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Type Package

Title Exploration of Multiple Biomarker Responses using Effect Size

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Suggests RProbSup (>= 3.0)

BugReports <https://github.com/phamdn/mbRes/issues>

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mbRes-package	<i>mbRes: Exploration of Multiple Biomarker Responses using Effect Size</i>
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Description

Summarize multiple biomarker responses of aquatic organisms to contaminants using Cliff's delta, as described in Pham & Sokolova (2023) [doi:10.1002/ieam.4676](https://doi.org/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

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

Beliaeff, B., & Burgeot, T. (2002). Integrated biomarker response: A useful tool for ecological risk assessment. *Environmental Toxicology and Chemistry*, 21(6), 1316–1322. doi:[10.1002/etc.5620210629](https://doi.org/10.1002/etc.5620210629).

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](#).

Value

blaise2002 returns a data frame of RSI.

References

Blaise, C., Gagné, F., Pellerin, J., Hansen, P.-D., & Trottier, S. (2002). Molluscan shellfish biomarker study of the Quebec, Canada, Saguenay Fjord with the soft-shell clam, *Mya arenaria*. *Environmental Toxicology*, 17(3), 170–186. doi:[10.1002/tox.10048](https://doi.org/10.1002/tox.10048).

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

Cliff, N. (1993). Dominance statistics: Ordinal analyses to answer ordinal questions. *Psychological Bulletin*, 114(3), 494–509. doi: [10.1037/00332909.114.3.494](https://doi.org/10.1037/00332909.114.3.494).

Vargha, A., & Delaney, H. D. (2000). A Critique and Improvement of the CL Common Language Effect Size Statistics of McGraw and Wong. *Journal of Educational and Behavioral Statistics*, 25(2), 101–132. doi: [10.3102/10769986025002101](https://doi.org/10.3102/10769986025002101).

Ruscio, J., & Mullen, T. (2012). Confidence Intervals for the Probability of Superiority Effect Size Measure and the Area Under a Receiver Operating Characteristic Curve. *Multivariate Behavioral Research*, 47(2), 201–223. doi: [10.1080/00273171.2012.658329](https://doi.org/10.1080/00273171.2012.658329).

See Also

[CalcA1](#).

Examples

```
cliff(unlist(sokolova2021[7:12, 2]), unlist(sokolova2021[1:6, 2]))
```

compare

Compare RSI, IBR, and Cliff's delta

Description

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

Usage

```
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

Blaise, C., Gagné, F., Pellerin, J., Hansen, P.-D., & Trottier, S. (2002). Molluscan shellfish biomarker study of the Quebec, Canada, Saguenay Fjord with the soft-shell clam, *Mya arenaria*. *Environmental Toxicology*, 17(3), 170–186. doi:10.1002/tox.10048.

Beliaeff, B., & Burgeot, T. (2002). Integrated biomarker response: A useful tool for ecological risk assessment. *Environmental Toxicology and Chemistry*, 21(6), 1316–1322. doi:10.1002/etc.5620210629.

Examples

```

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

```

ggbar*Make Bar Plot*

Description

ggbar creates bar plot of the ecological relevance. This is not meant to be called directly.

Usage

```
ggbar(dat, hax, vax, sub, env = parent.frame())
```

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.
sub	a numeric, mean ecological relevance.
env	an environment, to access outer scope variables.

Value

ggbar returns a ggplot object.

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

```
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	<i>Make Heatmap</i>
--------	---------------------

Description

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

Usage

```
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	<i>Compute Cliff's delta simplified</i>
-----------	---

Description

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

Usage

```
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

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

mbr.glass	<i>Compute Glass's delta simplified</i>
-----------	---

Description

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

Usage

```
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

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

perch

*Empirical Case Study Analysis***Description**

perch analyses the biomarker results of Hansson et al. (2014) <doi:10.1007/s00244-013-9974-5>.

Usage

```
perch()
```

Value

perch returns a list of length 3:

<code>tab</code>	a list of length 2 hansson2014 biomarker data reported by Hansson et al. (2014) percheco assigned ecological relevance of biomarkers
<code>fig</code>	a list of 5 ggplot objects SG length-corrected somatic growth SCI somatic condition index GSI time-corrected gonadosomatic index LSI time-corrected liver somatic index EROD liver ethoxyresorufin-O-deethylase activity
<code>est</code>	full results of our estimation method given by mbr

References

Hansson, T., Hansen, W., Tjärnlund, U., Balk, L., & Bengtsson, B.-E. (2014). Biomarker Investigations in Adult Female Perch (*Perca fluviatilis*) From Industrialised Areas in Northern Sweden in 2003. *Archives of Environmental Contamination and Toxicology*, 66(2), 237–247. doi:10.1007/s0024401399745.

plotsam	<i>Visualize Hypothetical Samples</i>
---------	---------------------------------------

Description

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

Usage

```
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

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

resampling	<i>Measure Statistical Uncertainty</i>
------------	--

Description

resampling performs randomization test and bootstrapping to calculate P-value and percentile bootstrap confidence interval of Cliff's delta.

Usage

```
resampling(v1, v0, nrand = 1999, nboot = 1999, conf.level = 0.95, seed = 1)
```

Arguments

<code>v1</code>	a vector, biomarker values from the treatment group.
<code>v0</code>	a vector, biomarker values from the control group.
<code>nrand</code>	an integer, the number of randomization samples. The default value is 1999.
<code>nboot</code>	an integer, the number of bootstrap samples. The default value is 1999.
<code>conf.level</code>	a numeric, the confidence level to calculate percentile bootstrap confidence interval. The default value is 0.95.
<code>seed</code>	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 four numerics:

<code>delta</code>	the Cliff's delta of the treatment group.
<code>pval</code>	the observed P-value p under the null hypothesis.
<code>sval</code>	the S-value s calculated from P-value p .
<code>se</code>	the standard error of Cliff's delta.
<code>ci.lower</code>	the lower bound of the confidence interval.
<code>ci.upper</code>	the upper bound of the confidence interval.
<code>ciw</code>	the width of the confidence interval.

References

Greenland, S. (2019). Valid P-Values Behave Exactly as They Should: Some Misleading Criticisms of P-Values and Their Resolution With S-Values. *The American Statistician*, 73(sup1), 106–114. doi: [10.1080/00031305.2018.1529625](https://doi.org/10.1080/00031305.2018.1529625).

Phipson, B., & Smyth, G. K. (2010). Permutation P-values Should Never Be Zero: Calculating Exact P-values When Permutations Are Randomly Drawn. *Statistical Applications in Genetics and Molecular Biology*, 9(1). doi: [10.2202/15446115.1585](https://doi.org/10.2202/15446115.1585).

Efron, B., & Tibshirani, R. (1993). *An introduction to the bootstrap*. Chapman & Hall.

Ruscio, J., & Mullen, T. (2012). Confidence Intervals for the Probability of Superiority Effect Size Measure and the Area Under a Receiver Operating Characteristic Curve. *Multivariate Behavioral Research*, 47(2), 201–223. doi: [10.1080/00273171.2012.658329](https://doi.org/10.1080/00273171.2012.658329).

See Also

[A1](#).

Examples

```
resampling(unlist(sokolova2021[7:12, 2]), unlist(sokolova2021[1:6, 2]))
```

setpop	<i>Define Hypothetical Populations</i>
--------	--

Description

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

Usage

```
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	<i>Generate Hypothetical Samples</i>
-------	--------------------------------------

Description

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

Usage

```
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.

sokolova2021

Biomarker Responses of the Blue Mussels to Organic UV Filters

Description

sokolova2021 contains the biomarker responses of the blue mussel *Mytilus edulis* to organic UV filters ensulizole and octocrylene. ecorelevance contains the ecological relevance of the biomarkers.

Usage

sokolova2021

ecorelevance

Format

sokolova2021 is a data frame with 30 rows and 31 variables:

Exposure 5 experimental groups:

CTRL control group

EN10 10 ug/L of ensulizole

EN100 100 ug/L of ensulizole

OC10 10 ug/L of octocrylene

OC100 100 ug/L of octocrylene

NRR lysosomal membrane stability

ROS reactive oxygen species generation

TBARSd lipid peroxidation in digestive gland

TBARSg lipid peroxidation in gills

PCd protein carbonylation in digestive gland

PCg protein carbonylation in gills

CPRd NADPH-P450 reductase activity in digestive gland

CPRg NADPH-P450 reductase activity in gills

ERODd 7-ethoxyresorufin-O-deethylase activity in digestive gland

ERODg 7-ethoxyresorufin-O-deethylase activity in gills

CEd carboxylesterase activity in digestive gland

CEg carboxylesterase activity in gills

GSTd glutathione-S-transferase activity in digestive gland

GSTg glutathione-S-transferase activity in gills

GRd glutathione reductase activity in digestive gland

GRg glutathione reductase activity in gills

CTSDTd total cathepsin D activity in digestive gland
CTSDTg total cathepsin D activity in gills
CTSDFd free cathepsin D activity in digestive gland
CTSDFg free cathepsin D activity in gills
Cas2 caspase 2
Cas3 caspase 3
BAX Bcl-2-associated X protein
Bcl-2 B-cell lymphoma 2
p53 tumor protein 53
GADD45 growth arrest and DNA-damage-inducible protein 45
NF-kB nuclear factor kB
IL-17 interleukin 17
COX-2 cyclooxygenase 2
ACC acetyl-CoA carboxylase

 ecorelevance is a data frame with 30 rows and 2 variables:
Biomarker 30 endpoints as documented in sokolova2021
Eco ecological relevance

Source

Sokolova, I. M., Falfushynska, H., & Sokolov, E. P. (2021). Biomarker responses of the blue mussels to organic UV filters [Data set]. Zenodo. doi: [10.5281/zenodo.5176087](https://doi.org/10.5281/zenodo.5176087).

visual	<i>Visualize Cliff's delta and S-value</i>
--------	--

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:

<code>fig.delta</code>	heatmap of Cliff's delta.
<code>fig.sval</code>	heatmap of S-value.
<code>fig.avg</code>	dot plot of the average of absolute Cliff's delta.
<code>mbr_fig</code>	combined heatmaps of Cliff's delta and S-value.

Examples

```
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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