Package ‘breathteststan’

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Type Package

Title Stan-Based Fit to Gastric Emptying Curves

Version 0.4.7

Description Stan-based curve-fitting function

for use with package 'breathtestcore' by the same author.

Stan functions are refactored here for easier testing.

License GPL (>= 3)

Encoding UTF-8

LazyData true

ByteCompile true

Depends R (>= 3.4.0), methods, Rcpp (>= 0.12.18)

Imports tibble, purrr, dplyr, rstan(>= 2.18.1), rstantools(>= 1.5.0),

stringr, tidyr

Suggests ggplot2, shinystan, bayesplot, testthat, covr, knitr,

rmarkdown, breathtestcore(>= 0.4.1.0)

LinkingTo StanHeaders (>= 2.18.0), rstan (>= 2.18.1), BH (>= 1.66.0-1), Rcpp (>= 0.12.18), RcppEigen (>= 0.3.3.4.0)

URL https://github.com/dmenne/breathteststan

BugReports https://github.com/dmenne/breathteststan/issues

NeedsCompilation yes

SystemRequirements GNU make, pandoc (>= 1.12.3), pandoc-citeproc

RoxygenNote 6.1.0

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as.matrix.coef_diff_by_group_stan

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as.matrix.coef_diff_by_group_stan

S3 as.matrix for result of coef_diff_by_group

Description

Generates a matrix that can be used with plotting functions from package MCMC-distributions.

Usage

```r
## S3 method for class 'coef_diff_by_group_stan'
as.matrix(x, ...)
```

Arguments

- `x` Result of a call to `coef_diff_by_group(fit)`
- `...` parameter name as string, e.g. "m", "k", "beta", "t50_bluck_coward". When missing, "t50_maes_ghoos" is assumed.

Value

mcmc array with columns of differences for use with functions from packages bayesplot or coda

Examples

```r
library(dplyr)
library(breathtestcore)
library(ggplot2)
data("usz_1Sc", package = "breathtestcore")
data = usz_1Sc %>%
dplyr::filter( patient_id %in% c("norm_PP1", "norm_PP2", "norm_PPS", "norm_PPT", "pat_PP1", "pat_PP2","pat_PPS")) %>%
cleanup_data()
fit = stan_group_fit(data, iter = 300, chains = 1)
cf = coef_diff_by_group(fit)
str(cf)
# Calling without parameters gives Maes/Ghoos t50
bayesplot::mcmc_hist(as.matrix(cf))
```
# Use a function from the bayesplot universe
dens = bayesplot::mcmc_dens(as.matrix(cf, parameter = "m"))
# use suppressMessages to avoid a message "another scale"
suppressMessages(
    dens + geom_vline(xintercept = 0) + scale_x_continuous(limits= c(-20,10)))

table_coef_by_group

Tabulates breath test parameter differences of groups from Stan group fit

Description

Given a Stan fit with grouping to 13C breath test curves, computes point estimated and Bayesian credible intervals for all group pair differences, for examples of the half emptying time t50.

Usage

c coef_diff_by_group(fit, mcp_group = NULL, reference_group = NULL, ...)

Arguments

fit Object of class breatheteststangroupfit from stan_fit
mcp_group Not used, always all pairs are compared
reference_group Not used
...

Value

A tibble of class coef_diff_by_group_stan with columns

<table>
<thead>
<tr>
<th>parameter</th>
<th>Parameter of fit, e.g. beta, k, m, t50</th>
</tr>
</thead>
<tbody>
<tr>
<td>method</td>
<td>Method used to compute parameter. exp_beta refers to primary fit parameters beta, k, m.</td>
</tr>
<tr>
<td>groups</td>
<td>Which pairwise difference, e.g solid - liquid</td>
</tr>
<tr>
<td>estimate</td>
<td>Point estimate (chain mean) of the difference</td>
</tr>
<tr>
<td>cred.low, cred.high</td>
<td>Lower and upper 95 percent credible interval of difference.</td>
</tr>
</tbody>
</table>

The chains of pairwise differences are returned as a attribute chain for use in plotting. See example below how to use these to display difference histograms.
Examples

```r
library(dplyr)
library(breathtestcore)
data("usz_1Sc", package = "breathtestcore")
data = usz_1Sc %>%
dplyr::filter(patient_id %in%
c("norm_PP1", "norm_PP2", "norm_PPS", "pat_001", "pat_002", "pat_003")
%>
cleanup_data()
fit = stan_group_fit(data, iter = 300, chains = 1) # Use more iterations!
cc = coef_diff_by_group(fit)
cc = attr(cc, "chain") %>
filter(key == "t50_maes_ghoos", abs(diff) < 200) %>
mute(
  groups = paste(group2, group1, sep = " - ")
)
str(cc)
if (require(ggplot2)) {
  ggplot(cc, aes(x = diff)) + geom_histogram() + facet_wrap(~groups)
}
# For comparison
fit = nlme_fit(data)
coef_diff_by_group(fit)
```

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**sigma.breathteststanfit**

_S3 method to extract the residual standard deviation_

**Description**

Functions for S3 method defined in breathtestcore for stan_fit and stan_group_fit.

**Usage**

```r
## S3 method for class 'breathteststanfit'
sigma(object, ...)
```

**Arguments**

- `object` A Stan-based fit
- `...` Not used

**Value**

A numeric value giving the sigma (= average residual standard deviation) term from the Stan fit.
stan_fit

Bayesian Stan fit to 13C Breath Data

Description

Fits exponential beta curves to 13C breath test series data using Bayesian Stan methods. See https://menne-biomed.de/blog/breath-test-stan for a comparison between single curve, mixed-model population and Bayesian methods.

Usage

stan_fit(data, dose = 100, sample_minutes = 15, student_t_df = 10, chains = 2, iter = 1000, model = "breath_test_1", seed = 4711)

Arguments

data Data frame or tibble as created by cleanup_data, with mandatory columns patient_id, group, minute and pdr. It is recommended to run all data through cleanup_data which will insert dummy columns for patient_id and minute if the data are distinct, and report an error if not. Since the Bayesian method is stabilized by priors, it is possible to fit single curves.
dose Dose of acetate or octanoate. Currently, only one common dose for all records is supported.
sample_minutes If mean sampling interval is < sampleMinutes, data are subsampled using a spline algorithm
student_t_df When student_t_df < 10, the student distribution is used to model the residuals. Recommended values to model typical outliers are from 3 to 6. When student_t_df >= 10, the normal distribution is used.
chains Number of chains for Stan
iter Number of iterations for each Stan chain
model Name of model; use names(stanmodels) for other models.
seed Optional seed for rstan

Value

A list of classes "breathteststanfit" and "breathtestfit" with elements

- coef Estimated parameters as data frame in a key-value format with columns patient_id, group, parameter, method and value. Has an attribute AIC.
- data The effectively analyzed data. If density of points is too high, e.g. with BreathId devices, data are subsampled before fitting.
- stan_fit The Stan fit for use with shinystan::launch_shiny or extraction of chains.

See Also

Base methods coef, plot, print; methods from package broom: tidy, augment.
Examples

```r
library(breathtestcore)
suppressPackageStartupMessages(library(dplyr))
d = breathtestcore::simulate_breathtest_data(n_records = 3) # default 3 records
data = breathtestcore::cleanup_data(d$data)
# Use more than 80 iterations and 4 chains for serious fits
fit = stan_fit(data, chains = 1, iter = 80)
plot(fit) # calls plot.breathtestfit
# Extract coefficients and compare these with those
# used to generate the data
options(digits = 2)
cf = coef(fit)
cf %>%
  filter(grepl("m|k|beta", parameter )) %>%
  select(-method, -group) %>%
  tidyr::spread(parameter, value) %>%
  inner_join(d$record, by = "patient_id") %>%
  select(patient_id, m_in = m.y, m_out = m.x,
         beta_in = beta.y, beta_out = beta.x,
         k_in = k.y, k_out = k.x)
# For a detailed analysis of the fit, use the shinystan library
library(shinystan)
# launch_shinystan(fit$stan_fit)

# The following plots are somewhat degenerate because
# of the few iterations in stan_fit
suppressPackageStartupMessages(library(rstan))
stan_plot(fit$stan_fit, pars = c("beta[1]","beta[2]","beta[3]"))
stan_plot(fit$stan_fit, pars = c("k[1]","k[2]","k[3]"))
stan_plot(fit$stan_fit, pars = c("m[1]","m[2]","m[3]"))
```

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**stan_group_fit**

*Bayesian Stan fit to 13C Breath Data in Multiple Groups*

---

**Description**

Fits exponential beta curves to 13C breath test series data using Bayesian Stan methods, by assuming fixed between group effects. This model is overly parsimonious. Do not use it unless you check the results carefully and understand why fits can be very bad.

**Usage**

```r
stan_group_fit(data, dose = 100, sample_minutes = 15,
               student_t_df = 10, chains = 2, iter = 1000,
               model = "breath_test_group_1")
```
Arguments

- **data**: Data frame or tibble as created by `cleanup_data`, with mandatory columns `patient_id`, `group`, `minute` and `pdr`. It is recommended to run all data through `cleanup_data` which will insert dummy columns for `patient_id` and `minute` if the data are distinct, and report an error if not. Since the Bayesian method is stabilized by priors, it is possible to fit single curves.

- **dose**: Dose of acetate or octanoate. Currently, only one common dose for all records is supported.

- **sample_minutes**: If mean sampling interval is < `sampleMinutes`, data are subsampled using a spline algorithm.

- **student_t_df**: When `student_t_df < 10`, the student distribution is used to model the residuals. Recommended values to model typical outliers are from 3 to 6. When `student_t_df >= 10`, the normal distribution is used.

- **chains**: Number of chains for Stan.

- **iter**: Number of iterations for each Stan chain.

- **model**: Name of model; use `names(stanmodels)` for other models.

Value

A list of classes "breathteststangroupfit", "breathteststanfit" and "breathtestfit" with elements

- **coef**: Estimated parameters as data frame in a key-value format with columns `patient_id`, `group`, `parameter`, `method` and `value`. Has an attribute AIC.

- **data**: The effectively analyzed data. If density of points is too high, e.g. with BreathId devices, data are subsampled before fitting.

- **stan_fit**: The Stan fit for use with `shinystan::launch_shiny` or extraction of chains.

See Also

Base methods `coef`, `plot`, `print`; methods from package `broom`: `tidy`, `augment`.

Examples

```R
library(breathtestcore)
library(dplyr)
data("usz_1Sc", package = "breathtestcore")
data = usz_1Sc %>%
dplyr::filter(patient_id %in%
c("norm_001", "norm_002", "norm_003", "norm_004", "pat_001", "pat_002","pat_003")) %>%
breathtestcore::cleanup_data()
fit = stan_group_fit(data, chains = 1, iter = 100)
plot(fit) # calls plot.breathtestfit
coe(fit)
```
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