Package 'gastempt'

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Version 0.7.0

Type Package

Title Analyzing Gastric Emptying from MRI or Scintigraphy

Description Fits gastric emptying time series from MRI or 'scintigraphic' measurements using nonlinear mixed-model population fits with 'nlme' and Bayesian methods with Stan; computes derived parameters such as t50 and AUC.

License GPL (>= 3)

NeedsCompilation yes

URL https://github.com/dmenne/gastempt, http://dmenne.github.io/gastempt/

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

Depends R (>= 4.3.0)

Imports nlme, Rcpp (>= 1.0.3), dplyr, methods, tibble (>= 3.1.0), ggplot2 (>= 3.3.0), rstan (>= 2.26.0), assertthat, stringr, shiny, utf8

Suggests rmarkdown, knitr, covr, testthat (>= 3.2.0), ragg, vdiffr, parallelly, rstantools

LinkingTo StanHeaders (>= 2.32.0), rstan (>= 2.32.0), BH (>= 1.80.0-1), Rcpp (>= 1.0.3), RcppEigen (>= 0.3.4.0.0), RcppParallel (>= 5.1.9)

VignetteBuilder knitr

RoxygenNote 7.3.2

Encoding UTF-8

SystemRequirements GNU make

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Description

Extract coefficients from nlme_gastempt result

Usage

```
## S3 method for class 'nlme_gastempt'
coef(object, ...)
```

Arguments

`object`	Result of a call to nlme_gastempt
`...`	other arguments

Value

a data frame with coefficients. See `nlme_gastempt` for an example.

coef.stan_gastempt *Extract coefficients from stan_gastempt result*

Description

Extract coefficients from stan_gastempt result

Usage

```
## S3 method for class 'stan_gastempt'
coef(object, ...)
```

Arguments

object	Result of a call to stan_gastempt
...	other arguments

Value

a data frame with coefficients. See nlme_gastempt for an example.

gastemptfunc *Functions for gastric emptying analysis*

Description

The linexp and the power exponential (powexp) functions can be used to fit gastric emptying curves.

Usage

```
linexp(t, v0 = 1, tempt = NULL, kappa = NULL, pars = NULL)

linexp_slope(t, v0 = 1, tempt = NULL, kappa = NULL, pars = NULL)

linexp_auc(v0 = 1, tempt = NULL, kappa = NULL, pars = NULL)

powexp(t, v0 = 1, tempt = NULL, beta = NULL, pars = NULL)

powexp_slope(t, v0 = 1, tempt = NULL, beta = NULL, pars = NULL)

linexp_log(t, v0 = 1, logtempt = NULL, logkappa = NULL, pars = NULL)

powexp_log(t, v0 = 1, logtempt = NULL, logbeta = NULL, pars = NULL)
```

Arguments

t	Time after meal or start of scan, in minutes; can be a vector.
v0	Initial volume at t=0.
tempt	Emptying time constant in minutes (scalar).
kappa	Overshoot term for linexp function (scalar).
pars	Default NULL. If not NULL, the other parameters with exception of t are not used and are retrieved as named parameters from the numeric vector pars instead.
beta	Power term for power exponential function (scalar).
logtempt	Logarithm of emptying time constant in minutes (scalar).
logkappa	Logarithm of overshoot term for linexp function (scalar).
logbeta	Logarithm of power term for power exponential function (scalar).

Details

The linexp function can have an initial overshoot to model secretion.

vol(t) = v0 * (1 + kappa * t / tempt) * exp(-t / tempt)

The powexp function introduced by Elashof et al. is montonously decreasing but has more freedom to model details in the function tail.

vol(t) = v0 * exp(-(t / tempt) ^ beta)

The _slope functions return the first derivatives of linexp and powexp. Use the _log functions to enforce positive parameters tempt and beta. Rarely required for gastric emptying curves.

Value

Vector of length(t) for computed volume.

Examples

```
t = seq(0,100, by=5)
kappa = 1.3
tempt = 60
v0 = 400
beta = 3
pars = c(v0 = v0, tempt = tempt, kappa = kappa)
oldpar = par(mfrow = c(1,3))
plot(t, linexp(t, v0, tempt, kappa), type = "l", ylab = "volume",
   main = "linexp\nkappa = 1.3 and 1.0")
lines(t, linexp(t, v0, tempt, 1), type = "l", col = "green")
# This should give the same plot as above
plot(t, linexp(t, pars = pars), type = "l", ylab = "volume",
   main = "linexp\nkappa = 1.3 and 1.0\nwith vectored parameters")
lines(t, linexp(t, v0, tempt, 1), type = "l", col = "green")
plot(t, powexp(t, v0, tempt, beta), type = "l", ylab = "volume",
  main = "powexp\nbeta = 2 and 1")
lines(t, powexp(t, v0, tempt, 1), type = "l", col = "green")
par(oldpar)
```

`nlme_gastempt` *Simplified population fit of gastric emptying data*

Description

Compute coefficients v0, tempt and kappa of a mixed model fit to a linexp function with one grouping variable

Usage

```
nlme_gastempt(d, pnlsTol = 0.001, model = linexp, variant = 1)
```

Arguments

`d`	A data frame with columns • `record` Record descriptor as grouping variable, e.g. patient ID • `minute` Time after meal or start of recording. • `vol` Volume of meal or stomach
`pnlsTol`	The value of pnlsTol at the initial iteration. See `nlmeControl` When the model does not converge, `pnlsTol` is multiplied by 5 and the iteration repeated until convergence or `pnlsTol >= 0.5`. The effective value of `pnlsTol` is returned in a separate list item. When it is known that a data set converges badly, it is recommended to set the initial `pnlsTol` to a higher value, but below 0.5, for faster convergence.
`model`	`linexp` (default) or `powexp`
`variant`	For both models, there are 3 variants • `variant = 1` The most generic version with independent estimates of all three parameters per record (`random = v0 + tempt + kappa ~ 1 | record`). The most likely to fail for degenerate cases. If this variant converges, use it. • `variant = 2` Diagonal random effects (`random = pdDiag(v0 + tempt + kappa) ~ 1; groups = ~record`). Better convergence in critical cases. Note: I never found out why I have to use the `groups` parameter instead of the `|`; see also p. 380 of Pinheiro/Bates. • `variant = 3` Since parameters `kappa` and `beta` respectively are the most difficult to estimate, these are fixed in this variant (`random = v0 + tempt ~ 1`). This variant converges in all reasonable cases, but the estimates of `kappa` and `beta` cannot be use for secondary between-group analysis. If you are only interested in `t50`, you can use this safe version.

Value

A list of class nlme_gastempt with elements `coef, summary, plot, pnlsTol, message`

- `coef` is a data frame with columns:

  - record Record descriptor, e.g. patient ID
  - v0 Initial volume at t=0
  - tempt Emptying time constant
  - kappa Parameter kappa for model = linexp
  - beta Parameter beta for model = powexp
  - t50 Half-time of emptying
  - slope_t50 Slope in t50; typically in units of ml/minute

  On error, coef is NULL

- nlme_result Result of the nlme fit; can be used for addition processing, e.g. to plot residuals or via summary to extract AIC. On error, nlme_result is NULL.
- plot A ggplot graph of data and prediction. Plot of raw data is returned even when convergence was not achieved.
- pnlsTol Effective value of pnlsTo after convergence or failure.
- message String "Ok" on success, and the error message of nlme on failure.

Examples

```
suppressWarnings(RNGversion("3.5.0"))
set.seed(4711)
d = simulate_gastempt(n_record = 10, kappa_mean = 0.9, kappa_std = 0.3,
                      model = linexp)$data
fit_d = nlme_gastempt(d)
# fit_d$coef # direct access
coef(fit_d) # better use accessor function
coef(fit_d, signif = 3) # Can also set number of digits
# Avoid ugly ggplot shading (not really needed...)
library(ggplot2)
theme_set(theme_bw() + theme(panel.spacing = grid::unit(0,"lines")))
# fit_d$plot  # direct access is possible
plot(fit_d) # better use accessor function
```

---

plot.nlme_gastempt *Plot data points and fit curve of an nlme_gastempt fit*

Description

Plot data points and fit curve of an nlme_gastempt fit

Usage

```
## S3 method for class 'nlme_gastempt'
plot(x, ...)
```

Arguments

x	Result of a call to nlme_gastempt
...	other arguments

Value

a ggplot object. Use `print()` if used non-interactively to show the curve

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`plot.stan_gastempt` *Plot data points and fit curve of an stan_gastempt fit*

Description

Plot data points and fit curve of an stan_gastempt fit

Usage

```
## S3 method for class 'stan_gastempt'
plot(x, ...)
```

Arguments

`x`	Result of a call to stan_gastempt
`...`	other arguments

Value

a ggplot object. Use `print()` if used non-interactively to show the curve

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`run_shiny` *Run shiny app demonstrating fit strategies with simulated data*

Description

Run shiny app demonstrating fit strategies with simulated data

Usage

```
run_shiny()
```

Value

Not used, starts shiny app

`simulate_gastempt` *Simulate gastric emptying data following a linexp or powexp function*

Description

Simulate gastric emptying data following a linexp or powexp function

Usage

```
simulate_gastempt(
  n_records = 10,
  v0_mean = 400,
  v0_std = 50,
  tempt_mean = ifelse(identical(model, linexp), 60, 120),
  tempt_std = tempt_mean/3,
  kappa_mean = 0.7,
  kappa_std = kappa_mean/3,
  beta_mean = 0.7,
  beta_std = beta_mean/3,
  noise = 20,
  student_t_df = NULL,
  missing = 0,
  model = linexp,
  seed = NULL,
  max_minute = NULL
)
```

Arguments

`n_records`	Number of records
`v0_mean`, `v0_std`	Mean and between record standard deviation of initial volume, typically in ml.
`tempt_mean`, `tempt_std`	Mean and between record standard deviation of parameter t_{empt}, typically in minutes.
`kappa_mean`, `kappa_std`	For linexp only: Mean and between-record standard deviation of overshoot parameter `kappa`. For values of `kappa` above 1, curve has an overshoot that can be used to follow volume time series with secretion.
`beta_mean`, `beta_std`	For powexp only: Mean and between-record standard deviation of the so called lag parameter.
`noise`	Standard deviation of normal noise when `student_t_df = NULL`; scaling of noise when student_t_df >= 2.
`student_t_df`	When NULL (default), Gaussian noise is added; when >= 2, Student_t distributed noise is added, which generates more realistic outliers. Values from 2 to 5 are useful, when higher values are used the result comes close to that of Gaussian noise. Values below 2 are rounded to 2.

missing	When 0 (default), all curves have the same number of data points. When > 0, this is the fraction of points that were removed randomly to simulate missing points. Maximum value is 0.5.
model	linexp(default) or powexp
seed	optional seed; not set if seed = NULL (default)
max_minute	Maximal time in minutes; if NULL, a sensible default rounded to hours is used

Value

A list with 3 elements:

record Data frame with columns `record(chr)`, `v0`, `tempt`, `kappa/beta` giving the effective `linexp` or `powexp` parameters for the individual record. `v0` is rounded to nearest integer.

data Data frame with columns `record(chr)`, `minute(dbl)`, `vol(dbl)` giving the time series and grouping parameters. `vol` is rounded to nearest integer.

stan_data A list for use as `data` in Stan-based fits with elements `prior_v0`, `n`, `n_record`, `record`, `minute`, `volume`.

A comment is attached to the return value that can be used as a title

Examples

```
suppressWarnings(RNGversion("3.5.0"))
set.seed(4711)
library(ggplot2)
vol_linexp = simulate_gastempt(n_records = 4, noise = 20)
ggplot(vol_linexp$data, aes(x = minute, y = vol)) + geom_point() +
  facet_wrap(~record) + ggtitle("linexp, noise = 0, no missing")

vol_powexp = simulate_gastempt(n_records = 4, missing = 0.2, student_t_df = 2)
ggplot(vol_powexp$data, aes(x = minute, y = vol)) + geom_point() +
  facet_wrap(~record) + ggtitle("powexp, noise = 10 (default), 20% missing,
  Student-t (df = 2) noise")
```

`stan_gastempt` *Fit gastric emptying curves with Stan*

Description

Fit gastric emptying curves with Stan

Usage

```
stan_gastempt(
  d,
  model_name = "linexp_gastro_2b",
  lkj = 2,
  student_df = 5L,
  init_r = 0.2,
  chains = 1,
  iter = 2000,
  ...
)
```

Arguments

d	A data frame with columns • rec Record descriptor as grouping variable, e.g. patient ID • minute Time after meal or start of recording. • vol Volume of meal or stomach
model_name	Name of predefined model in gastempt/exec. Use stan_model_names() to get a list of available models.
lkj	LKJ prior for kappa/tempt correlation, only required for model linexp_gastro_2b. Values from 1.5 (strong correlation) to 50 (almost independent) are useful.
student_df	Student-t degrees of freedom for residual error; default 5. Use 3 for strong outliers; values above 10 are close to gaussian residual distribution.
init_r	for stan, default = 0.2; Stan's own default is 2, which often results in stuck chains.
chains	for stan; default = 1
iter	A positive integer specifying the number of iterations for each chain (including warmup). The default is 2000.
...	Additional parameter passed to sampling and stan

Value

A list of class stan_gastempt with elements coef, fit, plot

- coef is a data frame with columns:
  - rec Record descriptor, e.g. patient ID
  - v0 Initial volume at t=0
  - tempt Emptying time constant
  - kappa Parameter kappa for model = linexp
  - beta Parameter beta for model = powexp
  - t50 Half-time of emptying
  - slope_t50 Slope in t50; typically in units of ml/minute On error, coef is NULL
- fit Result of class 'stanfit'
- plot A ggplot graph of data and prediction. Plot of raw data is returned even when convergence was not achieved.

Examples

```
# Runs 30+ seconds on CRAN
dd = simulate_gastempt(n_records = 6, seed = 471)
d = dd$data
ret = stan_gastempt(d)
print(ret$coef)
```

`stan_model_names` *Names and descriptions of precompiled Stan models*

Description

By default, line 2 and 3 of comments starting with # or // in Stan file are returned

Usage

```
stan_model_names(n_lines = 2, skip = 1, sep = "\n")
```

Arguments

`n_lines`	Number of comment lines to retrieve
`skip`	Number of lines to skip from beginning of Stan Model file
`sep`	separator for multiline strings

Value

A data frame with `model_name` and the first `n_lines` comment lines in model as description

---

`t50` *Compute half-emptying time from nlme parameters*

Description

No closed solution known for `linexp`, we use a Newton approximation.

Usage

```
t50(x)
```

Arguments

`x`	Result of a nlme fit, with named components ‘tempt, beta, logbeta, kappa, logkappa‘ depending on model. Function used ‘logbeta‘ when it is present, in ‘x‘, otherwise beta, and similar for logkappa/kappa.

Value

Half-emptying time. Name of evaluated function is returned as attribute `fun`. Negative of slope is returned as attribute `slope`.

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