Package ‘odeGUTS’

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Title Solve ODE for GUTS-RED-SD and GUTS-RED-IT Using Compiled Code

Version 1.0.3

Description Allows performing forwards prediction for the General Unified Threshold model of Survival using compiled ode code. This package was created to avoid dependency with the 'morse' package that requires the installation of 'JAGS'. This package is based on functions from the 'morse' package v3.3.1: Virgile Baudrot, Sandrine Charles, Marie Laure Delignette-Muller, Wandrille Duchemin, Benoit Goussen, Nils Kehrein, Guillaume Kon-Kam-King, Christelle Lopes, Philippe Ruiz, Alexander Singer and Philippe Veber (2021) <`https://CRAN.R-project.org/package=morse`>.

License GPL (>= 3)

Encoding UTF-8

LazyData true

RoxygenNote 7.3.2

URL `https://github.com/bgoussen/odeGUTS`

BugReports `https://github.com/bgoussen/odeGUTS/issues`

Imports deSolve, magrittr, stats, dplyr, zoo, tidyr

NeedsCompilation yes

Suggests morse

Depends R (>= 2.10)

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`fit_odeGUTS` *Model calibration results for a GUTS-SD theoretical species exposed to a compound.*

Description

Model calibration results for a GUTS-SD theoretical species exposed to a compound.

Usage

```
data(fit_odeGUTS)
```

Format

A list of class `survFit` constructed

`mcmc` A list of mcmc chain results

`model_type` A character string containing the type of GUTS model used (here 'SD').

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

Description

Function from the `morse v 3.3.1` package. It returns measures of goodness-of-fit for predictions.

Function from the `morse v 3.3.1` package. Provide various criteria for assessment of the model performance: (i) percentage of observation within the 95\ interval of the Posterior Prediction Check (PPC), the Normalised Root Mean Square Error (NRMSE) and the Survival Probability Prediction Error (SPPE) as recommended 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

Function from the `morse` v `3.3.1` package. 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.

Function from the `morse` v `3.3.1` package. 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.

Function from the `morse` v `3.3.1` package. 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

```
predict_ode(object, ...)

## S3 method for class 'survFit'
predict_ode(
```

```
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc_size = 1000,
  hb_value = FALSE,
  interpolate_length = 100,
  interpolate_method = "linear",
  hb_valueFORCED = 0,
  ...
)

predict_Nsurv_ode(
  object,
  data_predict,
  spaghetti,
  mcmc_size,
  hb_value,
  hb_valueFORCED,
  extend_time,
  interpolate_length,
  interpolate_method,
  ...
)

## S3 method for class 'survFit'
predict_Nsurv_ode(
  object,
  data_predict = NULL,
  spaghetti = FALSE,
  mcmc_size = 1000,
  hb_value = FALSE,
  hb_valueFORCED = 0,
  extend_time = 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 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 `FALSE`.
`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`. Default is `0`
`extend_time`	Length of time points interpolated with variable exposure profiles.

Value

The function returns an object of class `survFitPredict` or `survFitPredict_Nsurv` with two items:

`df_quantile`	Predicted quantiles (q50, qinf95, and qsup95)
`df_spaghetti`	Predicted survival curve (if spaghetti = `TRUE`)

Examples

```
library("odeGUTS")
data(fit_odeGUTS)

data_4prediction <- data.frame(time = 1:10,
                               conc = c(0,5,30,30,0,0,5,30,15,0),
                               replicate= rep("predict", 10))

predict_out <- predict_ode(object = fit_odeGUTS, data_predict = data_4prediction,
                           mcmc_size = 200, spaghetti = FALSE)
```

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