Package 'ggPMX'

November 30, 2023

Title 'ggplot2' Based Tool to Facilitate Diagnostic Plots for NLME Models

Description At Novartis, we aimed at standardizing the set of diagnostic plots used for modeling activities in order to reduce the overall effort required for generating such plots.

For this, we developed a guidance that proposes an adequate set of diagnostics and a toolbox, called 'ggPMX' to execute them. 'ggPMX' is a toolbox that can generate all diagnostic plots at a quality sufficient

for publication and submissions using few lines of code. This package focuses on plots recommended by ISoP

doi:10.1002/psp4.12161. While not required, you can get/install the 'R' 'lixoftConnectors' package in the 'Monolix' installation, as described at the following url

https://monolix.lixoft.com/monolix-api/lixoftconnectors_installation/.

When 'lixoftConnectors' is available 'P' can use 'Monolix' directly to greate the required.

When 'lixoftConnectors' is available, 'R' can use 'Monolix' directly to create the required Chart Data instead of exporting it from the 'Monolix' gui.

Version 1.2.11

URL https://github.com/ggPMXdevelopment/ggPMX

BugReports https://github.com/ggPMXdevelopment/ggPMX/issues

Depends R (>= 3.5)

Imports data.table, yaml, R6, gtable, ggplot2 (>= 3.4.0), ggforce, magrittr, stringr, assertthat, GGally, zoo, knitr, rmarkdown, tidyr, dplyr, purrr, readr, rlang, checkmate, scales

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Suggests testthat, xtable, vdiffr, rxode2, nlmixr2, nlmixr2data, lixoftConnectors, xgxr, withr, lifecycle

VignetteBuilder knitr

NeedsCompilation no

RoxygenNote 7.2.3

Encoding UTF-8

Author Amine Gassem [aut], Bruno Bieth [aut], Irina Baltcheva [aut],

Thomas Dumortier [aut],
Christian Bartels [aut],
Souvik Bhattacharya [aut],
Inga Ludwig [aut],
Ines Paule [aut],
Didier Renard [aut],
Matthew Fidler [aut, cre] (https://orcid.org/0000-0001-8538-6691),
Seid Hamzic [aut],
Benjamin Guiastrennec [ctb],
Kyle T Baron [ctb] (<https: 0000-0001-7252-5656="" orcid.org="">),</https:>
Qing Xi Ooi [ctb],
Novartis Pharma AG [cph]
Maintainer Matthew Fidler < matt.fidler@novartis.com>
Repository CRAN
Data/Publication 2022 11 20 16:10:06 UTC

R topics documented:

2

brev	 	4
ld_draft	 	5
neck_shrink	 	6
strib	 	6
a_cov	 	7
a_cov_plot	 	9
a_distribution_plot	 	12
a_pairs	 	15
ral_sym_parent_env	 	16
etPmxOption	 	17
et_abbrev	 	17
et_cats	 	18
et_conts	 	18
et_covariates	 	19
et_data	 	19
et_occ	 	20
et_plot	 	20
et_plot_config	 	21
et_strats	 	22
able_remove_grobs	 	22
dividual	 	23
put_finegrid	 	24
pmx_gpar	 	24
ad_config	 	25
ad_data_set	 	25
ad_source	 	26
left_join	 	26
pages	 	27
ram table	 	27

parse_mlxtran	28
pk_occ	
pk_pd	29
plots	29
plot_names	
plot_pmx	30
plot_pmx.distrib	31
plot_pmx.eta_cov	32
plot_pmx.eta_pairs	32
plot_pmx.individual	
plot_pmx.pmx_dens	
plot_pmx.pmx_gpar	
plot_pmx.pmx_qq	35
plot_pmx.residual	36
plot_shrink	
pmx	
pmxOptions	40
pmx_bloq	41
pmx_comp_shrink	
pmx_config	
pmx_copy	
pmx_cov	45
pmx_dens	
pmx_endpoint	
pmx_filter	
pmx_get_configs	49
pmx_gpar	
pmx_list_nm_tables	
pmx_manual_nm_import	
pmx_nlmixr	
pmx_nm	
pmx_plot	
pmx_plot_cats	57
pmx_plot_eta_matrix	
pmx_plot_individual	
pmx_plot_iwres_dens	
pmx_plot_vpc	66
pmx_qq	70
pmx_qq_plot	71
pmx_read_nm_files	74
pmx_read_nm_model	75
pmx_read_nm_tables	77
pmx_register_plot	78
pmx_report	79
pmx_report_template	81
pmx_settings	82
pmx_shrink	83
nmy sim	Q/

4 abbrev

	pmx_theme	85
	pmx_update	
	pmx_vpc	87
	pmx_vpc_bin	
	pmx_vpc_ci	
	pmx_vpc_obs	
	pmx_vpc_pi	90
	pmx_vpc_rug	91
	print.abbreviation	92
	print.configs	93
	print.pmxClass	93
	print.pmxConfig	94
	print.pmx_gpar	94
	read_extfile	95
	read_input	96
	read_mlx_ind_est	97
	read_mlx_par_est	97
	read_mlx_pred	98
	residual	98
	residual_scatter	00
	set_abbrev	04
	set_data	05
	set_plot	06
	theophylline	07
	wrap_formula	07
	[.pmx_gpar	08
Index	10	09

abbrev

Give the whole abbreviation definition

Description

Give the whole abbreviation definition

Usage

abbrev(param)

Arguments

param

abbreviation term

Value

character abbreviation definition

add_draft 5

Examples

```
abbrev("VPC")
```

 add_draft

Add draft layer annotation

Description

This function adds the word draft to certain graphics.

Usage

```
add_draft(
  label = "DRAFT",
  size = 10,
  colour = "grey50",
  x = Inf,
  y = -Inf,
  ...
)
```

Arguments

label	draft layer default to DRAFT
size	size of the annotation
colour	color of the annotation default to grey50
Х	numeric x coordinate of the draft label
У	numeric y coordinate of the draft label
	extra parameters to geom text used to annotate the draft

Value

ggplot2 annotation

6 distrib

 $check_shrink$

Performs checks of names in shrink list

Description

Performs checks of names in shrink list

Usage

```
check_shrink(shrink_list)
```

Arguments

```
shrink_list list list of shrink arguments
```

distrib

creates a graphic distribution object

Description

creates a graphic distribution object

Usage

```
distrib(
  labels,
  is.shrink,
  type = c("box", "hist"),
  is.jitter = FALSE,
  jitter = NULL,
  facets = NULL,
  histogram = NULL,
  shrink = NULL,
  dname = NULL,
  ...
)
```

Arguments

labels list of texts/titles used within the plot is.shrink logical if TRUE add shrinkage layer

type box for boxplot or histogram

is.jitter logical if TRUE add jitter operator for points

jitter list set jitter parameter

eta_cov 7

facets list set the facet setting in case of histogram plot

histogram list histogram graphical parameters

shrink pmxShrinkClass shrinkage graphical parameter or list coercible into one

dname name of dataset to be used

... others graphics arguments passed to pmx_gpar internal object.

Details

labels is a list that contains:

• title: plot title default "EBE distribution"

• subtitle: plot subtitle default empty

• x: x axis label default to "Etas"

• y: y axis label default to empty

• legend: legend title default to "random Effect"

shrink is a list that contains:

• fun: shrinkage function can be sd or var

size: shrinkage text sizecolor: shrinkage text color

• vjust: shrinkage position vertical adjustment

Value

distrib object

See Also

```
Other plot_pmx: eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

eta_cov	This creates an ETA covariance matrix which can be used to define the
	co-relation between the parameters and its shrinkage

Description

This creates an ETA covariance matrix which can be used to define the co-relation between the parameters and its shrinkage..

8 eta_cov

Usage

```
eta_cov(
  labels,
  type = c("cats", "conts"),
  dname = NULL,
  show.correl = TRUE,
  correl = NULL,
  facets = NULL,
  point = NULL,
  covariates = NULL,
  is.strat.color = FALSE,
  ...
)
```

Arguments

labels list of texts/titles used within the plot

type box for cats or conts

dname name of dataset to be used

show.correl logical if TRUE add correlation to the plot correl list correl geom text graphical parameter

facets list facetting graphical parameter point list geom point graphical parameter

is.strat.color logical if 'TRUE' use a different color for the spline stratification.

... others graphics arguments passed to pmx_gpar internal object.

Details

labels is a list that contains:

- title: plot title default "EBE vs. covariates"
- x: x axis label default to "Etas"
- y: y axis label default to empty

Value

```
eta_cov object
```

```
Other plot_pmx: distrib(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

eta_cov_plot 9

eta_cov_plot

Eta Covariates plots

Description

Eta Covariates plots

Relationships between (ETA) and categorical covariates

Relationships between (ETA) and continuous covariates

Usage

```
dummy(
  dname,
  show.correl,
  correl,
  point,
  facets,
  filter,
  strat.facet,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.smooth,
  smooth,
  is.band,
 band,
  is.draft,
  draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales
)
pmx_plot_eta_cats(ctr, ...)
pmx_plot_eta_conts(ctr, ...)
```

Arguments

 $\quad \text{dname} \quad$

character name of dataset to be used

10 eta_cov_plot

show.correl logical if TRUE add correlation to the plot
correl list correl geom text graphical parameter
point list geom point graphical parameter
facets list facetting graphical parameter

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx_gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.smooth logical if set to TRUE add smooth layer

smooth list geom_smooth graphical/smoothing fun parameters

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom_text graphical parameters.

is.identity_line

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters.

scale_x_log10 logical if TRUE use log10 scale for x axis. scale_y_log10 logical if TRUE use log10 scale for y axis.

scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

ctr pmx controller

... others graphics parameters passed :

- pmx_gpar internal function to customize shared graphical parameters
- eta_cov generic object for eta/covariates plots.
- pmx_update function.

eta_cov parameters

Value

ggplot2 object

eta_cov_plot

Examples

```
# basic use -----
ctr <- theophylline()</pre>
ctr %>% pmx_plot_eta_cats
ctr %>% pmx_plot_eta_conts
# update graphical parameter -----
## update labels
ctr %>% pmx_plot_eta_cats(
  labels = list(title = "New eta cats title")
)
## remove draft
ctr %>% pmx_plot_eta_cats(is.draft = FALSE)
## change text color line
ctr %>% pmx_plot_eta_conts(
  correl=list(colour="magenta")
  )
## set covariates custom labels
ctr %>% pmx_plot_eta_conts(
  covariates=pmx_cov(values=list("WT0","AGE0"),
                    labels=list("Weight","Age"))
)
## set effects and covaraites custom labels
ctr <- theophylline( settings = pmx_settings(</pre>
  effects=list( levels=c("ka", "V", "Cl"),
               labels=c("Concentration", "Volume", "Clearance")
  )
)
)
ctr %>% pmx_plot_eta_conts(
  covariates=pmx_cov(values=list("WT0","AGE0"),
                    labels=list("Weight","Age"))
)
```

12 eta_distribution_plot

```
eta_distribution_plot Eta distribution plots
```

Description

Eta distribution plots
Eta Distribution boxplot
Eta Distribution histogram plot

Usage

```
eta_distribution_plot(
  jitter,
  type,
  dname,
  is.shrink,
  shrink,
  is.jitter,
  histogram,
  filter,
  strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.smooth,
  smooth,
  is.band,
 band,
  is.draft,
  draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales,
)
pmx_plot_eta_box(ctr, ...)
pmx_plot_eta_hist(ctr, ...)
```

eta_distribution_plot 13

Arguments

jitter list set jitter parameter
type box for boxplot or histogram
dname name of dataset to be used

is.shrink logical if TRUE add shrinkage layer

shrink list parameters to control shrinkage, must contain "fun"

is. jitter logical if TRUE add jitter operator for points

histogram list histogram graphical parameters

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx_gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.smooth logical if set to TRUE add smooth layer

smooth list geom_smooth graphical/smoothing fun parameters

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom_text graphical parameters.

 $is.identity_line$

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters.
scale_x_log10 logical if TRUE use log10 scale for x axis.
scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

... others graphics parameters passed :

• pmx_gpar internal function to customize shared graphical parameters

• distrib generic object for distribution plots (histogram/boxplot).

• pmx_update function.

distrib parameters

ctr pmx controller

Value

ggplot2 object

Examples

```
# ******* basic use ********* -----
ctr <- theophylline()</pre>
## boxplot variation
p <- ctr %>% pmx_plot_eta_box()
## histogram variation
p <- ctr %>% pmx_plot_eta_hist()
# update graphical parameter -----
## add jitter
ctr %>%
 pmx_plot_eta_hist(is.jitter = TRUE, jitter = list(alpha = 0.4, color = "red"))
## remove shrinkage
ctr %>%
 pmx_plot_eta_hist(is.shrink = FALSE)
## update histogram graphical parameters
ctr %>%
 pmx_plot_eta_hist(
   histogram = list(
     color = NA,
     position = "fill",
     binwidth = 1 / 100
 )
# stratification -----
## categorical stratification color parameter
ctr %>% pmx_plot_eta_hist(is.jitter = TRUE, strat.facet = ~STUD, strat.color = ~SEX)
## categorical stratification facetting
ctr %>% pmx_plot_eta_hist(strat.facet = ~SEX)
## using formula categorical stratification facetting
ctr %>% pmx_plot_eta_hist(
 strat.facet = STUD ~ SEX,
 shrink = pmx_shrink(hjust = 0.5)
)
# subsetting -----
```

eta_pairs 15

```
## select a set of random effect
ctr %>% pmx_plot_eta_hist(filter = EFFECT %in% c("ka", "Cl"))
## filter and stratify by facets
ctr %>% pmx_plot_eta_hist(
  filter = EFFECT %in% c("ka", "Cl"), strat.facet = ~SEX
)
ctr %>% pmx_plot_eta_hist(
  filter = EFFECT %in% c("ka", "Cl"), strat.facet = ~SEX
)
```

eta_pairs

This creates an eta correlation which defines the relationship between parameters

Description

This creates an eta correlation which defines the relationship between parameters

Usage

```
eta_pairs(
  is.title,
  title,
  dname = NULL,
  type.eta = c("mode", "mean"),
  text_color = "black",
  is.shrink = TRUE,
  is.smooth = TRUE,
  smooth = NULL,
  point = NULL,
  shrink = NULL,
  is.hline = FALSE,
  hline = NULL,
  is.vreference_line = FALSE,
  vreference_line = list(colour = "orange", linetype = "longdash"),
)
```

Arguments

is.title	logical if TRUE then a title is used for the plot
title	character the plot title
dname	name of dataset to be used
type.eta	character type of eat can be 'mode' or 'mean'.'mode' by default
text_color	color of the correlation text in the upper matrix

eval_sym_parent_env

is. shrink logical if TRUE add shrinkage to the plot

is.smooth logical if TRUE add smoothing to lower matrix plots

smooth list geom_smooth graphical parameters
point list geom_point graphical parameter

shrink pmxShrinkClass shrinkage graphical parameter or list coercible into one

is.hline logical if TRUE add horizontal line to lower matrix plots

hline list geom_hline graphical parameters

is.vreference_line

logical if TRUE add the +- 1.96 lines

vreference_line

list geom_hline graphical parameters for the reference lines

... others graphics arguments passed to pmx_gpar internal object.

Value

ecorrel object

See Also

```
Other plot_pmx: distrib(), eta_cov(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

Description

Try to evaluate a symbol in the parent frame (on errorr eturn the symbol)

Usage

```
eval_sym_parent_env(x)
```

Arguments

x any object

getPmxOption 17

 ${\tt getPmxOption}$

Get ggPMX Option

Description

```
Get ggPMX Option
```

Usage

```
getPmxOption(name, default = NULL)
```

Arguments

name

Name of an option to get.

default

Value to be returned if the option is not currently set.

Examples

```
## Not run:
pmxOptions(myOption = 10)
getPmxOption("myOption")
## End(Not run)
```

get_abbrev

Get abbreviation definition by key

Description

Get abbreviation definition by key

Usage

```
get_abbrev(ctr, param)
```

Arguments

ctr pmxClass controller abbreviation term

Value

character abbreviation definition

18 get_conts

get_cats

Get category covariates

Description

Get category covariates

Usage

```
get_cats(ctr)
```

Arguments

ctr

the controller object

Value

a charcater vector

See Also

```
Other pmxclass: get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

get_conts

Get continuous covariates

Description

Get continuous covariates

Usage

```
get_conts(ctr)
```

Arguments

ctr

the controller object

Value

a charcater vector

```
Other pmxclass: get_cats(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

get_covariates 19

get_covariates

Get covariates variables

Description

Get covariates variables

Usage

```
get_covariates(ctr)
```

Arguments

ctr

the controller object

Value

a charcater vector

See Also

```
Other pmxclass: get_cats(), get_conts(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

get_data

Get controller data set

Description

Get controller data set

Usage

```
get_data(
  ctr,
  data_set = c("estimates", "predictions", "eta", "finegrid", "input", "sim",
        "individual")
)
```

Arguments

ctr the controller object data_set the data set name

Value

a data.table of the named data set if available.

20 get_plot

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

get_occ

Get controller occasional covariates

Description

Get controller occasional covariates

Usage

```
get_occ(ctr)
```

Arguments

ctr

the controller object

Value

a charcater vector

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

get_plot

Get plot object

Description

Get plot object

Usage

```
get_plot(ctr, nplot, which_pages = "all")
```

Arguments

ctr pmxClass controller object nplot character the plot name

which_pages integer vector (can be length 1), set page number in case of multi pages plot, or

character "all" to plot all pages.

get_plot_config 21

Value

ggplot object

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

Examples

```
library(ggPMX)
ctr <- theophylline()
p1 <- ctr %>% get_plot("iwres_ipred")
## get all pages or some pages
p2 <- ctr %>% get_plot("individual")
## returns one page of individual plot
p2 <- ctr %>% get_plot("individual", which_pages = 1)
p3 <- ctr %>% get_plot("individual", which_pages = c(1, 3))
## get distribution plot
pdistri <- ctr %>% get_plot("eta_hist")
```

get_plot_config

Get the plot config by name

Description

Get the plot config by name

Usage

```
get_plot_config(ctr, pname)
```

Arguments

ctr the controller object pname the plot name

Value

the config object

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

22 gtable_remove_grobs

Examples

```
ctr <- theophylline()
ctr %>% set_plot("IND", pname = "indiv1")
ctr %>% get_plot_config("distr1")
```

get_strats

Get extra stratification variables

Description

Get extra stratification variables

Usage

```
get_strats(ctr)
```

Arguments

ctr

the controller object

Value

a charcater vector

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), plot_names(), plots(), pmx_update(), set_data(), set_plot()
```

gtable_remove_grobs

Remove named elements from gtable

Description

Remove named elements from gtable

Usage

```
gtable_remove_grobs(table, names, ...)
```

Arguments

table The table from which grobs should be removed

names A character vector of the grob names (as listed in table\$layout) that should be

removed

... Other parameters passed through to gtable_filter.

individual 23

individual	This function can be used to obtain individual prediction and compare with observed data and population prediction for each individual separately

Description

This function can be used to obtain individual prediction and compare with observed data and population prediction for each individual separately

Usage

```
individual(
  labels,
  facets = NULL,
  dname = NULL,
  ipred_line = NULL,
  pred_line = NULL,
  point = NULL,
  bloq = NULL,
  is.legend,
  use.finegrid,
  ...
)
```

Arguments

```
labels
                  plot texts. labels, axis,
facets
                  list facets settings nrow/ncol
dname
                  name of dataset to be used
ipred_line
                  list some pred line geom properties aesthetics
pred_line
                  list some ipred line geom properties aesthetics
point
                  list some point geom properties aesthetics
bloq
                  pmxBL0Q object created by pmx_bloq
is.legend
                  logical if TRUE add a legend
use.finegrid
                  logical if FALSE use predictions data set
                  others graphics arguments passed to pmx_gpar internal object.
```

Value

individual fit object

is.pmx_gpar

See Also

```
plot_pmx.individual
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), plot_pmx.distrib(), plot_pmx.eta_cov(),
plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(),
plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

input_finegrid

Merge input and fingrid data sets

Description

Merge input and fingrid data sets

Usage

```
input_finegrid(input, finegrid)
```

Arguments

input data.table input data set finegrid data.table finegrid data set

Value

data.table

is.pmx_gpar

Check if an object is a pmx_gpar class

Description

Check if an object is a pmx_gpar class

Usage

```
is.pmx_gpar(x)
```

Arguments

x pmx_gpar object

Value

logical returns TRUE if it is a pmx_gpar object

load_config 25

 ${\tt load_config}$

Obtain the data source config

Description

Obtain the data source config

Usage

```
load_config(x, sys = c("mlx", "nm", "mlx18"))
```

Arguments

x the config name. sys can be mlx,nm,...

Value

a list :data configuration object

load_data_set

Load data set

Description

Load data set

Usage

```
load_data_set(x, path, sys, ...)
```

Arguments

x data set config

path character path to the directory

sys character mlx or nm

... extra parameter passed to special readers

Value

data.table

26 1_left_join

load_source

Load all/or some source data set

Description

Load all/or some source data set

Usage

```
load_source(sys, path, dconf, ...)
```

Arguments

sys type cane mlx/nom

path character directory path containing all sources.

dconf configuration object

... any extra parameters for readers

Value

list of data.table

 l_left_join

Merge 2 lists

Description

left join, the first list is updated by the seond one

Usage

```
l_left_join(base_list, overlay_list, recursive = TRUE)
```

Arguments

base_list list to update

overlay_list list used to update the first list

recursive logical if TRUE do the merge in depth

Value

list

n_pages 27

Description

This is a simple helper that returns the number of pages it takes to plot all panels when using facet_wrap_paginate. It partially builds the plot so depending on the complexity of your plot it might take some time to calculate...

Usage

```
n_pages(plot)
```

Arguments

plot

A ggplot object using either facet_wrap_paginate or facet_grid_paginate

Value

If the plot uses using either facet_wrap_paginate or facet_grid_paginate it returns the total number of pages. Otherwise it returns NULL

param_table	Creates parameter kable
hai aiii_rabie	Creates parameter kable

Description

Creates parameter kable

Usage

```
param_table(ctr, fun, return_table = FALSE, scientific = FALSE, digits = 2)
```

Arguments

ctr	Generated controller from e.g. pmx_mlx for Monolix.
fun	$character\ can\ be\ "sd"\ or\ "var"\ for\ shrinkage\ computation, see\ {\tt pmx_comp_shrink}$
return_table	If TRUE, returns the same table as in get_data('estimates') otherwise it returns a kable
scientific	logical set to TRUE to get scientific notation of parameter values, or FALSE otherwise
digits	integer the number of significant digits to use when rounding parameter values

pk_occ

Value

Returns a kable with the parameter estimates from get_data('estimates')

Examples

```
#ctr <- theophylline()
#my_params <- ctr %>% param_table(fun = "var")
```

parse_mlxtran

Parse MONOLIX mlxtran file

Description

Parse MONOLIX mlxtran file

Usage

```
parse_mlxtran(file_name)
```

Arguments

file_name

absolute path to mlxtran file

Value

list key/values to initialize ggPMX controller

pk_occ

Creates pmx controller using monlix data having Occasional variable

Description

Creates pmx controller using monlix data having Occasional variable

Usage

```
pk_occ()
```

Value

pmx controller

Examples

```
## Not run:
pk_occ()
## End(Not run)
```

pk_pd 29

pk_pd

Creates pkpd pmx controller using package internal data

Description

Creates pkpd pmx controller using package internal data

Usage

```
pk_pd(code = "3")
```

Arguments

code

can be 3 or 4

plots

Get plots description

Description

Get plots description

Usage

```
plots(ctr)
```

Arguments

ctr

pmxClass controller object

Value

data.frame of plots

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), pmx_update(), set_data(), set_plot()
```

30 plot_pmx

plot_names

Get plot names

Description

Get plot names

Usage

```
plot_names(ctr)
```

Arguments

ctr

pmxClass controller object

Value

list of plot names

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plots(), pmx_update(), set_data(), set_plot()
```

plot_pmx

This is a generic plot method that produces all plots by default described in pmx model evaluation guidance.

Description

This is a generic plot method that produces all plots by default described in pmx model evaluation guidance.

Usage

```
plot_pmx(x, dx, ...)
## S3 method for class 'pmx_vpc'
plot_pmx(x, dx, ...)
```

Arguments

x object to plot

dx data.table, plot source data
... extra argument (not used)

plot_pmx.distrib 31

See Also

```
pmx_gpar.
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual()
```

plot_pmx.distrib

Plot EBE distribution

Description

Plot EBE distribution

Usage

```
## S3 method for class 'distrib'
plot_pmx(x, dx, ...)
```

Arguments

x distribution object

dx data set

... not used for the moment

Value

ggplot2 plot

```
distrib
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

32 plot_pmx.eta_pairs

plot_pmx.eta_cov	This plots an ETA covariance matrix which can be used to define the co-relation between the parameters and its shrinkage
	co-retation between the parameters and its shrinkage

Description

This plots an ETA covariance matrix which can be used to define the co-relation between the parameters and its shrinkage

Usage

```
## S3 method for class 'eta_cov'
plot_pmx(x, dx, ...)
```

Arguments

```
x eta_cov object
dx data set
... not used for the moment
```

Value

```
ggplot2 plot
```

See Also

```
eta_cov
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

```
plot_pmx.eta_pairs
```

Plot random effect correlation plot

Description

Plot random effect correlation plot

Usage

```
## S3 method for class 'eta_pairs'
plot_pmx(x, dx, ...)
```

plot_pmx.individual 33

Arguments

x distribution object

dx data set

... not used for the moment

Value

ggpairs plot

See Also

```
distrib
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

plot_pmx.individual

This function can be used to plot individual prediction and compare with observed data and population prediction for each individual separately

Description

This function can be used to plot individual prediction and compare with observed data and population prediction for each individual separately

Usage

```
## S3 method for class 'individual'
plot_pmx(x, dx, ...)
```

Arguments

x individual object

dx data set

... not used for the moment

Value

a list of ggplot2

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

34 plot_pmx.pmx_gpar

plot_pmx.pmx_dens

This function plots EBE versus covariates using qq plots

Description

This function plots EBE versus covariates using qq plots

Usage

```
## S3 method for class 'pmx_dens'
plot_pmx(x, dx, ...)
```

Arguments

```
x eta_cov objectdx data set... not used for the moment
```

Value

```
ggplot2 plot
```

See Also

```
eta_cov
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

```
plot_pmx.pmx_gpar
```

The ggPMX base plot function

Description

This function should be called internally by other plots to set general settings like, smoothing, add band, labelling, theming,...

Usage

```
## S3 method for class 'pmx_gpar'
plot_pmx(x, dx, ...)
```

plot_pmx.pmx_qq 35

Arguments

x object of pmx_gpar type

dx plot

... ignored parameters

Value

ggplot2 object

See Also

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_qq(), plot_pmx.residual(), plot_pmx()
```

plot_pmx.pmx_qq

This function plot EBE versus covariates using qq plots

Description

This function plot EBE versus covariates using qq plots

Usage

```
## S3 method for class 'pmx_qq'
plot_pmx(x, dx, ...)
```

Arguments

x pmx_qq object

dx data set

... not used for the moment

Value

ggplot2 plot

```
eta_cov
```

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.residual(), plot_pmx()
```

36 plot_shrink

plot_pmx.residual	This function plots residual for each observed value by finding the difference between observed and predicted points. It also fits a distri-
	bution to the residual value.

Description

This function plots residual for each observed value by finding the difference between observed and predicted points. It also fits a distribution to the residual value.

Usage

```
## S3 method for class 'residual'
plot_pmx(x, dx, ...)
```

Arguments

x residual object dx data set

... not used for the moment

Value

ggplot2 object

See Also

residual

```
Other plot_pmx: distrib(), eta_cov(), eta_pairs(), individual(), plot_pmx.distrib(), plot_pmx.eta_cov(), plot_pmx.eta_pairs(), plot_pmx.individual(), plot_pmx.pmx_dens(), plot_pmx.pmx_gpar(), plot_pmx.pmx_qq(), plot_pmx()
```

plot_shrink

Plot shrink in eta matric

Description

Plot shrink in eta matric

Usage

```
plot_shrink(x, shrink.dx, shrink)
```

pmx 37

Arguments

Value

ggplot2 object

pmx

Create a pmx object

Description

Create a pmx object from a data source

```
pmx(
  config,
  sys = "mlx",
  directory,
  input,
  dν,
  dvid,
  cats = NULL,
  conts = NULL,
  occ = NULL,
  strats = NULL,
  settings = NULL,
  endpoint = NULL,
  sim = NULL,
 bloq = NULL,
  id = NULL,
  time = NULL,
  sim_blq = NULL
)
pmx_mlx(
  config,
  directory,
  input,
  dν,
  dvid,
  cats,
  conts,
```

38 pmx

```
occ,
 strats,
 settings,
 endpoint,
  sim,
 bloq,
 id,
  time,
  sim_blq
)
pmx_mlxtran(
  file_name,
 config = "standing",
 call = FALSE,
  endpoint,
 version = -1,
)
```

Arguments

config	Can be either: The complete path for the configuration file, the name of configuration within the built-in list of configurations, or a configuration object.
sys	the system name can "mlx" (for Monolix 2016) or "mlx18" (for Monolix 2018/19 and later)
directory	character modelling output directory.
input	character complete path to the modelling input file
dv	character the name of measurable variable used in the input modelling file
dvid	[Optional] character observation type parameter. This is mandatory in case of multiple endpoint (PKPD).
cats	[Optional]character vector of categorical covariates
conts	[Optional]character vector of continuous covariates
осс	[Optional]character occasional covariate variable name
strats	[Optional]character extra stratification variables
settings	[Optional]pmxSettingsClass pmx_settings shared between all plots
endpoint	<pre>pmxEndpointClass or integer or charcater default to NULL of the endpoint code. pmx_endpoint</pre>
sim	$\label{eq:pmxsimClass} $$ pmxSimClass default to NULL. $pmx_sim used for VPC, e.g.: sim = pmx_sim(file=vpc_file, irun="rep",idv="TIME") $$$
bloq	pmxBLOQClass default to NULL. pmx_bloq specify bloq, within controller: e.g. bloq=pmx_bloq(cens = "BLOQ_name", limit = "LIMIT_name")
id	[Optional] character the name of Indvidual variable used in the input modelling file

pmx 39

time [Optional] character Time variable.

sim_blq logical if TRUE uses sim_blq values for plotting. Only for Monolix 2018 and

later.

file_name character mlxtran file path.

call logical if TRUE the result is the parameters parsed

version integer Non-negative integer. Non-obligatory option, if you don't use a wild-

card in the file_name. Otherwise you MUST provide version and wildcard will be substituted with "version", which represents the mlxtran model version.

... extra arguments passed to pmx_mlx.

Details

pmx_mlx is a wrapper to mlx for the MONOLIX system (sys="mlx")

pmx_mlxtran parses mlxtran file and guess pmx_mlx arguments. In case of multi endpoint the first endpoint is selected. You can though set the endpoint through the same argument. When you set call=TRUE,no controller is created but only the parameters parsed by mlxtran. This can be very helpful, in case you would like to customize parameters (adding settings vi pmx_settings, chnag eth edefault endpoint.)

Value

pmxClass controller object.

Examples

```
## Example to create the controller using theophylline data
theophylline <- file.path(system.file(package = "ggPMX"), "testdata",
                           "theophylline")
WORK_DIR <- file.path(theophylline, "Monolix")</pre>
input_file <- file.path(theophylline, "data_pk.csv")</pre>
## using only mandatory variables
ctr <- pmx(
 sys="mlx",
 config = "standing",
 directory = WORK_DIR,
 input = input_file,
 dv = "Y",
 dvid ="DVID"
## Using covariates
ctr <- pmx(
 sys="mlx",
 config = "standing",
 directory = WORK_DIR,
 input = input_file,
 dv = "Y",
```

40 pmxOptions

```
dvid ="DVID",
 cats=c("SEX"),
 conts=c("WT0","AGE0"),
 strats="STUD"
)
## using settings parameter
ctr <- pmx(
 sys="mlx",
 config = "standing",
 directory = WORK_DIR,
 input = input_file,
 dv = "Y",
 dvid ="DVID",
 settings=list(is.draft=FALSE)
)
## using mlxtran file
mlxtran_file <-
 file.path(system.file(package = "ggPMX"),
    "testdata", "1_popPK_model", "project.mlxtran")
pmx_mlxtran(mlxtran_file)
## mlxtran , call =TRUE to get the pmx_mlx argument parsed by pmx_mlxtran
params <- pmx_mlxtran(mlxtran_file,call=TRUE)</pre>
str(params)
# $ directory: chr results_pathile
# $ input : chr observation file path
          : chr "DV"
# $ cats : chr [1:4] "SEX" "RACE" "DISE" "ILOW"
# $ conts : chr [1:4] "AGE0" "WT0" "HT0" "TRT"
# $ occ : chr "ISS"
# $ dvid : chr "YTYPE"
# $ endpoint :List of 5
# ..$ code : chr "1"
# ..$ label : chr ""
# ..$ unit : chr ""
# ..$ file.code: chr "1"
# ..$ trans : NULL
# ..- attr(*, "class")= chr "pmxEndpointClass"
# $ config : chr "standing"
```

pmxOptions

This function can be used to set ggPMX options

Description

getPmxOption retrieves the value of a ggPMX option. ggPMXOptions sets the value of ggPMX options; it can also be used to return a list of all currently-set ggPMX options.

pmx_bloq 41

Usage

```
pmxOptions(...)
```

Arguments

... Options to set, with the form name = value.

Details

There is a global option set, which is available by default.

Options used in ggPMX

• template_dir: path to template directory

Examples

```
## Not run:
pmxOptions(template_dir = PATH_TO_CUSTOM_CONFIGURATION)
## End(Not run)
```

pmx_bloq

Creates BLOQ object attributes

Description

Creates BLOQ object attributes

```
pmx_bloq(
  cens = "CENS",
  limit = "LIMIT",
  colour = "pink",
  size = 2,
  linewidth = 1,
  alpha = 0.9,
  show = TRUE,
  ...
)
```

42 pmx_comp_shrink

Arguments

cens character the censoring column name
limit character the limit column name (optional)

colour character the color of the geom
size numeric the size of the geom when using geom_point()
linewidth numeric the line width of the segment when using geom_segment()
alpha numeric the alpha of the geom
show logical if FALSE remove all censory observations

Details

. . .

To define that a measurement is censored, the observation data set should include a CENSORING column (default to 'CENS') and put 1 for lower limit or -1 for upper limit.

Optionally, data set can contain have a limit column (default to 'LIMIT') column to set the other limit.

pmx_comp_shrink

Compute Shrinkage

any other graphical parameter

Description

Compute Shrinkage

Usage

```
pmx_comp_shrink(
   ctr,
   fun = c("var", "sd"),
   strat.facet,
   strat.color,
   filter,
   ...
)
```

Arguments

ctr pmxClass controller object

fun character can be sd or var, var by default

strat.facet formula optional stratification parameter

strat.color character optional stratification parameter

filter optional filter which will be applied to plotting data

. . . others parameters not used for the moment

pmx_config 43

Value

```
data.table
```

pmx_config	This function can be used to define the pmx configuration used in plots.
	e.g. Monolix/Nonmem

Description

This function can be used to define the pmx configuration used in plots. e.g. Monolix/Nonmem

Usage

```
pmx_config(sys = "mlx", inputs, plots, ...)
```

Arguments

```
sys charcarter system used , monolix,nonmem,...

inputs charcater path to the inputs settings file (yaml format)

charcater path to the inputs settings file (yaml format)

extra arguments not used
```

Details

To create a controller user can create a pmxConfig object using

- either an input template file
- or a plot template file
- or both.

By default the 'standing' configuration will be used.

Value

```
pmxConfig object
```

Examples

44 pmx_copy

```
# create a controller with a custom plots template
ctr <- pmx_mlx(
  config = pmx_config(
   plots=file.path( system.file(package = "ggPMX"), "examples/plots.yaml"),
   inputs = system.file(package = "ggPMX", "examples/custom_inputs.yaml")
  ),
  directory = WORK_DIR,
  input = input_file,
  dv = "Y",
  dvid = "DVID",
  cats = c("SEX"),
  conts = c("WT0", "AGE0"),
  strats = "STUD"
## get the list of plots
ctr %>% plots
ctr %>% get_plot("custom_res_time")
ctr %>% get_plot("custom_npde_time")
```

pmx_copy

Creates a deep copy of the controller

Description

Creates a deep copy of the controller

Usage

```
pmx_copy(ctr, keep_globals = FALSE, ...)
```

Arguments

ctr pmxClass object
keep_globals logical if TRUE we keep the global parameters changed by pmx_settings
... extra parameters passed to pmx_settings

Details

The controller is an 'R6' object, it behaves like a reference object. Some functions (methods) can have a side effect on the controller and modify it internally. Technically speaking we talk about chaining not piping here. However, using pmx_copy user can work on a copy of the controller.

By default the copy does not keep global parameters set using pmx_settings.

Value

an object of pmxClass

pmx_cov 45

Examples

```
ctr <- theophylline()
cctr <- ctr %>% pmx_copy()
## Any change in the ctr has no side effect in the ctr and vice versa
```

pmx_cov

Select/Map covariates using human labels

Description

Select/Map covariates using human labels

Usage

```
pmx_cov(values, labels = NULL)
```

Arguments

values list of covariates to use to create the plot

labels list of covariates facets labels

Details

In case of 'pmx_plot_eta_cats' and 'pmx_plot_eta_conts' you can customize the covariates and covaraites labels using 'pmx_cov'.

Value

pmxCOVObject object

 ${\tt pmx_dens}$

Creates a density plot object

Description

Creates a density plot object

pmx_dens

Usage

```
pmx_dens(
    x,
    labels,
    dname = NULL,
    xlim = 3,
    var_line = NULL,
    snd_line = NULL,
    vline = NULL,
    is.legend = TRUE,
    ...
)
```

Arguments

X	character variable name to sample
labels	list of texts/titles used within the plot
dname	name of dataset to be used
xlim	numeric x axis limits
var_line	list variable density graphics parameters
snd_line	list normal density graphics parameters
vline	list vertical line graphics parameters
is.legend	logical whether to add a legend (defaults TRUE)
	others graphics arguments passed to pmx_gpar internal object.

Details

labels is a list that contains:

- title: plot title default "IWRES density plot"
- x: x axis label default to "Etas"
- y: y axis label default to empty

var_line is a list that contains:

linetype: default to 1color: default to blacklinewidth: default to 1

snd_line is a list that contains:

linetype: default to 2
color: default to black
linewidth: default to 1

vline is a list that contains:

pmx_endpoint 47

linetype: default to 3color: default to blacklinewidth: default to 1

pmx_endpoint Creates pmx endpoint object

Description

Creates pmx endpoint object

Usage

```
pmx_endpoint(code, label = "", unit = "", file.code = code, trans = NULL)
```

Arguments

code character endpoint code: used to filter observations DVID==code.

label character endpoint label: used to set title and axis labels

unit character endpoint unit: used to set title and axis labels

file.code character endpoint file code: used to set predictions and finegrid files extensions in case using code parameter is not enough.

trans list Transformation parameter not used yet.

Details

In case of multiple endpoints, pkpd case for example, we need to pass endpoint to the pmx call. Internally, ggPMX will filter the observations data set to keep only rows satisfying DVID==code. The code is also used to find the right predictions and or fingrid files. ggPMX use the configuration file to fine the path of the predictions file (like the single endpoint case) and then filter the right file using the code parameter.

For example:

- predictions{code}.txt for mlx16
- predictions{code}.txt and y{code}_residual for mlx18

For some tricky examples the code parameter is not enough to find the files. In that case the file.code parameter is used to distinguish the endpoint files.

48 pmx_filter

Examples

```
## Use file.code parameter
pk_pd_path <- file.path(system.file(package = "ggPMX"), "testdata","pk_pd")</pre>
WORK_DIR <- file.path(pk_pd_path, "RESULTS")</pre>
ep <- pmx_endpoint(</pre>
  code="4",
  file.code="2"
input_file <- file.path(pk_pd_path, "pk_pd.csv")</pre>
ctr <- pmx_mlx(</pre>
  config = "standing",
  directory = WORK_DIR,
  input = input_file,
  dv = "dv",
  dvid = "dvid",
  cats = "sex",
  conts = "wt",
  endpoint = ep
 )
## using mlxtran
ep <- pmx_endpoint(</pre>
  code="3",
 file.code="1"
)
mlxtran_file <- file.path(pk_pd_path, "pk_pd.mlxtran")</pre>
ctr <- pmx_mlxtran(mlxtran_file,endpoint=ep)</pre>
```

pmx_filter

filter data in a pmx controller

Description

filter data in a pmx controller

```
pmx_filter(
  ctr,
  data_set = c("estimates", "predictions", "eta", "finegrid", "shrink", "input",
        "individual", "sim_blq"),
```

pmx_get_configs 49

```
pmx_exp
)
```

Arguments

ctr A controller. An object of 'pmxClass'

data_set A data_set within the controller to apply a filter to.

pmx_exp A filter expression

Value

Returns a pmx controller with a filtered data set.

Examples

```
## example of global filter
ctr <- theophylline()
ctr %>% pmx_filter(data_set = "prediction", ID == 5 & TIME < 2)
ctr %>% get_data("prediction")
```

pmx_get_configs

Get List of built-in configurations

Description

Get List of built-in configurations

Usage

```
pmx_get_configs(sys = "mlx")
```

Arguments

sys

can be mlx, by default all configurations will be listed

Value

names of the config

Examples

```
pmx_get_configs()
```

50 pmx_gpar

pmx_gpar

Handling pmx Graphical parameters

Description

Handling pmx Graphical parameters

Usage

```
pmx_gpar(
  is.title,
  labels,
  axis.title,
 which_pages,
  print,
  axis.text,
  ranges,
  is.smooth,
  smooth,
  is.band,
 band,
  is.draft,
  draft,
  discrete,
  is.identity_line,
  identity_line,
  smooth_with_bloq,
  scale_x_log10,
  scale_y_log10,
  color.scales,
  is.legend,
  {\tt legend.position}
)
```

Arguments

is.title	logical if TRUE then a title is used for the plot
labels	list of labels, like title, subtitle, x, y
axis.title	list or element_text (same as ggplot2 axis.title theme)
which_pages	page(s) to display; if "all" display all pages, if 1 display first page, if $c(1,2)$ display first and second pages
print	if TRUE the ouptut will be a print not a ggplot2. This is useful for rmarkdwon output to avoid verbose list index print.
axis.text	list or element_text (same as ggplot2 axis.text theme)
ranges	limits of x/y ranges

pmx_list_nm_tables 51

is. smooth logical if set to TRUE add smooth layer

smooth smooth layer parameters

is.band logical if TRUE add horizontal band

band horizontal band parameters
is.draft logical if TRUE add draft layer

draft draft layer parameters

discrete logical if TRUE x axis is discrete(FALSE by default)

is.identity_line

logical if TRUE add y=x line

identity_line list y=x aes properties

smooth_with_bloq

logical if TRUE perform spline in plots with BLOQ data

scale_x_log10 logical if TRUE add scale_x_log10 layer scale_y_log10 logical if TRUE add scale_y_log10 layer

color.scales list define scales parameter in case of strat.color pmx_settings

is.legend logical if TRUE x axis is discrete(FALSE by default)

legend.position

charcater legend position it takes the same value as the equivalent ggplot2

parameter

Details

This object contains all general graphic settings. It used internally by all pmx_plot(generic function) to set the default behavior.

Value

An object of class "pmx_gpar".

Description

List NONMEM output tables file names from a nm_model object.

Usage

```
pmx_list_nm_tables(nm_model = NULL)
```

Arguments

nm_model An nm_model object generated with pmx_read_nm_model.

See Also

```
pmx_read_nm_model, pmx_read_nm_tables
```

Examples

```
## Not run:
pmx_read_nm_model(file = 'run001.lst') %>%
   pmx_list_nm_tables()
## End(Not run)
```

Description

Manually provide names of the table files to be imported.

Usage

Arguments

tab_names	Provide the name of the tables to import e.g. 'sdtab', 'patab', 'cotab', 'catab' for NONMEM.
tab_suffix	Default is ", but can be changed to any character string to be used as suffix in the table names.
sim_suffix	Default is 'sim', but can be changed to any character string to be used as suffix in the simulation table names e.g. sdtab001sim.

pmx_nlmixr 53

pmx_nlmixr	Creates pmx controller from an nlimxr fit object	

Description

Creates pmx controller from an nlimxr fit object

Usage

```
pmx_nlmixr(fit, dvid, conts, cats, strats, endpoint, settings, vpc = FALSE)
```

Arguments

fit	nlmixr object
dvid	[Optional] character observation type parameter.
conts	[Optional]character vector of continuous covariates
cats	[Optional]character vector of categorical covariates
strats	[Optional]character extra stratification variables
endpoint	${\sf pmxEndpointClass}$ or integer or charcater defalut to NULL of the endpoint code. ${\sf pmx_endpoint}$
settings	[Optional]pmxSettingsClass pmx_settings
vpc	[Optional] logical a boolean indiacting if vpc should be calculated (by default TRUE)

Value

pmxClass controller object.

pmx_nm	Creates pmx controller from NONMEM model outputs

Description

Creates pmx controller from NONMEM model outputs

54 pmx_nm

Usage

```
pmx_nm(
  file = NULL,
  directory = ".",
  runno = NULL,
  ext = ".lst",
  table_suffix = "",
  sim_suffix = "sim",
  simfile = NULL,
  prefix = "run",
 table_names = c("sdtab", "mutab", "patab", "catab", "cotab", "mytab", "extra", "xptab",
    "cwtab"),
 dvid = "DVID",
 pred = "PRED",
  time = "TIME",
  dv = "DV",
  conts,
  cats,
  npde,
  iwres,
  ipred,
  endpoint,
  strats = "",
  settings = pmx_settings(),
  vpc = TRUE,
  bloq = NULL,
 obs = FALSE,
  quiet = FALSE
)
```

Arguments

and ext.

file	A character vector of path to the files or a nm_table_list object created with pmx_list_nm_tables.
directory	directory of the model files.
runno	run number which is used for generating the model file name, or used for alternative import of NONMEM-output tables.
ext	Extension to be used to generate model file name. Should be one of '.lst' (default), '.out', '.res', '.mod' or '.ctl' for NONMEM.
table_suffix	suffix of the output tables, standard is "" (no suffix).
sim_suffix	suffix of the simulation output tables, standard is "sim" (e.g. stdab1sim).
simfile	Useful if the simulation is performed post-hoc and an additional simulation model file is generated e.g. "simulation.lst"; similar to "file" see above.
prefix	Prefix to be used to generate model file name. Used in combination with runno

pmx_nm 55

table_names	contains the names of the NONMEM-output tables e.g. "sdtab", "patab", "cotab", "catab".
dvid	[Optional] character observation type parameter, mandatory in case of multiple endpoint (PKPD). Standard = "DVID"
pred	$[Optional] \ character\ specifing\ variable\ name\ of\ the\ population\ prediction\ (standard\ ggPMX\ nomenclautre="PRED")$
time	$[Optional] \ character\ specifing\ variable\ name\ of\ time\ (standard\ ggPMX\ nomenclautre="TIME")$
dv	character the name of measurable variable used in the input modelling file (standard ggPMX nomenclautre = "DV")
conts	[Optional] character vector of continuous covariates (automatically detected if "cotab" is provided)
cats	[Optional] character vector of categorical covariates (automatically detected if "catab" is provided)
npde	[Optional] character specifing variable name of the normalized population predictor (standard ggPMX nomenclautre = "NPDE")
iwres	[Optional] character specifing variable name of the individual weighted residuals (standard ggPMX nomenclautre = "IWRES")
ipred	[Optional] character specifing variable name of the individual population prediction (standard ggPMX nomenclautre = "IPRED")
endpoint	$[Optional] \ {\tt pmxEndpointClass}$ or integer or charcater default to NULL of the endpoint code. ${\tt pmx_endpoint}$
strats	[Optional] character extra stratification variables
settings	pmxSettingsClass pmx_settings shared between all plots
vpc	logical a boolean indiacting if vpc should be calculated, simulation tables are required for VPC generation (by default TRUE)
bloq	pmxBLOQClass default to NULL. pmx_bloq specify bloq, within controller: e.g. bloq=pmx_bloq(cens = "BLOQ_name", limit = "LIMIT_name")
obs	logical if set to TRUE will filter dataset according to "MDV", default is FALSE
quiet	Logical, if FALSE messages are printed to the console.

Value

pmxClass controller object.

Author(s)

The ggPMX NONMEM reader (pmx_nm) is strongly based on NONMEM reading functions of the xpose package (v.0.4.11) (Thanks to Benjamin Guiastrennec) To avoid conflicts with the xpose package, the necessary xpose-based functions have been renamed with a "pmx_" prefix. If the user wants to use individual functions e.g. "read_nm_tables" please use the xpose-package

56 pmx_plot

Examples

```
## using only runnumber
# ctr <- pmx_nm(</pre>
# directory=model_dir,
# runno = "001"
## using a model file (e.g. run001.lst)
#ctr <- pmx_nm(</pre>
# directory=model_dir,
# file = "run001.lst"
#)
## if simulation was performed post-hoc, an additional simulation file can be loaded for VPC
#ctr <- pmx_nm(</pre>
# directory=model_dir,
# file = "run001.lst",
# simfile = "simulation.ctl"
## loading with individual table(s)-names
#ctr <- pmx_nm(directory = model_dir,</pre>
               runno = 3,
#
               table_names = "xptab")
#
```

pmx_plot

Generic pmx plot

Description

Generic pmx plot

Usage

```
pmx_plot(ctr, pname, ...)
```

Arguments

ctr pmxClass pmx controller
pname plot name
... others graphics parameters passed:

- pmx_gpar internal function to customize shared graphical parameters
- pmx_qq quantile-quantile plot object
- pmx_update function.

pmx_plot_cats 57

pmx_plot_cats

Generic pmx stratified plot

Description

Generic pmx stratified plot

Usage

```
pmx_plot_cats(ctr, pname, cats, chunk = "", print = TRUE, ...)
```

Arguments

```
ctr pmxClass pmx controller

pname plot name

cats list of categorical variables. By default all of them

chunk chunk name

print logical if TRUE print plots otherwise the list of plots is returned

others graphics parameters passed:

• pmx_gpar internal function to customize shared graphical parameters

• pmx_qq quantile-quantile plot object
```

• pmx_update function.

Description

Eta matrix plot

```
pmx_plot_eta_matrix(
   ctr,
   title,
   dname,
   type.eta,
   text_color,
   is.shrink,
   shrink,
   point,
   is.smooth,
   smooth,
```

58 pmx_plot_eta_matrix

```
is.hline,
 hline,
  is.vreference_line,
  vreference_line,
  filter,
  strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.band,
  band,
  is.draft,
  draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales,
)
```

Arguments

```
ctr
                 pmx controller
title
                 character the plot title
dname
                 name of dataset to be used
                 character type of eat can be 'mode' or 'mean'.'mode' by default
type.eta
text_color
                 color of the correlation text in the upper matrix
is.shrink
                 logical if TRUE add shrinkage to the plot
                 pmxShrinkClass shrinkage graphical parameter or list coercible into one
shrink
point
                 list geom_point graphical parameter
is.smooth
                 logical if TRUE add smoothing to lower matrix plots
smooth
                 list geom_smooth graphical parameters
is.hline
                 logical if TRUE add horizontal line to lower matrix plots
hline
                 list geom_hline graphical parameters
is.vreference_line
                 logical if TRUE add reference line to diag plots
vreference_line
                 list geom_vline graphical parameters
                 pmx_update parameters
```

pmx_plot_eta_matrix 59

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet_wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom_text graphical parameters.

is.identity_line

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters. scale_x_log10 logical if TRUE use log10 scale for x axis.

scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

... others graphics parameters passed :

• pmx_gpar internal function to customize shared graphical parameters

• eta_pairs ggPMX internal function for eta matrix plot.

• pmx_update function.

eta_pairs parameters

Value

ggplot2 object

Examples

```
# basic use ------
ctr <- theophylline()
```

```
p <- ctr %>% pmx_plot_eta_matrix
# update graphical parameter ------
## update labels
ctr %>% pmx_plot_eta_matrix(
 labels = list(title = "Eta matrix new title")
## remove draft
ctr %>% pmx_plot_eta_matrix(is.draft = FALSE)
## change text color line
ctr %>% pmx_plot_eta_matrix(
 text_color="red",
 shrink=pmx_shrink(mapping=aes(color="magenta"))
 )
## custom point aes and static parameters
## we can customize any geom_point parameter
ctr %>% pmx_plot_eta_matrix(
 point = list(color = "blue", shape = 4)
# stratification ------
## IGNORE continuous stratification
ctr %>% pmx_plot_eta_matrix(strat.color = "WT0")
## IGNORE categorical stratification
ctr %>% pmx_plot_eta_matrix(strat.facet = ~SEX)
# subsetting -----
## we can use any expression involving the data
ctr %>% pmx_plot_eta_matrix(filter = EFFECT%in% c("Cl","ka"))
```

Description

Individual plot

```
pmx_plot_individual(
  ctr,
```

```
which_pages = 1L,
 print = FALSE,
  dname,
  pred_line,
  ipred_line,
  point,
  is.legend,
  use.finegrid,
 bloq,
 filter,
 strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.smooth,
  smooth,
  is.band,
 band,
  is.draft,
 draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales,
)
```

Arguments

ctr	pmx controller
which_pages	integer page(s) to display, or character "all" to display all pages (argument previously called npage, now deprecated)
print	logical if TRUE the ouptut will be a print not a ggplot2. This is useful for rmarkdwon output to avoid verbose list index print.
dname	character name of dataset to be used. User can create his own dataset using set_data and pass it as dname to be plotted.
pred_line	list some ipred line geom properties aesthetics
ipred_line	list some pred line geom properties aesthetics
point	list some point geom properties aesthetics
is.legend	logical if TRUE add a legend

use.finegrid logical if FALSE use predictions data set bloq pmxBLOQ object created by pmx_bloq.

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet_wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx_gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x , y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.smooth logical if set to TRUE add smooth layer

smooth list geom_smooth graphical/smoothing fun parameters

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom_text graphical parameters.

is.identity_line

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters.

scale_x_log10 logical if TRUE use log10 scale for x axis.

scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

... others graphics parameters passed :

• pmx_gpar internal function to customize shared graphical parameters

• individual generic object for individual plots.

• pmx_update function.

individual parameters

Value

ggplot2 or list of ggplot2 objects

Examples

```
# basic use ------
ctr <- theophylline()</pre>
ctr %>% pmx_plot_individual(which_pages = 1)
## multiple pages
ctr %>% pmx_plot_individual(which_pages = c(1, 3))
## change faceting
ctr %>% pmx_plot_individual(facets = list(nrow = 5, ncol = 5), which_pages = 2)
# update graphical parameter ------
## update labels
ctr %>% pmx_plot_individual(
 labels = list(title = "Custom individual plot")
## remove draft
ctr %>% pmx_plot_individual(is.draft = FALSE)
## Customize ipred_line with any geom_line parameter
ctr %>% pmx_plot_individual(
 pred_line = list(color = "red", linetype = 20, alpha = 0.5)
)
## Customize ipred_line with any geom_line parameter
ctr %>% pmx_plot_individual(
 ipred_line = list(size = 5)
)
## Customize any geom_point parameter
ctr %>% pmx_plot_individual(
 point = list(aes(alpha = DV), color = "green", shape = 4)
## legend
p <- ctr %>% pmx_plot_individual(
 is.legend=TRUE,
 point=list(shape=20),
 pred_line=list(linetype=6)
)
# # stratification -----
# ## continuous stratification
ctr %>% pmx_plot_individual(strat.color = "WT0")
# # subsetting -----
```

```
# ## we can use any expression involving the data
# ## filter and stratify
ctr %>% pmx_plot_individual(
 filter = SEX == 1, strat.facet = ~SEX,
 facets = list(nrow = 5, ncol = 5))
# # transformation -----
# ## apply a log transformation in y
ctr %>% pmx_plot_individual(trans = "log10_y")
\# ## apply a custonm trsnformation to normalize axis between 0 and 1
## get a list of parameter
p <- ctr %>% pmx_plot_individual(
 which_pages="all",
 point=list(shape=4,color='blue',size=10),
 facets = list(nrow = 5, ncol = 5),
 labels = list(title = "My individuals",x='my time',y='PD data')
)
```

Description

IWRES density plot

```
pmx_plot_iwres_dens(
  ctr,
  sim_blq,
  dname,
  xlim,
  var_line,
  snd_line,
  vline,
  filter,
  strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
```

pmx_plot_iwres_dens 65

```
ranges,
is.smooth,
smooth,
is.band,
band,
is.draft,
draft,
is.identity_line,
identity_line,
scale_x_log10,
scale_y_log10,
color.scales,
...
)
```

Arguments

ctr pmx controller

sim_blq logical if TRUE uses sim_blq as dataset for plotting instead of predictions.

dname character name of dataset to be used. User can create his own dataset using

set_data and pass it as dname to be plotted.

xlim numeric x axis limits

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet_wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx_gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.smooth logical if set to TRUE add smooth layer

smooth list geom_smooth graphical/smoothing fun parameters

```
is.band
                  logical if TRUE add horizontal band
                  list horizontal band parameters. geom_hline graphical parameters.
band
is.draft
                  logical if TRUE add draft layer
draft
                 list draft layer parameters. geom_text graphical parameters.
is.identity_line
                  logical if TRUE add an identity line
identity_line
                 listgeom_abline graphical parameters.
scale_x_log10
                 logical if TRUE use log10 scale for x axis.
scale_y_log10
                 logical if TRUE use log10 scale for y axis.
color.scales
                  list define scales parameter in case of strat.color pmx_settings
                  others graphics parameters passed:
. . .
                    • pmx_gpar internal function to customize shared graphical parameters
                    • pmx_dens pmx density object.
                    • pmx_update function.
```

pmx_dens parameters

Value

ggplot2 or list of ggplot2 objects

pmx_plot_vpc

VPC plot

Description

VPC plot

```
pmx_plot_vpc(
   ctr,
   type,
   idv,
   obs,
   pi,
   ci,
   rug,
   bin,
   is.legend,
   sim_blq,
   dname,
   filter,
   strat.facet,
   facets,
```

```
strat.color,
  trans,
 pmxgpar,
 labels,
  axis.title,
 axis.text,
 ranges,
  is.smooth,
  smooth,
 is.band,
 band,
  is.draft,
 draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
 color.scales,
  is.footnote,
)
```

Arguments

ctr	pmx controller
type	charcater can be either percentile or scatter
idv	chracater individual variable
obs	pmx_vpc_obs object observation layer pmx_vpc_obs
pi	pmx_vpc_pi object percentile layer pmx_vpc_pi
ci	pmx_vpc_ci object confidence interval layer pmx_vpc_ci
rug	pmx_vpc_rug object rug layer pmx_vpc_rug. Note: consider not using a rug layer when bin[["within_strat"]]=TRUE, since the rugs plotted will not reflect the bins.
bin	pmx_vpc_bin object pmx_vpc_bin specify within pmx_plot_vpc() e.g.: bin = pmx_vpc_bin(style = "kmeans", n = 10)
is.legend	logical if TRUE add legend
sim_blq	logical if TRUE uses sim_blq values for plotting. Only for Monolix 2018 and later.
dname	added for compatibility with other ggPMX plots
	pmx_update parameters
filter	expression filter which will be applied to plotting data.
strat.facet	formula optional stratification parameter by facetting. This split plot by strats(each strat in a facet)
facets	list facet_wrap parameters.

character optional stratification parameter by grouping. This will split the plot strat.color by group (color) of strat. character define the transformation to apply on x or y or both variables trans a object of class pmx_gpar possibly the output of the pmxgpar pmx_gpar: Shared basic graphics parameters labels list list containing plot and/or axis labels: title, subtitle, x, y axis.title list containing element_text attributes to customize the axis title. (similar to ggplot2 axis.title theme) axis.text list containing element_text attributes to customize the axis text (similar to ggplot2 axis.text theme) list limits of x/y ranges ranges logical if set to TRUE add smooth layer is.smooth smooth list geom_smooth graphical/smoothing fun parameters is.band logical if TRUE add horizontal band band list horizontal band parameters. geom_hline graphical parameters. is.draft logical if TRUE add draft layer draft list draft layer parameters. geom_text graphical parameters. is.identity_line logical if TRUE add an identity line listgeom_abline graphical parameters. identity_line logical if TRUE use log10 scale for x axis. scale_x_log10 scale_y_log10 logical if TRUE use log10 scale for y axis. color.scales list define scales parameter in case of strat.color pmx_settings is.footnote logical if TRUE add footnote

- pmx_gpar internal function to customize shared graphical parameters
- pmx_vpc pmx vpc object.

others graphics parameters passed:

• pmx_update function.

pmx_vpc parameters

Details

You can use pmx_vpc_bin to set the bin parameters. In case of stratification, binning can be different for each strat level (case within_strat equal to FALSE).

Value

ggplot2 or list of ggplot2 objects

See Also

```
Other vpc: pmx_vpc_bin(), pmx_vpc_ci(), pmx_vpc_obs(), pmx_vpc_pi(), pmx_vpc_rug(), pmx_vpc()
```

Examples

```
library(ggPMX)
theo_path <- file.path(</pre>
  system.file(package = "ggPMX"), "testdata",
  "theophylline"
WORK_DIR <- file.path(theo_path, "Monolix")</pre>
input_file <- file.path(theo_path, "data_pk.csv")</pre>
vpc_file <- file.path(theo_path, "sim.csv")</pre>
ctr <- pmx_mlx(</pre>
  config = "standing",
  directory = WORK_DIR,
  input = input_file,
  dv = "Y",
  dvid = "dvid",
  cats = c("SEX"),
  conts = c("WT0", "AGE0"),
  strats = "STUD",
  settings = pmx_settings(
    use.labels=TRUE,
    cats.labels=list(
      SEX=c("0"="Male","1"="Female")
    )
  ),
  sim = pmx_sim(
    file = vpc_file,
    irun ="rep",
    idv="TIME"
)
ctr %>% pmx_plot_vpc(
  strat.facet=~SEX,
  facets=list(nrow=2),
  type="percentile",
  is.draft = FALSE,
  pi = pmx_vpc_pi(interval = c(0.1, 0.9),
              median=list(color="green"),
              extreme= list(color="green")),
  obs = pmx_vpc_obs(color="blue", shape=18, size=2),
  ci = pmx\_vpc\_ci(interval = c(0.1, 0.9),
              median=list(fill="pink")),
  bin=pmx_vpc_bin("kmeans", n=5)
)
ctr %>%
  pmx_plot_vpc(bin= pmx_vpc_bin(
     style = "fixed",
```

70 pmx_qq

```
fixedBreaks=c(-10,2, 5, 10,15,50))
)

# example with legend

ctr %>% pmx_plot_vpc(
   is.legend = TRUE,
   pi = pmx_vpc_pi(interval=c(0.02,0.98),median = list(linetype="dotted")),
   ci = pmx_vpc_ci(interval = c(0.05,0.95),median=list(fill="red"))
)
```

pmx_qq

This function creates a qq plot object

Description

This function creates a qq plot object

Usage

```
pmx_qq(
  х,
  labels,
 dname = NULL,
 point = NULL,
 xmax = TRUE,
  facets = NULL,
  is.reference_line = NULL,
  reference_line = NULL,
  is.shrink = NULL,
  shrink = NULL,
  is.hline = NULL,
 hline = NULL,
  is.vline = NULL,
  vline = NULL,
)
```

Arguments

x	character variable name to sample
labels	list of texts/titles used within the plot
dname	name of dataset to be used
point	list geom_point attributes color, shape,
xmax	logical if FALSE do not use max(aes(x)) as limits default to TRUE

pmx_qq_plot 71

facets list
is.reference_line

logical if TRUE add reference line to the plot

reference_line list geom_line attributes. Used only for pmx_plot_eta_qq

is.shrink logical if TRUE add shrinkage to the plot

shrink pmxShrinkClass shrinkage graphical parameter or list coercible into one

is.hline logical if TRUE add horizontal line y=0 (TRUE by default)

hline geom hline graphical parameters

is.vline logical if TRUE add vertical line x=0 (TRUE by default)

vline geom vline graphical parameters

... others graphics arguments passed to pmx_gpar internal object.

Details

labels is a list that contains:

• title: plot title default "EBE vs. covariates"

• x: x axis label default to "Etas"

• y: y axis label default to empty

point is a list that contains:

• shape: default to 1

• color: default to black

• size: default to 1

Value

pmx_qq object

pmx_qq_plot

Quantile-quantile plots

Description

Quantile-quantile plots

Quantile-quantile plot of IWRES

Quantile-quantile plot of eta variables

Quantile-quantile plot of NPDE

Quantile-quantile plot of NPD

Quantile-quantile plot of CWRES

72 pmx_qq_plot

```
pmx_qq_plot(
  dname,
  point,
  is.reference_line,
  reference_line,
  is.shrink,
  shrink,
  is.hline,
 hline,
  is.vline,
 vline,
  filter,
  strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.smooth,
  smooth,
  is.band,
 band,
  is.draft,
  draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales,
)
pmx_plot_iwres_qq(ctr, ...)
pmx_plot_eta_qq(ctr, ...)
pmx_plot_npde_qq(ctr, ...)
pmx_plot_npd_qq(ctr, ...)
pmx_plot_cwres_qq(ctr, ...)
```

pmx_qq_plot 73

Arguments

dname name of dataset to be used point list geom_point parameters.

is.reference_line

logical if TRUE add reference line to the plot

reference_line list geom_abline parameters.

is. shrink logical if TRUE add shrinkage to the plot

shrink pmxShrinkClass shrinkage graphical parameter or list coercible into one

is.hline logical if TRUE add horizontal line y=0 (TRUE by default)

hline list geom hline graphical parameters

is.vline logical if TRUE add vertical line x=0 (TRUE by default)

vline list geom vline graphical parameters

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet_wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar an object of class pmx_gpar

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is. smooth logical if set to TRUE add smooth layer

smooth list geom_smooth graphical/smoothing fun parameters

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom_text graphical parameters.

is.identity_line

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters. scale_x_log10 logical if TRUE use log10 scale for x axis.

scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

74 pmx_read_nm_files

... others graphics parameters passed :

- pmx_gpar internal function to customize shared graphical parameters
- pmx_qq quantile-quantile plot object.
- pmx_update function.

pmx_qq parameters

ctr pmx controller

Value

ggplot2 object

Examples

```
# ******** basic use ********* -----
ctr <- theophylline()</pre>
ctr %>% pmx_plot_eta_qq
ctr %>% pmx_plot_npde_qq
ctr %>% pmx_plot_iwres_qq
# update graphical parameter ------
## add reference line
ctr %>% pmx_plot_npde_qq(reference_line=list(color="blue"))
## remove reference line
ctr %>% pmx_plot_eta_qq(reference_line=NULL)
# stratification ------
## categorical stratification color parameter
ctr %>% pmx_plot_iwres_qq(strat.facet=~STUD,strat.color="SEX")
## categorical stratification facetting
ctr %>% pmx_plot_eta_qq(strat.facet = ~SEX)
## do not use symmetric axis
ctr %>% pmx_plot_npde_qq(xmax=FALSE,reference_line=list())
```

pmx_read_nm_files

NONMEM output file import function

Description

Quickly import NONMEM output files into R.

pmx_read_nm_model 75

Usage

```
pmx_read_nm_files(
  runno = NULL,
  prefix = "run",
  ext = c(".ext", ".cor", ".cov", ".phi", ".grd", ".shk"),
  file = NULL,
  dir = NULL,
  quiet = FALSE
)
```

Arguments

runno	Run number to be evaluated.
prefix	Prefix of the model file names.
ext	A vector of the file extension to import. By default '.ext', '.cor', '.cov', '.phi', '.grd', '.shk' files are listed.
file	Names of the model output file to be imported. Alternative argument to prefix, runno and ext.
dir	Location of the model files.
quiet	Logical, if FALSE messages are printed to the console.

Examples

```
## Not run:
# Using the `file` argument to import a model file:
ext_file <- pmx_read_nm_files(file = 'run001.ext', dir = 'models')

# Using the `runno` argument to import a model file:
ext_file <- pmx_read_nm_files(runno = '001', ext = '.ext', dir = 'models')

## End(Not run)</pre>
```

pmx_read_nm_model

NONMEM model file parser

Description

Parse NONMEM model files in R format

Usage

```
pmx_read_nm_model(
  runno = NULL,
  prefix = "run",
  ext = ".lst",
  file = NULL,
  dir = NULL
)
```

pmx_read_nm_model

Arguments

runno	run number which is used for generating the model file name
prefix	Prefix to be used to generate model file name. Used in combination with runno and ext.
ext	Extension to be used to generate model file name. Should be one of '.lst' (default), '.out', '.res', '.mod' or '.ctl' for NONMEM.
file	A character vector of path to the files or a nm_table_list object created with $list_nm_tables$.
dir	directory of the model files.

Value

A tibble of class model containing the following columns:

- problem: a numeric identifier for the \$PROBLEM associated with the code.
- level: a unique numeric identifier to each subroutine block associated with the code.
- **subroutine**: a character identifier named after the 3 first letters of the subroutine name e.g. '\$THETA' and '\$TABLE' will become 'the' and 'tab' respectively. In addition all output from the .lst is labeled 'lst', the general nonmem output e.g. NM-TRAN messages are labelled 'oth'. With priors thp, tpv, omp, opd, sip, spd abbreviations are given to the THETAP, THETAPV, OMEGAP, etc.
- **code**: the code without comments or subroutine names e.g. '\$THETA 0.5; TVCL' will return '0.5'.
- **comment**: the last comment of a record e.g. '0.5 ; Clearance (L/h) ; TVCL' will return 'TVCL'.

See Also

```
pmx_read_nm_tables
```

```
## Not run:
# Using the `file` argument to import a model file:
nm_model <- pmx_read_nm_model(file = 'run001.lst', dir = 'models')
# Using the `runno` argument to import a model file:
nm_model <- pmx_read_nm_model(runno = '001', ext = '.lst', dir = 'models')
## End(Not run)</pre>
```

pmx_read_nm_tables 77

pmx_read_nm_tables

NONMEM output table import function

Description

Quickly import NONMEM output tables into R. This function automatically detects the optimal settings to import the tables from nonmem. It is based on the read_nm_tables function of xpose. Slight adjustment were made for purposes of pmx_nm()

Usage

```
pmx_read_nm_tables(
    file = NULL,
    dir = NULL,
    combined = TRUE,
    rm_duplicates = TRUE,
    quiet = FALSE,
    simtab = NULL,
    ziptab = TRUE,
    user_mode = TRUE,
    ...
)
```

Arguments

tile	A character vector of path to the files or a nm_table_list object created with

list_nm_tables.

dir Location of the model files.

combined Logical value indicating whether multiple tables should be combined into a sin-

gle one. If the number of rows does not match an error will be returned.

rm_duplicates Logical value indicating whether duplicated columns should be removed.

quiet Logical, if FALSE messages are printed to the console.

simtab If TRUE only reads in simulation tables, if FALSE only reads estimation tables.

Default NULL reads all tables.

ziptab If TRUE search for the tables that have been compressed and renamed ??<file>.zip'.

user_mode Adjustment to the original code: usermode is set to "usermode = TRUE" in

order to improve this function for purposes of pmx_nm() (nonmem_reader.R), In order to use this function seperatly, the use of the original function in the

xpose package is advised.

... Additional arguments to be passed to the read_table or read_csv functions.

78 pmx_register_plot

Table format requirement

When using pmx_read_nm_tables with the combined argument set to FALSE an ID column must be present in all data tables. When combined is set to TRUE instead an ID column must be present in at least one table for each problem and for each 'firstonly' category. ID columns are required to properly combine/merge tables and removing NA records. If the ID column is missing from a table and combined = FALSE pmx_read_nm_tables will return the following warning: Unknown variables: `ID`. While the data is returned beware that NA records might be left in the data and the output should be checked carefully. If combined = TRUE pmx_read_nm_tables is more strict and will return the following warning instead: Dropped ` `due to missing required `ID` column..

Examples

pmx_register_plot

Register plot

Description

Register plot

Usage

```
pmx_register_plot(ctr, pp, pname = NULL)
```

Arguments

ctr pmxClass controller

pp ggplot2 plot

pname character plot nme

pmx_report 79

pmx_report

Generates ggpmX report from a pre-defined template

Description

Generates ggpmX report from a pre-defined template

Usage

```
pmx_report(
  contr,
  name,
  save_dir,
  plots_subdir = "ggpmx_GOF",
  output = c("all", "plots", "report"),
  template = "standing",
  footnote = output == "all",
  edit = FALSE,
  format = NULL,
  title,
  ...
)
```

Arguments

contr	pmxClass controller
name	character The report name
save_dir	Output directory. A directory to write the results files to
plots_subdir	Output folder name, ggpmx_GOF by default
output	character the result type, can be a standalone directory of plots or a report document as defined in the template (pdf, docx,) ,or both
template	character ggPMX predefined template or the path to a custom rmarkdown template. Use pmx_report_template to get the list of available templates
footnote	logical TRUE to add a footnote to the generated plots. The default footnote is to add the path where the plot is saved.
edit	logical TRUE to edit the template immediately
format	character The output document format. By default, a word report is generated. User can specify one or more formats from c("word","pdf","html","all"). format "all" to generate all formats.
title	character report title (optional)
• • •	extra parameters depending in the template used

pmx_report

Details

pmx_report uses pre-defined template .Rmd to generate the report. The idea is to pass the controller as a report argument using knitr params artifact.

```
library(ggPMX)
# you probably want to create the report in your own directory
# But using a temp directory allows for easy cleanup
## case1: generate a single report
withr::with_tempdir({
  ctr <- theophylline()</pre>
 ctr %>% pmx_report(
    name = "my_report",
    save_dir = getwd(),
    output="report"
})
## case2: generate standalone plots
withr::with_tempdir({
 ctr <- theophylline()</pre>
 ctr %>% pmx_report(
    name = "my_report",
    save_dir = getwd(),
    output="plots"
  )
})
## case3: generate both : reports + plots
## by default add footnote
## Note, you can force footnote to FALSE using footnote parameter
withr::with_tempdir({
  ctr <- theophylline()</pre>
  ctr %>% pmx_report(
    name="my_report",
    save_dir=getwd(),
    output="all"
  )
})
## case4 : generate standalone plots with footnotes
withr::with_tempdir({
  ctr <- theophylline()</pre>
 ctr %>% pmx_report(
    name="my_report",
```

pmx_report_template 81

```
save_dir=getwd(),
    footnote=TRUE,
    output="plots"
  )
})
## case6: dynamic edit
## uncomment to run
# ctr <- theophylline()</pre>
# ctr %>% pmx_report(
   save_dir = file.path(getwd(),"case6"),
   name="my_report",
   output="report",
   edit = TRUE)
## case7 : generate individual plots report
## ctr <- theophylline()</pre>
## ctr %>% pmx_report(
## name="report2",
## save_dir = getwd(),
## template="individual",
## format="all",
## which_pages=1:2
## )
```

pmx_report_template

Gets build-in report templates

Description

Gets build-in report templates

Usage

```
pmx_report_template()
```

Value

list of templates names

```
pmx_report_template()
```

82 pmx_settings

pmx_settings

Create controller global settings

Description

Create controller global settings

Usage

```
pmx_settings(
   is.draft = TRUE,
   use.abbrev = TRUE,
   color.scales = NULL,
   cats.labels = NULL,
   use.labels = FALSE,
   use.titles = FALSE,
   effects = NULL,
   ...
)
```

Arguments

```
is.draft
                 logical if FALSE any plot is without draft annotation
                  logical if FALSE use full description from abbreviation mapping for axis
use.abbrev
                  names
color.scales
                 list list containing elements of scale_color_manual
cats.labels
                 list list of named vectors for each factor
use.labels
                  logical if TRUE replace factor named by cats.labels
use.titles
                  logical FALSE to generate plots without titles
effects
                  list list of effects levels and labels
                  extra parameter not used yet
```

Value

pmxSettingsClass object

```
library(ggPMX)
library(ggplot2)
ctr <- theophylline(
   settings=
    pmx_settings(
      color.scales=list(</pre>
```

pmx_shrink 83

```
"Study",
       labels=c("Study 1","Study 2"),
        values=c("1"="lightyellow","2"="lightblue")),
      cats.labels=list(
       SEX=c("0"="M","1"="F"),
       STUD=c("1"="Study 1","2"="Study 2")
      ),
      use.abbrev=TRUE,
      is.draft=TRUE,
      use.labels=TRUE
)
ctr %>%
  pmx_plot_npde_time(strat.color="STUD",strat.facet=~SEX)
#
ctr %>%
  pmx_plot_eta_box(strat.color="STUD", strat.facet =~SEX)
ctr %>% pmx_plot_eta_hist
```

pmx_shrink

Create shrinkage parameter object

Description

Create shrinkage parameter object

Usage

```
pmx_shrink(
   fun = c("var", "sd"),
   size = 1,
   color = "green",
   vjust = 1.5,
   hjust = 0.5,
   ...
)
```

Arguments

fun list shrinkage function can be sd or var size numeric shrinkage text size

color character shrinkage text color

pmx_sim

```
vjust numeric shrinkage position vertical adjustment
hjust numeric shrinkage position horizontal adjustment
... any other parameter
```

Value

```
pmxShrinkClass object (list)
```

pmx_sim

Create simulation object

Description

Create simulation object

Usage

```
pmx_sim(file, data, irun, idv)
```

Arguments

```
file character path to the simulation file
data data.table simulation data
irun character name of the simulation column
idv character name of the ind. variable
```

```
library(ggPMX)
theo_path <- file.path(</pre>
  system.file(package = "ggPMX"), "testdata",
  "theophylline"
)
WORK_DIR <- file.path(theo_path, "Monolix")</pre>
input_file <- file.path(theo_path, "data_pk.csv")</pre>
vpc_file <- file.path(theo_path, "sim.csv")</pre>
ctr <- pmx_mlx(
  config = "standing",
  directory = WORK_DIR,
  input = input_file,
  dv = "Y",
  dvid = "dvid",
  cats = c("SEX"),
  conts = c("WT0", "AGE0"),
  strats = "STUD",
```

pmx_theme 85

```
settings = pmx_settings(
   use.labels=TRUE,
   cats.labels=list(
      SEX=c("0"="Male","1"="Female")
   )
  ),
  sim = pmx_sim(
   file = vpc_file,
   irun ="rep",
    idv="TIME"
  )
)
ctr %>% pmx_plot_vpc(
  strat.facet=~SEX,
  facets=list(nrow=2),
  type="percentile",
  is.draft = FALSE,
  pi = pmx_vpc_pi(interval = c(0.1,0.9),
              median=list(color="green"),
              extreme= list(color="green")),
  obs = pmx_vpc_obs(color="blue", shape=18, size=2),
  ci = pmx\_vpc\_ci(interval = c(0.1,0.9),
              median=list(fill="pink")),
  bin=pmx_vpc_bin("kmeans",n=5)
)
ctr %>%
  pmx_plot_vpc(bin= pmx_vpc_bin(
    style = "fixed",
     fixedBreaks=c(-10,2, 5, 10,15,50))
# example with legend
ctr %>% pmx_plot_vpc(
  is.legend = TRUE,
  pi = pmx_vpc_pi(interval=c(0.02,0.98),median = list(linetype="dotted")),
  ci = pmx\_vpc\_ci(interval = c(0.05, 0.95), median=list(fill="red"))
```

pmx_theme

Define ggPMX theme

Description

This theme is a simple wrapper gdoc theme from ggthems package.

pmx_update

Usage

```
pmx_theme(...)
```

Arguments

... can contain any valid argument of ggplot2 theme object.

pmx_update

Update plot object

Description

Update plot object

Usage

```
pmx_update(
   ctr,
   pname,
   strat.color = NULL,
   strat.facet = NULL,
   color.scales = NULL,
   filter = NULL,
   trans = NULL,
   ...,
   pmxgpar = NULL
)
```

Arguments

pmxClass controller object ctr character the plot name to update pname character optional stratification parameter strat.color strat.facet formula optional stratification parameter color.scales list can be used with strat.color to set scale_color_manual pmx_gpar function. filter optional filter which will be applied to plotting data character define the transformation to apply on x or y or both variables trans others graphical parameters given to set the plot a object of class pmx_gpar possibly the output of the pmxgpar

pmx_vpc 87

Details

trans is a transformation that user can apply to x, or y coordinates. The transformation is applied to the data before the plotting. This gives more felxiblilty to the user and also conserves all static positions like annotations (draft specially)

For example:

var_x apply variance to x coordinates the variance function

var_xy apply variance to both This mechanism is applied internally to scale log.

Value

controller object with the plot updated

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), set_data(), set_plot()
```

pmx_vpc

Creates vpc object

Description

Creates vpc object

Usage

```
pmx_vpc(
  type = c("percentile", "scatter"),
  idv = "TIME",
  obs = pmx_vpc_obs(),
  pi = pmx_vpc_pi(),
  ci = pmx_vpc_ci(),
  rug = pmx_vpc_rug(),
  bin = pmx_vpc_bin(),
  labels = NULL,
  facets = NULL,
  is.legend = TRUE,
  is.footnote = TRUE,
  dname = NULL,
  ...
)
```

pmx_vpc_bin

Arguments

charcater can be either percentile or scatter type idv chracater individual variable pmx_vpc_obs object observation layer pmx_vpc_obs obs pmx_vpc_pi object percentile layer pmx_vpc_pi рi pmx_vpc_ci object confidence interval layer pmx_vpc_ci ci pmx_vpc_rug object rug layer pmx_vpc_rug rug pmx_vpc_bin object pmx_vpc_bin bin labels list define title and axis labels is a list of parameters passed to facet_wrap in case of startification facets is.legend logical if TRUE add legend is.footnote logical if TRUE add footnote added for compatibility with other ggPMX plots dname extra parameters passed to base graphical parameters

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_bin(), pmx_vpc_ci(), pmx_vpc_obs(), pmx_vpc_pi(), pmx_vpc_rug()
```

|--|

Description

Creates vpc bins

Usage

```
pmx_vpc_bin(style, within_strat = TRUE, seed = 42, ...)
```

Arguments

style	character style chosen on of the: "fixed", "sd", "equal", "pretty", "quantile", "kmeans", "hclust" or "jenks"
within_strat	logical if TRUE compute the bining for each strat level. By default t is false and bining are equal for all stratifications levels.
seed	integer used in set. seed call to ensure reproducibility if style is "kmeans". Set to NULL if this is not desired.
	other classInt::classIntervals parameters excpet style and n

pmx_vpc_ci 89

Details

This is a wrapper to the bin based VPC

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_ci(), pmx_vpc_obs(), pmx_vpc_pi(), pmx_vpc_rug(), pmx_vpc()
```

pmx_vpc_ci

Sets vpc confidence interval layer

Description

Sets vpc confidence interval layer

Usage

```
pmx_vpc_ci(
    show = c("all", "median"),
    interval = c(0.025, 0.975),
    method = c("ribbon", "rectangle"),
    median = list(fill = "red", alpha = 0.3),
    extreme = list(fill = "#3388cc", alpha = 0.3)
)
```

Arguments

show

charcater how areas are displayed:

- **show="all"** areas will be displayed for each of the 3 percentiles.
- show="median" Show only median area.

interval

numeric quantiles values default to c(.05,.95)

method

charcater which areas are displayed:

- method="ribbon" areas are ribbons.
- method="rectangle" areas are horizontal rectangles.

median

list containing:

- fill character Color of the area representing the CI for the median. Default: "#3388cc".
- **alpha** numeric Transparency of the area representing the PI for the median. Default=0.3.

extreme

list containing:

- fill character Color of the area representing the CI for the extreme percentiles. Default: "#3388cc".
- **alpha** numeric Transparency of the area representing the PI for the extreme percentiles. Default=0.3.

90 pmx_vpc_pi

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_bin(), pmx_vpc_obs(), pmx_vpc_pi(), pmx_vpc_rug(), pmx_vpc()
```

pmx_vpc_obs

Sets vpc observation layer

Description

Sets vpc observation layer

Usage

```
pmx_vpc_obs(show = TRUE, color = "#000000", size = 1, alpha = 0.7, shape = 1)
```

Arguments

show	logical if TRUE show observation points
color	character Color of the observed endpoint values. Default: "#000000".
size	numeric Size of the observed endpoint values. Default: 1.
alpha	numeric Transparency of the observed endpoint values. Default: 0.7.
shape	numeric Shape of the observed endpoint values. Default: 1.

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_bin(), pmx_vpc_ci(), pmx_vpc_pi(), pmx_vpc_rug(), pmx_vpc()
```

pmx_vpc_pi

Sets vpc percentile layer

Description

Sets vpc percentile layer

Usage

```
pmx_vpc_pi(
    show = c("all", "median", "area"),
    interval = c(0.05, 0.95),
    median = list(color = "#000000", linewidth = 1, alpha = 0.7, linetype = "solid"),
    extreme = list(color = "#000000", linewidth = 1, alpha = 0.7, linetype = "dashed"),
    area = list(fill = "blue", alpha = 0.1)
)
```

pmx_vpc_rug 91

Arguments

show charcater how lines are displayed:

• **show=all** lines will be displayed for each of the 3 percentiles. with a shaded area.

- show=median Show only median line.
- show=area Show only median line and the shaded area

interval numeric quantiles values default to c(.05,.95)

median list containing:

- color charcater Color of the median percentile line. Default: "#000000".
- linewidth numeric Thickness of the median percentile line. Default: 1.
- alpha numeric Transparency of the median percentile line. Default: 0.7.
- linetype charcater Linetype of the median percentile line. Default: "solid".

extreme list containing:

- color charcater Color of the median percentile line. Default: "#000000".
- **linewidth** numeric Thickness of the median percentile line. Default: 1.
- alpha numeric Transparency of the median percentile line. Default: 0.7.
- linetype charcater Linetype of the median percentile line. Default: "solid"

area list containing:

- fill charcater Color of the shaded area. Default: "blue".
- alpha numeric Transparency of the sahded area. Default: 0.1.

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_bin(), pmx_vpc_ci(), pmx_vpc_obs(), pmx_vpc_rug(), pmx_vpc()
```

pmx_vpc_rug

Sets vpc rug layer

Description

Sets vpc rug layer

Usage

```
pmx_vpc_rug(show = TRUE, color = "#000000", linewidth = 1, alpha = 0.7, size)
```

92 print.abbreviation

Arguments

show logic	al If TRUE show bin ser	parators
------------	-------------------------	----------

color character Color of the rug. Default: "#000000".

linewidth numeric Thickness of the rug. Default: 1.

alpha numeric Transparency of the rug. Default: 0.7.

size numeric Depreciated thickness of the rug. Default: 1.

Details

When the vpc confidence interval layer method is rectangles we don't show rug separators.

See Also

```
Other vpc: pmx_plot_vpc(), pmx_vpc_bin(), pmx_vpc_ci(), pmx_vpc_obs(), pmx_vpc_pi(), pmx_vpc()
```

print.abbreviation

S3 print abbreviation

Description

S3 print abbreviation

Usage

```
## S3 method for class 'abbreviation' print(x, ...)
```

Arguments

x object of class configs

... pass additional options (not used presently)

Value

print abbreviation

print.configs 93

print.configs	This function can be used to print configuration of the defined object using S3 method.
	using 55 method.

Description

This function can be used to print configuration of the defined object using S3 method.

Usage

```
## S3 method for class 'configs' print(x, ...)
```

Arguments

x object of class configs

... pass additional options (not used presently)

Value

print result

print.pmxClass

Print pmxClass object

Description

Print pmxClass object

Usage

```
## S3 method for class 'pmxClass' print(x, ...)
```

Arguments

x pmxClass object

. . . additinal arguments to pass to print

Value

print object to screen

94 print.pmx_gpar

print.pmxConfig

S3 method print pmxConfig object

Description

S3 method print pmxConfig object

Usage

```
## S3 method for class 'pmxConfig'
print(x, ...)
```

Arguments

x pmxConfig object

... additional arguments to pass to print (unused currently)

Value

invisible object

print.pmx_gpar

Print pmx_gpar object

Description

Print pmx_gpar object

Usage

```
## S3 method for class 'pmx_gpar'
print(x, ...)
```

Arguments

x pmx_gpar object

... argument passed to print (to satisfy generic)

Value

a character description of graphical parameters

read_extfile 95

read_extfile	Reads .ext files generated by NONMEM
I COO_CX CI IIC	

Description

Reads .ext files generated by NONMEM

Usage

```
read_extfile(
  run = NA_real_,
  project = getwd(),
  file = paste0(run, ".ext"),
  path = NULL,
  read_fun = c("data.table", "read.table"),
  quiet
)
```

Arguments

run	run a run number or run identifier
project	project the NONMEM project directory
file	file the 'ext' file name
path	path full path and file name for 'ext' file
read_fun	read_fun function to read the 'ext' file
quiet	Logical, if FALSE messages are printed to the console.

Value

A list with param, omega, and sigma in a format ready to be used.

Author(s)

This function is based on read_nmext from mrgsolve, Original Author: Kyle T Baron. This function has some changes to the original code: Addition of param, "quiet", (option of pmx_msg function, from xpose package) (Line: 27) The code was slightly adjusted to check for multiple tables and also extract SE (ITERATION == 1000000001) (Line: 44-58, Line: 86-96, respectively) The output was also slightly adjusted to fit ggPMX output (df and df2) (Line: 105,106) as_bmat was replaced by bmat_like to create the diagonal matrix (Line 116:142)

```
#project <- system.file("nonmem", package = "mrgsolve")
#est <- read_nmext(1005, project = project)</pre>
```

96 read_input

read_input

Read Modelling input data

Description

Read Modelling input data

Usage

```
read_input(
  ipath,
  dv,
  dvid,
  cats = "",
  conts = "",
  strats = "",
  occ = "",
  endpoint = NULL,
  id = NULL,
  time = NULL
)
```

Arguments

ipath	full path of the input file
dv	character the name of measurable variable used in the input modelling file
dvid	character observation type parameter
cats	[Optional] character vector of categorical covariates
conts	[Optional] character vector of continuous covariates
strats	[Optional] character extra stratification variables
occ	[Optional] character inter individual occasion variables
endpoint	integer null in case of a single endpoint otherwise the index of endpoints.
id	character the name of identifier variable used in the input modelling file.
time	character the name of time variable used in the input modelling file

Value

data.table well formatted containing modelling input data

read_mlx_ind_est 97

read_mlx_ind_est

Read MONOLIX individual parameters

Description

Read MONOLIX individual parameters

Usage

```
read_mlx_ind_est(path, x, ...)
```

Arguments

path character path to the file

x dataset object

... extra parameter not used

Value

data.table object

read_mlx_par_est

Read MONOLIX parameter estimation file

Description

Read MONOLIX parameter estimation file

Usage

```
read_mlx_par_est(path, x, ...)
```

Arguments

path character path to the file

x dataset object

... extra parameter not used

Value

data.table object

98 residual

read_mlx_pred

Read MONOLIX model predictions

Description

Read MONOLIX model predictions

Usage

```
read_mlx_pred(path, x, ...)
```

Arguments

path character path to the file x dataset object ... extra parameter not used

Value

data.table object

residual

This function create a residual for each observed value and also generates a residual distribution

Description

This function create a residual for each observed value and also generates a residual distribution

Usage

```
residual(
    x,
    y,
    labels = NULL,
    point = NULL,
    is.hline = FALSE,
    hline = NULL,
    dname = NULL,
    facets = NULL,
    bloq = NULL,
    square_plot = TRUE,
    ...
)
```

residual 99

Arguments

x x axis aestheticsy y axis aesthetics

labels list that contain title, subtitle, axis labels

point geom point graphical parameters

is.hline logical if TRUE add horizontal line y=0 (TRUE by default)

hline geom hline graphical parameters

dname name of dataset to be used

facets list wrap facetting in case of strat.facet bloq pmxBLOQ object created by pmx_bloq square_plot square dv_pred plot (TRUE by default)

... others graphics arguments passed to pmx_gpar internal object.

Details

Some parameters are a list of parameters:

point is a list that contains:

• shape: default to 1

• color: default to black

• size: default to 1

labels is a list that contains:

• title: plot title default to AES_X versus AES_Y

• subtitle: plot subtitle default empty

• x: x axis label default to AES_X

• y: y axis label default to AES_Y

Value

a residual object

See Also

```
plot_pmx.residual
```

residual_scatter

Scatter residual plots

Description

```
Scatter residual plots
DV vs PRED plot
DV vs IPRED plot
IWRES vs IPRED plot
IWRESI vs IPRED plot
IWRESI vs TIME plot
IWRESI vs TIME plot
IWRES vs TIME plot
NPDE vs TIME plot
NPDE vs PRED plot
NPD vs TIME plot
NPD vs EPRED plot
NPD vs PRED plot
CWRES vs TIME plot
CWRES vs TIME plot
CWRES vs TIME plot
```

Usage

```
residual_scatter(
  sim_blq,
 point,
  is.hline,
 hline,
  dname,
 bloq,
 filter,
  strat.facet,
  facets,
  strat.color,
  trans,
  pmxgpar,
  labels,
  axis.title,
  axis.text,
  ranges,
  is.smooth,
  smooth,
```

```
is.band,
  band,
  is.draft,
  draft,
  is.identity_line,
  identity_line,
  scale_x_log10,
  scale_y_log10,
  color.scales,
)
pmx_plot_dv_pred(ctr, ...)
pmx_plot_dv_ipred(ctr, ...)
pmx_plot_iwres_ipred(ctr, ...)
pmx_plot_abs_iwres_ipred(ctr, ...)
pmx_plot_abs_iwres_time(ctr, ...)
pmx_plot_iwres_time(ctr, ...)
pmx_plot_npde_time(ctr, ...)
pmx_plot_npde_pred(ctr, ...)
pmx_plot_npd_time(ctr, ...)
pmx_plot_npd_epred(ctr, ...)
pmx_plot_npd_pred(ctr, ...)
pmx_plot_cwres_time(ctr, ...)
pmx_plot_cwres_cpred(ctr, ...)
pmx_plot_cwres_pred(ctr, ...)
```

Arguments

sim_blq	logical if TRUE uses sim_blq values for plotting. Only for Monolix 2018 and later.
point	list geom_point graphical parameters.
is.hline	logical if TRUE add horizontal line y=0 (TRUE by default).
hline	list geom_hline graphical parameters.

dname character name of dataset to be used. User can create his own dataset using

set_data and pass it as dname to be plotted.

bloq pmxBLOQ object created by pmx_bloq.

pmx_update parameters

filter expression filter which will be applied to plotting data.

strat.facet formula optional stratification parameter by facetting. This split plot by strats(each

strat in a facet)

facets list facet_wrap parameters.

strat.color character optional stratification parameter by grouping. This will split the plot

by group (color) of strat.

trans character define the transformation to apply on x or y or both variables

pmxgpar a object of class pmx_gpar possibly the output of the

pmx_gpar: Shared basic graphics parameters

labels list list containing plot and/or axis labels: title, subtitle, x, y

axis.title list containing element_text attributes to customize the axis title. (similar to

ggplot2 axis.title theme)

axis.text list containing element_text attributes to customize the axis text (similar to

ggplot2 axis.text theme)

ranges list limits of x/y ranges

is.smooth logical if set to TRUE add smooth layer

smooth list geom smooth graphical/smoothing fun parameters

is.band logical if TRUE add horizontal band

band list horizontal band parameters. geom_hline graphical parameters.

is.draft logical if TRUE add draft layer

draft list draft layer parameters. geom text graphical parameters.

is.identity_line

logical if TRUE add an identity line

identity_line listgeom_abline graphical parameters.

scale_x_log10 logical if TRUE use log10 scale for x axis.

scale_y_log10 logical if TRUE use log10 scale for y axis.

color.scales list define scales parameter in case of strat.color pmx_settings

... others graphics parameters passed :

• pmx_gpar internal function to customize shared graphical parameters

• residual generic object for all residual (scatter) plots .

• pmx_update function.

• aess can be used to change time variable within the plot (e.g. aess = list(x="TADQBW"))

residual parameters

ctr pmx controller

Value

ggplot2 object

```
# examples are availables for all residual plots:
# - pmx_plot_abs_iwres_ipred
# - pmx_plot_dv_ipred
# - pmx_plot_dv_pred
# - pmx_plot_iwres_ipred
# - pmx_plot_iwres_time
# - pmx_plot_npde_time
# basic use ------
ctr <- theophylline()</pre>
p <- ctr %>% pmx_plot_dv_pred()
## p is a ggplot2 object you can add any layer here
p + ggplot2::theme_minimal()
# update graphical parameter -----
## update labels
ctr %>% pmx_plot_dv_pred(
 labels = list(title = "DV versus PRED new title")
)
## remove draft
ctr %>% pmx_plot_dv_pred(is.draft = FALSE)
## remove horizontal line
ctr %>% pmx_plot_dv_pred(is.hline = FALSE)
## custom point aes and static parameters
## we can customize any geom_point parameter
ctr %>% pmx_plot_dv_pred(
 point = list(aes(alpha = DV), color = "green", shape = 4)
# stratification ------
## continuous stratification
ctr %>% pmx_plot_dv_pred(strat.color = ~WT0)
## categorical stratification
ctr %>% pmx_plot_dv_pred(strat.facet = ~SEX)
## using formula notation
ctr %>% pmx_plot_dv_pred(strat.facet = STUD~SEX)
```

104 set_abbrev

set_abbrev

update or add a new abbreviation

Description

update or add a new abbreviation

Usage

```
set_abbrev(ctr, ...)
```

Arguments

ctr pmxClass controller object... Options to set or add, with the form name = value.

```
ctr <- theophylline()
ctr %>% set_abbrev("new_param" = "new value")
ctr %>% get_abbrev("new_param")
```

set_data 105

set_data

Set a controller data set

Description

Set a controller data set

Usage

```
set_data(ctr, ..., envir = parent.frame())
```

Arguments

```
    the controller object
    a named list parameters (see example)
    the environment in which expr is to be evaluated. May also be NULL, a list, a data frame, a pairlist or an integer as specified to sys.call.
```

Details

This function can be used to set an existing data set or to create a new one. The basic idea is to change the built-in data set (change the factor level names, change some rows values or apply any other data set operation) and use the new data set using the dname parameter of pmx_plot family functions.

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_plot()
```

```
ctr <- theophylline()
dx <- ctr %>% get_data("eta")
dx <- dx[, EFFECT := factor(
    EFFECT,
    levels = c("ka", "V", "Cl"),
    labels = c("Concentration", "Volume", "Clearance")
)]
## update existing data set
ctr %>% set_data(eta = dx)
## or create a new data set
ctr %>% set_data(eta_long = dx)
```

106 set_plot

set_plot

Create a new plot of the desired type

Description

Create a new plot of the desired type

Usage

```
set_plot(
  ctr,
  ptype = c("IND", "DIS", "SCATTER", "ETA_PAIRS", "ETA_COV", "PMX_QQ", "VPC", "PMX_DENS"),
  pname,
  use.defaults = TRUE,
  filter = NULL,
  strat.color = NULL,
  strat.facet = NULL,
  color.scales = NULL,
  trans = NULL,
  ...
)
```

Arguments

```
pmxClass controller object
ctr
ptype
                  plot type can be:
                     • "IND" Individual plot type: individual
                     • "DIS" Distribution plot type: distrib
                     • "SCATTER" Residual plot type :residual
                  plot name, if missing it will be created using function aestetics
pname
use.defaults
                  logical if FALSE do not use defaults defined in yaml init files
filter
                  optional filter which will be applied to plotting data
strat.color
                  character
strat.facet
                   formula define categorical stratification as formula
color.scales
                  list can be used with strat.color to set scale_color_manual
trans
                  list transformation operator
                  other plot parameters to configure pmx_gpar.
. . .
```

Value

invisible ctr object

See Also

```
Other pmxclass: get_cats(), get_conts(), get_covariates(), get_data(), get_occ(), get_plot_config(), get_plot(), get_strats(), plot_names(), plots(), pmx_update(), set_data()
```

theophylline 107

theophylline

Creates pmx controller using theophylline data

Description

Creates pmx controller using theophylline data

Usage

```
theophylline(settings = NULL, ...)
```

Arguments

```
settings pmxSettings object
... other parameters of pmx_mlx like endpoint
```

Value

pmx controller

Examples

```
## Not run:
theophylline()
## End(Not run)
```

wrap_formula

merge facets formula with new formula

Description

merge facets formula with new formula

Usage

```
wrap_formula(x, origin = "lfacet")
```

Arguments

x formula object

origin the origin formula default to ~lfacets

Value

formula object

108 [.pmx_gpar

[.pmx_gpar

Method for subsetting "pmx_gpar" objects

Description

Method for subsetting "pmx_gpar" objects

Usage

```
## S3 method for class 'pmx_gpar'
x[index, ...]
```

Arguments

x pmx_gpar object

index can be character/integer of element

... other parameter (not used just for generic)

Value

if exists the parameter description

Index

```
* eta_cov_plot
                                                        residual_scatter, 100
    eta_cov_plot, 9
                                                   * vpc
                                                        pmx_plot_vpc, 66
* eta_distribution_plot
                                                        pmx_vpc, 87
    eta_distribution_plot, 12
                                                        pmx_vpc_bin, 88
* plot pmx
                                                        pmx_vpc_ci, 89
    distrib, 6
                                                        pmx_vpc_obs, 90
    eta_cov, 7
                                                        pmx_vpc_pi, 90
    eta_pairs, 15
                                                        pmx_vpc_rug, 91
    individual, 23
                                                   [.pmx_gpar, 108
    plot_pmx, 30
    plot_pmx.distrib, 31
                                                   abbrev, 4
    plot_pmx.eta_cov, 32
                                                   add_draft, 5
    plot_pmx.eta_pairs, 32
    plot_pmx.individual, 33
                                                   check_shrink, 6
    plot_pmx.pmx_dens, 34
    plot_pmx.pmx_gpar, 34
                                                   distrib, 6, 8, 13, 16, 24, 31-36, 106
    plot_pmx.pmx_qq, 35
                                                   dummy (eta_cov_plot), 9
    plot_pmx.residual, 36
                                                   environment, 105
* pmxclass functions
                                                   eta_cov, 7, 7, 10, 16, 24, 31-36
    print.pmxClass, 93
                                                   eta_cov_plot, 9
* pmxclass
                                                   eta_distribution_plot, 12
    get_cats, 18
                                                   eta_pairs, 7, 8, 15, 24, 31–36, 59
    get_conts, 18
                                                   eval_sym_parent_env, 16
    get_covariates, 19
    get_data, 19
                                                   facet_wrap_paginate, 27
    get_occ, 20
    get_plot, 20
                                                   get_abbrev, 17
    get_plot_config, 21
                                                   get_cats, 18, 18, 19-22, 29, 30, 87, 105, 106
    get_strats, 22
                                                   \mathtt{get\_conts}, 18, 18, 19–22, 29, 30, 87, 105, 106
    plot_names, 30
                                                   get_covariates, 18, 19, 20–22, 29, 30, 87,
    plots, 29
                                                            105, 106
    pmx_update, 86
                                                   get_data, 18, 19, 19, 20-22, 29, 30, 87, 105,
    set_data, 105
    set_plot, 106
                                                   get_occ, 18-20, 20, 21, 22, 29, 30, 87, 105,
* qq_plot
    pmx_qq, 70
                                                   get_plot, 18-20, 20, 21, 22, 29, 30, 87, 105,
* qqq
    pmx_qq_plot, 71
                                                   get_plot_config, 18-21, 21, 22, 29, 30, 87,
* residual
                                                            105, 106
```

INDEX

get_strats, 18-21, 22, 29, 30, 87, 105, 106	pmx_list_nm_tables, 51
getPmxOption, 17	<pre>pmx_manual_nm_import, 52</pre>
gtable_remove_grobs, 22	pmx_mlx, 27, 39
	pmx_mlx (pmx), 37
individual, 7, 8, 16, 23, 31–36, 62, 106	pmx_mlxtran (pmx), 37
<pre>input_finegrid, 24</pre>	pmx_nlmixr, 53
is.pmx_gpar, 24	pmx_nm, 53
	pmx_plot, 56
l_left_join, 26	pmx_plot_abs_iwres_ipred
load_config, 25	(residual_scatter), 100
load_data_set, 25	pmx_plot_abs_iwres_time
load_source, 26	(residual_scatter), 100
27	pmx_plot_cats, 57
n_pages, 27	pmx_plot_cwres_cpred
norm toble 27	(residual_scatter), 100
param_table, 27	<pre>pmx_plot_cwres_pred (residual_scatter),</pre>
parse_mlxtran, 28	100
pk_occ, 28	<pre>pmx_plot_cwres_qq(pmx_qq_plot), 71</pre>
pk_pd, 29	<pre>pmx_plot_cwres_time (residual_scatter),</pre>
plot_names, 18-22, 29, 30, 87, 105, 106	100
plot_pmx, 7, 8, 16, 24, 30, 31–36	<pre>pmx_plot_dv_ipred(residual_scatter),</pre>
plot_pmx.distrib, 7, 8, 16, 24, 31, 31, 32–36 plot_pmx.eta_cov, 7, 8, 16, 24, 31, 32, 33–36	100
plot_pmx.eta_cov, 7, 8, 10, 24, 31, 32, 33–30 plot_pmx.eta_pairs, 7, 8, 16, 24, 31, 32, 32,	<pre>pmx_plot_dv_pred(residual_scatter), 100</pre>
33–36	pmx_plot_eta_box
plot_pmx.individual, 7, 8, 16, 24, 31–33,	(eta_distribution_plot), 12
33, 34–36	pmx_plot_eta_cats (eta_cov_plot), 9
plot_pmx.pmx_dens, 7, 8, 16, 24, 31–33, 34,	pmx_plot_eta_conts (eta_cov_plot), 9
35, 36	pmx_plot_eta_hist
plot_pmx.pmx_gpar, 7, 8, 16, 24, 31–34, 34,	(eta_distribution_plot), 12
35, 36	pmx_plot_eta_matrix, 57
plot_pmx.pmx_qq, 7, 8, 16, 24, 31–35, 35, 36	pmx_plot_eta_qq(pmx_qq_plot), 71
plot_pmx.residual, 7, 8, 16, 24, 31–35, 36,	pmx_plot_individual, 60
99	pmx_plot_iwres_dens, 64
plot_shrink, 36	pmx_plot_iwres_ipred
plots, 18–22, 29, 30, 87, 105, 106	(residual_scatter), 100
pmx, 37	<pre>pmx_plot_iwres_qq(pmx_qq_plot), 71</pre>
pmx_bloq, 23, 38, 41, 55, 62, 99, 102	<pre>pmx_plot_iwres_time (residual_scatter),</pre>
pmx_comp_shrink, 27, 42	100
pmx_config, 43	<pre>pmx_plot_npd_epred (residual_scatter),</pre>
pmx_copy, 44	100
pmx_cov, 8, 45	<pre>pmx_plot_npd_pred (residual_scatter),</pre>
pmx_dens, 45, 66	100
pmx_endpoint, 38, 47, 53, 55	<pre>pmx_plot_npd_qq (pmx_qq_plot), 71</pre>
pmx_filter, 48	<pre>pmx_plot_npd_time (residual_scatter),</pre>
pmx_get_configs, 49	100
pmx_gpar, 7, 8, 10, 13, 16, 23, 31, 46, 50, 56,	<pre>pmx_plot_npde_pred (residual_scatter),</pre>
57, 59, 62, 66, 68, 71, 74, 86, 99,	100
102, 106	<pre>pmx_plot_npde_qq (pmx_qq_plot), 71</pre>

INDEX 111

```
pmx_plot_npde_time (residual_scatter),
                                                   tibble, 76
         100
                                                   wrap_formula, 107
pmx_plot_vpc, 66, 88-92
pmx_qq, 56, 57, 70, 74
pmx_qq_plot, 71
pmx_read_nm_files, 74
pmx_read_nm_model, 51, 52, 75
pmx_read_nm_tables, 52, 76, 77
pmx_register_plot, 78
pmx_report, 79
pmx_report_template, 79, 81
pmx_settings, 10, 13, 38, 51, 53, 55, 59, 62,
         66, 68, 73, 82, 102
pmx_shrink, 83
pmx_sim, 38, 84
pmx_theme, 85
pmx_update, 10, 13, 18-22, 29, 30, 56, 57, 59,
         62, 66, 68, 74, 86, 102, 105, 106
pmx_vpc, 68, 87, 89-92
pmx_vpc_bin, 67, 68, 88, 88, 90-92
pmx_vpc_ci, 67, 68, 88, 89, 89, 90-92
pmx_vpc_obs, 67, 68, 88-90, 90, 91, 92
pmx_vpc_pi, 67, 68, 88-90, 90, 92
pmx_vpc_rug, 67, 68, 88-91, 91
pmxOptions, 40
print.abbreviation, 92
print.configs, 93
print.pmx_gpar, 94
print.pmxClass, 93
print.pmxConfig, 94
read_csv, 77
read_extfile, 95
read_input, 96
read_mlx_ind_est, 97
read_mlx_par_est, 97
read_mlx_pred, 98
read_table, 77
residual, 36, 98, 102, 106
residual_scatter, 100
set_abbrev, 104
set_data, 18-22, 29, 30, 61, 65, 87, 102, 105,
         106
set_plot, 18-22, 29, 30, 87, 105, 106
sys.call, 105
theme, 86
theophylline, 107
```