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mbRes-package	<i>mbRes: Integrating Multiple Biomarker Responses in Aquatic Organisms using Effect Size, Statistical Uncertainty, and Ecological Relevance</i>
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Description

Compute and visualize the ps-index, a new integrated index for multiple biomarker responses, as described in Pham & Sokolova (2021, unpublished).

Guidelines

ps-index is a new integrated index for multiple biomarker responses. `mbr` is the main function to compute and visualize the ps-index. The others are helper functions and are not meant to be called directly by users. `sokolova2021` is provided as a sample dataset.

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Author(s)

Duy Nghia Pham & Inna M. Sokolova

cliff	<i>Compute Effect Size</i>
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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]))
```

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 ps-index. 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`*Make Heatmap*

Description

`ggheat` creates heatmaps of the Cliff's delta, surprisal, confidence interval width, and weighting factor. This is not meant to be called directly.

Usage

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

Arguments

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

Value

`ggheat` returns a `ggplot` object.

mbr	<i>Compute and Visualize ps-index</i>
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Description

mbr calculates the ps-index and visualizes the whole process.

Usage

```
mbr(df, df2 = NULL, rotate = FALSE, display = TRUE)
```

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.
df2	a data frame with the name of biomarkers as the first column and the ecological relevance as the second column.
rotate	a logical, whether to rotate the biomarker labels in figures.
display	a logical, whether to display cell values in heatmaps.

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.

The row order of biomarkers in df2 must match the column order of biomarkers in df. If df2 is missing, all biomarkers automatically have ecological relevance of only 1.

Value

mbr returns a list of length 4:

input	a list of 3 <ul style="list-style-type: none"> main the input biomarker data frame extra a data frame with 2 columns: <ul style="list-style-type: none"> biomarker individual biomarker eco the input ecological relevance eco.mean the mean ecological relevance
es	a data frame with 14 columns: <ul style="list-style-type: none"> treatment treatment groups or test sites control control group or reference site tm_size the sample size of treatment group ct_size the sample size of control group

	biomarker	individual biomarker
	delta	the Cliff's delta of treatment group
	delta.abs	the absolute Cliff's delta
	pval	the P-Value
	sval	the surprisal or S-Value
	se	the standard error of Cliff's delta
	ci.lower	the lower bound of the confidence interval
	ci.upper	the upper bound of the confidence interval
	ciw	the width of the confidence interval
	eco	the ecological relevance of the biomarker
	sval.cdf	the ascending rank of S-value by CDF method, see cume_dist
	ciw.cdf	the descending rank of confidence interval width by CDF method
	eco.cdf	the ascending rank of ecological relevance by CDF method
	weight	the total weighting factor
idx		a data frame with 2 columns:
	treatment	treatment groups or test sites
	ps	the ps-index
fig		a list of 6 ggplot objects
	delta	the Cliff's delta
	sval	the surprisal or S-value
	ciw	confidence interval width
	eco	the ecological relevance
	weight	the weighting factor
	ps	the ps-index

Examples

```
mbr(sokolova2021, ecorelevance, rotate = TRUE) #might take more than 5s in some machines
```

resampling

Measure Statistical Uncertainty

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]))
```

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).

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