Package 'bayesnec'

May 29, 2020

Title A Bayesian No-Effect-
Concentration (NEC) package. R package version 1. https://github.com/AIMS/bayesnec

Version 1.0

Description bayesnec is a No-Effect-Concentration estimation package that uses brms to fit concentration(dose)-response data using bayesiam methods for the purpose of estimating both ecx values, but more particularly nec. Please see ?bayesnec for more details.

Depends R (>= 3.6.0)

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.0

Imports brms, HDInterval

Suggests knitr, rmarkdown, plyr, dplyr, ggplot2

VignetteBuilder knitr

URL https://aims.github.io/bayesnec

BugReports https://github.com/aims/bayesnec/issues

Roxygen list(markdown = TRUE)

NeedsCompilation no

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R topics documented:

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check_data   *check_data*

Description

Check data input for a bayesian nec model fit

Usage

```
check_data(
  data,
  x_var,
  y_var,
  trials_var,
  x_type = NA,
  y_type = NA,
  over_disp,
  model
)
```

Arguments

data   a data.frame containing the data to use for the model

x_var   the column heading indicating the concentration (x) variable

y_var   the column heading indicating the response (y) variable

trials_var   the column heading indicating the column for the number of "trials" for binomial
                response data. If not supplied, the model may run but will not be the model you
                intended!

x_type   the statistical distribution to use for the x (concentration) data. This will be guess
                based on the characteristic of the input data if not supplied.

y_type   the statistical distribution to use for the y (response) data. This may currently be
                one of 'binomial', 'poisson',' 'gaussian', or 'gamma'. Others can be added as
                required, please contact the package maintainer. If not supplied, the appropriate
                distribution will be guessed based on the distribution of the input data.

over_disp   If an overdispersed model should be used. Only changes the model fit for pois-
                son and binomial y_type data. For poisson, a negative binomial model will be
                fit. For binomial a beta model will be fit.

model   The type of model to be fit. Currently takes values of "nec3param", "nec4param",
                "necsigmoidal", "nechorme", "ecx4param", "ecxwb1", or "ecxwb2".

Details

This is a wrapper function to test input data criteria and write the brms model file for use in a bayesnec model fit

Value

Modified elements of the bayesnec input data.

---

define_model *define_model*

Description

Writes an NEC model file for a three parameter model (top, beta and NEC) and generates a function for initial values to pass to jags

Usage

```
define_model(model, x_type, y_type, mod_dat)
```

Arguments

model	a character string indicating the model to fit
x_type	the statistical distribution to use for the x (concentration) data. This may currently be one of 'beta', 'gaussian', or 'gamma'. Others can be added as required, please contact the package maintainer.
y_type	the statistical distribution to use for the y (response) data. This may currently be one of 'binomial', 'beta', 'poisson', 'gaussian', 'negbin' or 'gamma'. Others can be added as required, please contact the package maintainer.
mod_dat	the model data to use for the NEC model fit

Value

a model formula, priors and the family to use

---

dispersion *Posterior dispersion*

Description

Calculates posterior dispersion metric

Usage

```
dispersion(model, summary = FALSE)
```

Arguments

`model`	An object of class `brmsfit` whose distribution family is either `gaussian`, `poisson` or `binomial`.
`summary`	Logical. Should summary stats be returned instead of full vector? Defaults to FALSE.

Details

This function calculates a dispersion metric which takes the ratio between the observed relative to simulated Pearson residuals sums of squares.

Value

If summary is FALSE, an n-long `numeric` vector containing the dispersion metric, where n is the number of post warm-up posterior draws from the `brmsfit` object. If TRUE, then a `data.frame` containing the summary stats (mean, median, 95% highest density intervals). of the dispersion metric.

Examples

```
## Not run:
library(brms)
set.seed(10)

dt <- data.frame(predictor = rpois(60, lambda = 15))
dt$response <- dt$predictor + round(rnorm(nrow(dt), 0, 1))
# mimic overdispersion
dt$response_od <- abs(dt$predictor + round(rnorm(nrow(dt), 0, 10)))
mod_pois <- brm(response ~ predictor, dt, family = poisson())
mod_pois_od <- brm(response_od~predictor, dt, family = poisson())

dispersion(mod_pois)
dispersion(mod_pois_od)

# compare with regular dispersion parameter
# from quasipoisson glm
dispersion(mod_pois, summary = TRUE)
summary(glm(response ~ predictor, data = dt, family = quasipoisson))
dispersion(mod_pois_od, summary = TRUE)
summary(glm(response_od ~ predictor, data = dt, family = quasipoisson))

## End(Not run)
```

---

extract_ecx	*extract_ecx*

Description

Extracts the predicted ecx value as desired from a bayesnec or a bayesmanec model fit.

Usage

```
extract_ecx(
  X,
  ecx_val = 10,
  precision = 1000,
  posterior = FALSE,
  type = "absolute",
  hormesis_def = "control",
  xform = NA,
  x_range = NA,
  prob_vals = c(0.5, 0.025, 0.975),
  link = "identity"
)
```

Arguments

X	a jag model fit as returned by a call to bayes from fit_bayesnec
ecx_val	the desired percentage effect value. This must be a value between 1 and 99 (for type = "relative" and "absolute"), defaults to 10.
precision	The number of unique x values over which to find ecx - large values will make the ecx estimate more precise.
posterior	A logical value indicating if the full posterior sample of calculated ecx values should be returned instead of just the median and 95 credible intervals
type	a character vector, taking values of "relative", "absolute" (the default) or "direct". Type "relative" is calculated as the percentage decrease from the maximum predicted value of the response (top) to the minimum predicted value of the response. Type "absolute" (the default) is calculated as the percentage decrease from the maximum value of the response (top) to 0 (or bot for a 4 parameter model fit). Type "direct" provides a direct estimate of the x value for a given y. Note that for the current version, ecx for an necHormesis model is estimated at a percent decline from the control
xform	A function to apply to the returned estimated concentration values
x_range	A range of x values over which to consider extracting ecx
prob_vals	A vector indicating the probability values over which to return the estimated ecx value. Defaults to 0.5 (median) and 0.025 and 0.975 (95 percent credible intervals).

Value

A vector containing the estimated ecx value, including upper and lower 95 percent Credible Interval bounds

---

extract_ecx.bayesmanecfit

extract_ecx.bayesmanec

Description

Extracts the predicted ecx value as desired from a bayesnec model fit obeject

Usage

```
extract_ecx.bayesmanecfit(
  X,
  ecx_val = 10,
  precision = 1000,
  posterior = FALSE,
  type = "absolute",
  hormesis_def = "control",
  xform = NA,
  x_range = NA,
  prob_vals = c(0.5, 0.025, 0.975)
)
```

Arguments

X	a fitted bayesmanec model object, containing a list of jag model fit as returned by a call to bayes from fit_bayesnec
ecx_val	the desired percentage effect value.
precision	The number of unique x values over which to find ecx.
posterior	A logical value indicating if the full posterior sample of calculated ecx values should be returned instead of just the median and 95 credible intervals.
type	a character vector indicating if relative or absolute values for the ecx should be calculated.
xform	A function to apply to the returned estimated concentration values
prob_vals	A vector indicating the probability values over which to return the estimated ecx value.

Value

A vector containing the estimated ecx value, including upper and lower 95 percent Credible Interval bounds

---

extract_ecx.bayesnecfit

extract_ecx.bayesnec

Description

Extracts the predicted ecx value as desired from a bayesnec model fit obeject

Usage

```
extract_ecx.bayesnecfit(
  X,
  ecx_val = 10,
  precision = 1000,
  posterior = FALSE,
  type = "absolute",
  hormesis_def = "control",
```

```
    x_range = NA,
    xform = NA,
    prob_vals = c(0.5, 0.025, 0.975)
)
```

Arguments

X	a jag model fit as returned by a call to bayes from fit_bayesnec
ecx_val	the desired percentage effect value.
precision	The number of unique x values over which to find ecx.
posterior	A logical value indicating if the full posterior sample of calculated ecx values should be returned instead of just the median and 95 credible intervals.
type	a character vector indicating if relative or absolute values for the ecx should be calculated.
xform	A function to apply to the returned estimated concentration values
prob_vals	A vector indicating the probability values over which to return the estimated ecx value.

Value

A vector containing the estimated ecx value, including upper and lower 95 percent Credible Interval bounds

---

extract_modstats   *extract_modstats*

Description

Extracts a range of statistics from a list of bayesnecfit model fits.

Usage

```
extract_modstats(mod_fits)
```

Arguments

mod_fits	a bayesMAnecfit mod_fits output list, as returned by fit.bayesMAnec

Value

A list of model statistical output derived from the input model list

---

extract_simdat   *extract_simdat*

Description

Extracts a range of statistics from a list of bayesnecfit model fits.

Usage

```
extract_simdat(modfit)
```

Arguments

modfit   a bayesnecfit, as returned by fit_bayesnec

Value

A list of model simulation statistics including iter, thin, warmup and chains

---

fit_bayesmanec   *fit_bayesmanec*

Description

Fits a variety of nec models using bayes and provides a model averaged predictions based on DIC
model weights

Usage

```
fit_bayesmanec(
  data,
  x_var,
  y_var,
  trials_var = NA,
  x_type = NA,
  y_type = NA,
  iter = 20000,
  over_disp = FALSE,
  model_set = "all",
  sig_val = 0.025,
  x_range = NA,
  ...
)
```

Arguments

data	A data.frame containing the data to use for the model
x_var	The column heading indicating the concentration (x) variable
y_var	The column heading indicating the response (y) variable
trials_var	The column heading indicating the column for the number of "trials" for binomial response data. If not supplied, the model may run but will not be the model you intended!
x_type	the statistical distribution to use for the x (concentration) data. This will be guess based on the characteristic of the input data if not supplied. As some concentration-response data will use zero concentration, and there is no distribution on the continuous scale from 0 to in (ie tweedie) available in bayes, a small offset is added (1/10^3 of the next lowest value) to zero values of concentration where these are gamma distributed.
y_type	the statistical distribution to use for the y (response) data. This may currently be one of 'binomial', 'poisson',' 'gaussian', or 'gamma'. Others can be added as required, please contact the package maintainer. If not supplied, the appropriate distribution will be guessed based on the distribution of the input data.
iter	the number of interations to for the brms fit. Defaults to 2e4.
over_disp	If an overdispersed model should be used. Only changes the model fit for poisson and binomial y_type data. For poisson, a negative binomial model will be fit. For binomial a beta model will be fit.
model_set	A vector of the names of model types to be fit. Currently defaults to all available model types. If "nec" is supplied, only the nec models will be fit. If "ecx" is supplied, only continuous curve models will be fit.
sig_val	Probability value to use as the lower quantile to test significance of the predictor posterior values against the control, to estimate nec as an interpolated NOec value from smooth ecx curves.

Value

All successully fitted bayes model fits, mod.stats a data.frame of model fit statistics, nec a model averaged posterior of the estimated nec, and pred.vals a list of model averaged predictions.

---

fit_bayesnec   *fit_bayesnec*

Description

Fits a concentration(dose)-response model using brms

Usage

```
fit_bayesnec(
  data,
  x_var,
  y_var,
  trials_var = NA,
  x_type = NA,
```

```
    y_type = NA,
    x_range = NA,
    precision = 1000,
    over_disp = FALSE,
    model = "nec3param",
    sig_val = 0.025,
    iter = 20000,
    warmup = floor(iter/5) * 4,
    ...
)
```

Arguments

data	a data.frame containing the data to use for the model fit
x_var	the column heading indicating the concentration (x) variable
y_var	the column heading indicating the response (y) variable
trials_var	the column heading indicating the column for the number of "trials" for binomial response data. If not supplied, the model may run but will not be the model you intended! #' @param x_type the statistical distribution to use for the x (concentration) data. This will be guess based on the characteristic of the input data if not supplied.
y_type	the statistical distribution to use for the y (response) data. This may currently be one of 'binomial', 'poisson',' 'gaussian', or 'gamma'. Others can be added as required, please contact the package maintainer. If not supplied, the appropriate distribution will be guessed based on the distribution of the input data.
x_range	The range of x values over which to obtain posterior predictions. Used for plot.bayesnecfit and to calculate nec for ecx models.
precision	The length of the x_seq to pass to posterior_predict as new data. Used for plot.bayesnecfit and to calculate nec for ecx models.
over_disp	If an overdispersed model should be used. Only changes the model fit for poisson and binomial y_type data. For poisson, a negative binomial model is used. For binomial a beta model is used.
model	The type of model to be fit. Currently takes values of "nec3param", "nec4param", "necsigm", "nechorme", "ecx4param", "ecxwb1", "ecxexp", "ecxlin", or "ecxwb2".
sig_val	Probability value to use as the lower quantile to test significance of the predictor posterior values against the control, to estimate nec as an interpolated NOEC value from smooth ecx curves.
iter	the number of interations for the brms fit. Defaults to 2e4.
warmup	the number of warmup iterations. Defaults to 4/5ths of iter.
...	further arguments to be passed to `brm`.

Details

As some concentration-response data will use zero concentration which can cause numerical estimation issues, a small offset is added (1/10th of the next lowest value) to zero values of concentration where x_var are gamma distributed.

All models provide an estimate for nec. For model types with "nec" as a prefix, nec is directly estimated as a paremeter in the model. Models with "ecx" as a prefix are continuous curve models, typically used for extracting ecx values from concentration response data. In this instance the

nec value is defined as the concentration at which there is a user supplied (see sig_val) percentage certainty (based on the Bayesian posterior estimate) that the response falls below the estimated value of the upper assymptote (top) of the response (i.e the response value is significantly lower than that expected in the case of no exposure).

Value

The fitted brms model, including an estimate of the nec value and predicted posterior values. A posterior sample of the nec is also available under $nec_posterior

---

modify   *modify*

Description

Modifies an existing bayesmanecfit object, for example, but adding or removing fitted models.

Usage

```
modify(object, model_set = NA, drop_models = NA, add_models = NA)
```

Arguments

object	a bayesmanecfit output list, as returned by fit.bayesmanec
model_set	A character vector containing the of names of model types to be included in the modified fit.
drop_models	A character vector containing the names of model types you which to drop for the modified fit.
add_models	A character vector containing the names of model types to add to the modified fit.

Value

All successully fitted bayesmanecfit model fit.

---

plot.bayesmanecfit   *plot.bayesmanecfit*

Description

Generates a plot of a fitted bayes nec model, as returned by fit.bayesnec.

Usage

```
## S3 method for class 'bayesmanecfit'
plot(
  X,
  CI = TRUE,
  add_nec = TRUE,
  position_legend = "topright",
  add_ec10 = FALSE,
  xform = NA,
  lxform = NA,
  jitter_x = FALSE,
  jitter_y = FALSE,
  ylab = "response",
  xlab = "concentration",
  x_lim = NA,
  y_lim = NA,
  xticks = NA,
  all_models = FALSE,
  ...
)
```

Arguments

X	the bayes nec model fit as returned by fit.bayesnec.
CI	a logical value indicating if confidence intervals on the model fit should be plotted, calculated as the upper and lower bounds of the individual predicted values from all posterior samples
add_nec	a logical value indicating if the estimated nec value and 95% credible intervals should be added to the plot.
position_legend	
	a vector indicating the location of the nec or ec10 legend, as per a call to legend.
add_ec10	a logical value indicating if an estimated ec10 value and 95% credible intervals should be added to the plot.
xform	a function to be applied as a transformation of the x data.
lxform	a function to be applied as a transformation only to axis labels and the annoted nec/ec10 values.
jitter_x	a logical value indicating if the x data points on the plot should be jittered.
jitter_y	a logical value indicating if the y data points on the plot should be jittered.
ylab	a character vector to use for the y-axis label
xlab	a character vector to use for the x-axis label
x_lim	a numeric vector of length two to use for the lower and uper limits of the x-axis range
y_lim	a numeric vector of length two to use for the lower and uper limits of the y-axis range
xticks	a numeric vector indicate where to place the tick marks of the x-axis
all_models	Logical indicating if all models in the model set should be plotted simultaneousl, or if a model average plot should be returned.

Value

a plot of the fitted model

---

plot.bayesnecfit   *plot.bayesnecfit*

Description

Generates a plot of a fitted bayes nec model, as returned by fit.bayesnec.

Usage

```
## S3 method for class 'bayesnecfit'
plot(
  X,
  CI = TRUE,
  add_nec = TRUE,
  position_legend = "topright",
  add_ec10 = FALSE,
  xform = NA,
  lxform = NA,
  jitter_x = FALSE,
  jitter_y = FALSE,
  ylab = "response",
  xlab = "concentration",
  x_lim = NA,
  y_lim = NA,
  xticks = NA,
  ...
)
```

Arguments

X	the bayes nec model fit as returned by fit.bayesnec.
CI	a logical value indicating if confidence intervals on the model fit should be plotted, calculated as the upper and lower bounds of the individual predicted values from all posterior samples
add_nec	a logical value indicating if the estimated nec value and 95% credible intervals should be added to the plot.
position_legend	
	a vector indicating the location of the nec or ec10 legend, as per a call to legend.
add_ec10	a logical value indicating if an estimated ec10 value and 95% credible intervals should be added to the plot.
xform	a function to be applied as a transformation of the x data.
lxform	a function to be applied as a transformation only to axis labels and the annoted nec/ec10 values.
jitter_x	a logical value indicating if the x data points on the plot should be jittered.
jitter_y	a logical value indicating if the y data points on the plot should be jittered.

ylab	a character vector to use for the y-axis label
xlab	a character vector to use for the x-axis label
x_lim	a numeric vector of length two to use for the lower and uper limits of the x-axis range
y_lim	a numeric vector of length two to use for the lower and uper limits of the y-axis range
xticks	a numeric vector indicate where to place the tick marks of the x-axis

Value

a plot of the fitted model

---

predict.bayesnecfit *predict.bayesnecfit*

Description

predict.bayesnecfit

Usage

```
## S3 method for class 'bayesnecfit'
predict(X, precision = 100, x_range = NA)
```

Arguments

X	the bayesnec model fit (as returned by fit_bayesnec)
precision	the number of x values over which to predict values
x_range	The range of x values over which to make predictions

Value

A list containing x and fitted y, with up and lw values

---

set_distribution *Sets distribution based on vector*

Description

Sets distribution based on vector

Usage

```
set_distribution(x, support_integer = FALSE, trials = NULL)
```

Arguments

x   a numeric vector.

support_integer

        Logical. Should integer vectors be supported? Defaults to FALSE.

trials   a numeric vector containing the number of trials. Defaults to NULL.

Details

Checks a vector and recommends a family distribution.

Value

a character vector.

Examples

```
library(bayesnec)
set_distribution(rpois(1000, lambda=10), support_integer = TRUE)
set_distribution(rnorm(1000))
set_distribution(x <- rgamma(1000, 2))
set_distribution(ifelse(x < 1, x, 1))
set_distribution(rbinom(1000, 10, 0.5), support_integer = TRUE, 10)
```

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