

# Package ‘nlmixr2plot’

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

**Version** 3.0.2

**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](https://doi.org/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](https://doi.org/10.1002/psp4.12052)>). This package is for 'ggplot2' plotting methods for 'nlmixr2' objects.

**License** GPL (>= 3)

**URL** <https://github.com/nlmixr2/nlmixr2plot>,  
<https://nlmixr2.github.io/nlmixr2plot/>

**BugReports** <https://github.com/nlmixr2/nlmixr2plot/issues/>

**Imports** ggplot2 (>= 3.4.0), nlmixr2est, nlmixr2extra, rxode2, utils,  
vpc, xgxr

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

**Config/testthat/edition** 3

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**NeedsCompilation** no

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|                     |                                      |
|---------------------|--------------------------------------|
| plot.nlmixr2AugPred | <i>Plot a.nlmixr2 augPred object</i> |
|---------------------|--------------------------------------|

---

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
    tc1 <- 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 sspecification and model specification
  model({
    ka <- exp(tka + eta.ka)
```

```

      c1 <- exp(tcl + eta.c1)
      v <- exp(tv + eta.v)
      d/dt(depot) = -ka * depot
      d/dt(center) = ka * depot - c1 / 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 (currently ignored) |

## Value

An nlmixr2PlotList object (a list of ggplot2 objects with easier plotting for all of them at the same time)

## Author(s)

Wenping Wang & Matthew Fidler

## Examples

```
library(nlmixr2est)
one.compartment <- function() {
  ini({
    tka <- 0.45
    tcl <- 1
    tv <- 3.45
    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)
    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, nBurn = 10, nEm = 20))

# 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 consists of an ini block that has initial estimates
one.compartment <- function() {
  ini({
    tka <- 0.45 # Log Ka
    tc1 <- 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 specification and model specification
  model({
    ka <- exp(tka + eta.ka)
    cl <- exp(tc1 + 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 = fit$dataUloq,
  lloq = fit$dataLloq,
  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,
  idv = "time",
  cens = FALSE
)

vpcPlotTad(..., idv = "tad")

vpcCensTad(..., cens = TRUE, idv = "tad")

vpcCens(..., cens = TRUE, idv = "time")

```

**Arguments**

|                   |                                                                                                                                                                                   |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>fit</code>  | nlmixr2 fit object                                                                                                                                                                |
| <code>data</code> | this is the data to use to augment the VPC fit. By default is the fitted data, (can be retrieved by <a href="#">getData</a> ), but it can be changed by specifying this argument. |
| <code>n</code>    | Number of VPC simulations                                                                                                                                                         |
| <code>bins</code> | 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 indicating 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 <a href="#">rxSolve</a>                                                                                                                                                                                        |
| seed                | an object specifying if and how the random number generator should be initialized                                                                                                                                           |
| idv                 | Name of independent variable. For vpcPlot() and vpcCens() the default is "time" for vpcPlotTad() and vpcCensTad() this is "tad"                                                                                             |
| cens                | is a boolean to show if this is a censoring plot or not. When cens=TRUE this is actually a censoring vpc plot (with vpcCens() and vpcCensTad()). When cens=FALSE this is traditional VPC plot (vpcPlot() and vpcPlotTad()). |

**Value**

Simulated dataset (invisibly)

**Author(s)**

Matthew L. Fidler

**Examples**

```
one.cmt <- function() {  
  ini({  
    tka <- 0.45; label("Ka")  
    tcl <- log(c(0, 2.7, 100)); label("Cl")  
    tv <- 3.45; label("V")  
    eta.ka ~ 0.6  
    eta.cl ~ 0.3  
    eta.v ~ 0.1  
    add.sd <- 0.7; label("Additive residual error")  
  })  
  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,  
    data = nlmixr2data::theo_sd,  
    est = "saem",  
    control = list(print = 0)  
  )  
  
vpcPlot(fit)
```

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