Package ‘nlmixr2plot’

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Title Nonlinear Mixed Effects Models in Population PK/PD, Plot Functions

Version 2.0.6

Description Fit and compare nonlinear mixed-effects models in differential equations with flexible dosing information commonly seen in pharmacokinetics and pharmacodynamics (Almquist, Leander, and Jirstrand 2015 <doi:10.1007/s10928-015-9409-1>). Differential equation solving is by compiled C code provided in the 'rxode2' package (Wang, Hallow, and James 2015 <doi:10.1002/psp4.12052>). This package is for 'ggplot2' plotting methods for 'nlmixr2' objects.

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URL `https://github.com/nlmixr2/nlmixr2plot`

BugReports `https://github.com/nlmixr2/nlmixr2plot/issues/`

Imports ggplot2, nlmixr2est, nlmixr2extra, rxode2, utils, vpc, xgxr

Suggests testthat (>= 3.0.0), dplyr, withr, nlmixr2data

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R topics documented:

plot.nlmixr2AugPred *Plot a nlmixr2 augPred object*

Description

Plot a nlmixr2 augPred object

Usage

```
## S3 method for class 'nlmixr2AugPred'
plot(x, y, ...)
```

Arguments

x	augPred object
y	ignored, used to mach plot generic
...	Other arguments (ignored)

Value

Nothing called for side effects

Examples

```
library(nlmixr2est)
## The basic model consiss of an ini block that has initial estimates
one.compartment <- function() {
  ini({
    tka <- 0.45 # Log Ka
    tcl <- 1 # Log Cl
    tv <- 3.45    # Log V
    eta.ka ~ 0.6
    eta.cl ~ 0.3
    eta.v ~ 0.1
    add.sd <- 0.7
  })
  # and a model block with the error sppecification and model specification
  model({
    ka <- exp(tka + eta.ka)
    cl <- exp(tcl + eta.cl)
    v <- exp(tv + eta.v)
    d/dt(depot) = -ka * depot
    d/dt(center) = ka * depot - cl / v * center
    cp = center / v
    cp ~ add(add.sd)
  })
}

## The fit is performed by the function nlmixr/nlmix2 specifying the model, data and estimate
fit <- nlmixr2est::nlmixr2(one.compartment, theo_sd,  est="saem", saemControl(print=0))

# augPred shows more points for the fit:

a <- nlmixr2est::augPred(fit)

# you can plot it with plot(augPred object)
plot(a)
```

plot.nlmixr2FitData *Plot a nlmixr2 data object*

Description

Plot some standard goodness of fit plots for the focei fitted object

Usage

```
## S3 method for class 'nlmixr2FitData'
plot(x, ...)
```

Arguments

x	a focei fit object
...	additional arguments

Value

Nothing, called for its side effects

Author(s)

Wenping Wang & Matthew Fidler

Examples

```
library(nlmixr2est)
## The basic model consiss of an ini block that has initial estimates
one.compartment <- function() {
  ini({
    tka <- 0.45 # Log Ka
    tcl <- 1 # Log Cl
    tv <- 3.45    # Log V
    eta.ka ~ 0.6
    eta.cl ~ 0.3
    eta.v ~ 0.1
    add.sd <- 0.7
  })
  # and a model block with the error sppecification and model specification
  model({
    ka <- exp(tka + eta.ka)
    cl <- exp(tcl + eta.cl)
    v <- exp(tv + eta.v)
    d/dt(depot) = -ka * depot
    d/dt(center) = ka * depot - cl / v * center
    cp = center / v
    cp ~ add(add.sd)
  })
}

## The fit is performed by the function nlmixr/nlmix2 specifying the model, data and estimate
fit <- nlmixr2(one.compartment, theo_sd,  est=”saem”, saemControl(print=0))

# This shows many goodness of fit plots
plot(fit)
```

traceplot *Produce trace-plot for fit if applicable*

Description

Produce trace-plot for fit if applicable

Usage

```
traceplot(x, ...)

## S3 method for class 'nlmixr2FitCore'
traceplot(x, ...)
```

Arguments

`x`	fit object
`...`	other parameters

Value

Fit traceplot or nothing.

Author(s)

Rik Schoemaker, Wenping Wang & Matthew L. Fidler

Examples

```
library(nlmixr2est)
## The basic model consiss of an ini block that has initial estimates
one.compartment <- function() {
  ini({
    tka <- 0.45 # Log Ka
    tcl <- 1 # Log Cl
    tv <- 3.45    # Log V
    eta.ka ~ 0.6
    eta.cl ~ 0.3
    eta.v ~ 0.1
    add.sd <- 0.7
  })
  # and a model block with the error sppecification and model specification
  model({
    ka <- exp(tka + eta.ka)
    cl <- exp(tcl + eta.cl)
    v <- exp(tv + eta.v)
    d/dt(depot) = -ka * depot
    d/dt(center) = ka * depot - cl / v * center
    cp = center / v
    cp ~ add(add.sd)
  })
}

## The fit is performed by the function nlmixr/nlmix2 specifying the model, data and estimate
fit <- nlmixr2(one.compartment, theo_sd,  est=”saem”, saemControl(print=0))

# This shows the traceplot of the fit (useful for saem)
traceplot(fit)
```

vpcPlot *VPC based on ui model*

Description

VPC based on ui model

Usage

```
vpcPlot(
  fit,
  data = NULL,
  n = 300,
  bins = "jenks",
  n_bins = "auto",
  bin_mid = "mean",
  show = NULL,
  stratify = NULL,
  pred_corr = FALSE,
  pred_corr_lower_bnd = 0,
  pi = c(0.05, 0.95),
  ci = c(0.05, 0.95),
  uloq = NULL,
  lloq = NULL,
  log_y = FALSE,
  log_y_min = 0.001,
  xlab = NULL,
  ylab = NULL,
  title = NULL,
  smooth = TRUE,
  vpc_theme = NULL,
  facet = "wrap",
  scales = "fixed",
  labeller = NULL,
  vpcdb = FALSE,
  verbose = FALSE,
  ...,
  seed = 1009
)
```

Arguments

`fit`	nlmixr2 fit object
`data`	this is the data to use to augment the VPC fit. By default is the fitted data, (can be retrieved by `getData`), but it can be changed by specifying this argument.
`n`	Number of VPC simulations. By default 100

`bins` either "density", "time", or "data", "none", or one of the approaches available in classInterval() such as "jenks" (default) or "pretty", or a numeric vector specifying the bin separators.

`n_bins` when using the "auto" binning method, what number of bins to aim for

`bin_mid` either "mean" for the mean of all timepoints (default) or "middle" to use the average of the bin boundaries.

`show` what to show in VPC (obs_dv, obs_ci, pi, pi_as_area, pi_ci, obs_median, sim_median, sim_median_ci)

`stratify` character vector of stratification variables. Only 1 or 2 stratification variables can be supplied.

`pred_corr` perform prediction-correction?

`pred_corr_lower_bnd`
lower bound for the prediction-correction

`pi` simulated prediction interval to plot. Default is c(0.05, 0.95),

`ci` confidence interval to plot. Default is (0.05, 0.95)

`uloq` Number or NULL indicating upper limit of quantification. Default is NULL.

`lloq` Number or NULL indicating lower limit of quantification. Default is NULL.

`log_y` Boolean indicting whether y-axis should be shown as logarithmic. Default is FALSE.

`log_y_min` minimal value when using log_y argument. Default is 1e-3.

`xlab` label for x axis

`ylab` label for y axis

`title` title

`smooth` "smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.

`vpc_theme` theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()

`facet` either "wrap", "columns", or "rows"

`scales` either "fixed" (default), "free_y", "free_x" or "free"

`labeller` ggplot2 labeller function to be passed to underlying ggplot object

`vpcdb` Boolean whether to return the underlying vpcdb rather than the plot

`verbose` show debugging information (TRUE or FALSE)

`...` Args sent to `rxSolve`

`seed` an object specifying if and how the random number generator should be initialized

Value

Simulated dataset (invisibly)

Author(s)

Matthew L. Fidler

Examples

```
one.cmt <- function() {
 ini({
   ## You may label each parameter with a comment
   tka <- 0.45 # Log Ka
   tcl <- log(c(0, 2.7, 100)) # Log Cl
   ## This works with interactive models
   ## You may also label the preceding line with label("label text")
   tv <- 3.45; label("log V")
   ## the label("Label name") works with all models
   eta.ka ~ 0.6
   eta.cl ~ 0.3
   eta.v ~ 0.1
   add.sd <- 0.7
 })
 model({
   ka <- exp(tka + eta.ka)
   cl <- exp(tcl + eta.cl)
   v <- exp(tv + eta.v)
   linCmt() ~ add(add.sd)
 })
}

fit <- nlmixr2est::nlmixr(one.cmt, nlmixr2data::theo_sd, est="focei")

vpcPlot(fit)
```

Index