Package: morse (via r-universe)

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```
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     risk assessment using Bayesian inference of survival and
     reproduction Data. Among others, it facilitates Bayesian
     inference of the general unified threshold model of survival
     (GUTS). See our companion paper Baudrot and Charles (2021)
     <doi:10.21105/joss.03200>, as well as complementary details in
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morse-package

MOdelling tools for Reproduction and Survival data in Ecotoxicology

Description

Provides tools for the analysis of survival/reproduction toxicity test data in quantitative environmental risk assessment. It can be used to explore/visualize experimental data, and to get estimates of LC_x (X% Lethal Concentration) or, EC_x (X% Effective Concentration) by fitting exposure-response curves. The LC_x , EC_x and parameters of the curve are provided along with an indication of the uncertainty of the estimation. morse can also be used to get an estimation of the NEC (No Effect Concentration) by fitting a Toxico-Kinetic Toxico-Dynamic (TKTD) model (GUTS: General Unified Threshold model of Survival). Within the TKTD-GUTS approach, LC(x,t), EC(x,t) and MF(x,t) (x% Multiplication Factors aka Lethal Profiles) can be explored in proportion x and time t.

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Details

Estimation procedures in morse can be used without a deep knowledge of their underlying probabilistic model or inference methods. Rather, they were designed to behave as well as possible without requiring a user to provide values for some obscure parameters. That said, morse models can also be used as a first step to tailor new models for more specific situations.

The package currently handles survival and reproduction data. Functions dedicated to survival (resp. reproduction) analysis start with a surv (resp. repro) prefix. morse provides a similar workflow in both cases:

- 1. create and validate a data set
- 2. explore a data set
- 3. plot a data set
- 4. fit a model on a data set and output the expected estimates
- 5. check goodness of fit with posterior preditive check plot (ppc)

More specifically, for survival data handles with TKTD 'GUTS' model, morse provides:

- 1. plot LC(x,t) and MF(x,t).
- 2. compute goodness-of-fit measures (PPC percent, NRMSE and SPPE)

Those steps are presented in more details in the "Tutorial" vignette, while a more formal description of the estimation procedures are provided in the vignette called "Models in morse package". Please refer to these documents for further introduction to the use of morse.

This reference manual is a detailed description of the functions exposed in the package.

Getting started The package uses the rjags package (Plummer, 2013), an R interface to the JAGS library for Bayesian model estimation. Note that the rjags package does not include a copy of the JAGS library: you need to install it separately. For instructions on downloading JAGS, see the home page at https://mcmc-jags.sourceforge.io. Once done, simply follow the steps described in the tutorial vignette.

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Type: Package
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References

Delignette-Muller, M.L., Ruiz P. and Veber P. (2017) Robust fit of toxicokinetic-toxicodynamic models using prior knowledge contained in the design of survival toxicity tests.

Delignette-Muller, M.L., Lopes, C., Veber, P. and Charles, S. (2014) *Statistical handling of reproduction data for exposure-response modelling*.

Forfait-Dubuc, C., Charles, S., Billoir, E. and Delignette-Muller, M.L. (2012) *Survival data analyses in ecotoxicology: critical effect concentrations, methods and models. What should we use?*

Plummer, M. (2013) *JAGS Version 4.0.0 user manual*. https://sourceforge.net/projects/mcmc-jags/files/Manuals/4.x/jags_user_manual.pdf/download

Baudrot, V., Preux, S., Ducrot, V., Pavé, A. and Charles, S. (2018) New insights to compare and choose TKTD models for survival based on an inter-laboratory study for Lymnaea stagnalis exposed to Cd.

EFSA PPR Scientific Opinion (2018) Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms https://www.efsa.europa.eu/en/efsajournal/pub/5377.

See Also

rjags, ggplot2

cadmium1

Reproduction and survival data sets for Daphnia magna exposed to cadmium during 21 days

Description

Reproduction and survival data sets of chronic laboratory toxicity tests with *Daphnia magna* freshwater invertebrate exposed to five concentrations of cadmium during 21 days. Five concentrations were tested, with four replicates per concentration. Each replicate contained 10 organisms. Reproduction and survival were monitored at 10 time points.

Usage

data(cadmium1)

Format

A data frame with 200 observations of the following five variables:

replicate A vector of class numeric with the replicate code (1 to 20).

conc A vector of class numeric with the cadmium concentrations in $\mu g.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

Nrepro A vector of class integer with the number of offspring at each time point for each concentration and each replicate.

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References

Billoir, E., Delhaye, H., Forfait, C., Clement, B., Triffault-Bouchet, G., Charles, S. and Delignette-Muller, M.L. (2012) Comparison of toxicity tests with different exposure time patterns: The added value of dynamic modelling in predictive ecotoxicology, *Ecotoxicology and Environmental Safety*, 75, 80-86.

cadmium2 Reproduction and survival data sets for Lymnaea stagnalis exposed to cadmium during 28 days

Description

Reproduction and survival data sets of chronic laboratory toxicity tests with snails (*Lymnaea stag-nalis*) exposed to six concentrations of cadmium during 28 days. Six concentrations were tested, with six replicates per concentration. Each replicate contained five organisms. Reproduction and survival were monitored at 17 time points.

Usage

data(cadmium2)

Format

A data frame with 612 observations of the following five variables:

replicate A vector of class numeric with the replicate code (1 to 36).

conc A vector of class integer with the cadmium concentrations in $\mu q.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

Nrepro A vector of class integer with the number of clutches at each time point for each concentration and each replicate.

References

Ducrot, V., Askem, C., Azam, D., Brettschneider, D., Brown, R., Charles, S., Coke, M., Collinet, M., Delignette-Muller, M.L., Forfait-Dubuc, C., Holbech, H., Hutchinson, T., Jach, A., Kinnberg, K.L., Lacoste, C., Le Page, G., Matthiessen, P., Oehlmann, J., Rice, L., Roberts, E., Ruppert, K., Davis, J.E., Veauvy, C., Weltje, L., Wortham, R. and Lagadic, L. (2014) Development and validation of an OECD reproductive toxicity test guideline with the pond snail Lymnaea stagnalis (Mollusca, Gastropoda), *Regulatory Toxicology and Pharmacology*, 70(3), 605-14.

Charles, S., Ducrot, V., Azam, D., Benstead, R., Brettschneider, D., De Schamphelaere, K., Filipe Goncalves, S., Green, J.W., Holbech, H., Hutchinson, T.H., Faber, D., Laranjeiro, F., Matthiessen, P., Norrgren, L., Oehlmann, J., Reategui-Zirena, E., Seeland-Fremer, A., Teigeler, M., Thome, J.P., Tobor Kaplon, M., Weltje, L., Lagadic, L. (2016) Optimizing the design of a reproduction toxicity

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test with the pond snail Lymnaea stagnalis, *Regulatory Toxicology and Pharmacology*, vol. 81 pp.47-56.

chlordan Reproduction and survival data sets for Daphnia magna exposed to chlordan during 21 days

Description

Reproduction and survival data sets of chronic laboratory toxicity tests with *Daphnia magna* freshwater invertebrate exposed to six concentrations of one organochlorine insecticide (chlordan) during 21 days. Six concentrations were tested, with 10 replicates per concentration. Each replicate contained one organism. Reproduction and survival were monitored at 22 time points.

Usage

data(chlordan)

Format

A data frame with 1320 observations of the following five variables:

replicate A vector of class numeric with the replicate code (1 to 60).

conc A vector of class numeric with the chlordan concentrations in $\mu g.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

Nrepro A vector of class integer with the number of offspring at each time point for each concentration and each replicate.

References

Manar, R., Bessi, H. and Vasseur, P. (2009) Reproductive effects and bioaccumulation of chlordan in Daphnia magna, *Environmental Toxicology and Chemistry*, 28, 2150-2159.

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copper Reproduction and survival data sets for Daphnia magna exposed to copper during 21 days	copper	
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Description

Reproduction and survival data sets of chronic laboratory toxicity tests with *Daphnia magna* freshwater invertebrate exposed to five concentrations of copper during 21 days. Five concentrations were tested, with three replicates per concentration. Each replicate contained 20 organisms. Reproduction and survival were monitored at 16 time points.

Usage

data(copper)

Format

A data frame with 240 observations of the following five variables:

replicate A vector of class numeric with the replicate code (1 to 15).

conc A vector of class numeric with the copper concentrations in $\mu g.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

Nrepro A vector of class integer with the number of offspring at each time point for each concentration and each replicate.

References

Billoir, E., Delignette-Muller, M.L., Pery, A.R.R. and Charles, S. (2008) A Bayesian Approach to Analyzing Ecotoxicological Data, *Environmental Science & Technology*, 42 (23), 8978-8984.

dichromate Survival data set for Daphnia magna exposed to dichromate during 21 days	
--	--

Description

Survival data set of chronic laboratory toxicity tests with *Daphnia magna* freshwater invertebrate exposed to six concentrations of one oxidizing agent (potassium dichromate) during 21 days. Six concentrations were tested with one replicate of 50 organisms per concentration. Survival is monitored at 10 time points.

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Usage

```
data(dichromate)
```

Format

A data frame with 60 observations on the following four variables:

replicate A vector of class numeric with the replicate code (1).

conc A vector of class numeric with dichromate concentrations in $mg.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

References

Bedaux, J., Kooijman, SALM (1994) Statistical analysis of toxicity tests, based on hazard modeling, *Environmental and Ecological Statistics*, 1, 303-314.

FOCUSprofile

A simulated exposure profile with 11641 time points.

Description

Exposure profile of 11641 time points used for prediction.

Usage

```
data(FOCUSprofile)
```

Format

A data frame with 11641 observations on the following two variables:

time A vector of class numeric.

conc A vector of class numeric with exposure concentrations.and

replicate A vector of class factor.

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Description

Test in a well-formed argument to function 'survData' if the concentration is constant and different from NA for each replicate (each time-serie)

Usage

```
is_exposure_constant(x)
```

Arguments

Х

an object of class data.frame

Value

a boolean TRUE if concentration in replicate is constant, or FALSE if the concentration in at least one of the replicates is time-variable, and/or if NA occures.

LCx

Predict X% Lethal Concentration at the maximum time point (default).

Description

Predict median and 95% credible interval of the x% Lethal Concentration.

The function LCx, x% Lethal Concentration (LC_x) , is use to compute the dose required to kill x% of the members of a tested population after a specified test duration (time_LCx) (default is the maximum time point of the experiment).

Mathematical definition of x% Lethal Concentration at time t, denoted LC(x,t), is:

$$S(LC(x,t),t) = S(0,t) * (1 - x/100),$$

where S(LC(x,t),t) is the survival probability at concentration LC(x,t) at time t, and S(0,t) is the survival probability at no concentration (i.e. concentration is 0) at time t which reflect the background mortality h_b :

$$S(0,t) = exp(-hb*t).$$

In the function LCx, we use the median of S(0,t) to rescale the x% Lethal Concentration at time t.

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Usage

```
LCx(object, ...)
## S3 method for class 'survFit'
LCx(object, X, time_LCx = NULL, conc_range = NULL, npoints = 100, ...)
```

Arguments

Details

When class of object is survFit, see LCx.survFit.

100 by default.

Value

returns an object of class LCx.

The function returns an object of class LCx, which is a list with the following information:

X_prop Survival probability of individuals surviving considering the median of the background mortality (i.e. S(0,t)*(1-x/100))

X_prop_provided

Survival probability of individuals surviving as provided in arguments (i.e. $\left(100-\right.$

X)/100)

time_LCx A number giving the time at which LC_x has to be estimated as provided in

arguments or if NULL, the latest time point of the experiment is used.

df_LCx A data. frame with quantiles (median, 2.5% and 97.5%) of LC_X at time time_LCx

for X% of individuals

df_dose A data.frame with four columns: concentration, and median q50 and 95%

credible interval (qinf95 and qsup95) of the survival probability at time time_LCx

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MFx

Predict the Multiplication Factor leading to x% of reduction in survival at a specific time.

Description

Generic method for MFx, a function denoted MF(x,t) for x% Multiplication Factor at time t.

The function MFx, x% Multiplication Factor at time t, (MF(x,t)), is used to compute the multiplication factor applied to the concentration exposure profile in order to reduce by x% (argument X) the survival probability at a specified test duration t (argument time_MFx) (default is the maximum time point of the experiment).

Mathematical definition of x% Multiplication Factor at time t (at the end of a time series $T = \{0, \ldots, t\}$), denoted MF(x, t), is given by:

```
S(MF(x,t) * C_w(\tau \in T), t) = S(C_w(\tau \in T), t) * (1 - x/100),
```

where $C_w(\tau \in T)$ is the initial exposure profile without multiplication factor. And so the expression $S(MF(x,t)*C_w(\tau \in T),t)$ is the survival probability after an exposure profile $MF(x,t)*C_w(\tau \in T)$ at time t.

This is a method to replace function MFx used on survFit object when computing issues happen. MFx_ode uses the deSolve library to improve robustness. However, time to compute may be longer.

The function MFx_ode, x% Multiplication Factor at time t, (MF(x,t)), is used to compute the multiplication factor applied to the concentration exposure profile in order to reduce by x% (argument X) the survival probability at a specified test duration t (argument time_MFx) (default is the maximum time point of the experiment).

Mathematical definition of x% Multiplication Factor at time t (at the end of a time series $T = \{0, \ldots, t\}$), denoted MF(x, t), is given by:

```
S(MF(x,t) * C_w(\tau \in T), t) = S(C_w(\tau \in T), t) * (1 - x/100),
```

where $C_w(\tau \in T)$ is the initial exposure profile without multiplication factor. And so the expression $S(MF(x,t)*C_w(\tau \in T),t)$ is the survival probability after an exposure profile $MF(x,t)*C_w(\tau \in T)$ at time t.

```
MFx(object, ...)
## S3 method for class 'survFit'
MFx(
  object,
  data_predict,
  X = 50,
  time_MFx = NULL,
  MFx_range = c(0, 1000),
  mcmc_size = 1000,
  hb_value = TRUE,
  spaghetti = FALSE,
```

MFx

```
accuracy = 0.01,
  quiet = FALSE,
  threshold_iter = 100,
  hb_valueFORCED = 0,
  ode = TRUE,
  interpolate_length = NULL,
  interpolate_method = "linear",
)
MFx_ode(object, ...)
## S3 method for class 'survFit'
MFx_ode(
  object,
  data_predict,
  X = 50,
  time_MFx = NULL,
  MFx_range = c(0, 1000),
  mcmc_size = 1000,
  hb_value = TRUE,
  spaghetti = FALSE,
  accuracy = 0.01,
  quiet = FALSE,
  threshold_iter = 100,
  hb_valueFORCED = 0,
  interpolate_length = NULL,
  interpolate_method = "linear",
)
```

Arguments

object	An object of class survFit.
	Further arguments to be passed to generic methods
data_predict	A dataframe with two columns time and conc.
X	Percentage of survival change (e.g., 50 for survival decrease of 50% , or -50 for survival increase of 50%). The default is 50 . Only time series computed during the adaptation using a binary search in $O(log(n))$ are returned. However, if NULL, all time series computed from the vector MFx_range are returned.
time_MFx	A number giving the time at which $MF(x,t)$ has to be estimated. If NULL, the latest time point of the profile is used.
MFx_range	A vector from which lower and upper bound of the range of the multiplication factor MFx are generated. The default is a vector c(0, 1000). If argument X is NULL, then all the time series generated with MFx_range are returned.
mcmc_size	Can be used to reduce the number of MCMC samples in order to speed up the computation. The default is 1000.

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hb_value If TRUE, the background mortality hb is taken into account from the posterior. If

FALSE, parameter hb is set to 0. The default is TRUE.

spaghetti If TRUE, return a set of survival curves using parameters drawn from the posterior

distribution.

accuracy Accuracy of the multiplication factor. The default is 0.01.

quiet If FALSE, print the evolution of accuracy.

threshold_iter Threshold number of iteration. hb_valueFORCED If hb_value is FALSE, it fix hb.

ode IF ode is TRUE, algo use predict_ode rather than predict. Default is TRUE.

interpolate_length

Length of the time sequence for which output is wanted.

interpolate_method

The interpolation method for concentration. See package deSolve for details.

Default is linear.

Details

When class of object is survFit, see MFx.survFit.

Value

returns an object of class MFx

The function returns an object of class MFx, which is a list with the following information:

X_prop Survival probability for X percent of reduction of the initial median survival

probability at time time_MFx.

X_prop_provided

A number giving the proportion of reduction in survival.

time_MFx A number giving the time at which MF(x,t) has to be estimated as provided in

arguments or if NULL, the latest time point of the profile is used.

df_MFx A data. frame with quantiles (median, 2.5% and 97.5%) of MF(x,t) at time t,

time_MFx, for x% of survival reduction.

df_dose A data.frame with quantiles (median, 2.5% and 97.5%) of survival probability

along the computed multiplication factor and at time time_MFx.

MFx_tested A vector of all multiplication factors computed.

1s_predict A list of all object of class survFitPredict obtained from computing survival

probability for every profiles build from the vector of multiplication factors

MFx_tested.

The function returns an object of class MFx, which is a list with the following information:

X_prop Survival probability for X percent of reduction of the initial median survival

probability at time time_MFx.

X_prop_provided

A number giving the proportion of reduction in survival.

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time_MFx	A number giving the time at which $MF(x,t)$ has to be estimated as provided in arguments or if NULL, the latest time point of the profile is used.
df_MFx	A data.frame with quantiles (median, 2.5% and 97.5%) of $MF(x,t)$ at time t , time_MFx, for $x\%$ of survival reduction.
df_dose	A data.frame with quantiles (median, 2.5% and 97.5%) of survival probability along the computed multiplication factor and at time time_MFx.
MFx_tested	A vector of all multiplication factors computed.
ls_predict	A list of all object of class survFitPredict obtained from computing survival probability for every profiles build from the vector of multiplication factors MFx_tested.

modelData	Create a list giving data to use in Bayesian inference.
-----------	---

Description

Create a data set to analyse a survDataCstExp object.

Create a data set to analyse a survDataVarExp object.

Usage

```
modelData(x, ...)
## S3 method for class 'survDataCstExp'
modelData(x, model_type = NULL, ...)
## S3 method for class 'survDataVarExp'
modelData(x, model_type = NULL, extend_time = 100, ...)
```

Arguments

X	An object of class survData
	Further arguments to be passed to generic methods
<pre>model_type</pre>	TKTD GUTS model type ('SD' or 'IT')
extend_time	Number of for each replicate used for linear interpolation (comprise between time to compute and fitting accuracy)

Value

A list for parameterization of priors for Bayesian inference.

A list for parameterization of priors for Bayesian inference.

A list for parameterization of priors for Bayesian inference.

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plot.LCx

Plotting method for LCx objects

Description

This is the generic plot S3 method for the LCx class. It plots the survival probability as a function of concentration.

Usage

```
## S3 method for class 'LCx'
plot(
    x,
    xlab = "Concentration",
    ylab = "Survival probability \n median and 95 CI",
    main = NULL,
    subtitle = NULL,
    ...
)
```

Arguments

```
x An object of class LCx.
xlab A label for the X-axis, by default Concentration.
ylab A label for the Y-axis, by default Survival probability median and 95 CI.
main A main title for the plot.
subtitle A subtitle for the plot
. . . Further arguments to be passed to generic methods.
```

Value

```
a plot of class ggplot
```

plot.MFx

Plotting method for MFx objects

Description

This is the generic plot S3 method for the MFx class. It plots the survival probability as a function of the multiplication factor applied or as a function of time.

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Usage

```
## S3 method for class 'MFx'
plot(
    x,
    x_variable = "MFx",
    xlab = NULL,
    ylab = "Survival probability \n median and 95 CI",
    main = NULL,
    log_scale = FALSE,
    ncol = 3,
    ...
)
```

Arguments

X	An object of class MFx.
x_variable	A character to define the variable for the X -axis, either "MFx" or "Time". The default is "MFx".
xlab	A label for the X -axis, by default NULL and depend on the argument $x_variable$.
ylab	A label for the Y -axis, by default Survival probability median and 95 CI.
main	A main title for the plot.
log_scale	If TRUE, the x-axis is log-scaled. Default is FALSE.
ncol	An interger for the number of columns when several panels are plotted.
	Further arguments to be passed to generic methods.

Value

a plot of class ggplot

plot.reproData Plotting method for reproData objects

Description

This is the generic plot S3 method for the reproData class. It plots the cumulated number of offspring as a function of time.

```
## S3 method for class 'reproData'
plot(
    x,
    xlab,
    ylab = "Cumulated Number of offspring",
    main = NULL,
```

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```
concentration = NULL,
style = "ggplot",
pool.replicate = FALSE,
addlegend = FALSE,
remove.someLabels = FALSE,
...
)
```

Arguments

x an object of class reproData

xlab label of the X-axis

ylab label of the Y-axis, by default Cumulated Number of offspring

main main title for the plot

concentration a numeric value corresponding to some concentration in data. If concentration

= NULL, draws a plot for each concentration

style graphical backend, can be 'ggplot' or 'generic'

pool.replicate if TRUE, the datapoints of each replicate are summed for a same concentration

addlegend if TRUE, adds a default legend to the plot

remove.someLabels

if TRUE, removes 3/4 of X-axis labels in 'ggplot' style to avoid the label overlap

... Further arguments to be passed to generic methods

Value

```
a plot of class ggplot
```

Note

```
When style = "generic", the function calls the generic function plot
```

When style = "ggplot", the function return an object of class gg and ggplot, see function ggplot

plot.reproFitTT Plotting method for reproFitTT objects

Description

This is the generic plot S3 method for the reproFitTT class. It plots the concentration-effect fit under target time reproduction analysis.

plot.reproFitTT 19

Usage

```
## S3 method for class 'reproFitTT'
plot(
 х,
 xlab = "Concentration",
 ylab = "Nb of offspring per ind/day",
 main = NULL,
 fitcol = "orange",
 fitlty = 1,
 fitlwd = 1,
 spaghetti = FALSE,
 cicol = "orange",
 cilty = 2,
 cilwd = 1,
 ribcol = "grey70",
 addlegend = FALSE,
 log.scale = FALSE,
 style = "ggplot",
)
```

Arguments

x	an object of class reproFitTT
xlab	a label for the X -axis, by default Concentration
ylab	a label for the Y -axis, by default Nb of offspring per ind/day
main	main title for the plot
fitcol	color of the fitted curve
fitlty	line type of the fitted curve
fitlwd	width of the fitted curve
spaghetti	if TRUE, the credible interval is represented by multiple curves
cicol	color of the 95 % credible limits
cilty	line type of the 95 % credible limits
cilwd	width of the 95 % credible limits
ribcol	color of the ribbon between lower and upper credible limits. Transparent if NULL
addlegend	if TRUE, adds a default legend to the plot
log.scale	if TRUE, displays X -axis in log-scale
style	graphical backend, can be 'ggplot' or 'generic'
	Further arguments to be passed to generic methods

Details

The fitted curve represents the **estimated reproduction rate** at the target time as a function of the chemical compound concentration. The function plots 95% credible intervals for the estimated reproduction rate (by default the grey area around the fitted curve). Typically a good fit is expected to display a large overlap between the two types of intervals. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. It consists of the representation of simulated curves using parameter values sampled in the posterior distribution (10% of the MCMC chains are randomly taken for this sample).

Value

```
a plot of class ggplot
```

Note

```
When style = "generic", the function calls the generic function plot

When style = "ggplot", the function return an object of class ggplot, see function ggplot
```

Description

This is the generic plot S3 method for the survData class. It plots the number of survivors as a function of time.

```
## S3 method for class 'survDataCstExp'
plot(
    x,
    xlab = "Time",
    ylab = "Number of survivors",
    main = NULL,
    concentration = NULL,
    style = "ggplot",
    pool.replicate = FALSE,
    addlegend = FALSE,
    remove.someLabels = FALSE,
    ...
)
```

plot.survDataVarExp 21

Arguments

```
an object of class survData
Х
                  a label for the X-axis, by default Time
xlab
ylab
                  a label for the Y-axis, by default Number of survivors
                  main title for the plot
main
concentration
                  a numeric value corresponding to some concentration(s) in data. If concentration
                  = NULL, draws a plot for each concentration
                  graphical backend, can be 'generic' or 'ggplot'
style
pool.replicate if TRUE, the datapoints of each replicate are summed for a same concentration
addlegend
                  if TRUE, adds a default legend to the plot
remove.someLabels
                  if TRUE, removes 3/4 of X-axis labels in 'ggplot' style to avoid label overlap
                  Further arguments to be passed to generic methods
```

Value

a plot of class ggplot

Note

When style = "ggplot" (default), the function calls function ggplot and returns an object of class ggplot.

plot.survDataVarExp Plotting method for survDataVarExp objects

Description

This is the generic plot S3 method for the survDataVarC class. It plots the number of survivors as a function of time.

```
## S3 method for class 'survDataVarExp'
plot(
    x,
    xlab = "Time",
    ylab = "Number of survivors",
    main = NULL,
    one.plot = FALSE,
    facetting_level = NULL,
    ...
)
```

22 plot.survFitCstExp

Arguments

```
x an object of class survDataVarExp

xlab a label for the X-axis, by default Time

ylab a label for the Y-axis, by default Number of survivors

main main title for the plot

one.plot if TRUE, draws all the points in one plot instead of one per replicate

facetting_level a vector of characters to rank replicates in the multi plot (i.e. one.plot == FALSE)

... Further arguments to be passed to generic methods
```

Value

an object of class ggplot, see function ggplot

```
plot.survFitCstExp Plotting method for survFit objects
```

Description

This is the generic plot S3 method for the survFit. It plots the fit obtained for each concentration of chemical compound in the original dataset.

```
## S3 method for class 'survFitCstExp'
plot(
    x,
    xlab = "Time",
    ylab = "Survival probability",
    main = NULL,
    concentration = NULL,
    spaghetti = FALSE,
    one.plot = FALSE,
    adddata = TRUE,
    addlegend = FALSE,
    style = "ggplot",
    ...
)
```

plot.survFitPredict 23

Arguments

Χ	An object of class survFit.
xlab	A label for the X -axis, by default Time.
ylab	A label for the Y -axis, by default Survival probability.
main	A main title for the plot.
concentration	A numeric value corresponding to some specific concentrations in data. If concentration = NULL, draws a plot for each concentration.
spaghetti	if TRUE, draws a set of survival curves using parameters drawn from the posterior distribution
one.plot	if TRUE, draws all the estimated curves in one plot instead of one plot per concentration.
adddata	if TRUE, adds the observed data to the plot with (frequentist binomial) confidence intervals $$
addlegend	if TRUE, adds a default legend to the plot.
style	graphical backend, can be 'generic' or 'ggplot'
	Further arguments to be passed to generic methods.

Details

The fitted curves represent the **estimated survival probability** as a function of time for each concentration. The black dots depict the **observed survival probability** at each time point. Note that since our model does not take inter-replicate variability into consideration, replicates are systematically pooled in this plot. The function plots both 95% credible intervals for the estimated survival probability (by default the grey area around the fitted curve) and 95% binomial confidence intervals for the observed survival probability (as black error bars if adddata = TRUE). Both types of intervals are taken at the same level. Typically a good fit is expected to display a large overlap between the two types of intervals. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (2% of the MCMC chains are randomly taken for this sample).

Value

a plot of class ggplot

plot.survFitPredict Plotting method for survFitPredict objects

Description

This is the generic plot S3 method for the survFitPredict. It plots the predicted survival probability for each concentration of the chemical compound in the provided dataset.

24 plot.survFitPredict

Usage

```
## S3 method for class 'survFitPredict'
plot(
    x,
    xlab = "Time",
    ylab = "Survival probability",
    main = NULL,
    spaghetti = FALSE,
    one.plot = FALSE,
    mcmc_size = NULL,
    ...
)
```

Arguments

X	An object of class survFitPredict.
xlab	A label for the X -axis, by default Time.
ylab	A label for the Y -axis, by default Survival probability.
main	A main title for the plot.
spaghetti	If TRUE, draws a set of survival curves using parameters drawn from the posterior distribution
one.plot	if TRUE, draws all the estimated curves in one plot instead of one plot per concentration.
mcmc_size	A numerical value referring by default to the size of the mcmc in object survFitPredict. This option is specific to survFitPredict objects for which computing time may be long. mcmc_size can be used to reduce the number of mcmc samples in order to speed up the computation.
	Further arguments to be passed to generic methods.

Details

The fitted curves represent the **predicted survival probability** as a function of time for each concentration. The function plots both the 95% credible band and the predicted survival probability over time. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (10% of the MCMC chains are randomly taken for this sample).

Value

```
a plot of class ggplot
```

```
plot.survFitPredict_Nsurv
```

Plotting method for survFitPredict_Nsurv objects.

Description

This is the generic plot S3 method for the survFitPredict_Nsurv. It plots the predicted survival probability for each concentration of the chemical compound in the provided dataset.

Usage

```
## $3 method for class 'survFitPredict_Nsurv'
plot(
    X,
    xlab = "Time",
    ylab = "Number of survivors",
    main = NULL,
    spaghetti = FALSE,
    one.plot = FALSE,
    mcmc_size = NULL,
    ...
)
```

Arguments

X	An object of class survFitPredict_Nsurv.
xlab	A label for the X -axis, by default Time.
ylab	A label for the Y -axis, by default Survival probability.
main	A main title for the plot.
spaghetti	If TRUE, draws a set of survival curves using parameters drawn from the posterior distribution
one.plot	if TRUE, draws all the estimated curves in one plot instead of one plot per concentration.
mcmc_size	A numerical value refering by default to the size of the mcmc in object survFitPredict. This option is specific to survFitPredict objects for which computing time may be long. mcmc_size can be used to reduce the number of mcmc samples in order to speed up the computation.
	Further arguments to be passed to generic methods.

Details

The fitted curves represent the **predicted survival probability** as a function of time for each concentration. The function plots both the 95% credible band and the predicted survival probability over time. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (10% of the MCMC chains are randomly taken for this sample).

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Value

```
a plot of class ggplot
```

 ${\tt plot.survFitTKTD} \qquad \qquad {\tt Plotting\ method\ for\ survFitTKTD\ objects}$

An object of class survFitTKTD.

Description

This is the generic plot S3 method for the survFitTKTD. It plots the fit obtained for each concentration of chemical compound in the original dataset.

Usage

```
## S3 method for class 'survFitTKTD'
plot(
    x,
    xlab = "Time",
    ylab = "Survival probablity",
    main = NULL,
    concentration = NULL,
    spaghetti = FALSE,
    one.plot = FALSE,
    adddata = FALSE,
    addlegend = FALSE,
    style = "ggplot",
    ...
)
```

Arguments ×

	·
xlab	A label for the X -axis, by default Time.
ylab	A label for the Y -axis, by default Survival probablity.
main	A main title for the plot.
concentration	A numeric value corresponding to some specific concentration in data. If concentration = NULL, draws a plot for each concentration.
spaghetti	if TRUE, draws a set of survival curves using parameters drawn from the posterior distribution
one.plot	if TRUE, draws all the estimated curves in one plot instead of one plot per concentration.
adddata	if TRUE, adds the observed data to the plot with (frequentist binomial) confidence intervals
addlegend	if TRUE, adds a default legend to the plot.
style	graphical backend, can be 'generic' or 'ggplot'
	Further arguments to be passed to generic methods.

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Details

The fitted curves represent the **estimated survival probablity** as a function of time for each concentration When adddata = TRUE the black dots depict the **observed survival probablity** at each time point. Note that since our model does not take inter-replicate variability into consideration, replicates are systematically pooled in this plot. The function plots both 95% credible intervals for the estimated survival probablity (by default the grey area around the fitted curve) and 95% binomial confidence intervals for the observed survival probablity (as black error bars if adddata = TRUE). Both types of intervals are taken at the same level. Typically a good fit is expected to display a large overlap between the two types of intervals. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (2% of the MCMC chains are randomly taken for this sample).

Value

a plot of class ggplot

plot.survFitTT

Plotting method for survFitTT objects

Description

This is the generic plot S3 method for the survFitTT class. It plots concentration-response fit under target time survival analysis.

```
## S3 method for class 'survFitTT'
plot(
  xlab = "Concentration".
  ylab = "Survival probability",
  main = NULL,
  fitcol = "orange",
  fitlty = 1,
  fitlwd = 1,
  spaghetti = FALSE,
  cicol = "orange",
  cilty = 2,
  cilwd = 1,
  ribcol = "grey70",
  adddata = FALSE,
  addlegend = FALSE,
  log.scale = FALSE,
  style = "ggplot",
)
```

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Arguments

X	an object of class survFitTT
xlab	a label for the X -axis, default is Concentration
ylab	a label for the Y -axis, default is Survival probability
main	main title for the plot
fitcol	color of the fitted curve
fitlty	line type of the fitted curve
fitlwd	width of the fitted curve
spaghetti	if TRUE, the credible interval is represented by multiple curves
cicol	color of the 95 % credible interval limits
cilty	line type for the 95 % credible interval limits
cilwd	width of the 95 % credible interval limits
ribcol	color of the ribbon between lower and upper credible limits. Transparent if \ensuremath{NULL}
adddata	if TRUE, adds the observed data with confidence intervals to the plot
addlegend	if TRUE, adds a default legend to the plot
log.scale	if TRUE, displays X -axis in log-scale
style	graphical backend, can be 'generic' or 'ggplot'
	Further arguments to be passed to generic methods

Details

The fitted curve represents the **estimated survival probability** at the target time as a function of the concentration of chemical compound; When adddata = TRUE the black dots depict the **observed survival probability** at each tested concentration. Note that since our model does not take inter-replicate variability into consideration, replicates are systematically pooled in this plot. The function plots both 95% credible intervals for the estimated survival probability (by default the grey area around the fitted curve) and 95% binomial confidence intervals for the observed survival probability (as black segments if adddata = TRUE). Both types of intervals are taken at the same level. Typically a good fit is expected to display a large overlap between the two intervals. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (10% of the MCMC chains are randomly taken for this sample).

Value

a plot of class ggplot

Note

When style = "ggplot", the function calls function ggplot and returns an object of class ggplot.

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plot.survFitVarExp

Plotting method for survFit *objects*

Description

This is the generic plot S3 method for the survFit. It plots the fit obtained for each concentration profile in the original dataset.

Usage

```
## S3 method for class 'survFitVarExp'
plot(
    X,
    xlab = "Time",
    ylab = "Survival probability",
    main = NULL,
    spaghetti = FALSE,
    one.plot = FALSE,
    adddata = TRUE,
    mcmc_size = NULL,
    scales = "fixed",
    addConfInt = TRUE,
    ...
)
```

Arguments

Χ	An object of class survFit.
xlab	A label for the X -axis, by default Time.
ylab	A label for the Y -axis, by default Survival probability.
main	A main title for the plot.
spaghetti	if TRUE, draws a set of survival curves using parameters drawn from the posterior distribution $$
one.plot	if TRUE, draws all the estimated curves in one plot instead of one plot per concentration.
adddata	if TRUE, adds the observed data to the plot.
mcmc_size	A numerical value refering by default to the size of the mcmc in object survFit. This option is specific to survFitVarExp objects for which computing time may be long. mcmc_size can be used to reduce the number of mcmc samples in order to speed up the computation.
scales	Shape the scale of axis. Default is "fixed", but can be "free", or free in only one dimension "free_x", "free_y". (See ggplot2 documentation for more details.)
addConfInt	If TRUE, add a 95% confidence interval on observed data from a binomial test
	Further arguments to be passed to generic methods.

30 plotDoseResponse

Details

The fitted curves represent the **estimated survival probability** as a function of time for each concentration profile. The black dots depict the **observed survival probability** at each time point. Note that since our model does not take inter-replicate variability into consideration, replicates are systematically pooled in this plot. The function plots both 95% binomial credible intervals for the estimated survival probability (by default the grey area around the fitted curve) and 95% binomial confidence intervals for the observed survival probability (as black segments if adddata = TRUE). Both types of intervals are taken at the same level. Typically a good fit is expected to display a large overlap between the two types of intervals. If spaghetti = TRUE, the credible intervals are represented by two dotted lines limiting the credible band, and a spaghetti plot is added to this band. This spaghetti plot consists of the representation of simulated curves using parameter values sampled in the posterior distribution (10% of the MCMC chains are randomly taken for this sample).

Value

```
a plot of class ggplot
```

plotDoseResponse

Plot dose-response from raw data

Description

Plots the response of the effect as a function of the concentration at a given target time.

Usage

```
plotDoseResponse(x, ...)
```

Arguments

- x an object used to select a method plotDoseRespons
- ... Further arguments to be passed to generic methods

Value

```
a plot of class ggplot
```

```
{\tt plotDoseResponse.reproData}
```

Plot dose-response from reproData objects

Description

This is the generic plotDoseResponse S3 method for the reproData class. It plots the number of offspring per individual-days as a function of concentration at a given target time.

Usage

Arguments

X	an object of class reproData	
xlab	a label for the X -axis, by default Concentration	
ylab	a label for the Y -axis, by default Nb of offspring per ind.day	
main	main title for the plot	
ylim	Y-axis limits	
target.time	a numeric value corresponding to some observed time points in data	
style	graphical backend, can be 'ggplot' or 'generic'	
log.scale	if TRUE, displays X -axis in log-scale	
remove.someLabels		
	if TRUE, removes 75% of X -axis labels in 'ggplot' style to avoid the label overlap	
axis	if TRUE displays ticks and label axis	
addlegend	if TRUE, adds a default legend to the plot	
	Further arguments to be passed to generic methods	

Details

The function plots the observed values of the reproduction rate (number of reproduction outputs per individual-day) at a given time point as a function of concentration. The 95 % Poisson confidence interval is added to each reproduction rate. It is calculated using function pois.exact from package epitools. As replicates are not pooled in this plot, overlapped points are shifted on the x-axis to help the visualization of replicates.

Value

```
a plot of class ggplot
```

Note

```
When style = "generic", the function calls the generic function plot
When style = "ggplot", the function return an object of class ggplot, see function ggplot
```

See Also

```
pois.exact
```

```
plotDoseResponse.survDataCstExp
```

Plot dose-response from survData objects

Description

This is the generic plotDoseResponse S3 method for the survData class. It plots the survival probability as a function of concentration at a given target time.

```
## S3 method for class 'survDataCstExp'
plotDoseResponse(
    x,
    xlab = "Concentration",
    ylab = "Survival probability",
    main = NULL,
    target.time = NULL,
    style = "ggplot",
    log.scale = FALSE,
    remove.someLabels = FALSE,
    addlegend = TRUE,
    ...
)
```

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Arguments

X	an object of class survData
xlab	a label for the X -axis, by default Concentration
ylab	a label for the Y -axis, by default Survival probability
main	main title for the plot
target.time	a numeric value corresponding to some observed time in data
style	graphical backend, can be 'ggplot' or 'generic'
log.scale	if TRUE, displays X -axis in log-scale
remove.someLab	els
	if TRUE, removes 75% of X-axis labels in 'ggplot' style to avoid the label overlap
addlegend	if TRUE, adds a default legend to the plot
	Further arguments to be passed to generic methods

Details

The function plots the observed values of the survival probability at a given time point as a function of concentration. The 95 % binomial confidence interval is added to each survival probability. It is calculated using function binom.test from package stats. Replicates are systematically pooled in this plot.

Value

```
a plot of class ggplot
```

Note

```
When style = "generic", the function calls the generic function plot
When style = "ggplot", the function return an object of class ggplot, see function ggplot
```

See Also

```
binom.test
```

plot_prior_post	Generic method to plot priors and posteriors.	
-----------------	---	--

Description

Plot priors and posteriors of a survFit object

```
plot_prior_post(x, ...)
```

Arguments

x an object used to select a method plot_prior_post... Further arguments to be passed to generic methods

Value

```
an object of class plot_prior_post
```

```
plot_prior_post.survFit

Plot posteriors vs priors
```

Description

Plot posteriors vs priors of a survFit object

Usage

```
## S3 method for class 'survFit'
plot_prior_post(x, size_sample = 1000, EFSA_name = FALSE, ...)
```

Arguments

x an object of class survFit used to select a method plot_prior_post
size_sample Size of the random generation of the distribution. Default is 1e3.

EFSA_name If TRUE, replace the current terminology by the one used in the recent EFSA PPR Scientific Opinion (2018).

Further arguments to be passed to generic methods

Value

```
a plot of class ggplot
```

References

EFSA PPR Scientific Opinion (2018) Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms https://www.efsa.europa.eu/en/efsajournal/pub/5377

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ppc

Posterior predictive check plot

Description

Plots posterior predictive check for reproFitTT, survFitTT, survFitTKTD, survFitCstExp and survFitVarExp objects.

This is the generic ppc S3 method for the reproFitTT class. It plots the predicted values with 95% credible intervals versus the observed values.

This is the generic ppc S3 method for the survFitCstExp class. It plots the predicted values along with 95% credible intervals versus the observed values for survFit objects.

This is the generic ppc S3 method for the survFitPredict_Nsurv class. It plots the predicted values along with 95% credible intervals versus the observed values for survFitPredict_Nsurv objects.

This is the generic ppc S3 method for the survFitTKTD class. It plots the predicted values along with 95% credible intervals versus the observed values for survFitTKTD objects.

This is the generic ppc S3 method for the survFitTT class. It plots the predicted values with 95 % credible intervals versus the observed values for survFitTT objects.

This is the generic ppc S3 method for the survFitVarExp class. It plots the predicted values along with 95% credible intervals versus the observed values for survFit objects.

```
ppc(x, ...)
## S3 method for class 'reproFitTT'
ppc(
    x,
    style = "ggplot",
    xlab = "Observed Cumul. Nbr. of offspring",
    ylab = "Predicted Cumul. Nbr. of offspring",
    main = NULL,
    ...
)

## S3 method for class 'survFitCstExp'
ppc(x, style = "ggplot", main = NULL, ...)

## S3 method for class 'survFitPredict_Nsurv'
ppc(
    x,
    xlab = "Observed nb of survivors",
    ylab = "Predicted nb of survivors",
    main = NULL,
```

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```
## S3 method for class 'survFitTKTD'
ppc(x, style = "ggplot", main = NULL, ...)
## S3 method for class 'survFitTT'
ppc(x, style = "ggplot", main = NULL, ...)
## S3 method for class 'survFitVarExp'
ppc(
    x,
    xlab = "Observed nb of survivors",
    ylab = "Predicted nb of survivors",
    main = NULL,
    ...
)
```

Arguments

X	An object of class survFitVarExp
	Further arguments to be passed to generic methods
style	graphical backend, can be 'generic' or 'ggplot'
xlab	A label for the X -axis, by default Observed nb of survivors.
ylab	A label for the Y -axis, by default Predicted nb of survivors.
main	A main title for the plot.

Details

Depending on the class of the object x see their links. for class reproFitTT: ppc.reproFitTT; for class survFitTT: ppc.survFitTT; for class survFitTKTD: ppc.survFitTKTD; for class survFitCstExp: ppc.survFitCstExp and for class survFitVarExp: ppc.survFitVarExp.

The coordinates of black points are the observed values of the cumulated number of reproduction outputs for a given concentration (X-scale) and the corresponding predicted values (Y-scale). 95% prediction intervals are added to each predicted value, colored in green if this interval contains the observed value and in red in the other case. As replicates are not pooled in this plot, overlapped points are shifted on the X-axis to help the visualization of replicates. The bisecting line (y = x) is added to the plot in order to see if each prediction interval contains each observed value. As replicates are shifted on the X-axis, this line may be represented by steps.

The black points show the observed number of survivors (pooled replicates, on X-axis) against the corresponding predicted number (Y-axis). Predictions come along with 95% prediction intervals, which are depicted in green when they contain the observed value and in red otherwise. Samples with equal observed value are shifted on the X-axis. For that reason, the bisecting line (y = x), is represented by steps when observed values are low. That way we ensure green intervals do intersect the bisecting line.

For survFitPredict_Nsurv object, PPC is based on times series simulated for each replicate. In addition, the black points show the observed number of survivors (on *X*-axis) against the corre-

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sponding predicted number (Y-axis). Predictions come along with 95% prediction intervals, which are depicted in green when they contain the observed value and in red otherwise.

The black points show the observed number of survivors (pooled replicates, on X-axis) against the corresponding predicted number (Y-axis). Predictions come along with 95% prediction intervals, which are depicted in green when they contain the observed value and in red otherwise. Samples with equal observed value are shifted on the X-axis. For that reason, the bisecting line (y = x), is represented by steps when observed values are low. That way we ensure green intervals do intersect the bisecting line.

The coordinates of black points are the observed values of the number of survivors (pooled replicates) for a given concentration (X-axis) and the corresponding predicted values (Y-axis). 95% prediction intervals are added to each predicted value, colored in green if this interval contains the observed value and in red otherwise. The bisecting line (y = x) is added to the plot in order to see if each prediction interval contains each observed value. As replicates are shifted on the x-axis, this line is represented by steps.

The black points show the observed number of survivors (on X-axis) against the corresponding predicted number (Y-axis). Predictions come along with 95% prediction intervals, which are depicted in green when they contain the observed value and in red otherwise.

Value

a plot of class ggplot

predict.survFit

Predict method for survFit objects

Description

This is the generic predict S3 method for the survFit class. It provides simulation for "SD" or "IT" models under constant or time-variable exposure.

It provides the simulated number of survivors for "SD" or "IT" models under constant or time-variable exposure.

It provides the simulated number of survivors for "SD" or "IT" models under constant or time-variable exposure.

This is a method to replace function predict_Nsurv used on survFit object when computing issues happen. predict_nsurv_ode uses the deSolve library to improve robustness. However, time to compute may be longer.

38 predict.survFit

```
## S3 method for class 'survFit'
predict(
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc_size = NULL,
 hb_value = TRUE,
  ratio_no.NA = 0.95,
 hb\_valueFORCED = NA,
  extend_time = 100,
)
predict_Nsurv(object, ...)
## S3 method for class 'survFit'
predict_Nsurv(
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc_size = NULL,
  hb_value = TRUE,
  hb\_valueFORCED = NA,
  extend_time = 100,
)
predict_Nsurv_ode(
  object,
  data_predict,
  spaghetti,
 mcmc_size,
  hb_value,
  hb_valueFORCED,
  extend_time,
  interpolate_length,
  interpolate_method,
  . . .
)
## S3 method for class 'survFit'
predict_Nsurv_ode(
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc\_size = 1000,
 hb_value = TRUE,
```

predict.survFit 39

```
hb_valueFORCED = NA,
extend_time = 100,
interpolate_length = NULL,
interpolate_method = "linear",
...
)
```

Arguments

object An object of class survFit.

data_predict A dataframe with three columns time, conc and replicate used for prediction.

If NULL, prediction is based on x object of class survFit used for fitting.

spaghetti If TRUE, return a set of survival curves using parameters drawn from the posterior

distribution.

mcmc_size Can be used to reduce the number of mcmc samples in order to speed up the

computation. mcmc_size is the number of selected iterations for one chain.

Default is 1000. If all MCMC is wanted, set argument to NULL.

hb_value If TRUE, the background mortality hb is taken into account from the posterior. If

FALSE, parameter hb is set to 0. The default is TRUE.

ratio_no.NA A numeric between 0 and 1 standing for the proportion of non-NA values re-

quired to compute quantile. The default is 0.95.

hb_valueFORCED If hb_value is FALSE, it fix hb.

extend_time Length of time points interpolated with variable exposure profiles.

... Further arguments to be passed to generic methods

interpolate_length

Length of the time sequence for which output is wanted.

interpolate_method

The interpolation method for concentration. See package deSolve for details.

Default is linear.

Value

a list of data.frame with the quantiles of outputs in df_quantiles or all the MCMC chaines df_spaghetti

an object of class predict_Nsurv.

The function returns an object of class survFitPredict_Nsurv, which is a list with the two following data.frame:

df_quantile

A data.frame with 10 columns, time, conc, replicate, Nsurv (observed number of survivors) and other columns with median and 95% credible interval of the number of survivors computed with 2 different way refers as check and valid: Nsurv_q50_check, Nsurv_qinf95_check, Nsurv_qsup95_check, Nsurv_q50_valid, Nsurv_qinf95_valid, Nsurv_qsup95_valid. The _check refers to the number of survivors at time t predicted using the observed number of survivors at time t-1, while the _valid refers to the number of survivors predicted at time t based on the predicted number of survivors at time t-1.

40 predict_Nsurv_check

 ${\tt df_spaghetti} \qquad {\tt NULL} \ if \ arguement \ {\tt spaghetti} = {\tt FALSE}. \ With \ {\tt spaghetti} = {\tt TRUE}, \ it \ returns \ a$

dataframe with all simulations based on MCMC parameters from a survFit object.

an object of class predict_Nsurv_ode.

a list of data.frame with the quantiles of outputs in df_quantiles or all the MCMC chaines df_spaghetti

Description

It returns measures of goodness-of-fit for predictions.

Provide various criteria for assessment of the model performance: (i) percentage of observation within the 95% credible interval of the Posterior Prediction Check (PPC), the Normalised Root Mean Square Error (NRMSE) and the Survival Probability Prediction Error (SPPE) as reccommended by the recent Scientific Opinion from EFSA (2018).

Usage

```
predict_Nsurv_check(object, ...)
## S3 method for class 'survFitPredict_Nsurv'
predict_Nsurv_check(object, ...)
```

Arguments

object an object of class survFitPredict_Nsurv

. . . Further arguments to be passed to generic methods

Value

return a list of data.frame.

The function return a list with three items:

PPC The criterion, in percent, compares the predicted median numbers of survivors

associated to their uncertainty limits with the observed numbers of survivors. Based on experience, PPC resulting in less than 50% of the observations within the uncertainty limits indicate poor model performance. A fit of 100% may hide

too large uncertainties of prediction (so covering all data).

PPC_global percentage of PPC for the whole data set by gathering replicates.

predict_ode 41

NRMSE The criterion, in percent, is based on the classical root-mean-square error (RMSE),

used to aggregate the magnitudes of the errors in predictions for various timepoints into a single measure of predictive power. In order to provide a criterion expressed as a percentage, NRMSE is the normalised RMSE by the mean of the

observations.

NRMSE_global NRMSE for the whole data set by gathering replicates.

SPPE The SPPE indicator, in percent, is negative (between 0 and -100%) for an un-

derestimation of effects, and positive (between 0 and 100) for an overestimation of effects. An SPPE value of 0 means an exact prediction of the observed sur-

vival probability at the end of the exposure profile.

@references EFSA PPR Scientific Opinion (2018) Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms https://www.efsa.europa.eu/en/efsajournal/pub/5377

predict_ode

Predict method for survFit objects

Description

This is a method to replace function predict used on survFit object when computing issues happen. predict_ode uses the deSolve library to improve robustness. However, time to compute may be longer.

Usage

```
predict_ode(object, ...)
```

Arguments

object an object used to select a method ppc

... Further arguments to be passed to generic methods

Value

an object of class predict_ode

42 predict_ode.survFit

```
predict_ode.survFit Predict method for survFit objects
```

Description

This is the generic predict S3 method for the survFit class. It provides predicted survival rate for "SD" or "IT" models under constant or time-variable exposure.

Usage

```
## S3 method for class 'survFit'
predict_ode(
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc_size = 1000,
  hb_value = TRUE,
  interpolate_length = 100,
  interpolate_method = "linear",
  hb_valueFORCED = NA,
  ...
)
```

Arguments

	object	An object of class survFit.
	data_predict	A dataframe with three columns time, conc and replicate used for prediction. If NULL, prediction is based on x object of class $survFit$ used for fitting.
	spaghetti	If TRUE, return a set of survival curves using parameters drawn from the posterior distribution.
	mcmc_size	Can be used to reduce the number of mcmc samples in order to speed up the computation. mcmc_size is the number of selected iterations for one chain. Default is 1000. If all MCMC is wanted, set argument to NULL.
	hb_value	If TRUE, the background mortality hb is taken into account from the posterior. If FALSE, parameter hb is set to a fixed value. The default is TRUE.
interpolate_length		
		Length of the time sequence for which output is wanted.
	interpolate_method	
		The interpolation method for concentration. See package deSolve for details. Default is linear.
	hb_valueFORCED	If hb_value is FALSE, it fix hb.
		Further arguments to be passed to generic methods

print.msgTable 43

Value

a list of data.frame with the quantiles of outputs in df-quantiles or all the MCMC chaines df-spaghetti

print.msgTable

Print msgTables objects

Description

Print in the REPL the msgTables

Usage

```
## S3 method for class 'msgTable'
print(x, ...)
```

Arguments

- x an object of class msgTables
- ... Further arguments to be passed to generic methods

Value

Print in the REPL the msgTables

print.reproFitTT

Print of reproFitTT object

Description

This is the generic print S3 method for the reproFitTT class. It prints the underlying JAGS model and some information on the Bayesian inference procedure.

Usage

```
## S3 method for class 'reproFitTT'
print(x, ...)
```

Arguments

- x An object of class reproFitTT
- ... Further arguments to be passed to generic methods

Value

print the model text and the Jags Computing information

44 print.survFitTKTD

Description

This is the generic print S3 method for the survFitCstExp class. It prints the underlying JAGS model and some information on the Bayesian inference procedure.

Usage

```
## S3 method for class 'survFitCstExp'
print(x, ...)
```

Arguments

x An object of class survFitCstExp

... Further arguments to be passed to generic methods.

Value

print the model text and the Jags Computing information

print.survFitTKTD Print of survFitTKTD object

Description

This is the generic print S3 method for the survFitTKTD class. It prints the underlying JAGS model and some information on the Bayesian inference procedure.

Usage

```
## S3 method for class 'survFitTKTD'
print(x, ...)
```

Arguments

x An object of class survFitTKTD

... Further arguments to be passed to generic methods.

Value

print the model text and the Jags Computing information

print.survFitTT 45

Description

This is the generic print S3 method for the survFitTT class. It prints the underlying JAGS model and some information on the Bayesian inference procedure.

Usage

```
## S3 method for class 'survFitTT'
print(x, ...)
```

Arguments

x An object of class survFitTT

... Further arguments to be passed to generic methods

Value

print the model text and the Jags Computing information

print.survFitVarExp Print of survFitVarExp object

Description

This is the generic print S3 method for the survFitVarExp class. It prints the underlying JAGS model and some information on the Bayesian inference procedure.

Usage

```
## S3 method for class 'survFitVarExp'
print(x, ...)
```

Arguments

x An object of class survFitVarExp

... Further arguments to be passed to generic methods.

Value

print the model text and the Jags Computing information

Description

Return a data. frame with prior density distributions of parameters used in object.

Usage

```
priors_distribution(object, ...)
```

Arguments

object An object used to select a method

... Further arguments to be passed to generic methods

Details

When the object is of class survFit, see priors_distribution.survFit

Value

```
an object of class priors_distribution
```

```
priors_distribution.survFit
```

Density distribution of priors from a survFit object.

Description

Return a data. frame with priors distribution of parameters used in object.

Usage

```
## S3 method for class 'survFit'
priors_distribution(object, size_sample = 1000, EFSA_name = FALSE, ...)
```

Arguments

object An object of class survFit.

size_sample Size of the random generation of the distribution. Default is 1e3.

EFSA_name If TRUE, replace the current terminology by the one used in the recent EFSA

PPR Scientific Opinion (2018).

. . . Further arguments to be passed to generic methods.

priors_survData 47

Value

a data. frame with prio distribution.

References

EFSA PPR Scientific Opinion (2018) Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms https://www.efsa.europa.eu/en/efsajournal/pub/5377.

priors_survData

Create a list of scalars giving priors to use in Bayesian inference.

Description

Create a list of scalars giving priors to use in Bayesian inference.

Usage

```
priors_survData(x, model_type = NULL)
```

Arguments

x An object of class survData
model_type TKTD model type ('SD' or 'IT')

Value

A list for parameterization of priors for Bayesian inference with JAGS.

propiconazole	Survival data set for Gammarus pulex exposed to propiconazole dur-
	ing four days

Description

Survival data set of chronic laboratory toxicity tests with *Gammarus pulex* freshwater invertebrate exposed to eight concentrations of one fungicide (propiconazole) during four days. Eight concentrations were tested with two replicates of 10 organisms per concentration. Survival is monitored at five time points.

```
data(propiconazole)
```

Format

A dataframe with 75 observations on the following four variables:

replicate A vector of class factor with the replicate code (SC for the control and A1 to G2 for other profiles).

conc A vector of class numeric with propiconazole concentrations in $\mu mol.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

References

Nyman, A.-M., Schirmer, K., Ashauer, R., (2012) Toxicokinetic-toxicodynamic modelling of survival of *Gammarus pulex* in multiple pulse exposures to propiconazole: model assumptions, calibration data requirements and predictive power, *Ecotoxicology*, (21), 1828-1840.

propiconazole_pulse_exposure

Survival data set for Gammarus pulex exposed to propiconazole during 10 days with time-variable exposure concentration (non-standard pulsed toxicity experiments)

Description

Survival data set of laboratory toxicity tests with *Gammarus pulex* freshwater invertebrates exposed to several profiles of concentrations (time-variable concentration for each time series) of one fungicide (propiconazole) during 10 days.

Usage

data(propiconazole_pulse_exposure)

Format

A data frame with 74 observations on the following four variables:

replicate A vector of class factor with the replicate code (varControl, varA, varB and varC). conc A vector of class numeric with propiconazole concentrations in $\mu mol.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

propiconazole_split 49

References

Nyman, A.-M., Schirmer, K., Ashauer, R., (2012) Toxicokinetic-toxicodynamic modelling of survival of *Gammarus pulex* in multiple pulse exposures to propiconazole: model assumptions, calibration data requirements and predictive power, *Ecotoxicology*, (21), 1828-1840.

 ${\it propiconazole_split} \qquad {\it Survival\ data\ set\ for\ Gammarus\ pulex\ exposed\ to\ propiconazole\ during\ four\ days}$

Description

Survival data set of chronic laboratory toxicity tests with *Gammarus pulex* freshwater invertebrate exposed to eight concentrations of one fungicide (propiconazole) during four days. Eight concentrations were tested with two replicates of 10 organisms per concentration. Survival is monitored at five time points.

Usage

data(propiconazole_split)

Format

A dataframe with 75 observations on the following four variables:

replicate A vector of class factor with the replicate code (SC for the control and A1 to G2 for other profiles).

conc A vector of class numeric with propiconazole concentrations in $\mu mol.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

References

Nyman, A.-M., Schirmer, K., Ashauer, R., (2012) Toxicokinetic-toxicodynamic modelling of survival of *Gammarus pulex* in multiple pulse exposures to propiconazole: model assumptions, calibration data requirements and predictive power, *Ecotoxicology*, (21), 1828-1840.

50 reproDataCheck

, , , , , , , , , , , , , , , , , , , ,	reproData	Creates a dataset for reproduction toxicity analysis
---	-----------	--

Description

This function creates a reproData object from experimental data provided as a data. frame. The resulting object can then be used for plotting and model fitting. The reproData class is a sub-class of survData, meaning that all functions and method available for survival analysis can be used with reproData objects.

Usage

reproData(x)

Arguments

Χ

a dataframe as expected by survData containing one additional Nrepro column of class integer with positive values only. This column should provide the number of offspring produced since the last observation.

Details

The x argument contains the experimental data, and should have the same structure than the argument of survData, plus a single additional column providing the total number of offspring observed since the last time point. The function fails if x does not meet the expected requirements. Please run reproDataCheck to ensure x is well-formed.

Note that experimental data with time-variable exposure are not supported.

Value

An object of class reproData.

reproDataCheck Checks if an object can be analysis	be used to perform reproduction toxicity data
--	---

Description

The reproDataCheck function can be used to check if an object containing data from a reproduction toxicity assay meets the expectations of the function reproData.

```
reproDataCheck(data, diagnosis.plot = TRUE)
```

reproFitTT 51

Arguments

```
data any object diagnosis.plot if TRUE, produces a diagnosis plot
```

Details

Since in morse' reproduction data sets are a special case of survival data sets, reproDataCheck performs the same verifications than survDataCheck plus additional ones that are specific to reproduction data.

Value

The function returns a data.frame similar to the one returned by survDataCheck, except that it may contain the following additional error ids:

- NreproInteger: column Nrepro contains values of class other than integer
- Nrepro0T0: Nrepro is not 0 at time 0 for each concentration and each replicate
- Nsurvt0Nreprotp1P: at a given time T, the number of alive individuals is null and the number of collected offspring is not null for the same replicate and the same concentration at time T+1

Note

If an error of type dataframeExpected or missingColumn is detected, the function reproDataCheck is stopped. When no error is detected the reproDataCheck function returns an empty dataframe.

See Also

reproData

reproFitTT

Fits a Bayesian concentration-effect model for target-time reproduction analysis

Description

This function estimates the parameters of a concentration-effect model for target-time reproduction analysis using Bayesian inference. In this model the endpoint is the cumulated number of reproduction outputs over time, with potential mortality all along the experiment.

```
reproFitTT(
  data,
  stoc.part = "bestfit",
  target.time = NULL,
  ecx = c(5, 10, 20, 50),
  n.chains = 3,
  quiet = FALSE
)
```

52 reproFitTT

Arguments

data an object of class reproData

stoc.part stochastic part of the model. Possible values are "bestfit", "poisson" and

"gammapoisson"

target.time defines the target time point at which to analyse the repro data. By default the

last time point

ecx desired values of x (in percent) for which to compute EC_x

n.chains number of MCMC chains. The minimum required number of chains is 2

quiet if TRUE, does not print messages and progress bars from JAGS

Details

Because some individuals may die during the observation period, the reproduction rate alone is not sufficient to account for the observed number of offspring at a given time point. In addition, we need the time individuals have stayed alive during this observation period. The reproFitTT function estimates the number of individual-days in an experiment between its start and the target time. This covariable is then used to estimate a relation between the chemical compound concentration and the reproduction rate *per individual-day*.

The reproFitTT function fits two models, one where inter-individual variability is neglected ("Poisson" model) and one where it is taken into account ("gamma-Poisson" model). When setting stoc.part to "bestfit", a model comparison procedure is used to choose between both. More details are presented in the vignette accompanying the package.

Value

The function returns an object of class reproFitTT which is a list of the following objects:

DIC DIC value of the selected model

estim.ECx a table of the estimated 5, 10, 20 and 50 % effective concentrations (by default)

and their 95 % credible intervals

estim.par a table of the estimated parameters as medians and 95 % credible intervals

mcmc an object of class mcmc.list with the posterior distribution

model a JAGS model object

warnings a data.frame with warning messages

model.label a character string, "P" if the Poisson model is used, "GP" if the gamma-Poisson

is used

parameters a list of the parameter names used in the model

n.chains an integer value corresponding to the number of chains used for the MCMC

computation

n.iter a list of two indices indicating the beginning and the end of monitored iterations

n. thin a numerical value corresponding to the thinning interval

jags.data a list of the data passed to the jags model

transformed.data

the survData object passed to the function

dataTT the dataset with which the parameters are estimated

summary.reproData 53

summary.reproD	sta Summary of reproData ob	bject

Description

This is the generic summary S3 method for the reproData class. It provides information about the structure of the data set and the experimental design.

Usage

```
## S3 method for class 'reproData'
summary(object, quiet = FALSE, ...)
```

Arguments

object an object of class reproData quiet if TRUE, does not print

... Further arguments to be passed to generic methods

Value

The function returns a list with the same information than summary.survDataCstExp plus an additional one:

NboffTimeConc nb of offspring for all concentrations and time points

```
summary.reproFitTT Summary of reproFitTT object
```

Description

This is the generic summary S3 method for the reproFitTT class. It shows the quantiles of priors and posteriors on parameters and the quantiles of the posterior on the ECx estimates.

Usage

```
## S3 method for class 'reproFitTT'
summary(object, quiet = FALSE, ...)
```

Arguments

```
object an object of class reproFitTT quiet when TRUE, does not print
```

. . . Further arguments to be passed to generic methods

Value

The function returns a list with the following information:

Qpriors quantiles of the model priors

Qposteriors quantiles of the model posteriors

QECx quantiles of ECx estimates

summary.survDataCstExp

 $Summary\ of\ survDataCstExp\ object$

Description

The generic summary S3 method for the survDataCstExp class provides information about the structure of the data set and the experimental design.

Usage

```
## S3 method for class 'survDataCstExp'
summary(object, quiet = FALSE, ...)
```

Arguments

object an object of class survDataCstExp

quiet when TRUE, does not print

... Further arguments to be passed to generic methods

Value

The function returns a list with the following information:

NbrepTimeConc nb of replicates for all concentrations and time points

NbsurvTimeConc nb of survivors. for all concentrations and time points

```
summary.survDataVarExp
```

Summary of survDataVarExp object

Description

The generic summary S3 method for the survDataVarExp class provides information about the structure of the data set and the experimental design.

Usage

```
## S3 method for class 'survDataVarExp'
summary(object, quiet = FALSE, ...)
```

Arguments

object an object of class survDataVarExp

quiet when TRUE, does not print

... Further arguments to be passed to generic methods

Value

The function returns a list with the following information:

OccRepTime Occurence of replicates for all time points

NbsurvTimeRep nb of survivors. for all replicates and time points

ConcTimeRep Concentration for all replicates and time points

summary.survFit Summary of survFit object

Description

This is the generic summary S3 method for the survFit class. It shows the quantiles of priors and posteriors on parameters.

```
## S3 method for class 'survFit'
summary(object, quiet = FALSE, EFSA_name = FALSE, ...)
```

Arguments

object An object of class survFit. quiet When TRUE, does not print.

EFSA_name If TRUE, the current terminology by the one used in the recent EFSA PPR Sci-

entific Opinion (2018).

... Further arguments to be passed to generic methods.

Value

The function returns a list with the following information:

Qpriors quantiles of the model priors

Qposteriors quantiles of the model posteriors

References

EFSA PPR Scientific Opinion (2018) Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms https://www.efsa.europa.eu/en/efsajournal/pub/5377.

summary.survFitTKTD Summary of survFitTKTD object

Description

This is the generic summary S3 methode for the survFitTKTD class. It shows the quantiles of priors and posteriors on parameters.

Usage

```
## S3 method for class 'survFitTKTD'
summary(object, quiet = FALSE, ...)
```

Arguments

object an object of class survFitTKTD quiet when TRUE, does not print

... Further arguments to be passed to generic methods.

Value

The function returns a list with the following information:

Qpriors quantiles of the model priors

Qposteriors quantiles of the model posteriors

summary.survFitTT 57

y of survFitTT object

Description

This is the generic summary S3 method for the survFitTT class. It shows the quantiles of priors and posteriors on parameters and the quantiles of the posteriors on the LCx estimates.

Usage

```
## S3 method for class 'survFitTT'
summary(object, quiet = FALSE, ...)
```

Arguments

object an object of class survFitTT quiet when TRUE, does not print

... Further arguments to be passed to generic methods

Value

The function returns a list with the following information:

Qpriors quantiles of the model priors

Qposteriors quantiles of the model posteriors

QLCx quantiles of LCx estimates

survData

Creates a data set for survival analysis

Description

This function creates a survData object from experimental data provided as a data.frame. The resulting object can then be used for plotting and model fitting. It can also be used to generate *individual-time* estimates.

The survDataCheck function can be used to check if an object containing survival data is formatted according to the expectations of the survData function.

```
survData(x)
survDataCheck(data, diagnosis.plot = FALSE)
```

58 survData

Arguments

x a data. frame containing the following four columns:

- replicate: a vector of any class numeric, character or factor for replicate identification. A given replicate value should identify the same group of individuals followed in time
- conc: a vector of class numeric with tested concentrations (positive values, may contain NAs)
- time: a vector of class integer with time points, minimal value must be 0
- Nsurv: a vector of class integer providing the number of alive individuals at each time point for each concentration and each replicate (may contain NAs)

data any object

diagnosis.plot if TRUE, the function may produce diagnosis plots

Details

Survival data sets can be under either constant or time-variable exposure profile. The resulting object, in addition to its survData class, inherits the class survDataCstExp or survDataVarExp respectively.

The x argument describes experimental results from a survival toxicity test. Each line of the data. frame corresponds to one experimental measurement, that is a number of alive individuals at a given concentration at a given time point and in a given replicate. Note that either the concentration or the number of alive individuals may be missing. The data set is inferred to be under constant exposure if the concentration is constant for each replicate and systematically available. The function survData fails if x does not meet the expected requirements. Please run survDataCheck to ensure x is well-formed.

Value

A dataframe of class survData and column replicate as factor.

The function returns a dataframe of class msgTable and data.frame with two columns: id and msg of character strings. When no error is detected the object is empty. Here is the list of possible error ids with their meaning:

dataframeExpected an object of class data. frame is expected at least one expected column heading is missing missingColumn firstTime0 the first time point for some (concentration, replicate) couples is not 0 concNumeric column conc contains a value of class other than numeric timeNumeric column time contains a value of class other than numeric column Nsurv contains a value of class other than integer NsurvInteger tablePositive some data are negative Nsurv0T0 Nsurv is 0 at time 0 for some (concentration, replicate) there are two identical (replicate, time) couples duplicateID NsurvIncrease Nsurv increases at some time point of some (concentration, replicate) maxTimeDiffer maximum time for concentration is lower than maximum time for survival survData_join 59

Note

If an error of type dataframeExpected or missingColumn is detected, the function survDataCheck is stopped before looking for other errors.

See Also

survDataCheck
survData

survData_join

Joins a concentration with a survival data set into an argument for 'survData' when the concentration varies over time

Description

This function joins two data sets, one for exposure measurements, the other for survival measurements, into a single dataframe that can be used with the survData function.

Usage

```
survData_join(x, y)
```

Arguments

x a data. frame containing the following three columns:

- replicate: a vector of class integer or factor for replicate identification
- time: a vector of class integer with time points, \min value must be $\boldsymbol{0}$
- Nsurv: a vector of class integer providing the number of alive individuals at some or all time points for each replicate

y a data. frame containing the following three columns:

- replicate: a vector of class integer or factor for replicate identification
- time: a vector of class integer with time points, min value must be 0
- conc: a vector of class numeric providing the concentration at some or all time points for each replicate

Value

a dataframe suitable for 'survData'

60 survFit

survFit

Fits a TKTD model for survival analysis using Bayesian inference

Description

This function estimates the parameters of a TKTD model ('SD' or 'IT') for survival analysis using Bayesian inference. In this model, the survival rate of individuals is modeled as a function of the chemical compound concentration with a mechanistic description of the effects on survival over time.

```
survFit(
 data,
 model_type,
 quiet,
 n.chains,
 n.adapt,
  n.iter,
  n.warmup,
  thin.interval,
  limit.sampling,
  dic.compute,
  dic.type,
 hb_value,
  hb_valueFIXED,
)
## S3 method for class 'survDataCstExp'
survFit(
 data,
 model_type = NULL,
 quiet = FALSE,
 n.chains = 3,
  n.adapt = 3000,
  n.iter = NULL,
  n.warmup = NULL,
  thin.interval = NULL,
  limit.sampling = TRUE,
  dic.compute = FALSE,
  dic.type = "pD",
 hb_value = TRUE,
  hb\_valueFIXED = NA,
)
```

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```
## S3 method for class 'survDataVarExp'
survFit(
 data,
 model_type = NULL,
 quiet = FALSE,
 n.chains = 3,
 n.adapt = 1000,
 n.iter = NULL,
 n.warmup = NULL,
 thin.interval = NULL,
 limit.sampling = TRUE,
 dic.compute = FALSE,
 dic.type = "pD",
 hb_value = TRUE,
 hb\_valueFIXED = NA,
 extend_time = 100,
)
```

Arguments

data	An object of class survDataCstExp or survDataVarExp.
model_type	Can be "SD" or "IT" to choose between "Stochastic Death" or "Individual Tolerance" models (resp.). See the modeling vignette for details.
quiet	If FALSE, prints logs and progress bar from JAGS.
n.chains	A positive integer specifying the number of MCMC chains. The minimum required number of chains is 2.
n.adapt	A positive integer specifying the number of iterations for adaptation. If n adapt $= 0$ then no adaptation takes place.
n.iter	A positive integer specifying the number of iterations to monitor for each chain.
n.warmup	A positive integer specifying the number of warmup (aka burnin) iterations per chain.
thin.interval	A positive integer specifying the period to monitor.
limit.sampling	if FALSE (default is TRUE), there is no limit to the number of iterations in MCMC imposed by the raftery.diag test.
dic.compute	if TRUE (default is FALSE), it generates penalized deviance samples to compute the Deviance Information Criterion (DIC) with the rjags package
dic.type	type of penalty to use. A string identifying the type of penalty: pD or popt (see function dic.samples)
hb_value	If TRUE, the background mortality hb is taken into account. If FALSE, parameter hb is set to 0. The default is TRUE.
hb_valueFIXED	If hb_value is FALSE, then hb_valueFiXED is the value to fix hb. If hb_value is FALSE and hb_valueFiXED is NA, then hb is fixed to 0.
	Further arguments to be passed to generic methods
extend_time	Number of for each replicate used for linear interpolation (comprise between time to compute and fitting accuracy)

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Details

The function survFit returns the parameter estimates of Toxicokinetic-toxicodynamic (TKTD) models SD for 'Stochastic Death' or IT fo 'Individual Tolerance'. TKTD models, and particularly the General Unified Threshold model of Survival (GUTS), provide a consistent process-based framework to analyse both time and concentration dependent datasets. In GUTS-SD, all organisms are assumed to have the same internal concentration threshold (denoted z), and, once exceeded, the instantaneous probability to die increases linearly with the internal concentration. In GUTS-IT, the threshold concentration is distributed among all the organisms, and once exceeded in one individual, this individual dies immediately.

When class of object is survDataCstExp, see survDataCstExp; and for a survDataVarExp, see survFit.survDataVarExp.

Value

an object of class survFit

The function returns an object of class survFitCstExp, which is a list with the following information:

estim.par a table of the estimated parameters as medians and 95% credible intervals

mcmc an object of class mcmc.list with the posterior distribution

model a JAGS model object

dic return the Deviance Information Criterion (DIC) if dic.compute is TRUE

warnings a table with warning messages

parameters a list of parameter names used in the model

n.chains an integer value corresponding to the number of chains used for the MCMC

computation

mcmcInfo a table with the number of iterations, chains, adaptation, warmup and the thin-

ning interval.

jags.data a list of the data passed to the JAGS model model_type the type of TKTD model used: SD or IT

The function returns an object of class survFitVarExp, which is a list with the following information:

estim.par a table of the estimated parameters as medians and 95% credible intervals

mcmc an object of class mcmc.list with the posterior distribution

model a JAGS model object

dic return the Deviance Information Criterion (DIC) if dic.compute is TRUE

warnings a table with warning messages

parameters a list of parameter names used in the model

n.chains an integer value corresponding to the number of chains used for the MCMC

computation

mcmcInfo a table with the number of iterations, chains, adaptation, warmup and the thin-

ning interval

jags.data a list of the data passed to the JAGS model model_type the type of TKTD model used: SD or IT

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References

Jager, T., Albert, C., Preuss, T. G. and Ashauer, R. (2011) General unified threshold model of survival-a toxicokinetic-toxicodynamic framework for ecotoxicology, *Environmental Science and Technology*, 45, 2529-2540. 303-314.

survFitTKTD	Fits a TKTD for survival analysis using Bayesian inference for
	survDataTKTD <i>object</i>

Description

This function estimates the parameters of a TKTD model for survival analysis using Bayesian inference. In this model, the survival rate of individuals is modeled as a function of the chemical compound concentration with a mechanistic description of the effects on survival over time.

Usage

```
survFitTKTD(data, n.chains = 3, quiet = FALSE)
```

Arguments

data An object of class survData.

n. chains Number of MCMC chains. The minimum required number of chains is 2.

quiet If FALSE, prints logs and progress bar from JAGS.

Value

The function returns an object of class survFitTKTD, which is a list with the following information:

estim.par a table of the estimated parameters as medians and 95% credible intervals

mcmc an object of class mcmc.list with the posterior distribution

warnings a table with warning messages

model a JAGS model object

parameters a list of parameter names used in the model

n.chains an integer value corresponding to the number of chains used for the MCMC

computation

n.iter a list of two indices indicating the beginning and the end of monitored iterations

n.thin a numerical value corresponding to the thinning interval

jags.data a list of data passed to the JAGS model

References

Delignette-Muller ML, Ruiz P and Veber P (2017). Robust fit of toxicokinetic-toxicodynamic models using prior knowledge contained in the design of survival toxicity tests.

Bedaux, J., Kooijman, SALM (1994) Statistical analysis of toxicity tests, based on hazard modeling, *Environmental and Ecological Statistics*, 1, 303-314.

survFitTT

Fits a Bayesian concentration-response model for target-time survival analysis

Description

Fits a Bayesian concentration-response model for target-time survival analysis

Usage

```
survFitTT(data, ...)
```

Arguments

data an object used to select a method 'survFitTT'
... Further arguments to be passed to generic methods

Value

an object of class survFitTT

```
survFitTT.survDataCstExp
```

Fits a Bayesian concentration-response model for target-time survival analysis

Description

This function estimates the parameters of an concentration-response model for target-time survival analysis using Bayesian inference. In this model, the survival rate of individuals at a given time point (called target time) is modeled as a function of the chemical compound concentration. The actual number of surviving individuals is then modeled as a stochastic function of the survival rate. Details of the model are presented in the vignette accompanying the package.

```
## S3 method for class 'survDataCstExp'
survFitTT(
  data,
  target.time = NULL,
  lcx = c(5, 10, 20, 50),
  n.chains = 3,
  quiet = FALSE,
   ...
)
```

Arguments

data an object of class survData

target.time the chosen endpoint to evaluate the effect of the chemical compound concentra-

tion, by default the last time point available for all concentrations

lcx desired values of x (in percent) for which to compute LC_x .

n. chains number of MCMC chains, the minimum required number of chains is 2

quiet if TRUE, does not print messages and progress bars from JAGS

... Further arguments to be passed to generic methods

Details

The function returns parameter estimates of the concentration-response model and estimates of the so-called LC_x , that is the concentration of chemical compound required to get an (1 - x/100) survival rate.

Value

The function returns an object of class survFitTT, which is a list with the following information:

estim.LCx a table of the estimated LC_x along with their 95% credible intervals

estim.par a table of the estimated parameters (medians) and 95% credible intervals

det.part the name of the deterministic part of the used model

mcmc an object of class mcmc.list with the posterior distribution

warnings a table with warning messages

model a JAGS model object

parameters a list of parameter names used in the model

n.chains an integer value corresponding to the number of chains used for the MCMC

computation

n.iter a list of two indices indicating the beginning and the end of monitored iterations

n.thin a numerical value corresponding to the thinning interval

jags.data a list of the data passed to the JAGS model

transformed.data

the survData object passed to the function

dataTT the dataset with which the parameters are estimated

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zinc	Reproduction and survival data sets for Daphnia magna exposed to zinc during 21 days
	·

Description

Reproduction and survival data sets of a chronic laboratory toxicity tests with *Daphnia magna* freshwater invertebrate exposed to four concentrations of zinc during 21 days. Four concentrations were tested with three replicates per concentration. Each replicate contained 20 organisms. Reproduction and survival were monitored at 15 time points.

Usage

data(zinc)

Format

A data frame with 180 observations on the following five variables:

replicate A vector of class numeric with the replicate code (1 to 12).

conc A vector of class numeric with zinc concentrations in $mg.L^{-1}$.

time A vector of class integer with the time points (in days from the beginning of the experiment t=0).

Nsurv A vector of class integer with the number of alive individuals at each time point for each concentration and each replicate.

Nrepro A vector of class integer with the number of offspring at each time point for each concentration and each replicate.

References

Billoir, E., Delignette-Muller, M.L., Pery, A.R.R. and Charles S. (2008) A Bayesian Approach to Analyzing Ecotoxicological Data, *Environmental Science & Technology*, 42 (23), 8978-8984.

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