

Package ‘rPBK’

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Title Inference and Prediction of Generic Physiologically-Based Kinetic Models

Version 0.2.5

BugReports <https://gitlab.in2p3.fr/mosaic-software/rPBK/-/issues>

URL <https://gitlab.in2p3.fr/mosaic-software/rPBK/>

Description Fit and simulate any kind of physiologically-based kinetic ('PBK') models whatever the number of compartments. Moreover, it allows to account for any link between pairs of compartments, as well as any link of each of the compartments with the external medium. Such generic PBK models have today applications in pharmacology (PBPK models) to describe drug effects, in toxicology and ecotoxicology (PBTk models) to describe chemical substance effects. In case of exposure to a parent compound (drug or chemical) the 'rPBK' package allows to consider metabolites, whatever their number and their phase (I, II, ...). Last but not least, package 'rPBK' can also be used for dynamic flux balance analysis (dFBA) to deal with metabolic networks. See also Charles et al. (2022) <[doi:10.1101/2022.04.29.490045](https://doi.org/10.1101/2022.04.29.490045)>.

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Biarch true

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Author Virgile Baudrot [aut, cre],
 Sandrine Charles [aut],
 Christelle Lopes [aut],
 Ophélie Gestin [ctb],
 Dominique Lamonica [ctb],
 Aurélie Siberchicot [ctb]
Maintainer Virgile Baudrot <virgile.baudrot@qonfluens.com>
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Contents

dataCompartment4	2
dataMaleGammarusSingle	3
dataPBK	3
df_quant95_	5
export_interpolate	6
fitPBK	6
fitPBK_C4	7
plot.fitPBK	8
ppc	8
Index	10

dataCompartment4	<i>An example data set with 4 compartment</i>
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Description

A dataset containing an example with 4 compartments.

Usage

data(dataCompartment4)

Format

A data frame with 21 rows and 7 variables:

- temps** vector of time
- condition** exposure concentration
- replicat** replicate of experiment
- intestin** compartiment 'intestin'

caecum compartment 'caecum'
cephalon compartment 'cephalon'
reste compartment 'reste'##

dataMaleGammarusSingle

An example data set with 1 compartment

Description

A dataset containing an example with a single compartment.

Usage

```
data(dataMaleGammarusSingle)
```

Format

A data frame with 22 rows and 4 variables:

time vector of time
expw exposure concentration
replicate replicat of experiment
conc internal measured concentration##

dataPBK

Create a list giving data and parameters to use in the model inference.

Description

Create a list giving data and parameters to use in the model inference.

Usage

```
dataPBK(object, ...)

## S3 method for class 'data.frame'
dataPBK(
  object,
  col_time = NA,
  col_replicate = NA,
  col_exposure = NA,
  col_compartment = NA,
  time_accumulation = NA,
```

```

    ku_nest = NA,
    ke_nest = NA,
    k_nest = NA,
    ...
)

nested_model(object)

## S3 method for class 'stanPBKdata'
nested_model(object)

```

Arguments

<code>object</code>	An object of class <code>stanPBKdata</code> (from <code>dataPBK()</code> function).
<code>...</code>	Further arguments to be passed to generic methods
<code>col_time</code>	Column name of the time column
<code>col_replicate</code>	Column name of the replicate column
<code>col_exposure</code>	Column name of the exposure column.
<code>col_compartment</code>	Column names of the compartment column. If several columns, give a vector with the column names.
<code>time_accumulation</code>	A scalar giving accumulation time.
<code>ku_nest</code>	Vector of binary (0 or 1) to select the uptake route. Use the <code>nested_model()</code> on the <code>stanPBKdata</code> object to check it.
<code>ke_nest</code>	Vector of binary (0 or 1) to select the excretion route. Use the <code>nested_model()</code> on the <code>stanPBKdata</code> object to check it.
<code>k_nest</code>	Matrix of binary (0 or 1) to select interaction routes. Use the <code>nested_model()</code> on the <code>stanPBKdata</code> object to check it.

Value

A list with data and parameters require for model inference.

Examples

```

# (1) load data file
data("dataCompartment4")
# (2) prepare data set
dataPBK_C4 <- dataPBK(
  object = dataCompartment4,
  col_time = "temps",
  col_replicate = "replicat",
  col_exposure = "condition",
  col_compartment = c("intestin", "reste", "caecum", "cephalon"),
  time_accumulation = 7)

# (1) load data file

```

```

data("dataCompartment4")
# (2) prepare data set
dataPBK_C4 <- dataPBK(
  object = dataCompartment4,
  col_time = "temps",
  col_replicate = "replicat",
  col_exposure = "condition",
  col_compartment = c("intestin", "reste", "caecum", "cephalon"),
  time_accumulation = 7)
# (3) check nesting
nested_model(dataPBK_C4)
# (2bis)
dataPBK_C42 <- dataPBK(
  object = dataCompartment4,
  col_time = "temps",
  col_replicate = "replicat",
  col_exposure = "condition",
  col_compartment = c("intestin", "reste", "caecum", "cephalon"),
  time_accumulation = 7,
  ku_nest = c(1,1,1,1), # No Change here
  ke_nest = c(1,1,1,1), # No Change here
  k_nest = matrix(c(
    c(0,1,1,1),
    c(0,0,1,1),
    c(0,0,0,0),
    c(0,0,0,0)),
    ncol=4,nrow=4,byrow=TRUE) # Remove
)
# (3bis) re-checking nesting
nested_model(dataPBK_C42)

```

df_quant95_

*Compute 95 credible intervals***Description**

Compute quantiles 95 credible intervals

Usage

```
df_quant95_(x, ...)
```

Arguments

x	An object of class <code>fitPBK</code>
...	Additional arguments

Value

An object of class `data.frame` returning median and 95 credible interval

export_interpolate	<i>Interpolate function implemented in Stan only export for checking</i>
--------------------	--

Description

This function export the linear interpolation implemented in Stan. It can be use to re-sample the exposure profiles.

Usage

```
export_interpolate(x, xpt, ypt, chain = 1, iter = 1, ...)
```

Arguments

x	interpolation point x
xpt	a vector of x axis (has to be same size as ypt vector)
ypt	a vector of y axis (has to be same size as ypt vector)
chain	number of chain
iter	number of iteration
...	Arguments passed to <code>rstan::sampling</code>

Value

A sample of a stanfit object returning a linear interpolation

fitPBK	<i>Bayesian inference of TK model with Stan</i>
--------	---

Description

Bayesian inference of TK model with Stan

Usage

```
fitPBK(stanPBKdata, ...)

## S3 method for class 'stanPBKdata'
fitPBK(stanPBKdata, ...)
```

Arguments

stanPBKdata	List of Data require for computing
...	Arguments passed to <code>rstan::sampling</code> (e.g. iter, chains).

Value

An object of class `fitPBK` containing two object: `stanPBKdata` the data set used for inference and `stanfit` returned by `rstan::sampling`

Examples

```
# (1) load data file
data("dataCompartment4")
# (2) prepare data set
dataPBK_C4 <- dataPBK(
  object = dataCompartment4,
  col_time = "temps",
  col_replicate = "replicat",
  col_exposure = "condition",
  col_compartment = c("intestin", "reste", "caecum", "cephalon"),
  time_accumulation = 7)
# (3) run Bayesian fitting: <5 sec to be executed
# 1 chain and 10 iterations is fast to run but provide
# bad goodness-of-fit
fitPBK_C4_FASTbadGOF <- fitPBK(dataPBK_C4, chains = 1, iter = 10)

# (3) run Bayesian fitting: > 5 sec to be executed
# 4 chains and 2000 iterations provides better estimates
fitPBK_C4 <- fitPBK(dataPBK_C4, chains = 4, iter = 2000)
```

fitPBK_C4

An example of fitPBK object

Description

A `fitPBK` object containing Bayesian inference of the `dataCompartment4` data set.

Usage

```
data(fitPBK_C4)
```

Format

A `fitPBK` object with:

stanPBKdata original data frame wrap in a formatted list for inference

stanfit a `stanfit` object resulting from inference with `stan`

<code>plot.fitPBK</code>	<i>Plotting method for fitPBK objects</i>
--------------------------	---

Description

This is the generic plot S3 method for the `fitTK`. It plots the fit obtained for each variable in the original dataset.

Usage

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

Arguments

<code>x</code>	And object returned by <code>fitPBK</code>
<code>...</code>	Additional arguments

Value

a plot of class `ggplot`

Examples

```
# (1) load a fitPBK object
data("fitPBK_C4")
# (2) plot result of bayesian fitting
plot(fitPBK_C4)
```

<code>ppc</code>	<i>Posterior predictive check plot</i>
------------------	--

Description

Plots posterior predictive check for `fitPBK`

Usage

```
ppc(x, ...)

## S3 method for class 'fitPBK'
ppc(x, ...)
```


Arguments

<code>x</code>	an object used to select a method <code>ppc</code>
<code>...</code>	Further arguments to be passed to generic methods

Value

a plot of class `ggplot`

Examples

```
# (1) load a fitPBK object
data("fitPBK_C4")
# (2) plot ppc of bayesian fitting
ppc(fitPBK_C4)
```

Index

* **datasets**

- dataCompartment4, [2](#)
- dataMaleGammarusSingle, [3](#)
- fitPBK_C4, [7](#)

- dataCompartment4, [2](#)
- dataMaleGammarusSingle, [3](#)
- dataPBK, [3](#)
- df_quant95_, [5](#)

- export_interpolate, [6](#)

- fitPBK, [6](#)
- fitPBK_C4, [7](#)

- nested_model (dataPBK), [3](#)

- plot.fitPBK, [8](#)
- ppc, [8](#)