Package ‘simode’

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R topics documented:

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confint.profile.simode

Calculates confidence intervals for the model parameters

Description

Calculates confidence intervals for the model parameters, based on the given likelihood profiles

Usage

```r
## S3 method for class 'profile.simode'
confint(object, parm = NULL, level = 0.95, ...)
```

Arguments

- `object`: A fitted model object: `profile.simode` object returned by a call to `profile`.
- `parm`: A specification of which parameters are to be given confidence intervals (named vector). If missing, all parameters are considered.
- `level`: The confidence level required.
- `...`: Additional argument(s) for methods.

Value

The confidence intervals.
**plot.confint.simode**  
*Plot confidence intervals for the model parameters*

Description

Plot confidence intervals for the model parameters of a simode object, calculated based on likelihood profiles.

Usage

```r
## S3 method for class 'confint.simode'
plot(
  x,
  which = NULL,
  pars_true = NULL,
  legend = FALSE,
  cols = list(fit = "blue", true = "black"),
  ...
)
```

Arguments

- `x`: confint.simode object returned by a call to `confint`
- `which`: Which parameters to plot the confidence intervals for. If empty, the plot will include all of the parameters in `x`.
- `pars_true`: The true parameter values (if are known).
- `legend`: Whether or not to add a figure legend.
- `cols`: List of colors for each element of the plot.
- `...`: Additional argument(s) for methods.

---

**plot.list.simode**  
*Plot the fit/estimates of a list.simode object*

Description

Plot the fit or parameter estimates obtained from a call to simode with `obs_sets>1`. 
Usage

## S3 method for class 'list.simode'
plot(
  x,
  type = c("fit", "est"),
  show = c("nls", "im", "both"),
  which = NULL,
  pars_true = NULL,
  time = NULL,
  plot_mean_sd = FALSE,
  plot_im_smooth = FALSE,
  legend = FALSE,
  mfrow = par("mfrow"),
  cols = list(nls_fit = "blue", im_fit = "green", true = "black", obs = "red",
              im_smooth = "magenta"),
  ...
)

Arguments

x list.simode object.

type Type of plot - 'fit' to plot the fitted equations and 'est' to plot the parameter estimates.

show Whether to plot the fit/estimates obtained using nonlinear least squares ('nls'), integral-matching ('im') or both ('both').

which Which variables to plot in case type='fit', or which parameters to plot in case type='est'. If empty, the plot will include all of the variables/parameters in x.

pars_true The true parameter values (if are known). Should be named using the parameter names. If given, the true values for the variables/parameters will be added to the plot.

time The time points to use for the fitted curves (relevant only for type='fit'). If not given then the time points of the observations in x will be used.

plot_mean_sd Plot the mean and standard deviation for the fit/estimates of the simode objects in x. To be used when x is the result of fitting monte-carlo simulations.

plot_im_smooth Whether or not to plot the smoothed curves created and used by the integral-matching procedure (relevant only for type='fit').

legend Whether or not to add a figure legend.

mfrow A vector of the form c(nr,nc) setting the layout of subplots in one plot (see also par).

cols List of colors for each element of the plot.

... Additional argument(s) for methods.
plot.profile.simode

Plot the likelihood profiles for the model parameters

Description

Plot the likelihood profiles for the model parameters.

Usage

```r
## S3 method for class 'profile.simode'
plot(
  x,
  which = NULL,
  mfrow = par("mfrow"),
  cols = list(fit = "blue", threshold = "red"),
  ...
)
```

Arguments

- `x` profile.simode object returned by a call to `profile`.
- `which` Which parameters to plot the likelihood profiles for. If empty, the plot will include all of the parameters in `x`.
- `mfrow` A vector of the form c(nr,nc) setting the layout of subplots in one plot (see also `par`).
- `cols` List of colors for each element of the plot.
- `...` Additional argument(s) for methods.

plot.simode

Plot the fit/estimates of a simode object

Description

Plot the fit or parameter estimates obtained from a call to `simode`.

Usage

```r
## S3 method for class 'simode'
plot(
  x,
  type = c("fit", "est"),
  show = c("nls", "im", "both"),
  which = NULL,
  pars_true = NULL,
```
time = NULL,
plot_im_smooth = FALSE,
legend = FALSE,
mfrow = par("mfrow"),
cols = list(nls_fit = "blue", im_fit = "green", true = "black", obs = "red",
           im_smooth = "magenta"),
...)
)

Arguments

x simode object returned by a call to simode.

type Type of plot - 'fit' to plot the fitted variables and 'est' to plot the parameter estimates.

show Whether to plot the fit/estimates obtained using nonlinear least squares ('nls'), integral-matching ('im') or both ('both').

which Which variables to plot in case type='fit', or which parameters to plot in case type='est'. If empty, the plot will include all of the variables/parameters in x.

pars_true The true parameter values (if are known). Should be named using the parameter names. If given, the true values for the variables/parameters will be added to the plot.

time The time points to use for the fitted curves (relevant only for type='fit'). If not given then the time points of the observations in x will be used.

plot_im_smooth Whether or not to plot the smoothed curves created and used by the integral-matching procedure (relevant only for type='fit').

legend Whether or not to add a figure legend.

mfrow A vector of the form c(nr,nc) setting the layout of subplots in one plot (see also par).

cols List of colors for each element of the plot.

... Additional argument(s) for methods.

plot_trace  Plot optimization trace of a call to simode

Description

Plot a trace of the loss values and parameter estimates during the integral-matching/nonlinear least squares optimization within a call to simode. For the traces to exist, the arguments save_im_trace and/or save_nls_trace in simode.control should be set to true, when calling simode.
**Usage**

```r
plot_trace(
  x,
  show = c("nls", "im", "both"),
  which = NULL,
  mfrow = par("mfrow"),
  cols = list(nls_fit = "blue", im_fit = "green"),
  ...
)
```

**Arguments**

- `x` simode object returned by a call to `simode`.
- `show` Whether to plot the estimates obtained using nonlinear least squares (`nls`), integral-matching (`im`) or both (`both`).
- `which` Which parameters' traces to plot. If NULL, the trace for all the parameters in `x` will be plotted.
- `mfrow` A vector of the form c(nr,nc) setting the layout of subplots in one plot (see also `par`).
- `cols` List of colors for each element of the plot.
- `...` Additional argument(s) for methods.

**Description**

Print method for `confint.simode` objects

**Usage**

```r
## S3 method for class 'confint.simode'
print(x, ...)
```

**Arguments**

- `x` The `confint.simode` object.
- `...` Additional argument(s) for methods.
print.profile.simode  Print method for profile.simode objects

Description
Print method for profile.simode objects

Usage
## S3 method for class 'profile.simode'
print(x, ...)

Arguments
x  The profile.simode object.
...  Additional argument(s) for methods.

print.simode  Print method for simode objects

Description
Print method for simode objects

Usage
## S3 method for class 'simode'
print(x, ...)

Arguments
x  The simode object.
...  Additional argument(s) for methods.
print.summary.simode  

Print method for summary.simode objects

Description

Print method for summary.simode objects

Usage

## S3 method for class 'summary.simode'
print(x, ...)

Arguments

x  
  The summary.simode object.

...  
  Additional argument(s) for methods.

profile.simode  

Calculate likelihood profiles for the model parameters

Description

Calculate likelihood profiles for the model parameters

Usage

## S3 method for class 'simode'
profile(
  fitted,
  which = NULL,
  optim_type = c("nls", "both"),
  step_size,
  max_steps = 100,
  alpha = 0.05,
  skip_err = TRUE,
  trace = 0,
  save_to_log = FALSE,
  ...
)

Arguments

- **fitted**: simode object returned by a call to simode.
- **which**: Which parameters to estimate the profile for.
- **optim_type**: Whether to calculate the profiles based on maximum-likelihood optimization only ('nls') or based on integral-matching followed by maximum-likelihood optimization ('both').
- **step_size**: Step size for profiling (one value for all parameters or a value for each parameter in which).
- **max_steps**: Maximum number of steps to take in each direction.
- **alpha**: Maximum (two-sided) likelihood ratio test confidence level to find.
- **skip_err**: Whether on not to stop the calculation if encountering a problem with one point in the profile.
- **trace**: Report level (0-4), with higher values producing more tracing information.
- **save_to_log**: Whether to redirect output to log file. The log file will be saved to tempdir().
- **...**: Additional argument(s) for methods.

Details

If the call to simode, which returned the fitted object given to this method, included a user-defined likelihood function (with the calc_nll argument), then the likelihood profiles will be calculated using this function. Otherwise, the profiles will be calculated using a likelihood based on a Gaussian distribution with fixed sigma, where sigma will be estimated in the background together with the rest of the model parameters.

Value

The likelihood profiles.

---

simode: Statistical inference of ordinary differential equations using separable integral-matching

Description

Estimating the parameters of an ODE system in two stages: 1) Estimate the parameters using separable integral-matching. 2) Estimate the parameters using nonlinear least squares starting from the values obtained in stage 1.
Usage

```r
simode(
  equations,
  pars,
  time,
  obs,
  obs_sets = 1,
  nlin_pars = NULL,
  likelihood_pars = NULL,
  fixed = NULL,
  start = NULL,
  lower = NULL,
  upper = NULL,
  im_method = c("separable", "non-separable"),
  decouple_equations = FALSE,
  gen_obs = NULL,
  calc_nll = NULL,
  scale_pars = NULL,
  simode_ctrl = simode.control(),
  ...
)
```

Arguments

- **equations**: Named vector. The equations describing the ODE system. Each element of the vector should contain a character representation of the right-hand side of an equation, and should be named according to the left-hand side of the equation (i.e., the variable name). An equation can contain parameters appearing in `pars`, variables appearing in the equations names, observed non-modeled variables appearing in `obs`, and/or any function of `t`, which is a reserved symbol for the time domain.

- **pars**: The names of the parameters and initial conditions to be estimated. An initial condition name for a certain variable is the name given to the relevant equation in `equations` (e.g., if an equation is named 'x' than its initial condition should be named 'x' as well). Note: The symbol 't' is reserved for the time domain and cannot be used as a parameter name.

- **time**: Time points of the observations. Either a vector, if the same time points were used for observing all variables, or a list of vectors the length of `obs`, of which each element is the length of the relevant element in `obs`.

- **obs**: Named list. The observations. When `obs_sets`=1, `obs` should contain a list of vectors with observations of either a variable described by one of the equations (named according to the relevant equation name) or a non-modeled variable appearing in one of the equations. Each observations vector should be the length of the relevant time vector. When `obs_sets`>1, `obs` should contain a list, where each list member is a list that fits the description in the case of `obs_sets`=1.

- **obs_sets**: Number of observations sets. When `obs_sets`>1, the function will fit the set of observations according to the value of `obs_sets_fit` in `simode_ctrl`.
nlin_pars  Names of parameters or initial conditions that will be estimated in stage 1 using nonlinear least squares optimization. The parameter names in nlin_pars must appear in pars.

likelihood_pars  Names of likelihood parameters not appearing in the ODE system, which are needed for the the user-defined function calc_nll. The parameter names in likelihood_pars must appear in pars.

fixed  Named vector. Fixed values for one or more of the ODE system parameters or initial conditions. Parameters in this list will not be estimated.

start  Named vector. Starting values for optimization of parameters/initial conditions. Must contain starting values for all the parameters in nlin_pars and likelihood_pars. If im_method="non-separable", can optionally contain starting values for any other parameter/initial condition.

lower  Named vector. Lower bounds for any parameter/initial condition.

upper  Named vector. Upper bounds for any parameter/initial condition.

im_method  The method to use for integral-matching. Default "separable" means that linear parameters are estimated directly while "non-separable" means that linear parameters are estimated using nonlinear least squares optimization. If none of the parameters are linear then the default can be used.

decouple_equations  Whether to fit each equation separately in the integral-matching stage.

gen_obs  An optional user-defined function for completing missing observations (see Details).

calc_nll  An optional user-defined function for calculating negative log-likelihood for the model (see Details).

scale_pars  An optional user-defined function for scaling transformations of parameters estimated using non-linear optimization (see Details).

simode_ctrl  Various control parameters. See simode.control.

...  Additional arguments passed to optim, gen_obs and calc_nll

Details

gen_obs can be used in cases of a partially observed system, for which observations of the missing variables can be generated given values for the system parameters. The function will be called during the optimization using integral-matching.

It must be defined as gen_obs <- function(equations, pars, x0, time, obs, ...), where:

- equations the ODE equations
- pars the parameter values
- x0 the initial conditions
- time the timing of the observations (vector or list)
- obs the observations
- ... additional parameters passed from the call to simode

The function should return a list with two items:
time the vector or list of time points of the observations
• obs the list of observations with the newly generated observations
calc_nll allows the user to pass his own likelihood function to be used in the optimization in
the second stage (if not defined, the default nonlinear least squares optimization will be used).
The likelihood function will also be used in a following call to profile, for the calculation of
likelihood profiles. It must be defined as calc_nll <- function(pars, time, obs, model_out,
...), where:

• pars the parameter values
• time the timing of the observations (vector or list)
• obs the observations
• model_out the model output returned from a call to solve_ode. If time is a list with possibly
different times for each variable then model_out will contain a union of all these times.
• ... additional parameters passed from the call to simode

The function should return the negative log-likelihood.
scale_pars allows the user to pass a function for rescaling transformations of some/all of the
parameters estimated using non-linear optimization. The function will be called at each step of
the optimization with the current values of the parameters, as the optimization algorithm sees them,
and will return rescaled parameters values to be used in estimation of the direct parameters (stage 1)
and in solving the ODE equations (stage 2). It must be defined as scale_pars <- function(pars,
...), where:

• pars the parameter values
• ... additional parameters passed from the call to simode

The function should return the rescaled parameter values.

Value

If obs_sets=1, the function returns a simode object containing the parameter estimates and solu-
tions after integral-matching (stage 1) and after nonlinear least squares optimization (stage 2). If
obs_sets>1 and obs_sets_fit!="together" in simode_ctrl, the function returns a list.simode
object which is a list of simode objects the length of obs_sets.

References

Equations Linear in Functions of the Parameters, Electronic Journal of Statistics, Vol. 9, No. 2,

Dattner, Miller, Petrenko, Kadouriz, Jurkevitch & Huppert (2017). Modelling and Parameter In-
ference of Predator-prey Dynamics in Heterogeneous Environments Using The Direct Integral Ap-
Examples

```r
## ==============================================================
## Predator-Prey Lotka-Volterra model
## ==============================================================

## generate model equations and parameters (X=Prey,Y=Predator)
pars <- c('alpha','beta','gamma','delta')
vars <- c('X','Y')
eq_X <- 'alpha*X-beta*X*Y'
eq_Y <- 'delta*X*Y-gamma*Y'
equations <- c(eq_X,eq_Y)
names(equations) <- vars
x0 <- c(0.9,0.9)
names(x0) <- vars
theta <- c(2/3,4/3,1,1)
names(theta) <- pars

## generate observations
n <- 50
time <- seq(0,25,length.out=n)
model_out <- solve_ode(equations,theta,x0,time)
x_det <- model_out[,vars]
set.seed(1000)
sigma <- 0.05
obs <- list()
for(i in 1:length(vars)) {
  obs[[i]] <- pmax(0, rnorm(n,x_det[,i],sigma))
}
names(obs) <- vars

## estimate model parameters with known initial conditions
simode_fit1 <- simode(equations=equations, pars=pars, fixed=x0, time=time, obs=obs)
plot(simode_fit1, type='fit', time=seq(0,25,length.out=100), pars_true=theta, mfrow=c(2,1))
plot(simode_fit1, type='est', pars_true=theta)

## estimate model parameters and initial conditions
simode_fit2 <- simode(equations=equations, pars=c(pars,vars), time=time, obs=obs)
plot(simode_fit2, type='fit', time=seq(0,25,length.out=100), pars_true=c(theta,x0), mfrow=c(2,1))
plot(simode_fit2, type='est', pars_true=c(theta,x0))
profiles_fit2 <- profile(simode_fit2,step_size=0.01,max_steps=50)
plot(profiles_fit2,mfrow=c(2,3))
ci_fit2 <- confint(profiles_fit2)
ci_fit2
plot(ci_fit2,pars_true=c(theta,x0),legend=TRUE)
```
simode.control

Class containing control parameters for a call to simode

Description

Class containing control parameters for a call to simode

Usage

```r
simode.control(
  optim_type = c("both", "im", "nls"),
  im_optim_method = c("BFGS", "Nelder-Mead", "CG", "L-BFGS-B", "SANN", "Brent", 
                      "Rcgmin", "Rvmmin"),
  nls_optim_method = c("BFGS", "Nelder-Mead", "CG", "L-BFGS-B", "SANN", "Brent", 
                      "Rcgmin", "Rvmmin"),
  im_optim_control = list(),
  nls_optim_control = list(),
  ode_control = list(method = "lsoda"),
  im_smoothing = c("splines", "kernel", "none"),
  im_grid_size = 0,
  bw_factor = 1.5,
  use_pars2vars_mapping = FALSE,
  trace = 0,
  save_im_trace = FALSE,
  save_nls_trace = FALSE,
  obs_sets_fit = c("separate", "separate_x0", "together"),
  parallel = FALSE,
  save_to_log = FALSE
)
```

Arguments

- **optim_type** Controls what optimization will be performed: either only integral-matching ('im'), only nonlinear least squares ('nls') or both (the default, i.e., first integral-matching then nonlinear least squares starting from the integral-matching estimates).

- **im_optim_method** Method for optimization during the integral-matching stage. Accepted values are any method supported by the `method` argument in `optim`, as well as \`Rvmmin\` and \`Rcgmin\`, if the relevant packages are installed.

- **nls_optim_method** Method for optimization during the nonlinear least squares stage. Accepted values are the same as in `im_optim_method`.

- **im_optim_control** A list with control parameters for optimization during the integral-matching stage. Can include anything that would appear in the `control` argument in
simode.control

- **optim/Rvmmin/Rcgmin** (depending on the choice of `im_optim_method`). See `optim`, `Rvmmin`, `Rcgmin`.

  - **nls_optim_control**
    - Control parameters for optimization during the nonlinear least squares stage (as in `im_optim_control`).

  - **ode_control**
    - A list with control parameters for the ODE solver. Can include the argument method appearing in the arguments to `ode`, as well as any other control parameters accepted as additional parameters in the call to `ode`.

  - **im_smoothing**
    - Choice of type of smoothing during the integral-matching stage (see Details).

  - **im_grid_size**
    - Number of points used in integral-matching grid (not relevant when `im_smoothing='kernel'`). Value <=0 means the grid size will be set according to maximum number of observations for any of the equations in the call to `simode`.

  - **bw_factor**
    - Controls the bandwidth when `im_smoothing='kernel'`. The bandwidth for each equation will be bw_factor*the maximum time interval between two observations (should be >= 1).

  - **use_pars2vars_mapping**
    - Whether to use pars2vars mapping (see Details).

  - **trace**
    - Report level (0-4), with higher values producing more tracing information (see Details).

  - **save_im_trace**
    - Whether to save trace information of integral-matching optimization, which can then be plotted using `plot_trace`.

  - **save_nls_trace**
    - Whether to save trace information of nonlinear least squares optimization, which can then be plotted using `plot_trace`.

  - **obs_sets_fit**
    - Controls the way multiple observation sets are fitted: either "separate" (each set can be fitted with its own parameter values and initial conditions), "separate_x0" (same parameter values fitted for all sets while initial conditions may be different for each set) or "together" (fitting the mean of all observations sets).

  - **parallel**
    - Controls whether to fit sequentially or in parallel multiple observation sets (obs_sets>1 in the call to `simode`) that are fitted separately (obs_sets_fit="separate"). Fitting in parallel requires that the parallel package will be installed. When running in parallel, output will not be displayed regardless of the trace level. Instead, one can set `save_to_log` to true to save the output to a log file.

  - **save_to_log**
    - Controls whether to redirect output to a log file. If true, output will be saved to the file 'simode.log' in tempdir.

**Details**

Possible values for `im_smoothing` are 'splines' (the default), in which case smoothing will be performed using `smooth.spline` with generalized cross-validation, 'kernel', using own kernel smoother function, or 'none' (using the observations as is, with interpolation if necessary). `use_pars2vars_mapping` controls whether to use a mapping of which equations are affected by each of the parameters. When set to true, previous matrices computed as part of the integral-matching estimation are stored during the integral-matching optimization, and are updated only for the equations that were affected by the change in the parameter estimates from the previous iteration. When the number of equations is large and some of the parameters affect only a few equations, setting this option to true can significantly reduce the optimization time during the integral-matching stage (while increasing the storage...
usage). This is especially true with derivative based optimization methods (such as \BFGS\ of optim) which updates only one of the optimized parameters in each iteration. trace has 5 possible levels:

With trace=0, there would be no output displayed if there are no errors.
With trace=1, a message will be displayed at the beginning and end of each optimization stage.
With trace=2, non-critical errors occurring during the optimization iterations will be displayed.
With trace=3, non-critical warnings occurring during the optimization iterations will be displayed.
With trace=4, the calculated loss value for each iteration of the integral-matching and nonlinear least squares optimizations will be displayed.

---

**sir_example**  
*Example dataset for a multi-group SIR model*

---

**Description**

A model for the spread of a seasonal influenza epidemics in two groups over five seasons.

**Usage**

`sir_example`

**Format**

A list containing the following variables:

- **equations** The ODE equations describing the system, including ten equations for the susceptible dynamics (2 groups * 5 seasons) and ten equations for the infected dynamics.
- **beta** The 2x2 transmission matrix parameters (in time unit of weeks).
- **gamma** The recovery rate parameter (in time unit of weeks).
- **kappa** The relative infectiousness of seasons 2-5 compared to season 1.
- **S0** The initial conditions for the susceptible variables.
- **I0** The initial conditions for the infected variables.
- **time** Times in which the observations were made (in weeks).
- **obs** A list of observations of the infected variables, generated using Gaussian measurement error with sigma=1e-3.
**solve_ode**

*Ordinary differential equations solver*

**Description**

A wrapper for the `ode` function that solves a system of ordinary differential equations described using symbolic equations.

**Usage**

```r
solve_ode(equations, pars, x0, time, xvars = NULL, ...)
```

**Arguments**

- `equations` The equations describing the ODE system. See `simode`.
- `pars` The parameter values. Named according to their names in `equations`.
- `x0` The initial conditions. Named according to the names of `equations`.
- `time` The time points for which the ODE variables’ values will be computed.
- `xvars` External observations of time-dependant variables referred to in `equations`.
- `...` Additional argument(s) for methods.

**Value**

A matrix whose first column contains the given time points and subsequent columns hold the computed ODE equations’ values at these time points.

**solve_ode2**

*Ordinary differential equations solver using a simode object*

**Description**

A wrapper for the `ode` function that solves a system of ordinary differential equations described using symbolic equations.

**Usage**

```r
solve_ode2(x, type = c("both", "im", "nls"))
```

**Arguments**

- `x` A simode object returned from a call to `simode`.
- `type` Which solution to generate (`both`, `im`, `nls`).

**Value**

A matrix whose first column contains the given time points and subsequent columns hold the computed ODE equations’ values at these time points.
### summary.list.simode

**Summary method for list.simode objects**

#### Description

Summary method for list.simode objects

#### Usage

```r
## S3 method for class 'list.simode'
summary(
  object,
  sum_mean_sd = FALSE,
  pars_true = NULL,
  digits = max(3,getOption("digits") - 3),
  ...  
)
```

#### Arguments

- `object`: list.simode object returned by a call to `simode` with `obs_sets>1`
- `sum_mean_sd`: Whether to calculate mean and standard deviation for the parameter estimates in the fits included in the given object. To be used when `object` is the result of fitting monte-carlo simulations.
- `pars_true`: The true parameter values (relevant only for when `sum_mean_sd=TRUE`). When given, the summary will also include the bias and RMSE for each parameter estimate.
- `digits`: The number of significant digits to use.
- `...`: Additional argument(s) for methods.

#### Value

The mean and standard deviation for the loss values and parameter estimates obtained from the integral-matching and nonlinear least squares optimizations. If `pars_true` is given, then will also calculate bias and RMSE for the parameter estimates.

### summary.simode

**Summary method for simode objects**

#### Description

Summary method for simode objects
Usage

```r
## S3 method for class 'simode'
summary(object, digits = max(3, getOption("digits") - 3), ...)
```

Arguments

- `object`: The simode object.
- `digits`: The number of significant digits to use.
- `...`: Additional argument(s) for methods.
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