrap-based test.

Usage

```
test.rocs(x0, x1, z0, z1, B = 1000, do.plot = TRUE)
```

Arguments

x0	Vector; the raw data of the true-negative class in study 1.
x1	Vector; the raw data of the true-positive class in study 1.
z0	Vector; the raw data of the true-negative class in study 2.
z1	Vector; the raw data of the true-positive class in study 2.
B	The number of bootstrap samples to be used in order to estimate the spread of the distribution under the null hypothesis.
do.plot	Whether to plot the spread based on bootstrap samples.

Value

The p-value of the test is returned.

Author(s)

Tianwei Yu. Email: tianwei.yu@emory.edu.

References

Yu T (2012) ROCS: Receiver Operating Characteristic Surface for Class-Skewed High-Throughput Data. PLoS ONE 7(7): e40598.

Examples

```
x0<-rnorm(1000, mean=0, sd=1.5)
x1<-rnorm(100, mean=3, sd=1)
```

```
z0<-rnorm(800, mean=0, sd=1.5)
z1<-rnorm(80, mean=3.25, sd=1)
```

```
test.rocs(x0, x1, z0,z1, B=1000)
```

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