Package 'morse'

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Description Tools for ecotoxicologists and regulators dedicated to the mathematical and statistical modelling of toxicity test data. They use advanced and innovative methods for a valuable quantitative environmental risk assessment. See also Delignette-Muller et al. (2017) <doi:10.1021/acs.est.6b05326>. and Baudrot et al. (2018) <doi:10.1021/acs.est.7b05464>.

Depends R (>= 3.5.0)

SystemRequirements JAGS (>= 4.0.0) (see http://mcmc-jags.sourceforge.net)

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morse-package . . . 3
cadmium1 . . . 5
cadmium2 . . . 6
chlordan . . . 7
copper . . . 8
dichromate . . . 8
FOCUSprofile . . . 9
is_exposure_constant . . . 10
LCx . . . 10
MFx . . . 12
modelData . . . 16
modelData.survDataCstExp . . . 17
modelData.survDataVarExp . . . 17
plot.LCx . . . 18
plot.MFx . . . 19
plot.reproData . . . 20
plot.reproFitTT . . . 22
plot.survDataCstExp . . . 24
plot.survDataVarExp . . . 25
plot.survFitCstExp . . . 26
plot.survFitPredict . . . 27
plot.survFitPredict_Nsurv . . . 28
plot.survFitTKTD . . . 29
plot.survFitTT . . . 31
plot.survFitVarExp . . . 33
plotDoseResponse . . . 35
plotDoseResponse.reproData . . . 35
plotDoseResponse.survDataCstExp . . . 37
plot_prior_post . . . 39
plot_prior_post.survFit . . . 39
ppc . . . 40
predict.survFit . . . 44
predict_Nsurv_check . . . 47
predict_ode . . . 48
predict_ode.survFit . . . 48
print.reproFitTT . . . 50
print.survFitCstExp . . . 50

print.survFitTKTD . . . 51
print.survFitTT . . . 52
print.survFitVarExp . . . 53
priors_distribution . . . 54
priors_distribution.survFit . . . 54
priors_survData . . . 55
propiconazole . . . 55
propiconazole_pulse_exposure . . . 56
propiconazole_split . . . 57
reproData . . . 58
reproDataCheck . . . 59
reproFitTT . . . 60
summary.reproData . . . 62
summary.reproFitTT . . . 63
summary.survDataCstExp . . . 64
summary.survDataVarExp . . . 65
summary.survFit . . . 66
summary.survFitTKTD . . . 67
summary.survFitTT . . . 68
survData . . . 69
survData_join . . . 71
survFit . . . 72
survFitTKTD . . . 77
survFitTT . . . 79
survFitTT.survDataCstExp . . . 79
zinc . . . 81

Index **82**

`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.

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 `http://mcmc-jags.sourceforge.net`. Once done, simply follow the steps described in the tutorial vignette.

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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*. https://pubs.acs.org/doi/10.1021/acs.est.6b05326

Delignette-Muller, M.L., Lopes, C., Veber, P. and Charles, S. (2014) *Statistical handling of reproduction data for exposure-response modelling*. https://pubs.acs.org/doi/abs/10.1021/es502009r?journalCode=esthag.

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

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* https://pubs.acs.org/doi/abs/10.1021/acs.est.6b05326

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*. https://pubs.acs.org/doi/abs/10.1021/acs.est.7b05464.

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.

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 stagnalis*) 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 $\mu g.L^{-1}$.

`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 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 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.

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

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.

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`.

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

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

x	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.

Examples

```
# (1) Load the survival data set and test if concentration in replicates is constant
data("propiconazole")
is_exposure_constant(propiconazole)
is_exposure_constant(survData(propiconazole))

 # (1) Load the survival data set and test if concentration in replicates is constant
data("propiconazole_pulse_exposure")
is_exposure_constant(propiconazole_pulse_exposure)
```

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.

Usage

```
LCx(object, ...)

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

Arguments

`object`	An object of class `survFit`
`...`	Further arguments to be passed to generic methods
`X`	Percentage of individuals dying (e.g., 50 for LC_{50}, 10 for LC_{10}, ...)
`time_LCx`	A number giving the time at which LC_x has to be estimated. If NULL, the latest time point of the experiment is used.
`conc_range`	A vector of length 2 with minimal and maximal value of the range of concentration. If NULL, the range is define between 0 and the highest tested concentration of the experiment.
`npoints`	Number of time point in `conc_range` between 0 and the maximal concentration. 100 by default.

Details

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

Value

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. $(100 - X)/100$)

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

Examples

```
# (1) Load the data
data("propiconazole")

# (2) Create an object of class 'survData'
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with model_type SD (or IT)
out_SD <- survFit(dataset, model_type = "SD")

# (4) estimate LC50 at time 4
LCx(out_SD, X = 50, time_LCx = 4)

## End(Not run)
```

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.

Usage

```
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,
  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 = FALSE,
  spaghetti = FALSE,
  accuracy = 0.01,
```

```
  quiet = FALSE,
  threshold_iter = 100,
  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.
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

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.
`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`.

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.
`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`.

Examples

```
# (1) Load the data
data("propiconazole")

# (2) Create an object of class 'survData'
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with model_type SD (or IT)
```

```
out_SD <- survFit(dataset, model_type = "SD")

# (4) data to predict
data_4prediction <- data.frame(time = 1:10, conc = c(0,0.5,3,3,0,0,0.5,3,1.5,0))

# (5) estimate MF(x=30, t=4), that is for 30% reduction of survival at time 4
MFx_SD_30.4 <- MFx(out_SD, data_predict = data_4prediction , X = 30, time_MFx = 4)

# (5bis) estimate MF(x,t) along the MF_range from 5 to 10 (50) (X = NULL)
MFx_SD_range <- MFx(out_SD, data_predict = data_4prediction ,
                    X = NULL, time_MFx = 4, MFx_range = seq(5, 10, length.out = 50))

## End(Not run)



# (1) Load the data
data("propiconazole")

# (2) Create an object of class 'survData'
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with model_type SD (or IT)
out_SD <- survFit(dataset, model_type = "SD")

# (4) data to predict
data_4prediction <- data.frame(time = 1:10, conc = c(0,0.5,3,3,0,0,0.5,3,1.5,0))

# (5) estimate MF(x=30, t=4), that is for 30% reduction of survival at time 4
MFx_SD_30.4 <- MFx_ode(out_SD, data_predict = data_4prediction , X = 30, time_MFx = 4)

# (5bis) estimate MF(x,t) along the MF_range from 5 to 10 (50) (X = NULL)
MFx_SD_range <- MFx_ode(out_SD, data_predict = data_4prediction ,
                    X = NULL, time_MFx = 4, MFx_range = seq(5, 10, length.out = 50))

## End(Not run)
```

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

Description

Create a list giving data to use in Bayesian inference.

Usage

```
modelData(x, ...)
```

Arguments

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

Value

A list for parameterization of priors for Bayesian inference.

---

modelData.survDataCstExp

Create a data set to analyse a survDataCstExp *object.*

Description

Create a data set to analyse a survDataCstExp object.

Usage

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

Arguments

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

---

modelData.survDataVarExp

Create a data set to analyse a survDataVarExp *object.*

Description

Create a data set to analyse a survDataVarExp object.

Usage

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

Arguments

x	An object of class survData
model_type	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)
...	Further arguments to be passed to generic methods

plot.LCx *Plotting method for* LCx *objects*

Description

This is the generic plot S3 method for the \codeLCx 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.

Examples

```
# (1) Load the data
data("propiconazole")

# (2) Create an object of class 'survData'
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with model_type SD (or IT)
out_SD <- survFit(dataset, model_type = "SD")

# (4) estimate LC50 at time 4
LCx_SD <- LCx(out_SD, X = 50, time_LCx = 4)

# (5) plot the object of class 'LCx'
plot(LCx_SD)
```

```
## End(Not run)
```

---

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.

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.

Examples

```
# (1) Load the data
data("propiconazole")

# (2) Create an object of class 'survData'
dataset <- survData(propiconazole)
```

```
## Not run:
# (3) Run the survFit function with model_type SD (or IT)
out_SD <- survFit(dataset, model_type = "SD")

# (4) data to predict
data_4prediction <- data.frame(time = 1:10, conc = c(0,0.5,3,3,0,0,0.5,3,1.5,0))

# (5) estimate MF for 30% reduction of survival at time 4
MFx_SD_30.4 <- MFx(out_SD, data_predict = data_4prediction , X = 30, time_MFx = 4)

# (6) plot the object of class 'MFx'
plot(MFx_SD_30.4)

# (6bis) plot with log-scale of x-axis
plot(MFx_SD_30.4, log_scale = TRUE)

# (6ter) plot with "Time" as the x-axis
plot(MFx_SD_30.4, x_variable = "Time")

# (7) plot when X = NULL and along a MFx_range from 5 to 10:
MFx_SD_range <- MFx(out_SD, data_predict = data_4prediction ,
                    X = NULL, time_MFx = 4, MFx_range = seq(5, 10, length.out = 50))
plot(MFx_SD_range)
plot(MFx_SD_range, x_variable = "Time", ncol = 10)

## End(Not run)
```

`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.

Usage

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

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class 'reproData'
cadmium1 <- reproData(cadmium1)

# (3) Plot the reproduction data
plot(cadmium1)

# (4) Plot the reproduction data for a fixed concentration
plot(cadmium1, concentration = 4.36, style = "generic")
```

`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.

Usage

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

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class "reproData"
dataset <- reproData(cadmium1)

## Not run:
# (3) Run the reproFitTT function with the log-logistic gamma-Poisson model
out <- reproFitTT(dataset, stoc.part = "gammapoisson",
                  ecx = c(5, 10, 15, 20, 30, 50, 80), quiet = TRUE)


# (4) Plot the fitted curve with generic style
plot(out, xlab = expression("Concentration in" ~ mu~g.L^{-1}),
     fitcol = "blue", cicol = "lightblue",
     main = "Log-logistic response to concentration")

## End(Not run)
```

`plot.survDataCstExp` *Plotting method for* `survData` *objects*

Description

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

Usage

```
## 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,
  ...
)
```

Arguments

`x`	an object of class `survData`
`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
`concentration`	a numeric value corresponding to some concentration(s) in `data`. If `concentration = NULL`, draws a plot for each concentration
`style`	graphical backend, can be `'generic'` or `'ggplot'`
`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

Note

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

Examples

```
# (1) Load the data
data(zinc)
zinc <- survData(zinc)

# (2) Plot survival data with a ggplot style
plot(zinc)

# (3) Plot the survival data for one specific concentration
plot(zinc, concentration = 0.66)
```

`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.

Usage

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

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.

Usage

```
## 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",
  ...
)
```

Arguments

`x`	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).

`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.

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 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).

Examples

```
# (1) Load the survival data
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function
out <- survFit(dataset , model_type = "SD")

# (4) Create a new data table for prediction
data_4prediction <- data.frame(time = 1:10, conc = c(0,5,5,5,0,0,5,5,5,5),
 replicate= rep("predict", 10))

# (5) Predict on a new dataset
predict_out <- predict(out, data_predict = data_4prediction, spaghetti = TRUE)

# (6) Plot the predicted curve
plot(predict_out)
plot(predict_out, spaghetti = TRUE)

## End(Not run)
```

---

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

```
## S3 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).

---

plot.survFitTKTD *Plotting method for* survFitTKTD *objects*

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

x	An object of class survFitTKTD.
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.

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).

Examples

```
# (1) Load the survival data
data(propiconazole)

# (2) Create an object of class "survData"
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function ('SD' model only)
out <- survFitTKTD(dataset)

# (4) Plot the fitted curves in one plot
plot(out)

# (5) Plot one fitted curve per concentration with credible limits as
# spaghetti, data and confidence intervals
# and with a ggplot style
plot(out, spaghetti = TRUE , adddata = TRUE, one.plot = FALSE,
     style = "ggplot")

# (6) Plot fitted curve for one specific concentration
plot(out, concentration = 36, style = "ggplot")

## End(Not run)
```

`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.

Usage

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

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 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).

Note

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class "survData"
dat <- survData(cadmium1)

## Not run:
# (3) Run the survFitTT function with the log-logistic
#     binomial model
out <- survFitTT(dat, lcx = c(5, 10, 15, 20, 30, 50, 80),
                 quiet = TRUE)

# (4) Plot the fitted curve
plot(out, log.scale = TRUE, adddata = TRUE)

# (5) Plot the fitted curve with ggplot style
plot(out, xlab = expression("Concentration in" ~ mu~g.L^{-1}),
     fitcol = "blue", adddata = TRUE, cicol = "blue",
     style = "ggplot")

## End(Not run)
```

`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

x	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.

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).

Examples

```
# (1) Load the survival data
data("propiconazole_pulse_exposure")
```

```
# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function
out <- survFit(dataset , model_type = "SD")

# (4) Summary look the estimated values (parameters)
summary(out)

# (5) Plot the fitted curve
plot(out, adddata = FALSE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE)

## End(Not run)
```

`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

`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

```
## S3 method for class 'reproData'
plotDoseResponse(
  x,
  xlab = "Concentration",
  ylab = "Nb of offspring per ind.day",
  main = NULL,
  ylim = NULL,
  target.time = NULL,
  style = "ggplot",
  log.scale = FALSE,
  remove.someLabels = FALSE,
  axis = TRUE,
  addlegend = TRUE,
  ...
)
```

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.

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

Examples

```
# (1) Load the data
data(zinc)

# (2) Create an object of class 'reproData'
zinc_rpr <- reproData(zinc)

# (3) Plot dose-response
plotDoseResponse(zinc_rpr)

# (4) Plot dose-response with a generic style
plotDoseResponse(zinc_rpr, style = "generic")
```

---

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.

Usage

```
## 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,
  ...
)
```

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.someLabels	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.

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

Examples

```
library(ggplot2)

# (1) Load the data
data(zinc)

# (2) Create an object of class 'survData'
zinc <- survData(zinc)

# (3) Plot dose-response
plotDoseResponse(zinc)

# (4) Plot dose-respo nse with a generic style
plotDoseResponse(zinc, style = "generic")
```

plot_prior_post *Generic method to plot priors and posteriors.*

Description

Plot priors and posteriors of a `survFit` object

Usage

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

Arguments

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

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

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

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.

Usage

```
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,
  ...
```

```
)

## 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-

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.

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class "reproData"
dataset <- reproData(cadmium1)

## Not run:
# (3) Run the reproFitTT function with the log-logistic gamma-Poisson model
out <- reproFitTT(dataset, stoc.part = "gammapoisson",
ecx = c(5, 10, 15, 20, 30, 50, 80), quiet = TRUE)

# (4) Plot observed versus predicted values
ppc(out)

## End(Not run)


# (1) Load the data
data(propiconazole)

# (2) Create an object of class "survData"
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function with the TKTD model ('SD' or 'IT')
out <- survFit(dataset, model_type = "SD")

# (4) Plot observed versus predicted values
ppc(out)
```

```
## End(Not run)


# (1) Load the data
data(propiconazole)

# (2) Create an object of class "survData"
dat <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function with the TKTD model ('SD' only)
out <- survFitTKTD(dat)

# (4) Plot observed versus predicted values
ppc(out)

## End(Not run)


# (1) Load the data
data(cadmium1)

# (2) Create an object of class "survData"
dat <- survData(cadmium1)

## Not run:
# (3) Run the survFitTT function with the log-logistic binomial model
out <- survFitTT(dat, lcx = c(5, 10, 15, 20, 30, 50, 80),
quiet = TRUE)

# (4) Plot observed versus predicted values
ppc(out)

## End(Not run)


# (1) Load the data
data(propiconazole_pulse_exposure)

# (2) Create an object of class "survData"
dat <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFitTKTD function with the TKTD model ('SD' or 'IT')
out <- survFit(dat, model_type = "SD")

# (4) Plot observed versus predicted values
ppc(out)

## End(Not run)
```

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.

Usage

```
## 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,
  ...
)
```

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 required 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

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 $t-1$.

df_spaghetti NULL if arguement spaghetti = FALSE. With spaghetti = TRUE, it returns a dataframe with all simulations based on MCMC parameters from a survFit object.

Examples

```
# (1) Load the survival data
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function
out <- survFit(dataset , model_type = "SD")

# (4) Create a new data table for prediction
data_4prediction <- data.frame(time = 1:10,
                               conc = c(0,5,30,30,0,0,5,30,15,0),
                               replicate= rep("predict", 10))

# (5) Predict on a new dataset
predict_out <- predict(object = out, data_predict = data_4prediction, spaghetti = TRUE)


## End(Not run)



# (1) Load the survival data
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function
out <- survFit(dataset , model_type = "SD")

# (4) Create a new data table for prediction
data_4prediction <- data.frame(time = 1:10,
                               conc = c(0,5,30,30,0,0,5,30,15,0),
                               replicate= rep("predict", 10),
                               Nsurv = c(20,20,17,16,15,15,15,14,13,12))

# (5) Predict Nsurv on a new data set
predict_out <- predict_Nsurv(object = out, data_predict = data_4prediction, spaghetti = TRUE)


## End(Not run)
```

predict_Nsurv_check *Checking goodness-of-fit method for* survFitPredict *and* survFitPredict_Nsurv *objects*

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

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.
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 time-points 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 underestimation 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 survival 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

`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

Examples

```
# (1) Load the survival data
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function
out <- survFit(dataset , model_type = "SD")

# (4) Create a new data table for prediction
data_4prediction <- data.frame(time = 1:10,
                               conc = c(0,5,30,30,0,0,5,30,15,0),
                               replicate= rep("predict", 10))

# (5) Predict on a new data set
predict_out <- predict_ode(object = out, data_predict = data_4prediction,
                           mcmc_size = 1000, spaghetti = TRUE)


## End(Not run)
```

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class 'reproData'
cadmium1 <- reproData(cadmium1)

## Not run:
# (3) Run the reproFitTT function with the log-logistic
# model
out <- reproFitTT(cadmium1, ecx = c(5, 10, 15, 20, 30, 50, 80),
quiet = TRUE)

# (4) Print the reproFitTT object
print(out)

## End(Not run)
```

print.survFitCstExp *Print of* survFit *object*

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.

Examples

```
# (1) Load the data
data(propiconazole)

# (2) Create an object of class 'survData'
dat <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dat, quiet = TRUE, model_type="SD")

# (4) Print the survFit object
print(out)

## End(Not run)
```

---

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.

Examples

```
# (1) Load the data
data(propiconazole)

# (2) Create an object of class 'survData'
dat <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function
out <- survFitTKTD(dat, quiet = TRUE)

# (4) Print the survFitTKTD object
print(out)

## End(Not run)
```

---

print.survFitTT *Print of* survFitTT *object*

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class 'survData'
cadmium1 <- survData(cadmium1)

## Not run:
# (3) Run the survFitTT function with the log-logistic
# binomial model
out <- survFitTT(cadmium1, lcx = c(5, 10, 15, 20, 30, 50, 80),
                 quiet = TRUE)
```

```
# (4) Print the survFitTT object
print(out)

## End(Not run)
```

`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.

Examples

```
# (1) Load the data
data(propiconazole_pulse_exposure)

# (2) Create a survData object
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dataset, model_type="SD")

# (4) Print the survFit object
print(out)

## End(Not run)
```

priors_distribution *Density distribution of priors.*

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

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.

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.

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create a survData object
dat <- survData(cadmium1)

# (3) Create priors for SD model_type
priors_survData(dat, model_type = "SD")

# (4) Create priors for IT model_type
priors_survData(dat, model_type = "IT")
```

propiconazole — *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)
```

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.

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_split` *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.

`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

`x`	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`.

Examples

```
# (1) Load reproduction dataset
data(cadmium1)

# (2) Create an object of class "reproData"
dat <- reproData(cadmium1)
class(dat)
```

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

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.

Usage

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

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

Examples

```
# Run the check data function
data(copper)
reproDataCheck(copper)

# Now we insert an error in the data set, by setting a non-zero number of
# offspring at some time, although there is no surviving individual in the
# replicate from the previous time point.
copper[148, "Nrepro"] <- as.integer(1)
reproDataCheck(copper)
```

`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.

Usage

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

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class "reproData"
dataset <- reproData(cadmium1)

## Not run:
```

```
# (3) Run the reproFitTT function with the log-logistic gamma-Poisson model
out <- reproFitTT(dataset, stoc.part = "gammapoisson",
                  ecx = c(5, 10, 15, 20, 30, 50, 80), quiet = TRUE)

## End(Not run)
```

`summary.reproData` *Summary of* `reproData` *object*

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create a reproData object
cadmium1 <- reproData(cadmium1)

# (3) Summarize the data set
summary(cadmium1)
```

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create a reproData object
cadmium1 <- reproData(cadmium1)

## Not run:
# (3) Run the reproFitTT function with the log-logistic
# model
out <- reproFitTT(cadmium1, ecx = c(5, 10, 15, 20, 30, 50, 80),
quiet = TRUE)

# (4) summarize the reproFitTT object
summary(out)

## End(Not run)
```

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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create a survDataCstExp object
dat <- survData(cadmium1)

# (3) Summarize the data set
summary(dat)
```

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

Examples

```
# (1) Load the data
data(propiconazole_pulse_exposure)

# (2) Create a survDataVarExp object
out <- survData(propiconazole_pulse_exposure)

# (3) Summarize the data set
summary(out)
```

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.

Usage

```
## 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 Scientific 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.

Examples

```
# (1) Load the data
data(propiconazole)

# (2) Create a survData object
dat <- survData(propiconazole)

## Not run:
# (3) Run the survFit function
out <- survFit(dat, model_type = "SD")

# (4) summarize the survFit object
summary(out)
```

```
## End(Not run)
```

`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

Examples

```
# (1) Load the data
data(propiconazole)

# (2) Create a survData object
dat <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function
out <- survFitTKTD(dat)

# (4) summarize the survFitTKTD object
summary(out)

## End(Not run)
```

summary.survFitTT *Summary 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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create a survData object
cadmium1 <- survData(cadmium1)

## Not run:
# (3) Run the survFitTT function with the log-logistic
# binomial model
out <- survFitTT(cadmium1, lcx = c(5, 10, 15, 20, 30, 50, 80),
                 quiet = TRUE)

# (4) summarize the survFitTT object
summary(out)

## End(Not run)
```

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.

Usage

```
survData(x)

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

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
missingColumn	at least one expected column heading is missing
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
NsurvInteger	column Nsurv contains a value of class other than integer
tablePositive	some data are negative
Nsurv0T0	Nsurv is 0 at time 0 for some (concentration, replicate)
duplicateID	there are two identical (replicate, time) couples
NsurvIncrease	Nsurv increases at some time point of some (concentration, replicate)
maxTimeDiffer	maximum time for concentration is lower than maximum time for survival

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

Examples

```
# (1) Load the survival data set
data(zinc)

# (2) Create an objet of class 'survData'
dat <- survData(zinc)
class(dat)

# Run the check data function
data(zinc)
survDataCheck(zinc)

# Now we insert an error in the dataset, by artificially increasing the
# number of survivors at a given time point, in such a way that the number
# of indivuals increases in the corresponding replicate
zinc[25, "Nsurv"] <- as.integer(20)
survDataCheck(zinc, diagnosis.plot = TRUE)
```

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 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'

Examples

```
# (1) Load the two survival data sets
data(propiconazole_pulse_exposure)
exposure <- propiconazole_pulse_exposure[,c("replicate", "time", "conc")]
survival <- propiconazole_pulse_exposure[,c("replicate", "time", "Nsurv")]

# (2) Create an objet of class 'survData'
dat_join <- survData(survData_join(exposure, survival))
class(dat_join)
```

`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.

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.

This function estimates the parameters of a TKTD ('SD' or 'IT') 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

```
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,
  ...
)

## 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 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)

Details

The function survFit return 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 survFit.survDataCstExp ; and for a survDataVarExp, see survFit.survDataVarExp.

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Value

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

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.

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.

Examples

```
# (1) Load the survival data
data(propiconazole)

# (2) Create an object of class "survData"
dataset  <- survData(propiconazole)

## Not run:
```

```
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dataset , model_type = "SD")

# (4) Summarize look the estimated parameters
summary(out)

# (5) Plot the fitted curve
plot(out, adddata = TRUE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE , adddata = TRUE)

## End(Not run)

# When the data set include variable exposure profile, time for inference is longer

# (1) Load the survival data with variable exposure profile
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dataset , model_type = "SD")

# (4) Summarize look the estimated parameters
summary(out)

# (5) Plot the fitted curve
plot(out, adddata = FALSE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE)

## End(Not run)



# (1) Load the survival data
data(propiconazole)

# (2) Create an object of class "survData"
dataset  <- survData(propiconazole)

## Not run:
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dataset , model_type = "SD")

# (4) Summarize look the estimated parameters
summary(out)

# (5) Plot the fitted curve
```

```
plot(out, adddata = TRUE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE , adddata = TRUE)

## End(Not run)


# (1) Load the survival data
data("propiconazole_pulse_exposure")

# (2) Create an object of class "survData"
dataset <- survData(propiconazole_pulse_exposure)

## Not run:
# (3) Run the survFit function with TKTD model 'SD' or 'IT'
out <- survFit(dataset , model_type = "SD")

# (4) Summarize look the estimated parameters
summary(out)

# (5) Plot the fitted curve
plot(out, adddata = FALSE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE)

## End(Not run)
```

`survFitTKTD` *Fits a TKTD for survival analysis using Bayesian inference for* `survDataTKTD` *object*

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.

Examples

```
# (1) Load the survival data
data(propiconazole)

# (2) Create an object of class "survData"
dataset <- survData(propiconazole)

## Not run:
# (3) Run the survFitTKTD function
out <- survFitTKTD(dataset)

# (4) Summarize look the estimated parameters
summary(out)

# (5) Plot the fitted curve
plot(out, adddata = TRUE)

# (6) Plot the fitted curve with ggplot style and CI as spaghetti
plot(out, spaghetti = TRUE , adddata = TRUE,
     style = "ggplot")

## End(Not run)
```

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

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.

Usage

```
## 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 concentration, 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

Examples

```
# (1) Load the data
data(cadmium1)

# (2) Create an object of class "survData"
dat <- survData(cadmium1)
```

```
## Not run:
# (3) Run the survFitTT function with the log-logistic
#     binomial model
out <- survFitTT(dat, lcx = c(5, 10, 15, 20, 30, 50, 80),
                 quiet = TRUE)

## End(Not run)
```

`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.

Index

∗ **check**
reproDataCheck, 59
∗ **data**
cadmium1, 5
cadmium2, 6
chlordan, 7
copper, 8
dichromate, 8
FOCUSprofile, 9
propiconazole, 55
propiconazole_pulse_exposure, 56
propiconazole_split, 57
zinc, 81
∗ **estimation**
reproFitTT, 60
survFit, 72
survFitTKTD, 77
survFitTT.survDataCstExp, 79
∗ **plot**
plot.LCx, 18
plot.MFx, 19
plot.reproData, 20
plot.reproFitTT, 22
plot.survDataCstExp, 24
plot.survDataVarExp, 25
plot.survFitCstExp, 26
plot.survFitPredict, 27
plot.survFitPredict_Nsurv, 28
plot.survFitTKTD, 29
plot.survFitTT, 31
plot.survFitVarExp, 33
plotDoseResponse.reproData, 35
plotDoseResponse.survDataCstExp, 37
∗ **print**
print.reproFitTT, 50
print.survFitCstExp, 50
print.survFitTKTD, 51
print.survFitTT, 52
print.survFitVarExp, 53
∗ **set**
cadmium1, 5
cadmium2, 6
chlordan, 7
copper, 8
dichromate, 8
FOCUSprofile, 9
propiconazole, 55
propiconazole_pulse_exposure, 56
propiconazole_split, 57
zinc, 81
∗ **summary**
summary.reproData, 62
summary.reproFitTT, 63
summary.survDataCstExp, 64
summary.survDataVarExp, 65
summary.survFit, 66
summary.survFitTKTD, 67
summary.survFitTT, 68
∗ **transformation**
reproData, 58
survData, 69

binom.test, *38*

cadmium1, 5
cadmium2, 6
chlordan, 7
copper, 8

dic.samples, *74*
dichromate, 8

FOCUSprofile, 9

ggplot, *21*, *23–25*, *33*, *36*, *38*
ggplot2, *5*

is_exposure_constant, 10

LCx, 10
LCx.survFit, *11*

MFx, 12
MFx.survFit, *14*
MFx_ode *(*MFx*)*, 12
modelData, 16
modelData.survDataCstExp, 17
modelData.survDataVarExp, 17
morse *(*morse-package*)*, 3
morse-package, 3

plot, *21*, *23*, *36*, *38*
plot.LCx, 18
plot.MFx, 19
plot.reproData, 20
plot.reproFitTT, 22
plot.survDataCstExp, 24
plot.survDataVarExp, 25
plot.survFitCstExp, 26
plot.survFitPredict, 27
plot.survFitPredict_Nsurv, 28
plot.survFitTKTD, 29
plot.survFitTT, 31
plot.survFitVarExp, 33
plot_prior_post, 39
plot_prior_post.survFit, 39
plotDoseResponse, 35
plotDoseResponse.reproData, 35
plotDoseResponse.survDataCstExp, 37
pois.exact, *36*, *37*
ppc, 40
ppc.reproFitTT, *41*
ppc.survFitCstExp, *41*
ppc.survFitTKTD, *41*
ppc.survFitTT, *41*
ppc.survFitVarExp, *41*
predict.survFit, 44
predict_Nsurv *(*predict.survFit*)*, 44
predict_Nsurv_check, 47
predict_Nsurv_ode *(*predict.survFit*)*, 44
predict_ode, 48
predict_ode.survFit, 48
print.reproFitTT, 50
print.survFitCstExp, 50
print.survFitTKTD, 51
print.survFitTT, 52
print.survFitVarExp, 53
priors_distribution, 54
priors_distribution.survFit, *54*, 54
priors_survData, 55
propiconazole, 55
propiconazole_pulse_exposure, 56
propiconazole_split, 57

reproData, 58, *59*
reproDataCheck, *58*, 59
reproFitTT, 60
rjags, *5*

summary.reproData, 62
summary.reproFitTT, 63
summary.survDataCstExp, *62*, 64
summary.survDataVarExp, 65
summary.survFit, 66
summary.survFitTKTD, 67
summary.survFitTT, 68
survData, 69, *70*
survData_join, 71
survDataCheck, *59*, *69*, *70*
survDataCheck *(*survData*)*, 69
survFit, 72
survFit.survDataCstExp, *74*
survFit.survDataVarExp, *74*
survFitTKTD, 77
survFitTT, 79
survFitTT.survDataCstExp, 79

zinc, 81