

Package ‘fitode’

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Type Package

Title Tools for Ordinary Differential Equations Model Fitting

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Description Methods and functions for fitting ordinary differential equations (ODE) model in 'R'. Sensitivity equations are used to compute the gradients of ODE trajectories with respect to underlying parameters, which in turn allows for more stable fitting. Other fitting methods, such as MCMC (Markov chain Monte Carlo), are also available.

License GPL (>= 2)

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blowfly

Nicholson's blowfly data

Description

...

Usage

blowfly

Format

A data frame containing 361 rows comprising:

eggs number of eggs

nonemerging ?

emerging ?

deaths ?

total ?

coef,fitode-method	<i>Extract model coefficients from fitode objects</i>
--------------------	---

Description

Extracts estimated parameters (either on response scales or link scales)

Usage

```
## S4 method for signature 'fitode'
coef(object, type = c("response", "links"))
```

Arguments

object	fitode object
type	type of coefficients. The default (type=response) is on the response scale; this is the scale on which the model parameters are defined. Alternatively, type=link can be used to obtain parameters on the estimated scale.

Value

The estimated coefficients of the fitode object

coef,fitodeMCMC-method	<i>Extract model coefficients from fitodeMCMC objects</i>
------------------------	---

Description

Extracts estimated parameters (median of the marginal posterior distributions)

Usage

```
## S4 method for signature 'fitodeMCMC'
coef(object)
```

Arguments

object fitodeMCMC object

Value

The estimated median coefficients of the fitodeMCMC object

confint, fitode-method *Calculate confidence intervals from fitode objects for model parameters and their transformations*

Description

Calculate confidence intervals for model parameters and their transformations using (1) delta method, (2) profile likelihood, and (3) importance sampling.

Usage

```
## S4 method for signature 'fitode'
confint(
  object,
  parm,
  level = 0.95,
  method = c("delta", "profile", "impsamp", "wmvrnorm"),
  nsim = 1000,
  seed,
  ...
)
```

Arguments

object fitode object

parm character vector specifying model parameters or list of formuals specifying transformations

level the confidence level required

method method for calculating confidence intervals

nsim number of simulations to be used for importance sampling

seed seed

... extra arguments passed to profiling method

Value

The confidence intervals for model parameters and their transformations of the fitode object

 confint,fitodeMCMC-method

Calculate credible intervals from fitodeMCMC objects for model parameters and their transformations

Description

Calculate credible intervals for model parameters and their transformations from posterior samples.

Usage

```
## S4 method for signature 'fitodeMCMC'
confint(object, parm, level = 0.95)
```

Arguments

object	fitodeMCMC object
parm	character vector specifying model parameters or list of formulas specifying transformations
level	the credible level required

Value

The credible intervals of the fitodeMCMC object

 fitode

Fit ordinary differential equations model

Description

This function fits ordinary differential equations models to a uni- or multi-variate time series by maximum likelihood. It relies on sensitivity equations to compute gradients of the estimated trajectory with respect to model parameters. This allows one to use gradient-based optimization algorithms, which can provide more robust estimation.

Usage

```
fitode(
  model,
  data,
  start,
  tcol = "times",
  method = "BFGS",
  optimizer = "optim",
  link,
```

```

fixed = list(),
prior = list(),
prior.density = TRUE,
control = list(maxit = 1e+05),
solver.opts = list(method = "rk4"),
solver = ode,
skip.hessian = FALSE,
force.hessian = FALSE,
use.ginv = TRUE,
quietly = FALSE,
...
)

```

Arguments

model	odemodel object
data	data frame with a time column and observation columns
start	named vector of starting parameter values
tcol	(character) time column
method	optimization method
optimizer	optimizer
link	named vector or list of link functions for model parameters
fixed	named vector or list of model parameters to fix and their values
prior	list of formulas specifying prior distributions
prior.density	(logical) should priors represent probability distributions?
control	see optim
solver.opts	options for ode integration. See ode
solver	ode solver
skip.hessian	skip hessian calculation
force.hessian	(logical) calculate the hessian numerically instead of taking the jacobian of the gradients based on sensitivity equations
use.ginv	(logical) use generalized inverse (ginv) to compute approximate vcov
quietly	suppress progress messages?
...	mle2 arguments

Value

An object of class “fitode” as described in [fitode-class](#).

See Also

[mle2](#)

fitode-class	<i>Class "fitode". Result of ode fitting based on Maximum Likelihood Estimation</i>
--------------	---

Description

Class "fitode". Result of ode fitting based on Maximum Likelihood Estimation

Slots

call (language) The call to [fitode](#)
model odemodel object
data the time series data
coef estimated parameters
vcov estimated variance-covariance matrix
min minimum negative log-likelihood
mle2 mle2 object
link list of link functions for model parameters
fixed list of fixed parameters
prior list of priors

See Also

[mle2-class](#)

fitodeMCMC	<i>Fit ordinary differential equations model using MCMC</i>
------------	---

Description

This function fits ordinary differential equations models to a uni- or multi-variate time series by MCMC using the Metropolis-Hastings update rule. It searches through the parameter space on link scales, which can provide more efficient posterior sampling.

Usage

```
fitodeMCMC(  
  model,  
  data,  
  start,  
  tcol = "times",  
  proposal.vcov,  
  prior = list(),
```

```

chains = 1,
iter = 2000,
burnin = iter/2,
thin = 1,
refresh = max(iter/10, 1),
prior.only = FALSE,
link,
fixed = list(),
solver.opts = list(method = "rk4"),
solver = ode,
...
)

```

Arguments

model	ode model
data	data frame with time column and observation column
start	named vector of starting parameter values
tcol	time column
proposal.vcov	variance-covariance matrix of a multivariate normal proposal distribution
prior	list of formulas specifying prior distributions
chains	(numeric) number of chains
iter	(numeric) number of iterations per chain
burnin	(numeric) number of burnin iterations
thin	(numeric) thinning interval between consecutive observations
refresh	(numeric) refresh interval
prior.only	(logical) sample from prior distribution only?
link	named vector or list of link functions for model parameters
fixed	named vector or list of model parameters to fix and their values
solver.opts	options for ode integration. See ode
solver	ode solver
...	additional arguments (unused)

Value

An object of class “fitodeMCMC” as described in [fitodeMCMC-class](#).

fitodeMCMC-class	<i>Class "fitodeMCMC". Result of ode fitting based on Markov Chain Monte Carlo (MCMC)</i>
------------------	---

Description

Class "fitodeMCMC". Result of ode fitting based on Markov Chain Monte Carlo (MCMC)

Slots

call (language) The call to `fitodeMCMC`
 model odemodel object
 data the time series data
 coef estimated parameters (posterior median)
 vcov estimated variance-covariance matrix
 mcmc mcmc.list object containing posterior samples
 lp mcmc.list object containing log-posterior values of posterior samples
 link list of link functions for model parameters
 fixed list of fixed parameters
 prior list of priors
 details a list containing miscellaneous objects for internal uses

initialize, odemodel-method	<i>Constructor method of "odemodel" class</i>
-----------------------------	---

Description

Constructor method of "odemodel" class

Usage

```
## S4 method for signature 'odemodel'
initialize(
  .Object,
  name,
  model,
  observation,
  initial,
  par,
  link,
  diffnames,
  keep_sensitivity = TRUE,
  call
)
```

Arguments

.Object	object
name	name of the model
model	ode model
observation	observation model
initial	initial values
par	model parameters
link	link functions for parameters (log links are used as default)
diffnames	optional character vector specifying the names of a variable for which the consecutive difference needs to be calculated
keep_sensitivity	(logical) maintain the Jacobian as a part of the model object?
call	original function call

Value

An object of class “odemodel” as described in [odemodel-class](#).

Examples

```
SI_model <- odemodel(
  name = "SI",
  model = list(
    S ~ - beta*S*I/N,
    I ~ beta*S*I/N - gamma*I
  ),
  observation = list(
    susceptible ~ dnorm(mean=S, sd=sigma1),
    infected ~ dnorm(mean=I, sd=sigma2)
  ),
  initial = list(
    S ~ N * (1 - i0),
    I ~ N * i0
  ),
  par = c("beta", "gamma", "N", "i0", "sigma1", "sigma2"),
  link = c(i0="logit")
)
```

logLik, fitode-method *Extract log-likelihood*

Description

Extract log-likelihood of a fit

Usage

```
## S4 method for signature 'fitode'
logLik(object)
```

Arguments

object fitode object

Value

The log-likelihood of the fitode object

loglik.ode-class	<i>Class representing log-likelihood models used to fit ode models</i>
------------------	--

Description

Class representing log-likelihood models used to fit ode models

Slots

name name of the distribution
 expr an expression specifying the model
 observation observation variable name
 mean mean variable name
 par additional parameter names
 grad the gradient with respect to the parameters

plot, fitode, missing-method	<i>Plot a fitode object</i>
------------------------------	-----------------------------

Description

Plot a fitode object

Usage

```
## S4 method for signature 'fitode,missing'
plot(
  x,
  level,
  data,
  which,
  method = c("delta", "impsamp", "wmvnorm"),
  onepage = TRUE,
  xlim,
  ylim,
  xlabs,
  ylabs,
  col.traj = "black",
  lty.traj = 1,
  col.conf = "black",
  lty.conf = 4,
  add = FALSE,
  nsim = 1000,
  ...
)
```

Arguments

<code>x</code>	fitode object
<code>level</code>	the confidence level required
<code>data</code>	(FIXME)
<code>which</code>	which to plot
<code>method</code>	confidence interval method
<code>onepage</code>	(logical) print all figures on one page?
<code>xlim</code>	x coordinates range
<code>ylim</code>	y coordinates range
<code>xlabs</code>	a label for the x axis
<code>ylabs</code>	a label for the y axis
<code>col.traj</code>	colour of the estimated trajectory
<code>lty.traj</code>	line type of the estimated trajectory
<code>col.conf</code>	colour of the confidence intervals
<code>lty.conf</code>	line type of the confidence intervals
<code>add</code>	add to another plot?
<code>nsim</code>	number of simulations for mvrnorm, wmvnorm methods
<code>...</code>	additional arguments to be passed on to the plot function

Value

No return value, called for side effects

```
plot,fitodeMCMC,missing-method
```

Plot a fitodeMCMC object

Description

Plot a fitodeMCMC object

Usage

```
## S4 method for signature 'fitodeMCMC,missing'
plot(
  x,
  level,
  data,
  which,
  onepage = TRUE,
  xlim,
  ylim,
  xlab,
  ylab,
  col.traj = "black",
  lty.traj = 1,
  col.conf = "black",
  lty.conf = 4,
  add = FALSE,
  ...
)
```

Arguments

x	fitodeMCMC object
level	the confidence level required
data	(FIXME)
which	which to plot
onepage	(logical) print all figures on one page?
xlim	x coordinates range
ylim	y coordinates range
xlab	a label for the x axis
ylab	a label for the y axis
col.traj	colour of the estimated trajectory
lty.traj	line type of the estimated trajectory
col.conf	colour of the confidence intervals

lty.conf	line type of the confidence intervals
add	add to another plot?
...	additional arguments to be passed on to the plot function

Value

No return value, called for side effects

plot_internal	<i>Internal function for plotting methods</i>
---------------	---

Description

Internal function for plotting methods

Usage

```
plot_internal(
  pred,
  data,
  onepage = TRUE,
  xlim,
  ylim,
  xlab,
  ylab,
  col.traj = "black",
  lty.traj = 1,
  col.conf = "black",
  lty.conf = 4,
  add = FALSE,
  ...
)
```

Arguments

pred	prediction objects
data	observed data
onepage	(logical) print all figures on one page?
xlim	x coordinates range
ylim	y coordinates range
xlab	a label for the x axis
ylab	a label for the y axis
col.traj	colour of the estimated trajectory
lty.traj	line type of the estimated trajectory

col.conf	colour of the confidence intervals
lty.conf	line type of the confidence intervals
add	add to another plot?
...	additional arguments to be passed on to the plot function

predict,fitode-method *Prediction function for fitode objects*

Description

Computes estimated trajectories and their confidence intervals (using either the delta method or importance sampling).

Usage

```
## S4 method for signature 'fitode'
predict(
  object,
  level,
  times,
  method = c("delta", "impsamp", "wmvrnorm"),
  nsim = 1000
)
```

Arguments

object	fitode object
level	the confidence level required
times	time vector to predict over. Default is set to the time frame of the data.
method	confidence interval method. Default is set to Delta method.
nsim	number of simulations for mvnrm, wmvrnorm methods

Value

The estimated trajectories and their confidence intervals of the fitode object

predict, fitodeMCMC-method

Prediction function for fitodeMCMC objects

Description

Computes estimated trajectories and their credible intervals. The estimated trajectories are obtained by taking the median trajectories from the posterior samples.

Usage

```
## S4 method for signature 'fitodeMCMC'
predict(object, level, times, simplify = TRUE)
```

Arguments

object	fitodeMCMC object
level	the credible level required
times	time vector to predict over. Default is set to the time frame of the data.
simplify	(logical) simplify output to return estimated trajectories and their credible intervals? If simplify=FALSE, all posterior trajectories will be returned

Value

Estimated trajectories and their credible intervals of the fitodeMCMC object

prior.ode-class

Class representing prior models used to fit ode models

Description

Class representing prior models used to fit ode models

Slots

name	name of the distribution
expr	an expression specifying the model
observation	observation variable name
par	additional parameter names
keep_grad	keep gradient?
grad	the gradient with respect to the parameters

profile,fitode-method *Profile fitode objects*

Description

Profile fitode objects

Usage

```
## S4 method for signature 'fitode'
profile(fitted, which = 1:p, alpha = 0.05, trace = FALSE, ...)
```

Arguments

fitted	fitted model object
which	which parameter(s) to profile? (integer value)
alpha	critical level
trace	trace progress of computations?
...	additional arguments passed to mle2 profiling method

Value

The log-likelihood profile of the fitode object

SierraLeone2014 *Data from 2014 Sierra Leone Ebola epidemic*

Description

Ebola case reports ...

Usage

```
SierraLeone2014
```

Format

A data frame with 67 rows comprising:

times decimal dates (year + fraction of year)

confirmed confirmed cases

 simulate,fitode-method

simulate fitode objects

Description

simulate fitode objects

Usage

```
## S4 method for signature 'fitode'
simulate(object, nsim = 1, seed = NULL, times, parms, y, observation = TRUE)
```

Arguments

object	fitode object
nsim	number of simulations
seed	random-number seed
times	time vector
parms	named vector of parameter values
y	initial values
observation	(logical) propagate observation error?

Value

The numerical simulation of the object

 simulate,odemodel-method

simulate model objects

Description

simulate model objects

Usage

```
## S4 method for signature 'odemodel'
simulate(
  object,
  nsim = 1,
  seed = NULL,
  times,
  parms,
```

```

    y,
    solver.opts = list(method = "rk4"),
    solver = ode,
    observation = TRUE
  )

```

Arguments

object	odemodel object
nsim	number of simulations
seed	random-number seed
times	time vector
parms	named vector of parameter values
y	initial values
solver.opts	options for ode solver
solver	ode solver (must take y, times, func, and parms arguments)
observation	(logical) propagate observation error?

Value

The numerical simulation of the object

simulate_internal	<i>Internal function for simulation models</i>
-------------------	--

Description

Simulates deterministic trajectories and propagates observation error

Usage

```

simulate_internal(
  model,
  times,
  parms,
  y,
  solver.opts = list(method = "rk4"),
  solver = ode,
  observation = TRUE,
  nsim = 1,
  seed = NULL
)

```

Arguments

model	odemodel object
times	time vector
parms	named vector of parameter values
y	initial values
solver.opts	options for ode solver
solver	ode solver (must take y, times, func, and parms arguments)
observation	(logical) propagate observation error?
nsim	number of simulations
seed	seed

stdEr, fitode-method	<i>Extract standard error from fitode objects</i>
----------------------	---

Description

Calculates standard error by taking the square root of the diagonal matrix

Usage

```
## S4 method for signature 'fitode'
stdEr(x, type = c("response", "links"))
```

Arguments

x	fitode object
type	type of standard error. The default (type=response) is on the response scale; this is the scale on which the model parameters are defined. Alternatively, type=link can be used to obtain standard errors on the estimated scale.

Value

The standard error of the fitode object

`stdEr,fitodeMCMC-method`*Extract standard error from fitodeMCMC objects*

Description

Calculates standard error by taking the square root of the diagonal of the variance-covariance matrix

Usage

```
## S4 method for signature 'fitodeMCMC'  
stdEr(x)
```

Arguments

x fitodeMCMC object

Value

The standard error of the fitodeMCMC object

`summary,fitode-method` *Summarize fitode object*

Description

Summarize fitode objects; returns estimate, standard error, and confidence intervals

Usage

```
## S4 method for signature 'fitode'  
summary(object)
```

Arguments

object fitode object

Value

The summary of the fitode object

```
summary, fitodeMCMC-method
```

Summarize fitodeMCMC object

Description

Summarize fitodeMCMC object; returns estimate, standard error, credible intervals, effective sample sizes, and gelman-rubin diagnostic

Usage

```
## S4 method for signature 'fitodeMCMC'
summary(object)
```

Arguments

object fitodeMCMC object

Value

The summary of the fitodeMCMC object

See Also

[effectiveSize](#) [gelman.diag](#)

```
tumorgrowth
```

Tumor growth data

Description

...

Usage

```
tumorgrowth
```

Format

A data frame containing 14 rows comprising:

day

volume

update,fitode-method *Update fitode fits*

Description

Update fitode fits

Usage

```
## S4 method for signature 'fitode'
update(object, observation, initial, par, link, ...)
```

Arguments

object	fitode objects
observation	observation model
initial	initial values
par	model parameters
link	link functions for parameters (log links are used as default)
...	additional arguments to be passed to fitode

Value

An object of class “fitode” as described in [fitode-class](#).

update,fitodeMCMC-method
Update fitodeMCMC fits

Description

Update fitodeMCMC fits

Usage

```
## S4 method for signature 'fitodeMCMC'
update(object, observation, initial, par, link, ...)
```

Arguments

object	fitodeMCMC objects
observation	observation model
initial	initial values
par	model parameters
link	link functions for parameters (log links are used as default)
...	additional arguments to be passed to fitode

Value

An object of class “fitode” as described in [fitodeMCMC-class](#).

vcov,fitode-method	<i>Extract variance-covariance matrix from fitode objects</i>
--------------------	---

Description

Extracts variance-covariance matrix (either on response scales or link scales)

Usage

```
## S4 method for signature 'fitode'
vcov(object, type = c("response", "links"))
```

Arguments

object	fitode object
type	type of covariance matrix. The default (type=response) is on the response scale; this is the scale on which the model parameters are defined. Alternatively, type=link can be used to obtain the covariance matrix on the estimated scale.

Value

The variance-covariance matrix of the fitode object

vcov,fitodeMCMC-method	<i>Extract variance-covariance matrix from fitodeMCMC objects</i>
------------------------	---

Description

Calculates variance-covariance matrix from posterior samples

Usage

```
## S4 method for signature 'fitodeMCMC'
vcov(object)
```

Arguments

object	fitodeMCMC object
--------	-------------------

Value

The variance-covariance matrix of the fitodeMCMC object

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