Package ‘GUTS’

February 26, 2022

Type  Package

Title  Fast Calculation of the Likelihood of a Stochastic Survival Model

Version  1.2.3

Date  2022-02-25

Author  Carlo Albert <carlo.albert@eawag.ch>, Sören Vogel <soeren.vogel@posteo.ch>, Oliver Jakoby <oliver.jakoby@rifcon.de>, Alexander Singer <alexander.singer@rifcon.de> and Dirk Nickisch <dirk.nickisch@rifcon.de>

Maintainer  Oliver Jakoby <oliver.jakoby@rifcon.de>

Description  Given exposure and survival time series as well as parameter values, GUTS allows for the fast calculation of the survival probabilities as well as the logarithm of the corresponding likelihood (see Albert, C., Vogel, S. and Ashauer, R. (2016) <doi:10.1371/journal.pcbi.1004978>).

License  GPL (>= 2)

Depends  R (>= 3.5.0), methods, Rcpp (>= 0.12.16)

LinkingTo  Rcpp

LazyLoad  yes

LazyData  no

Encoding  UTF-8

Suggests  knitr, rmarkdown, adaptMCMC, xlsx, drc, testthat

VignetteBuilder  knitr

Repository  CRAN

Repository/R-Forge/Project  guts

Repository/R-Forge/Revision  82

Repository/R-Forge/DateTimeStamp  2022-02-25 10:21:02

Date/Publication  2022-02-25 23:30:20 UTC

NeedsCompilation  yes
R topics documented:

GUTS-package ................................................. 2
diazinon ................................................... 3
GUTS .................................................................. 4

Index 11

GUTS-package  Fast Calculation of the Likelihood of a Stochastic Survival Model

Description

GUTS (General Unified Threshold model of Survival) is a stochastic survival model for ecotoxicology. The package allows for the definition of exposure and survival time series as well as parameter values, and the fast calculation of the survival probabilities as well as the logarithm of the corresponding likelihood.

Details

Package: GUTS
Type: Package
License: GPL (>= 2)

A GUTS object is a special list of class “GUTS”. Functions guts_setup, guts_calc_loglikelihood and guts_calc_survivalprobs are available to create and work with GUTS objects. A data set diazinon is also included. See links for more details.

Author(s)

Carlo Albert <carlo.albert@eawag.ch>, Sören Vogel <soeren.vogel@posteo.ch>, Oliver Jakoby <oliver.jakoby@rifcon.de>, Alexander Singer <alexander.singer@rifcon.de> and Dirk Nickisch <dirk.nickisch@rifcon.de>

Maintainer: Oliver Jakoby <oliver.jakoby@rifcon.de>

References


**diazinon**

**See Also**

`guts_setup, guts_calc_loglikelihood, guts_calc_survivalprobs, guts_report_damage, diazinon, Rcpp`

---

**diazinon**  
*GUTS data set with Gammarus pulex exposed to diazinon*

**Description**

Data of 3 pulsed toxicity tests with the freshwater crustacean Gammarus pulex and diazinon, an organophosphate insecticide.

**Usage**

```r
data("diazinon")
```

**Format**

A list containing 12 data vectors.

**Author(s)**

Carlo Albert <carlo.albert@eawag.ch>, Sören Vogel <soeren.vogel@posteo.ch>, Oliver Jakoby <oliver.jakoby@rifcon.de>, Alexander Singer <alexander.singer@rifcon.de> and Dirk Nickisch <dirk.nickisch@rifcon.de>  
Maintainer: Oliver Jakoby <oliver.jakoby@rifcon.de>

**Source**


**See Also**

GUTS
**Description**

GUTS (General Unified Threshold model of Survival) is a stochastic survival model for ecotoxicology. The package allows for the definition of exposure and survival time series as well as parameter values, and the fast calculation of the survival probabilities as well as the logarithm of the corresponding likelihood.

The package implements the GUTS-SIC (also called GUTS-RED) variants that assume a one-compartment model with first-order toxicokinetics.

**Usage**

```r
guts_setup(C, Ct, y, yt, dist = "lognormal", 
            model = "Proper", 
            N = 1000L, 
            MF = 100L, 
            M = max( 
                5000L, 
                as.integer(ceiling(MF * length(union(Ct, yt)))), 
                as.integer(ceiling(MF * max(union(Ct, yt)))) 
            ), 
            SVR = 1L, 
            study = "" , Clevel = ""
            )

guts_calc_loglikelihood(gobj, par, external_dist = NULL, 
                       use_multinomial_coefficient = FALSE)

guts_calc_survivalprobs(gobj, par, external_dist = NULL)

guts_report_damage(gobj)

guts_report_sppe(gobj)

guts_report_squares(gobj)
```

**Arguments**

- **C**: Numeric vector of concentrations. Vector must contain at least 2 values and be of the same length as `Ct`.
- **Ct**: Numeric vector of concentration time points. Vector must contain at least 2 values and be of the same length as `C`. Time points must start at 0, and contain unique values in ascending order.
y  Integer vector (counts) of survivors. Vector must contain at least 2 values and be of the same length as yt. y must not be ascending.

yt Numeric vector of survivor time points. Vector must contain at least 2 values and be of the same length as y. Time points must start at 0, and contain unique values in ascending order. Survivor information at time points later than the latest concentration time point will be disregarded (with a warning).

dist Distribution as character, either “lognormal” (default), “loglogistic”, “external” or “delta”.

model Model as character, either “Proper” (for full model, the default), “IT” (for individual tolerance), or “SD” (for stochastic death).

MF Integer. Multiplication factor for M. Must be greater than 1. MF is used only if “model = ‘SD’” or “model = ‘Proper’” and M is not specified. Setting MF automatically ensures that the number of points for time discretization M is at least the number of measurement time steps or the measurement time (which ever is larger) multiplied by MF. A minimum of $M = 5000$ is ensured.

M Integer. Desired number of points for time discretization. Must be greater than 1. M is used only if “model = ‘SD’” or “model = ‘Proper’”

N Integer. Sample length of individual tolerance thresholds. Must be greater than 2. N is used only if “model = ‘Proper’”

study string with the name of the study

Clevel character vector with names for each of the concentration levels

SVR Numeric surface-volume-ratio. A multiplication factor to kd.

gobj GUTS object. The object to be updated (and used for the calculation).

par Numeric vector of parameters. See details below.

external_dist Numeric vector containing the distribution of individual thresholds. Only used if dist = ‘external’. See details below.

use_multinomial_coefficient

Details

Functions:
Use guts_setup to define (or alter) a GUTS object. Various checks are applied to the data. On success, a GUTS object will be created.

Use guts_calc_loglikelihood to calculate the survival probabilities and the corresponding loglikelihood for a given set of parameters. The function is very fast and can be used in routines for parameter estimation. The function returns the loglikelihood, however it also updates the fields par, S, D, SPPE, squares, zt and LL of the GUTS-object.

guts_calc_survivalprobs is a convenience wrapper that can be used for predictions; it returns the survival probabilities, however it also updates the fields par, S, D, SPPE, squares, zt and LL of the GUTS-object.

guts_report_damage returns a data.frame with time grid points and the damage for each of these. The function reports the damage that was calculated in the previous call to guts_calc_loglikelihood or guts_calc_survivalprobs.
guts_report_squares returns the sum of squares. The function reports the sum of squares that was calculated in the previous call to guts_calc_loglikelihood or guts_calc_survivalprobs. guts_report_sppe returns the survival-probability prediction error (SPPE). The function reports the SPPE that was calculated in the previous call to guts_calc_loglikelihood or guts_calc_survivalprobs.

Models, Parameters, and Distributions:
The GUTS package provides three model types:

- **Proper**: a GUTS-SIC-Propers (also called GUTS-RED-Propers) model using random individual tolerances and a stochastic death process, when individual tolerances are exceeded.
- **IT**: a GUTS-SIC-IT (GUTS-RED-IT) individual tolerance model using random individual tolerances. If an individual’s tolerance threshold is exceeded, the individual dies.
- **SD**: a GUTS-SIC-SD (GUTS-RED-SD) stochastic death model using a stochastic death process above a population-wide tolerance threshold. The tolerance-threshold is the same for all individuals.

The Proper GUTS model requires the following parameters \( \text{par} \), while variants IT and SD are based on a reduced subset (as indicated in brackets). Parameter values in \( \text{par} \) must be ordered as listed here:

- **hb**: background mortality rate (Proper, IT, SD)
- **ke**: dominant rate constant (Proper, IT, SD)
- **kk**: killing rate (Proper, SD)
- **further parameters** for the tolerance threshold (in SD) or the threshold distribution \( \text{dist} \) (in Proper and IT)

For model type “SD” (stochastic death), required parameters \( \text{par}[1:4] \) are \( \text{hb} \), \( \text{ke} \), \( \text{kk} \) and \( \text{mn} \), which is the population-wide tolerance threshold. For backwards compatibility this model type can be initiated setting \( \text{dist} = \text{"Delta"} \) and \( \text{model} = \text{"Proper"} \).

For model type “IT” (individual tolerance), required parameters \( \text{par}[1:2] \) are \( \text{hb} \), \( \text{ke} \), as well as respective distribution parameters (from \( \text{par}[3] \) onwards). Parameter (\( \text{kk} \)) is set internally to infinity and does not need to be provided.

For model type “Proper”, all parameters are needed. \( \text{par}[1:3] \) take \( \text{hb} \), \( \text{ke} \), \( \text{kk} \), distribution parameters follow (from \( \text{par}[4] \) onwards).

For model types “Proper” and “IT” individual tolerance thresholds are created internally. Individual tolerances are drawn from the specified distribution \( \text{dist} \). The parameter values required depend on the specified \( \text{dist} \):

- **"lognormal"**: requires the parameters \( \text{mn} \) and \( \text{sd} \) which are the mean and standard deviation of the lognormal random distribution. In contrast to parameters \( \text{meanlog} \) and \( \text{sdlog} \) of function \text{dlnorm}, these parameters are not on the logscale. They relate in the following way:

  \[
  \text{sdlog} = \sqrt{\ln \frac{1 + \text{sd}^2}{\text{mn}^2}}
  \]
  \[
  \text{meanlog} = \ln \text{mn} - \frac{1}{2} \ast \text{sdlog}^2
  \]

- **"loglogistic"**: requires the parameters \( \text{mn} = \text{scale} = \text{median} \) and \( \text{beta} = \text{shape} \).

- **"external"**: uses random variates provided to \text{external_dist}. With this option GUTS can be run with arbitrarily distributed individual tolerance thresholds. With the option “external” only parameters \( \text{hb} \), \( \text{ke} \) and \( \text{kk} \) (Proper only) are required. Further, the thresholds sample length \( N \) is internally adjusted to the length of the external vector of random variates \text{external_dist}. The adjustment of \( N \) is notified by a warning.
For performance reasons the implemented distributions “lognormal” and “loglogistic” are approximated using importance sampling. The option “external” generally performs well, but might require a larger thresholds sample (i.e. length(external_dist) should be large).

The number of parameters is checked according to dist and model. Wrong number of parameters invokes an error, wrong parameter values (e.g., negative values) invoke a warning, and the loglikelihood is set to -Inf.

Field and Attribute Access:
Fields and attributes of an object of class “GUTS” are read-only. It is not possible to directly modify single elements of the GUTS object. Instead use function guts_setup to create GUTS objects or modify fields on existing GUTS objects. Functions guts_calc_loglikelihood and guts_calc_survivalprobs update an object’s fields par (parameters), D (damage), squares (sum of squares), SPPE (survival-probability prediction error), S (survival probabilities) and LL (the loglikelihood).

Value

guts_setup returns a list of class “GUTS” with the following fields:

- C: Concentrations.
- Ct: Concentration time points.
- y: Survivors.
- yt: Survivor time points.
- dist: Distribution.
- model: Model.
- N: Sample length.
- M: Time grid points.
- par: Parameters.
- S: Vector of survivor probabilities.
- D: Vector of internal damage for each of the M time grid points.
- squares: Sum of squares.
- SPPE: Survival-probability prediction error.
- LL: The loglikelihood.

guts_calc_loglikelihood returns the loglikelihood.
guts_calc_survivalprobs returns the survival probabilities.
guts_report_damage returns the damage.
guts_report_squares returns the sum of squares.
guts_report_sppe returns the survival-probability prediction error (SPPE).

Note

The GUTS project web site can be found here: http://guts.r-forge.r-project.org. For questions and discussion, please subscribe to the mailing list there.
Author(s)

Carlo Albert <carlo.albert@eawag.ch>, Sören Vogel <soeren.vogel@posteo.ch>, Oliver Jakoby <oliver.jakoby@rifcon.de>, Alexander Singer <alexander.singer@rifcon.de> and Dirk Nickisch <dirk.nickisch@rifcon.de>

Maintainer: Oliver Jakoby <oliver.jakoby@rifcon.de>

References


See Also
diazinon, GUTS-package and the package vignettes for examples on how to calibrate and project GUTS-models.

Examples

data(diazinon)

# create GUTS object to calculate the Proper model
# using a log-normal distribution of tolerance thresholds
gts.lognormal <- guts_setup(
  C = diazinon$C1, Ct = diazinon$Ctl,
y = diazinon$y1, yt = diazinon$yt1,
   dist = "lognormal", model = "Proper")

# calculate likelihood of Proper model using log-normal distribution
guts_calc_loglikelihood(
   gts.lognormal,
   c(0.051, 0.126, 1.618, 19.099, 6.495))
gts.lognormal # show GUTS object

# repeating calculation above
# with threshold values from an external log-normal distribution.
# Note, we need to account for the different parametrisations
# used in the GUTS-package and in rlnorm
sigma2 <- log(1 + 6.495^2 / 19.099^2)
mu <- log(19.099) - 0.5 * sigma2
lognormal.thresholds <- rlnorm(1000, meanlog = mu, sdlog = sqrt(sigma2))
gts.external <- guts_setup(
   C = diazinon$C1, Ct = diazinon$Ct1,
   y = diazinon$y1, yt = diazinon$yt1,
   dist = "external", model = "Proper")
guts_calc_loglikelihood(
   gts.external,
   c(0.051, 0.126, 1.618), external_dist = lognormal.thresholds)
# -> Results using external and internal distributions are comparable

# create GUTS object to calculate the Proper model
# using a log-logistic distribution of tolerance thresholds
gts.loglogistic <- guts_setup(
   C = diazinon$C1, Ct = diazinon$Ct1,
   y = diazinon$y1, yt = diazinon$yt1,
   dist = "loglogistic", model = "Proper")
guts_calc_survivalprobs(# returning survival probabilities
   gts.loglogistic,
   c(0.01, 0.2, 0.3, 3, 2))

str(guts_report_damage(gts.loglogistic)) # returning damage

# calculate survival probabilities with IT model
# using a log-logistic distribution of tolerance thresholds

# calculate survival probabilities with an SD model with a fixed tolerance threshold
## Not run: guts_calc_survivalprobs(gts.external, rep(.5, 3))
# Warning and no result, because no external distribution was specified

## Not run: guts_calc_survivalprobs(gts.loglogistic, 1:4) # Error.

## Not run: gts.loglogistic["C"] <- 1:3 # Error.
Index

* datasets
  diazinon, 3
  [[<-.GUTS (GUTS-package), 2
  $<-:.GUTS (GUTS-package), 2
  attr<-:.GUTS (GUTS-package), 2
  attributes<-:.GUTS (GUTS-package), 2
  diazinon, 2, 3, 3, 8
  dlnorm, 6
  GUTS, 3, 4
  guts (GUTS), 4
  GUTS-package, 2
  guts_calc_loglikelihood, 2, 3
  guts_calc_loglikelihood (GUTS), 4
  guts_calc_survivalprobs, 2, 3
  guts_calc_survivalprobs (GUTS), 4
  guts_report_damage, 3
  guts_report_damage (GUTS), 4
  guts_report_sppe (GUTS), 4
  guts_report_squares (GUTS), 4
  guts_setup, 2, 3
  guts_setup (GUTS), 4
  modguts (GUTS-package), 2
  mostattributes<-.GUTS (GUTS-package), 2
  print.GUTS (GUTS-package), 2
  Rcpp, 3