Package: odeGUTS (via r-universe)

August 23, 2024

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

Version 1.0.2.9000

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

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

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)

Repository https://bgoussen.r-universe.dev

RemoteUrl https://github.com/bgoussen/odeguts

RemoteRef HEAD

RemoteSha ac2d1cddd6e348bdb4b54011b25183ccc655ed07

Contents

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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').

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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

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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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