Package ‘mbRes’

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mbRes-package

mbRes: Exploration of Multiple Biomarker Responses using Effect Size

Description

Summarize multiple biomarker responses of aquatic organisms to contaminants using Cliff’s delta, as described in Pham & Sokolova (2022) doi:10.1002/ieam.4676.

Guidelines

mbr and visual are the main functions to compute and visualize Cliff’s delta and S-value which are results of cliff and resampling. setpop, simul, and plotsam simulate and visualize a hypothetical dataset. compare compares the results of Cliff’s delta and two other integrated indices published earlier (i.e., RSI and IBR, see blaise2002 and beliaeff2002). The others (ggheat and ggdot) are helper functions and are not meant to be called directly by users.

Updates

mbr.cliff and mbr.glass simply compute and visualize Cliff’s delta and Glass’s delta.

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**beliaeff2002**

**Compute Integrated Biomarker Index**

**Author(s)**
Duy Nghia Pham & Inna M. Sokolova

**Description**

beliaeff2002 calculates IBR in the hypothetical case study. This is not meant to be called directly.

**Usage**

beliaeff2002(sam_mean)

**Arguments**

* sam_mean a data frame, the third output of simul.

**Value**

beliaeff2002 returns a data frame of IBR.

**References**


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**blaise2002**

**Compute Rank Sum Biomarker Index**

**Description**

blaise2002 calculates RSI in the hypothetical case study. This is not meant to be called directly.

**Usage**

blaise2002(sam, sam_mean)

**Arguments**

* sam a data frame, the first output of simul.
* sam_mean a data frame, the third output of simul.
cliff

Value

blaise2002 returns a data frame of RSI.

References


cliff

Compute Effect Size

Description

cliff calculates Cliff’s delta statistic using the rank sum method.

Usage

cliff(v1, v0)

Arguments

v1 a vector, biomarker values from the treatment group.
v0 a vector, biomarker values from the control group.

Value

cliff returns a numeric that is the Cliff’s delta of the treatment group.

References


See Also

CalcA1.
**compare**

**Examples**

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
cliff(subset(temp$sam, Site == "S1", Bmk1, drop = TRUE),
      subset(temp$sam, Site == "S0", Bmk1, drop = TRUE))
```

**Description**

`compare` calculates RSI assigned values, IBR translated scores, and Cliff’s delta in the hypothetical case study.

**Usage**

```r
compare(sam, sam_mean)
```

**Arguments**

- `sam`: a data frame, the first output of `simul`.
- `sam_mean`: a data frame, the third output of `simul`.

**Value**

`compare` returns a list of length 5:

- `blaise`: RSI assigned values and final RSI.
- `beliaeff`: IBR translated scores and final IBR.
- `pham`: Cliff’s delta and the average of absolute Cliff’s delta.
- `fig1`: ggplot object of comparisons among RSI assigned values, IBR translated scores, and Cliff’s delta.
- `fig2`: ggplot object of comparison among RSI, IBR, and the average of absolute Cliff’s delta.

**References**


Examples

```r
cat.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
compare(temp$sam, temp$sam_mean)
#might take more than 5s in some machines
```

---

**ggdot**  
*Make Dot Plot*

**Description**

`ggdot` creates dot plot of the average of absolute Cliff’s delta. This is not meant to be called directly.

**Usage**

```r
ggdot(dat, hax, vax)
```

**Arguments**

- `dat`: a data frame with at least two columns.
- `hax`: a character, name of the column to be used as the horizontal axis.
- `vax`: a character, name of the column to be used as the vertical axis.

**Value**

`ggdot` returns a ggplot object.

---

**ggheat**  
*Make Heatmap*

**Description**

`ggheat` creates heatmaps of the Cliff’s delta and S-value. This is not meant to be called directly.
**Usage**

```r
ggheat(
  dat,
  hax,
  vax,
  cell,
  nm,
  lim,
  lo,
  hi,
  diverging = FALSE,
  env = parent.frame()
)
```

**Arguments**

- `dat` a data frame with at least three columns.
- `hax` a character, name of the column to be used as the horizontal axis.
- `vax` a character, name of the column to be used as the vertical axis.
- `cell` a character, name of the column to be used as the cells.
- `nm` a character, name of the heatmap.
- `lim` a numeric vector, limits of the color scale.
- `lo` a character, color of the color scale low end.
- `hi` a character, color of the color scale high end.
- `diverging` a logical, whether to use diverging color gradient.
- `env` an environment, to access outer scope variables.

**Value**

`ggheat` returns a ggplot object.

---

**mbr**

*Compute Cliff’s delta and S-value*

**Description**

`mbr` summarizes Cliff’s delta and S-value for multiple groups and multiple biomarkers.

**Usage**

`mbr(df)`
Arguments

df       a data frame with the name of experimental groups or biomonitoring sites as the first column and the measurement of biomarkers as the remaining columns.

Details

The header of the first column can be any character, for example, ‘group’ or ‘site’. The first name appearing in the first column will determine the control group or the reference site. The other names will be treatment groups or test sites. The header of the remaining columns will define the list of biomarkers.

Value

mbr returns a list of length 3:

mess       a list of length 3 confirms the information about df.
es        a data frame with 9 columns:
test_site  treatment groups or test sites.
ref_site   control group or reference site.
t_size     the sample size of treatment group or test sites.
r_size     the sample size of control group or reference site.
biomarker  individual biomarker.
delta      the Cliff’s delta of treatment group or reference site.
delta.abs  the absolute Cliff’s delta.
pval       the P-Value.
sval       the surprisal or S-Value.
idx        a data frame summarizes delta.abs and their average.

Examples

set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
mbr(temp$sam)
#might take more than 5s in some machines
**mbr.cliff**

*Compute Cliff’s delta simplified*

**Description**

*mbr.cliff* summarizes Cliff’s delta for multiple groups and multiple biomarkers.

**Usage**

```r
mbr.cliff(df)
```

**Arguments**

- `df`: a data frame with the name of experimental groups or biomonitoring sites as the first column and the measurement of biomarkers as the remaining columns.

**Examples**

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
mbr.cliff(temp$sam)
#might take more than 5s in some machines
```

---

**mbr.glass**

*Compute Glass’s delta simplified*

**Description**

*mbr.glass* summarizes Glass’s delta for multiple groups and multiple biomarkers.

**Usage**

```r
mbr.glass(df)
```

**Arguments**

- `df`: a data frame with the name of experimental groups or biomonitoring sites as the first column and the measurement of biomarkers as the remaining columns.
Examples

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
mbr.glass(temp$sam)
# might take more than 5s in some machines
```

---

**plotsam**

*Visualize Hypothetical Samples*

**Description**

plotsam plots the sample dataset of biomarker responses. This is used for the hypothetical case study.

**Usage**

```r
plotsam(pop_mean_long, pop_profile, sam_long)
```

**Arguments**

- `pop_mean_long`: a data frame, the second output of `setpop`.
- `pop_profile`: a data frame, the third output of `setpop`.
- `sam_long`: a data frame, the second output of `simul`.

**Value**

plotsam returns a ggplot object.

**Examples**

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
plotsam(setting$pop_mean_long, setting$pop_profile, temp$sam_long)
```
Description

resampling performs randomization test to calculate P-value and S-value.

Usage

resampling(v1, v0, nrand = 1999, seed = 1)

Arguments

v1 a vector, biomarker values from the treatment group.
v0 a vector, biomarker values from the control group.
nrand an integer, the number of randomization samples. The default value is 1999.
seed an integer, the seed for random number generation. Setting a seed ensures the reproducibility of the result. See set.seed for more details.

Value

resampling returns a one-row data frame with 3 numerics:

delta the Cliff’s delta of the treatment group.
pval the observed P-value p under the null hypothesis.
sval the S-value s calculated from P-value p.

References


See Also

A1.
Examples

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
resampling(subset(temp$sam, Site == "S1", Bmk1, drop = TRUE),
subset(temp$sam, Site == "S0", Bmk1, drop = TRUE))
```

---

### setpop

**Define Hypothetical Populations**

**Description**

setpop sets the true means of biomarker responses in populations. This is used for the hypothetical case study.

**Usage**

```r
setpop()
```

**Value**

setpop returns a list of length 3:

- `pop_mean` true means of biomarker responses in populations.
- `pop_mean_long` true means of biomarker responses in long format.
- `pop_profile` profile of biomarkers.

---

### simul

**Generate Hypothetical Samples**

**Description**

simul yields a sample dataset of biomarker responses. This is used for the hypothetical case study.

**Usage**

```r
simul(pop_mean, size = 75)
```

**Arguments**

- `pop_mean` a data frame, the first output of setpop.
- `size` an integer, the sample size.
Value

simul returns a list of length 3:

- `sam`: sample dataset.
- `sam_long`: sample dataset in long format.
- `sam_mean`: sample means of biomarker responses.

visual: Visualize Cliff’s delta and S-value

Description

visual plots Cliff’s delta and S-value for multiple groups and multiple biomarkers.

Usage

visual(rs, rotate = FALSE, display = TRUE)

Arguments

- `rs`: a list, output of `mbr`.
- `rotate`: a logical, whether to rotate the biomarker labels in figures.
- `display`: a logical, whether to display cell values in heatmaps.

Value

visual returns a list of ggplot objects:

- `fig.delta`: heatmap of Cliff’s delta.
- `fig.sval`: heatmap of S-value.
- `fig.avg`: dot plot of the average of absolute Cliff’s delta.
- `mbr_fig`: combined heatmaps of Cliff’s delta and S-value.

Examples

```r
set.seed(1)
setting <- setpop()
temp <- simul(setting$pop_mean)
mbr_result <- mbr(temp$sam)
visual(mbr_result)
# might take more than 5s in some machines
```
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