

Package ‘deBInfer’

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Type Package

Title Bayesian Inference for Differential Equations

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BugReports <https://github.com/pboesu/debinfer/issues>

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Description A Bayesian framework for parameter inference in differential equations.

This approach offers a rigorous methodology for parameter inference as well as modeling the link between unobservable model states and parameters, and observable quantities. Provides templates for the DE model, the observation model and data likelihood, and the model parameters and their prior distributions. A Markov chain Monte Carlo (MCMC) procedure processes these inputs to estimate the posterior distributions of the parameters and any derived quantities, including the model trajectories. Further functionality is provided to facilitate MCMC diagnostics and the visualisation of the posterior distributions of model parameters and trajectories.

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LazyData TRUE

RoxygenNote 7.1.2

Depends R (>= 3.5.0), deSolve

Imports truncdist, coda, RColorBrewer, MASS, stats, mvtnorm, graphics, grDevices, plyr, PBSddesolve, methods

Suggests testthat, knitr, rmarkdown, devtools, R.rsp, beanplot

VignetteBuilder knitr, R.rsp

NeedsCompilation no

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Contents

chytrid	2
debinfer_cov	3
debinfer_par	3
deinits	5
depars	5
de_mcmc	6
is.debinfer_parlist	7
is.debinfer_result	7
logd_prior	8
logistic	8
log_post_params	9
log_prior_params	9
pairs.debinfer_result	10
plot.debinfer_result	10
plot.post_sim_list	11
post_prior_densplot	11
post_sim	12
prior_draw_rev	13
propose_joint_rev	13
propose_single_rev	14
reshape_post_sim	14
setup_debinfer	15
solve_de	15
summary.debinfer_result	16
update_sample_rev	17
Index	19

chytrid	<i>Chytrid fungus data set</i>
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Description

Replicated spore counts of an experimental culture of the chytrid fungus *Batrachochytrium dendrobatidis*. This dataset is a subset of the observations from the experimental study conducted by Voyles et al. (2012).

Format

A data.frame with 76 rows and two columns

time days since the start of the experiment

count count of zoospores (x 1e4)

References

Voyles et al. 2012, Ecol Evol 9:2241-2249 doi:[10.1002/ece3.334](https://doi.org/10.1002/ece3.334)

debinfer_cov	<i>debinfer_cov</i>
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Description

debinfer_cov

Usage

```
debinfer_cov(var.names, sigma = diag(length(names)), name, samp.type = "rw")
```

Arguments

var.names	names of the parameters that are to be proposed together
sigma	covariance matrix
name	name of the joint block
samp.type	character; type of sampler. currently only "rw" = Normal random walk is implemented for multivariate proposals

Value

a debinfer_cov object

debinfer_par	<i>debinfer_par</i>
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Description

Creates an object containing all the necessary bits for a parameter i.e. initial values, prior distributions, hyper-parameters, tuning parameters, etc. to set up a debinfer analysis

Usage

```
debinfer_par(
  name,
  var.type,
  fixed,
  value,
  joint = NULL,
  prior = NULL,
  hypers = NULL,
  prop.var = NULL,
  samp.type = NULL
)
```

Arguments

name	character vector; name of the variable
var.type	character vector; type of the variable "de" = parameter for the differential equation, "obs" = parameter of the observation model, "init" = initial condition for a state variable in the differential equation
fixed	boolean; TRUE = parameter is taken to be fixed, FALSE = parameter is to be estimated by MCMC
value	numeric; parameter value. For fixed parameters this is the value used in the analysis for free parameters this is the starting value used when setting up the MCMC chain
joint	integer; number of block for joint proposal; NULL means the parameter is not to be jointly proposed
prior	character; name of the probability distribution for the prior on the parameter. Must conform to standard R naming of d/r function pairs, e.g. beta (foo = beta), binomial binom, Cauchy cauchy, chi-squared chisq, exponential exp, Fisher F f, gamma gamma, geometric geom, hypergeometric hyper, logistic logis, lognormal lnorm, negative binomial nbinom, normal norm, Poisson pois, Student t t, uniform unif, Weibull weibull. Priors from the truncdist package are available by default. User priors can be provided but must be available in the environment from which de_mcmc is called.
hypers	list of numeric vectors, hyperparameters for the prior; mean only for mvnorm. Can include trunc for truncated pdfs from package truncdist.
prop.var	numeric; tuning parameters. For Normal proposals ('samp.type="rw"' or 'samp.type="rw-ref"'), this must be a positive number representing the standard deviation of the proposal distribution for each parameter. For the asymmetric uniform proposal distribution ('samp.type="rw-unif"') two positive numeric values are required and the proposal will then have the bounds 'prop.var[1]/prop.var[2]*current_proposal' and 'prop.var[2]/prop.var[1]*current_proposal'. See Boersch-Supan et al. (2016).
samp.type	character; type of sampler: "rw" = Normal random walk, "ind" = independence, "rw-unif" = asymmetric uniform distribution, "rw-ref" = reflecting random walk sampler on the bounds of the prior support (cf. Hoff 2009, Chapter 10.5.1; Yang and Rodriguez 2013)

Value

returns an object of class `debinfer_par` to be fed to the `mcmc` setup function

References

- Boersch-Supan et al. 2016, MEE 8:511-518 [doi:10.1111/2041210X.12679](https://doi.org/10.1111/2041210X.12679)
- Hoff 2009, A First Course in Bayesian Statistical Methods, Springer
- Yang and Rodriguez 2013, PNAS 110:19307-19312 [doi:10.1073/pnas.1311790110](https://doi.org/10.1073/pnas.1311790110)

deinits	<i>Get starting/fixed values of DE initial values</i>
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Description

Accessor function for initial values

Usage

```
deinits(x)
```

Arguments

x a debinfer_result or debinfer_parlist object

Value

a named numeric vector

depars	<i>Get starting/fixed values of DE parameters</i>
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Description

Accessor function for parameters

Usage

```
depars(x)
```

Arguments

x a debinfer_result or debinfer_parlist object

Value

a named numeric vector

de_mcmc

*de_mcmc***Description**

Bayesian inference for a deterministic DE model (with models solved via an DE solver) with an observation model.

Usage

```
de_mcmc(
  N,
  data,
  de.model,
  obs.model,
  all.params,
  ref.params = NULL,
  ref.inits = NULL,
  Tmax,
  data.times,
  cnt = 10,
  plot = TRUE,
  sizestep = 0.01,
  solver = "ode",
  verbose.mcmc = TRUE,
  verbose = FALSE,
  ...
)
```

Arguments

N	integer, number of MCMC iterations
data	data.frame of time course observations to fit the model to. The observations must be ordered ascending by time.
de.model	a function defining a DE model, compliant with the solvers in deSolve or PBSSolve
obs.model	a function defining an observation model. Must be a function with arguments 'data', 'sim.data', 'samp'.
all.params	debinfer_parlist containing all model, MCMC, and observation
ref.params	an optional named vector containing a set of reference parameters, e.g. the true parameters underlying a simulated data set
ref.inits	an optional named vector containing a set of reference initial values, e.g. the true initial values underlying a simulated data set
Tmax	maximum timestep for solver
data.times	time points for which observations are available

<code>cnt</code>	integer interval at which to print and possibly plot information on the current state of the MCMC chain
<code>plot</code>	logical, plot traces for all parameters at the interval defined by <code>cnt</code>
<code>sizestep</code>	timestep for solver to return values at, only used if <code>data.times</code> is missing
<code>solver</code>	the solver to use. 1 or "ode" = <code>deSolve::ode</code> ; 2 or "dde" = <code>PBSddesolve::dde</code> ; 3 or "dede" = <code>deSolve::dde</code>
<code>verbose.mcmc</code>	logical display MCMC progress messages
<code>verbose</code>	logical display verbose solver output
<code>...</code>	further arguments to the solver

Value

a `debinfer_result` object containing input parameters, data and MCMC samples

`is.debinfer_parlist` *is.debinfer_parlist*

Description

Check `debinfer_parlist` class

Usage

`is.debinfer_parlist(x)`

Arguments

`x` an object

`is.debinfer_result` *is.debinfer_result*

Description

Check `debinfer_result` class

Usage

`is.debinfer_result(x)`

Arguments

`x` an object

logd_prior	<i>logd_prior</i>
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Description

Evaluates the log probability density of value given a name of a prior pdf and the corresponding hyperparameters

Usage

```
logd_prior(x, pdf, hypers)
```

Arguments

x	numeric; vector of values.
pdf	character; name of a probability function. Must conform to base R nomenclature of d/r function pairs. Can include trunc for truncated pdfs from package truncdist.
hypers	list; a list of parameters to be passed to the density function.

Value

the value of the log density function evaluated at x

logistic	<i>Logistic growth data set</i>
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Description

Simulated data from the logistic growth model with $N_0=0.1$, $r=0.1$ and $K=10$

Format

A data.frame with 36 rows and 3 columns

time time since start of the model

N_true Numerical solution of N_t

N_noisy N_t with the addition of log-normal noise, where $sdlog = 0.05$

log_post_params	<i>log_post_params</i>
-----------------	------------------------

Description

evaluate the likelihood given the data, the current deterministic model solution and the observation model

Usage

```
log_post_params(samp, w.p, data, pdfs, hyper, sim.data, obs.model)
```

Arguments

samp	named numeric; current sample
w.p	character; parameter names
data	data
pdfs	character, prior pdf names
hyper	list, hyper parameters for the priors
sim.data	solver output
obs.model	function containing the observation model

log_prior_params	<i>log_prior_params</i>
------------------	-------------------------

Description

evaluate prior density at current parameter values

Usage

```
log_prior_params(samp, pdfs, w.p, hyper)
```

Arguments

samp	named numeric; current sample
pdfs	character, prior pdf names
w.p	character; parameter names
hyper	list of named hyper parameters for the priors

pairs.debinfer_result *Pairwise posterior marginals*

Description

Plots pairwise correlations of posterior marginals

Usage

```
## S3 method for class 'debinfer_result'
pairs(x, trend = FALSE, scatter = FALSE, burnin = NULL, medians = TRUE, ...)
```

Arguments

x	a deBInfer_result object
trend	logical, add loess smooth
scatter	logical, add scatterplot of posterior samples
burnin	integer, number of samples to discard from start of chain before plotting
medians	logical, plot marginal medians on contour plot
...	further arguments to plot.default (the call that draws the scatter/contour plot)

plot.debinfer_result *Plot inference outputs*

Description

Plots the inference results from a debinfer_result object

Usage

```
## S3 method for class 'debinfer_result'
plot(x, plot.type = "coda", burnin = 1, ...)
```

Arguments

x	a deBInfer_result object
plot.type	character, which type of plot. Options are "coda" for coda::plot.mcmc, "post_prior" for deBInfer::post_prior_densplot.
burnin	numeric, number of samples to discard before plotting
...	further arguments to methods

See Also

[post_prior_densplot](#), [plot.mcmc](#), [pairs.debinfer_result](#)

plot.post_sim_list *Plot posterior trajectory*

Description

Plots the inference results from a `debinfer_result` object

Usage

```
## S3 method for class 'post_sim_list'
plot(
  x,
  plot.type = "medianHDI",
  col = c("red", "darkgrey"),
  lty = c(1, 2),
  auto.layout = TRUE,
  panel.first = NULL,
  ...
)
```

Arguments

<code>x</code>	a <code>post_sim</code> or <code>post_sim_list</code> object
<code>plot.type</code>	character, which type of plot. Options are "ensemble" and "medianHDI".
<code>col</code>	color, for <code>plot.type = "medianHDI"</code> the first element is used for the median, the second for the HDI
<code>lty</code>	line type, for <code>plot.type = "medianHDI"</code> the first element is used for the median, the second for the HDI
<code>auto.layout</code>	logical, should the layout for <code>plot.type = "medianHDI"</code> be determined automatically?
<code>panel.first</code>	an expression to be evaluated after the plot axes are set up but before any plotting takes place. This can be useful for adding data points.
<code>...</code>	further arguments to methods

post_prior_densplot *Plot posterior marginals and corresponding priors*

Description

Plots posterior densities and the densities of the corresponding priors. The prior density is automatically evaluated for the range given by the x-axis limits of the plot (which defaults to the posterior support).

Usage

```
post_prior_densplot(
  result,
  param = "all",
  burnin = NULL,
  prior.col = "red",
  n = 1000,
  ...
)
```

Arguments

result	a deBInfer_result object
param	character, name of parameter to plot. "all" (default) plots all parameters
burnin	numeric, number of samples to discard before plotting
prior.col	character color for prior density
n	integer, number of points at which to evaluate the prior density.
...	further arguments to coda::densplot

 post_sim

post_sim

Description

post_sim

Usage

```
post_sim(x, n = 100, times, output = "all", burnin = NULL, prob = 0.95, ...)
```

Arguments

x	debinfer_result object
n	number of simulations
times	numeric a vector of times at which the ODE is to be evaluated. Defaults to NULL.
output	character, "sims", "all", "HDI"
burnin	integer, number of samples to discard from the start of the mcmc chain
prob	A numeric scalar in the interval (0,1) giving the target probability content of the intervals. The nominal probability content of the intervals is the multiple of 1/nrow(obj) nearest to prob.
...	additional arguments to solver

Value

a post_sim object containing a list of de solutions or summaries thereof

prior_draw_rev *prior_draw_rev*

Description

draw from prior

Usage

```
prior_draw_rev(b, hypers, prior.pdf)
```

Arguments

b	current value of a parameter
hypers	list of hyper parameters, named appropriately for the corresponding prior.pdf
prior.pdf	string name of probability distribution following base R conventions, or those of additionally loaded packages

propose_joint_rev *propose_joint*

Description

joint proposal function

Usage

```
propose_joint_rev(samps, s.ps, cov.mat)
```

Arguments

samps	current sample of the MCMC chain
s.ps	debinfer_parlist object representing the parameters that are to be proposed
cov.mat	debinfer_cov object; covariance matrix for the proposal

Details

Function to jointly propose parameters using a multivariate normal proposal distribution

propose_single_rev *propose_single_rev*

Description

propose a parameter individually

Usage

propose_single_rev(samps, s.p)

Arguments

samps current sample of the MCMC chain
s.p debinfer_par object representing the parameter that is to be proposed

reshape_post_sim *Reshape posterior model solutions*

Description

Take a list of DE model solutions and transform into a list of matrices, one for each state variable, where each row is an iteration, and each column is a time point

Usage

reshape_post_sim(x)

Arguments

x a post_sim object

setup_debinfer	<i>setup_debinfer</i>
----------------	-----------------------

Description

Creates an object of class `debinfer_parlist` containing initial values, parameters, prior distributions, hyperparameters tuning parameters etc. to set up a `debinfer` analysis

Usage

```
setup_debinfer(...)
```

Arguments

... `debinfer_par` objects to be combined into a `debinfer_parlist`

Value

returns an S3 object of class `debinfer_parlist` to be fed to the `mcmc` function

solve_de	<i>solve_de</i>
----------	-----------------

Description

`solve_de`

Usage

```
solve_de(  
  sim,  
  params,  
  inits,  
  Tmax,  
  numsteps = 10000,  
  solver = "ode",  
  sizestep = NULL,  
  verbose = FALSE,  
  data.times = NULL,  
  method = "lsoda",  
  ...  
)
```

Arguments

sim	function; solver compatible specification of the DE
params	numeric; named vector of parameter values
inits	numeric; initial values. Must be in the same order as specified within sim!
Tmax	numeric; maximum timestep
numsteps	numeric
solver	Choice of solver to use 1 or "ode" = deSolve::ode, 2 or "dde" = PBSddesolve::dde, 3 or "dede" = deSolve::dede
sizestep	for solver
verbose	passed to deSolve::ode
data.times	numeric a vector of times at which the ODE is to be evaluated. Defaults to NULL. If value is supplied it takes precedence over any value supplied to numsteps or sizesteps.
method	solver method
...	additional arguments to solver

Value

integrated ode object. Data structure depends on the employed solver.

summary.debinfer_result

Summary of the inference results

Description

A wrapper for coda::summary.mcmc

Usage

```
## S3 method for class 'debinfer_result'
summary(object, ...)
```

Arguments

object	a deBInfer_result object
...	further arguments to summary.mcmc

See Also

[summary.mcmc](#)

update_sample_rev *update_sample_rev*

Description

This is the workhorse of the MCMC algorithm

Usage

```
update_sample_rev(
  samps,
  samp.p,
  cov.mats,
  data,
  sim,
  out,
  Tmax,
  sizestep,
  data.times,
  l,
  solver,
  i,
  cnt,
  obs.model,
  pdfs,
  hyper,
  w.p,
  verbose.mcmc,
  verbose,
  is.de,
  is.single,
  joint.blocks,
  ...
)
```

Arguments

samps	row vector of samples from the previous mcmc iteration
samp.p	the parlist created by setup_debinfer
cov.mats	the covariance matrices
data	the observation
sim	the de.model
out	list containing the initial or previous update i.e. list(s=samps[i-1,], inits=inits, p=params, sim.old=sim.start)
Tmax	maximum timestep for solver

sizestep	sizestep for solver when not using data.times
data.times	times with observations
l	number of parameters to be proposed
solver	solver choice
i	current MCMC iteration
cnt	interval for printing/plotting information on chains
obs.model	function containing obs model
pdfs	names of prior pdfs
hyper	list of hyperparameters
w.p	names of free parameters
verbose.mcmc	logical print MCMC progress messages
verbose	logical, print additional information from solver
is.de	logical, parameter is an input for the solver
is.single	parameter is to be proposed individually
joint.blocks	names of joint blocks
...	further arguments to solver

Index

* data

- chytrid, 2
- logistic, 8

chytrid, 2

de_mcmc, 6
debinfer_cov, 3
debinfer_par, 3
deinits, 5
depars, 5

is.debinfer_parlist, 7
is.debinfer_result, 7

log_post_params, 9
log_prior_params, 9
logd_prior, 8
logistic, 8

pairs.debinfer_result, 10, 10
plot.debinfer_result, 10
plot.mcmc, 10
plot.post_sim_list, 11
post_prior_densplot, 10, 11
post_sim, 12
prior_draw_rev, 13
propose_joint_rev, 13
propose_single_rev, 14

reshape_post_sim, 14

setup_debinfer, 15
solve_de, 15
summary.debinfer_result, 16
summary.mcmc, 16

update_sample_rev, 17