Package 'ssd4mosaic'

March 19, 2024

Title Web Application for the SSD Module of the MOSAIC Platform

Version 1.0.1

Description Web application using 'shiny' for the SSD (Species
Sensitivity Distribution) module of the MOSAIC (MOdeling and
StAtistical tools for ecotoxICology) platform. It estimates the
Hazardous Concentration for x% of the species (HCx) from toxicity
values that can be censored and provides various plotting options for
a better understanding of the results. See our companion paper
Kon Kam King et al. (2014) <doi:10.48550/arXiv.1311.5772>.

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URL https://gitlab.in2p3.fr/mosaic-software/mosaic-ssd,
https://mosaic.univ-lyon1.fr/

BugReports https://gitlab.in2p3.fr/mosaic-software/mosaic-ssd/-/issues

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R topics documented:

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add_CI_plot   *Add confidence interval(s) to an existing fitted distribution ggplot*

Description

Add confidence interval(s) to an existing fitted distribution ggplot

Usage

```
add_CI_plot(base_plot, bts, logscale, CI.level = 0.95)
```

Arguments

base_plot	A ggplot object that depicts the fit(s) of the bootstrap(s).
bts	A list of bootdist or bootdistcens objects.
logscale	if TRUE, uses a logarithmic scale for the x-axis
CI.level	A strictly positive numeric smaller than 1. The level of the confidence interval(s).

Value

A ggplot object.

---

base_cdf	*Graphical representation of fitted distribution(s)*

Description

base_cdf plots an empirical cdf of the toxicity values against one or several fitted distributions'
cdf. It works for both censored and non censored data.

Usage

```
base_cdf(fits, unit, logscale, names = NULL, horizontals = TRUE, xlim = NULL)
```

Arguments

fits	A list of fits of class fitdist or fitdistcens computed from the same toxicity data.
unit	A character vector, the unit of the toxicity data
logscale	if TRUE, uses a logarithmic scale for the x-axis
names	Label vector for data points (only for non censored data)
horizontals	If TRUE, draws horizontal lines for the step empirical cumulative distribution function (ecdf). See also plot.stepfun.
xlim	The x-limits of the plot.

Value

A ggplot object.

---

bootdist_fun   *Determines the appropriate bootstrap function based on a fit object*

Description

Determines the appropriate bootstrap function based on a fit object

Usage

```
bootdist_fun(x, ft, niter = 200)
```

Arguments

x	Not used
ft	A `fitdist` or `fitdistcens` object
niter	An integer. The number of iterations set for the bootstrap function

Value

An appropriate bootstrap function.

---

cens_lines_plot   *Graphical representation of censored data*

Description

`cens_lines_plot` create a plot representing each interval of toxicity values with a horizontal line, or a point if the bounds of the interval are equal. It is possible to color the lines by a grouping indicator.

Usage

```
cens_lines_plot(
  data,
  unit,
  logscale,
  fits = NULL,
  leftNA = 0,
  rightNA = Inf,
  color_group = FALSE
)
```

Arguments

data	A data.frame containing censored toxicity values. It must have columns left, right, and label if color_group = TRUE. Censored values are indicated with NA.
unit	A character vector, the unit of the toxicity data
logscale	if TRUE, uses a logarithmic scale for the x-axis
fits	A list of fits of class fitdist or fitdistcens computed from the same toxicity data.
leftNA	The value to replace censored left values. Default to 0 because toxicity values are concentrations.
rightNA	The value to replace censored right values.
color_group	if TRUE, color the elements of the plot by the group label of the data (column label).

Value

A ggplot object.

---

code_r_ssd	*Generate a script according to user in-app inputs*

Description

Generate a script according to user in-app inputs

Usage

```
code_r_ssd(
  data,
  distributions,
  censored = FALSE,
  logscale = TRUE,
  unit = "arbitrary unit",
  names = FALSE,
  groups = FALSE,
  CI.level = 0.95
)
```

Arguments

data	If censored = TRUE, a data.frame with columns left and right. If censored = FALSE, a data.frame with a column conc.
distributions	A list of the names of the distributions to apply (e.g., 'lnorm', 'llogis')
censored	A Boolean, whether the given data is to be interpreted as censored

logscale	A logical
unit	A character string
names	A logical
groups	A logical
CI.level	A numerical

Value

A character string containing a R script.

---

combine_boot_samples	*Combine several bootstrap samples into a single* bootdist *or* bootdistcens *object*

Description

Combine several bootstrap samples into a single bootdist or bootdistcens object

Usage

```
combine_boot_samples(bs)
```

Arguments

bs	A list of bootdist or bootdistcens objects obtained from the same fit object.

Value

A bootdist or bootdistcens object with a number of samples equal to the sum of number of samples of each bootstrap from the list input.

---

custom_theme	*Custom ggplot theme created for MOSAIC bioacc overwriting* theme_bw

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Description

Custom ggplot theme created for MOSAIC bioacc overwriting theme_bw

Usage

```
custom_theme()
```

| endosulfan | *Summary of 48 to 96-hour acute toxicity values for endosulfan* |

Description

Summary of 48 to 96-hour acute toxicity values (LC50 and EC50 values) for exposure of Australian and Non-Australian taxa to endosulfan.

Usage

```
endosulfan
```

Format

endosulfan

A data frame with 88 rows and 3 columns:

conc Lethal or effective concentration in μg/L.

name Specie's name for each concentration.

group Classification by geographical origin and type: fish or arthropod.

Source

https://pubmed.ncbi.nlm.nih.gov/15499502/

| fluazinam | *48-hour acute toxicity values for fluazinam* |

Description

48-hour acute toxicity values (EC50 values) for exposure of macroinvertebrates and zooplancton to fluazinam.

Usage

```
fluazinam
```

Format

fluazinam

A data frame with 14 rows and 4 columns:

left, right Lower & higher bounds of the effective concentration interval in μg/L.

name Specie's name for each effective concentration.

group Classification of the specie, not all rows use the same taxonomic rank.

Source

<https://pubmed.ncbi.nlm.nih.gov/19837458/>

---

get_bootstrap	*Generate bootstrap sample(s) for a list of fit(s) and check their convergence*

Description

Generate bootstrap sample(s) for a list of fit(s) and check their convergence

Usage

```
get_bootstrap(fits)
```

Arguments

fits	A list of `fitdist` or `fitdistcens` objects

Value

A list of two lists. The first list contains the bootstrap sample(s) and the second one the logical value of convergence.

---

get_fits	*Fit the specified distributions to the given data*

Description

Fit the specified distributions to the given data

Usage

```
get_fits(data, distributions, censored)
```

Arguments

data	If censored = TRUE, a data.frame with columns `left` and `right`. If censored = FALSE, a data.frame with a column `conc`.
distributions	A list of the names of the distributions to apply (e.g., `'lnorm'`, `'llogis'`)
censored	A Boolean, whether the given data is to be interpreted as censored

Value

A list containing the fit object(s) of class `fitdist` or `fitdistcens`.

get_HCx_table   *Get HCx values from fit or bootstrap*

Description

Get HC5, HC10, HC20 and HC50 for each fit provided, with confidence intervals if the corresponding bootstraps were provided.

Usage

```
get_HCx_table(fits, distributions, bootstrap = NULL, CI.level = 0.95)
```

Arguments

fits	A list of fits of class `fitdist` or `fitdistcens` computed from the same toxicity data.
distributions	A list of the names of the distributions to apply (e.g., `'lnorm'`, `'llogis'`)
bootstrap	A list of `bootdist` or `bootdistcens` objects corresponding to the fits provided.
CI.level	A numeric, either 0.95 or 0.9. The level of the confidence interval(s).

Value

A data.frame with different HCx as rows and different fits as columns.

get_parameters_html   *Get fit(s) parameters in HTML format for shiny outputs*

Description

Get fit(s) parameters in HTML format for shiny outputs. Should do nothing if the fit is not ready, and should display limited information if the bootstrap is not done.

Usage

```
get_parameters_html(fits = NULL, bootstrap = NULL, CI.level = 0.95)
```

Arguments

fits	A list of fits of class `fitdist` or `fitdistcens` computed from the same toxicity data.
bootstrap	A list of `bootdist` or `bootdistcens` objects corresponding to the fits provided.
CI.level	A numeric, either 0.95 or 0.9. The level of the confidence interval(s).

Details

The output should look like: (once bootstrap is done)

Log normal distribution

(log-likelihood = -161.8)

meanlog: 1.1 [0.66 ; 1.5]

sdlog: 1.6 [1.3 ; 1.9]

Value

A character string with HTML formatting.

---

get_xlab   *Create a label for x axis based on concentration unit and log scale*

Description

Create a label for x axis based on concentration unit and log scale

Usage

```
get_xlab(unit, logscale)
```

Arguments

unit	A character vector, the unit of the toxicity data
logscale	if TRUE, uses a logarithmic scale for the x-axis

Value

A character vector.

---

group_cdf_censored   *Graphical representation of grouped toxicity censored data*

Description

Create an empirical cdf representation colored according to a "group" attribute. The fitted distribution is also represented.

Usage

```
group_cdf_censored(fits, unit, logscale, data)
```

Arguments

`fits`	A list of fits of class `fitdist` or `fitdistcens` computed from the same toxicity data.
`unit`	A character vector, the unit of the toxicity data
`logscale`	if TRUE, uses a logarithmic scale for the x-axis
`data`	A data.frame with columns `left`, `right` and `group`

Details

The plot represents each interval of toxicity values with a horizontal line, or a point if the bounds of the interval are equal, using function `cens_lines_plot()`.

Value

A ggplot object.

`group_cdf_uncensored`	*Graphical representation of grouped toxicity uncensored data*

Description

Add a group coloration to a provided empirical cdf representation according to a "group" column in data.

Usage

```
group_cdf_uncensored(data, p)
```

Arguments

`data`	A data.frame with columns `conc` and `group`.
`p`	a ggplot object showing the empirical cumulative distribution function of the uncensored data provided.

Value

A ggplot object.

---

my_CIcdfplot	*Create a pretty confidence interval ggplot*

Description

Create a pretty confidence interval ggplot

Usage

```
my_CIcdfplot(b, logscale, CI.level)
```

Arguments

b	One "bootdist" object.
logscale	if TRUE, uses a logarithmic scale for the x-axis
CI.level	A strictly positive numeric smaller than 1. The level of the confidence interval(s).

Value

A ggplot with 7 or 8 layers.

Note

With a bootdist, the plot created has 8 layers. With a bootdistcens object, the plot created has 7 layers. The ribbon and its delimiting lines are always the last 3 layers.

---

name_plot_censored	*Graphical representation of named toxicity censored data*

Description

Add names to a provided empirical cumulative distribution function ggplot (i.e.,species names).

Usage

```
name_plot_censored(data, p, leftNA = 0, rightNA = Inf)
```

Arguments

data	A data.frame with column conc if uncensored data, with left and right if censored data. In any case, must contain a column name.
p	A ggplot object showing the empirical cumulative distribution function of the censored data provided.
leftNA	The value to replace censored left values. Default to 0 because toxicity values are concentrations.
rightNA	The value to replace censored right values.

Details

The positions of the names on the plot are based on the raw data visualization and not the non parametric maximum likelihood estimation (NPMLE) representation, but they can be added to both types of plot.

Compatible with plots colored by group labels.

Value

A ggplot object.

---

name_plot_uncensored   *Graphical representation of named toxicity uncensored data*

Description

Create an empirical cumulative distribution function ggplot with a name (i.e. species names) associated to each observation.

Usage

```
name_plot_uncensored(fits, unit, logscale, data, horizontals = TRUE)
```

Arguments

fits	A list of fits of class `fitdist` or `fitdistcens` computed from the same toxicity data.
unit	A character vector, the unit of the toxicity data
logscale	if `TRUE`, uses a logarithmic scale for the x-axis
data	A data.frame with column `conc` if uncensored data, with `left` and `right` if censored data. In any case, must contain a column `name`.
horizontals	If `TRUE`, draws horizontal lines for the step empirical cumulative distribution function (ecdf). See also `plot.stepfun`.

Value

A ggplot object.

---

options_plot	*Graphical representation of toxicity data with additional elements*

Description

Create an empirical cdf representation with the options to color data according to a group label and to display a name label for each observation.

Usage

```
options_plot(
  fits,
  unit,
  logscale,
  data,
  use_names = FALSE,
  use_groups = FALSE,
  horizontals = TRUE,
  lines_display = TRUE
)
```

Arguments

fits	A list of fits of class `fitdist` or `fitdistcens` computed from the same toxicity data.
unit	A character vector, the unit of the toxicity data
logscale	if TRUE, uses a logarithmic scale for the x-axis
data	A data.frame with column `conc` if uncensored data, with `left` and `right` if censored data, column `name` if the names are to be displayed and column `group` if the groups are to be displayed.
use_names	if TRUE, name labels are added to the plot.
use_groups	if TRUE, data in the plot is colored by group.
horizontals	A boolean. In case of uncensored data, whether to draw horizontal lines for the step of the cumulative distribution function. Should be set to FALSE when `use_group = TRUE` for a better visual.
lines_display	A boolean. In case of censored data, whether to display the raw data or the non parametric maximum likelihood estimation (NPMLE) representation. Ignored when `use_groups = TRUE`. Raw data give a better visual with name labels.

Value

A ggplot object.

---

order_cens_data | *Take a data.frame of censored toxicity data and order them like* `fitdistrplus` *plots*

Description

Take a data.frame of censored toxicity data and order them like `fitdistrplus` plots

Usage

```
order_cens_data(data)
```

Arguments

data   A data.frame of censored data with columns `left` and `right`

Value

A data.frame with ordered toxicity values.

Note

Left censored data are put in first, based on the value of their right bound, then non censored data are ordered based on their average value. The right censored data are put in last, ordered among themselves by their left bound.

---

run_app | *Run the Shiny Application*

Description

Run the Shiny Application

Usage

```
run_app(
  onStart = NULL,
  options = list(),
  enableBookmarking = NULL,
  uiPattern = "/",
  ...
)
```

Arguments

onStart	A function that will be called before the app is actually run. This is only needed for shinyAppObj, since in the shinyAppDir case, a global.R file can be used for this purpose.
options	Named options that should be passed to the runApp call (these can be any of the following: "port", "launch.browser", "host", "quiet", "display.mode" and "test.mode"). You can also specify width and height parameters which provide a hint to the embedding environment about the ideal height/width for the app.
enableBookmarking	
	Can be one of "url", "server", or "disable". The default value, NULL, will respect the setting from any previous calls to enableBookmarking(). See enableBookmarking() for more information on bookmarking your app.
uiPattern	A regular expression that will be applied to each GET request to determine whether the ui should be used to handle the request. Note that the entire request path must match the regular expression in order for the match to be considered successful.
...	arguments to pass to golem_opts. See '?golem::get_golem_options' for more details.

Value

No return value, called for side effects

---

salinity_family	*72-hour acute salinity tolerance of macro-invertebrates grouped by family.*

Description

72-hour acute salinity tolerance (LC50 values) of riverine macro-invertebrates grouped by taxonomic family.

Usage

```
salinity_family
```

Format

Salinity_order

A data frame with 108 rows and 3 columns:

left, right Lower & higher bounds of the lethal concentration interval in mS/cm^2.

group Family of each tested specie.

Source

<https://cdnsciencepub.com/doi/abs/10.1139/f06-080>

---

salinity_order	*72-hour acute salinity tolerance of macro-invertebrates grouped by order.*

Description

72-hour acute salinity tolerance (LC50 values) of riverine macro-invertebrates grouped by taxonomic order.

Usage

```
salinity_order
```

Format

```
Salinity_order
```

A data frame with 108 rows and 3 columns:

left, right Lower & higher bounds of the lethal concentration interval in mS/cm^2.

group Order of each tested specie.

Source

<https://cdnsciencepub.com/doi/abs/10.1139/f06-080>

---

switchInput	*Custom toggle switch input for shiny UI*

Description

Custom toggle switch input for shiny UI

Usage

```
switchInput(id, aria_label, checked = TRUE)
```

Arguments

id	The `input` slot that will be used to access the value.
aria_label	An invisible label for screen readers.
checked	Whether to create the switch as ON.

Value

A toggle switch control that can be added to a UI definition.

---

test_conv   *Test the approximate equality of the quantiles from several bootstrap*
                                       samples

Description

Test the approximate equality of the quantiles from several bootstrap samples

Usage

```
test_conv(bs, probs)
```

Arguments

bs	A list of `bootdist` or `bootdistcens` objects obtained from the same fit object.
probs	A numeric vector of probabilities with values in [0,1]

Value

A logical.

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