

Package ‘vpc’

July 22, 2025

Title Create Visual Predictive Checks

Version 1.2.2

Date 2021-01-11

Author Ron Keizer <ronkeizer@gmail.com>

Maintainer Ron Keizer <ronkeizer@gmail.com>

Description Visual predictive checks are a commonly used diagnostic plot in pharmacometrics, showing how certain statistics (percentiles) for observed data compare to those same statistics for data simulated from a model. The package can generate VPCs for continuous, categorical, censored, and (repeated) time-to-event data.

Depends R (>= 3.1.0)

Imports classInt, dplyr, MASS, survival, ggplot2, readr, stringr, tidyrr

License MIT + file LICENSE

LazyData true

URL <https://github.com/ronkeizer/vpc>

Suggests knitr, testit

RoxygenNote 7.1.0

NeedsCompilation no

Repository CRAN

Date/Publication 2021-01-11 20:20:02 UTC

Contents

vpc-package	2
add_noise	3
add_sim_index_number	3
add_stratification	4
auto_bin	4
bin_data	5
check_stratification_columns_available	5

compute_kaplan	6
compute_kmmc	6
create_vpc_theme	7
define_data_columns	7
draw_params_mvr	8
loq_perc	8
new_vpc_theme	9
pk_iv_1cmt	10
pk_oral_1cmt	11
plot_vpc	12
quantile_cens	13
read_table_nm	13
replace_list_elements	14
rtte_obs_nm	15
rtte_sim_nm	15
show_default	16
show_default_tte	16
simple_data	16
sim_data	17
theme_empty	18
theme_plain	18
triangle_to_full	19
vpc	19
vpc_cat	22
vpc_cens	24
vpc_tte	26

Index	29
--------------	-----------

vpc-package	<i>VPC package</i>
-------------	--------------------

Description

Create Visual Predictive Checks in R

Author(s)

Ron Keizer <ronkeizer@gmail.com>

add_noise	<i>Add noise / residual error to data</i>
-----------	---

Description

Add noise / residual error to data

Usage

```
add_noise(x, ruv = list(proportional = 0, additive = 0, exponential = 0))
```

Arguments

x	data
ruv	list describing the magnitude of errors. List arguments: "proportional", "additive", "exponential".

Examples

```
library(dplyr)
ipred <- c(10, 8, 6, 4, 2, 0) %>% add_noise(ruv = list(proportional = 0.1, additive = 0.2))
```

add_sim_index_number	<i>Add sim index number</i>
----------------------	-----------------------------

Description

Add simulation index number to simulation when not present

Usage

```
add_sim_index_number(sim, id = "id", sim_label = "sim")
```

Arguments

sim	a data.frame containing the simulation data
id	character specifying the column name in the data.frame
sim_label	label to indicate simulation index (if available)

add_stratification	<i>Adds stratification to data set</i>
--------------------	--

Description

Adds stratification to data set

Usage

```
add_stratification(dat, strat, verbose = FALSE)
```

Arguments

dat	data.frame
strat	vector of stratification variables
verbose	verbosity ('TRUE' or 'FALSE')

auto_bin	<i>Calculate appropriate bin separators for vpc</i>
----------	---

Description

This function calculates bin separators either using R's native binning approaches available in the classInt library such as 'kmeans', 'jenks', 'pretty' etc. Alternatively, a custom approach is available which is based on finding the nadirs in the density functions for the independent variable. Default approach is k-means clustering.

Usage

```
auto_bin(dat, type = "kmeans", n_bins = 8, verbose = FALSE, ...)
```

```
## S3 method for class 'numeric'
```

```
auto_bin(dat, type = "kmeans", n_bins = 8, verbose = FALSE, ...)
```

```
## S3 method for class 'data.frame'
```

```
auto_bin(dat, type = "kmeans", n_bins = 8, verbose = FALSE, ...)
```

Arguments

dat	data frame
type	auto-binning type: "density", "time", or "data"
n_bins	number of bins to use; either a positive integer or "auto". For "density" the function might not return a solution with the exact number of bins.
verbose	show warnings and other messages (TRUE or FALSE)
...	arguments passed on to underlying binning functions

Value

A vector of bin separators

bin_data	<i>Function to bin data based on a vector of bin separators, e.g. for use in VPC</i>
----------	--

Description

Function to bin data based on a vector of bin separators, e.g. for use in VPC

Usage

```
bin_data(x, bins = c(0, 3, 5, 7), idv = "time", labeled = F)
```

Arguments

x	data
bins	numeric vector specifying bin separators
idv	variable in the data specifies the independent variable (e.g. "time")
labeled	whether a labeled factor instead of integers should be returned

check_stratification_columns_available	<i>Check whether stratification columns are available</i>
--	---

Description

Check whether stratification columns are available

Usage

```
check_stratification_columns_available(data, stratify, type = "observation")
```

Arguments

data	‘data.frame’ with observation or simulation data
stratify	vector of stratification columns
type	either ‘observation’ or ‘simulation’

compute_kaplan	<i>Compute Kaplan-Meier statistics</i>
----------------	--

Description

Compute Kaplan-Meier statistics

Usage

```
compute_kaplan(
  dat,
  strat = "strat",
  reverse_prob = FALSE,
  rtte_conditional = TRUE,
  ci = NULL
)
```

Arguments

dat	data.frame with events
strat	vector of stratification variables
reverse_prob	reverse the probability (i.e. return '1-probability')?
rtte_conditional	'TRUE' (default) or 'FALSE'. Compute the probability for each event newly ('TRUE'), or calculate the absolute probability ('FALSE', i.e. the "probability of a 1st, 2nd, 3rd event etc" rather than the "probability of an event happening").
ci	confidence interval to calculate, numeric vector of length 2

compute_kmmc	<i>Compute KMMC statistics</i>
--------------	--------------------------------

Description

Kaplan-Meier Mean Covariate plots are a simulation-based diagnostic to study the influence of covariates and identify potential model misspecification.

Usage

```
compute_kmmc(dat, strat = NULL, reverse_prob = FALSE, kmmc = "DOSE")
```

Arguments

dat	data.frame with events
strat	vector of stratification variables
reverse_prob	reverse the probability (i.e. return '1-probability')?
kmmc	variable to create the KMMC plot for.

create_vpc_theme	Create new vpc theme
------------------	----------------------

Description

Create new vpc theme

Usage

create_vpc_theme(...)

Arguments

... pass arguments to 'new_vpc_theme'

define_data_columns	Define data column defaults for various softwares
---------------------	---

Description

Define data column defaults for various softwares

Usage

define_data_columns(sim, obs, sim_cols, obs_cols, software_type)

Arguments

- | | |
|---------------|---|
| sim | simulated data |
| obs | observed data |
| sim_cols | list for mapping simulation data columns, e.g. 'list(dv = "DV", id = "ID", idv = "TIME", pred="PRED")' |
| obs_cols | list for mapping observation data columns, e.g. 'list(dv = "DV", id = "ID", idv = "TIME", pred="PRED")' |
| software_type | software type, one of 'nonmem', 'phoenix', 'PKPDsim' |

draw_params_mvr	<i>Draw parameters from multivariate distribution</i>
-----------------	---

Description

Draw parameters from multivariate distribution

Usage

```
draw_params_mvr(ids, n_sim, theta, omega_mat, par_names = NULL)
```

Arguments

ids	vector of id numbers
n_sim	number of simulations
theta	theta vector
omega_mat	omega matrix
par_names	parameter names vector

loq_perc	<i>Calculate percentiles below / above lloq / uloq</i>
----------	--

Description

Calculate percentiles below / above lloq / uloq

Usage

```
loq_perc(x, limit = 1, cens = "left")
```

Arguments

x	data
limit	censoring limit
cens	censoring direction (left/right)

new_vpc_theme	<i>Create a customized VPC theme</i>
---------------	--------------------------------------

Description

Create a customized VPC theme

Usage

```
new_vpc_theme(update = NULL)
```

Arguments

update	list containing the plot elements to be updated. Run 'new_vpc_theme()' with no arguments to show an overview of available plot elements.
--------	--

Details

This function creates a theme that customizes how the VPC looks, i.e. colors, fills, transparencies, linetypes and sizes, etc. The following arguments can be specified in the input list:

- obs_color: color for observations points
- obs_size: size for observation points
- obs_median_color: color for median observation line
- obs_median_linetype: linetype for median observation line
- obs_median_size: size for median observation line
- obs_ci_fill: color for observation CI fill
- obs_ci_color: color for observation CI lines
- obs_ci_linetype: linetype for observation CI lines
- obs_ci_size: size for observations CI lines
- sim_pi_fill: fill color for simulated prediction interval areas
- sim_pi_alpha: transparency for simulated prediction interval areas
- sim_pi_color: color for simulated prediction interval lines
- sim_pi_linetype: linetype for simulated prediction interval lines
- sim_pi_size: size for simulated prediction interval lines
- sim_median_fill: fill color for simulated median area
- sim_median_alpha: transparency for simulated median area
- sim_median_color: color for simulated median line
- sim_median_linetype: linetype for simulated median line
- sim_median_size: size for simulated median line
- bin_separators_color: color for bin separator lines, NA for don't plot
- bin_separators_location: where to plot bin separators ("t" for top, "b" for bottom)
- loq_color: color of line showing limit of quantification

Value

A list with vpc theme specifiers

Examples

```
theme1 <- new_vpc_theme(update = list(
  obs_color = "red",
  obs_ci_color = "#aa0000",
  obs_alpha = .3,
  sim_pi_fill = "#cc8833",
  sim_pi_size = 2
))
vpc(simple_data$sim, simple_data$obs, vpc_theme = theme1)
```

pk_iv_1cmt

Simulate PK data from a 1-compartment iv model

Description

Simulate PK data from a 1-compartment iv model

Usage

```
pk_iv_1cmt(
  t,
  t_inf = 1,
  tau = 24,
  dose = 120,
  CL = 0.345,
  Vc = 1.75,
  ruv = NULL
)
```

Arguments

t	Time after dose
t_inf	Infusion length
tau	Dosing interval
dose	Dose
CL	Clearance
Vc	Volume of distribution
ruv	Residual variability

Value

A vector of predicted values, with or without added residual variability

Examples

```
dat1 <- vpc::pk_iv_1cmt(t = c(0:72), tau = 24, dose = 120,
  CL = 5, Vc = 50)
dat2 <- vpc::pk_iv_1cmt(t = c(0:72), tau = 24, dose = 120,
  CL = 5, Vc = 50,
  ruv = list(proportional = 0.1, additive = 0.1))
```

pk_oral_1cmt

*Simulate PK data from a 1-compartment oral model***Description**

Simulate PK data from a 1-compartment oral model

Usage

```
pk_oral_1cmt(t, tau = 24, dose = 120, ka = 1, ke = 1, cl = 10, ruv = NULL)
```

Arguments

t	Time after dose
tau	Dosing interval
dose	Dose
ka	Absorption rate
ke	Elimination rate
cl	Clearance
ruv	Residual variability

Value

A vector of predicted values, with or without added residual variability

Examples

```
dat1 <- vpc::pk_oral_1cmt(t = c(0:72), tau = 24, dose = 120,
  ka = 1, ke = 1, cl = 10)
dat2 <- vpc::pk_oral_1cmt(t = c(0:72), tau = 24, dose = 120,
  ka = 1, ke = 1, cl = 10,
  ruv = list(proportional = 0.1, additive = 0.1))
```

plot_vpc	<i>VPC plotting function</i>
----------	------------------------------

Description

This function performs no parsing of data, it just plots the already calculated statistics generated using one of the 'vpc' functions.

Usage

```
plot_vpc(
  db,
  show = NULL,
  vpc_theme = NULL,
  smooth = TRUE,
  log_x = FALSE,
  log_y = FALSE,
  xlab = NULL,
  ylab = NULL,
  title = NULL,
  verbose = FALSE
)
```

Arguments

db	object created using the 'vpc' function
show	what to show in VPC (obs_dv, obs_ci, pi, pi_as_area, pi_ci, obs_median, sim_median, sim_median_ci)
vpc_theme	theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()
smooth	"smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.
log_x	Boolean indicting whether x-axis should be shown as logarithmic. Default is FALSE.
log_y	Boolean indicting whether y-axis should be shown as logarithmic. Default is FALSE.
xlab	label for x axis
ylab	label for y axis
title	title
verbose	verbosity (T/F)

See Also

[sim_data](#), [vpc_cens](#), [vpc_tte](#), [vpc_cat](#)

Examples

```
## See vpc.ronkeizer.com for more documentation and examples

library(vpc)
vpc_db <- vpc(sim = simple_data$sim, obs = simple_data$obs, vpcdb = TRUE)
plot_vpc(vpc_db, title = "My new vpc", x = "Custom x label")
```

quantile_cens	<i>Calculate quantiles respecting the censored data</i>
---------------	---

Description

Calculate quantiles respecting the censored data

Usage

```
quantile_cens(x, p = 0.5, limit = 1, cens = "left")
```

Arguments

x	data
p	quantile
limit	censoring limit
cens	censoring direction (left/right)

read_table_nm	<i>NONMEM output table import function</i>
---------------	--

Description

Quickly import NONMEM output tables into R. Function taken from ‘modelviz’ package by Benjamin Guiastrennec. When both skip and header are NULL, read_nmstab will automatically detect the optimal settings to import the tables. When more than one files are provided for a same NONMEM run, they will be combined into a single data.frame.

Usage

```
read_table_nm(
  file = NULL,
  skip = NULL,
  header = NULL,
  rm_duplicates = FALSE,
  nonmem_tab = TRUE
)
```

Arguments

file	full file name
skip	number of lines to skip before reading data
header	logical value indicating whether the file contains the names of the variables as its first line
rm_duplicates	logical value indicating whether duplicated columns should be removed
nonmem_tab	logical value indicating to the function whether the file is a table or a nonmem additional output file.

Value

A data.frame

Examples

```
## Not run:  
data <- read_table_nm(file = '../models/pk/sdtab101')  
  
## End(Not run)
```

replace_list_elements *Replace list elements by name*

Description

Replace list elements by name

Usage

```
replace_list_elements(list, replacement)
```

Arguments

list	original list
replacement	replacement list

Details

Finds and replaces list elements by name and throws an error if an element is not available in the original list. This is a local duplicate of the PKPDmisc copy for the VPC package to reduce dependency on PKPDmisc at this time.

Examples

```
## Not run:
list <- list(ipred = "ipred", dv = "dv", idv = "idv", "pred" = "pred")
replacement <- list(dv = "conc", idv = "time")
list <- replace_list_elements(list, replacement)

## End(Not run)
```

rtte_obs_nm	<i>Simulated RTTE data (1x)</i>
-------------	---------------------------------

Description

An example dataset with simulated repeated time-to-event data

Usage

```
rtte_obs_nm
```

Format

An object of class `data.frame` with 573 rows and 6 columns.

rtte_sim_nm	<i>Simulated RTTE data (100x)</i>
-------------	-----------------------------------

Description

An example dataset with simulated repeated time-to-event data (100 simulations)

Usage

```
rtte_sim_nm
```

Format

An object of class `data.frame` with 2000000 rows and 7 columns.

show_default	<i>Defaults for show argument</i>
--------------	-----------------------------------

Description

Defaults for show argument

Usage

show_default

Format

An object of class list of length 11.

show_default_tte	<i>Defaults for show argument for TTE VPC</i>
------------------	---

Description

Defaults for show argument for TTE VPC

Usage

show_default_tte

Format

An object of class list of length 11.

simple_data	<i>A small rich dataset</i>
-------------	-----------------------------

Description

A small rich dataset

Usage

simple_data

Format

An object of class list of length 2.

Details

a list containing the obs and sim data for an example dataset to run a simple vpc.

Examples

```
## Not run:
vpc(sim_data$sim, sim_data$obs)

## End(Not run)
```

sim_data

Simulate data based on a model and parameter distributions

Description

Simulate data based on a model and parameter distributions

Usage

```
sim_data(
  design = cbind(id = c(1, 1, 1), idv = c(0, 1, 2)),
  model = function(x) { return(x$alpha + x$beta) },
  theta,
  omega_mat,
  par_names,
  par_values = NULL,
  draw_iiv = "mvrnorm",
  error = list(proportional = 0, additive = 0, exponential = 0),
  n = 100
)
```

Arguments

design	a design dataset. See example
model	A function with the first argument the simulation design, i.e. a dataset with the columns ... The second argument to this function is a dataset with parameters for every individual. This can be supplied by the user, or generated by this sim_data if theta and omega_mat are supplied.
theta	vector of fixed effect parameters
omega_mat	vector of between subject random effects, specified as lower triangle
par_names	A character vector linking the parameters in the model to the variables in the dataset. See example.
par_values	parameter values
draw_iiv	draw between subject random effects?
error	see example
n	number of simulations to perform

Details

This function generates the simulated dependent values for use in the VPC plotting function.

Value

a vector of simulated dependent variables (for use in the VPC plotting function)

See Also

[vpc](#)

theme_empty	<i>Empty ggplot2 theme</i>
-------------	----------------------------

Description

Empty ggplot2 theme

Usage

```
theme_empty()
```

Examples

```
vpc(simple_data$sim, simple_data$obs) + theme_empty()
```

theme_plain	<i>A nicer default theme for ggplot2</i>
-------------	--

Description

A nicer default theme for ggplot2

Usage

```
theme_plain()
```

Examples

```
vpc(simple_data$sim, simple_data$obs) + theme_plain()
```

triangle_to_full	<i>Lower to full triangle</i>
------------------	-------------------------------

Description

Convert the lower triangle of a covariance matrix to a full matrix object

Usage

```
triangle_to_full(vect)
```

Arguments

vect	the lower triangle of a covariance matrix
------	---

vpc	<i>VPC function</i>
-----	---------------------

Description

Creates a VPC plot from observed and simulation data

Usage

```
vpc(sim, ...)
```

Default S3 method:

```
vpc(sim, ...)
```

```
vpc_vpc(
  sim = NULL,
  obs = NULL,
  psn_folder = NULL,
  bins = "jenks",
  n_bins = "auto",
  bin_mid = "mean",
  obs_cols = NULL,
  sim_cols = NULL,
  software = "auto",
  show = NULL,
  stratify = NULL,
  pred_corr = FALSE,
  pred_corr_lower_bnd = 0,
  pi = c(0.05, 0.95),
  ci = c(0.05, 0.95),
```

```

    uloc = NULL,
    lloc = NULL,
    log_y = FALSE,
    log_y_min = 0.001,
    xlab = NULL,
    ylab = NULL,
    title = NULL,
    smooth = TRUE,
    vpc_theme = NULL,
    facet = "wrap",
    scales = "fixed",
    labeller = NULL,
    vpcdb = FALSE,
    verbose = FALSE,
    ...
  )

```

Arguments

<code>sim</code>	this is usually a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm . However it can also be an object like a nlmixr or xpose object
<code>...</code>	Other arguments sent to other methods (like xpose or nlmixr); Note these arguments are not used in the default vpc and are ignored by the default method.
<code>obs</code>	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
<code>psn_folder</code>	instead of specifying "sim" and "obs", specify a PsN-generated VPC-folder
<code>bins</code>	either "density", "time", or "data", "none", or one of the approaches available in <code>classInterval()</code> such as "jenks" (default) or "pretty", or a numeric vector specifying the bin separators.
<code>n_bins</code>	when using the "auto" binning method, what number of bins to aim for
<code>bin_mid</code>	either "mean" for the mean of all timepoints (default) or "middle" to use the average of the bin boundaries.
<code>obs_cols</code>	observation dataset column names (list elements: "dv", "idv", "id", "pred")
<code>sim_cols</code>	simulation dataset column names (list elements: "dv", "idv", "id", "pred", "sim")
<code>software</code>	name of software platform using (e.g. nonmem, phoenix)
<code>show</code>	what to show in VPC (obs_dv, obs_ci, pi, pi_as_area, pi_ci, obs_median, sim_median, sim_median_ci)
<code>stratify</code>	character vector of stratification variables. Only 1 or 2 stratification variables can be supplied.
<code>pred_corr</code>	perform prediction-correction?
<code>pred_corr_lower_bnd</code>	lower bound for the prediction-correction

pi	simulated prediction interval to plot. Default is c(0.05, 0.95),
ci	confidence interval to plot. Default is (0.05, 0.95)
uloq	Number or NULL indicating upper limit of quantification. Default is NULL.
lloq	Number or NULL indicating lower limit of quantification. Default is NULL.
log_y	Boolean indicating whether y-axis should be shown as logarithmic. Default is FALSE.
log_y_min	minimal value when using log_y argument. Default is 1e-3.
xlab	label for x axis
ylab	label for y axis
title	title
smooth	"smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.
vpc_theme	theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()
facet	either "wrap", "columns", or "rows"
scales	either "fixed" (default), "free_y", "free_x" or "free"
labeller	ggplot2 labeller function to be passed to underlying ggplot object
vpcdb	Boolean whether to return the underlying vpcdb rather than the plot
verbose	show debugging information (TRUE or FALSE)

Value

a list containing calculated VPC information (when vpcdb=TRUE), or a ggplot2 object (default)

See Also

[sim_data](#), [vpc_cens](#), [vpc_tte](#), [vpc_cat](#)

Examples

```
## See vpc.ronkeizer.com for more documentation and examples
library(vpc)

# Basic commands:
vpc(sim = simple_data$sim, obs = simple_data$obs)
vpc(sim = simple_data$sim, obs = simple_data$obs, lloq = 20)
```

vpc_cat

*VPC function for categorical***Description**

Creates a VPC plot from observed and simulation data for categorical variables.

Usage

```
vpc_cat(
  sim = NULL,
  obs = NULL,
  psn_folder = NULL,
  bins = "jenks",
  n_bins = "auto",
  bin_mid = "mean",
  obs_cols = NULL,
  sim_cols = NULL,
  software = "auto",
  show = NULL,
  ci = c(0.05, 0.95),
  uloq = NULL,
  lloq = NULL,
  xlab = NULL,
  ylab = NULL,
  title = NULL,
  smooth = TRUE,
  vpc_theme = NULL,
  facet = "wrap",
  labeller = NULL,
  plot = TRUE,
  vpcdb = FALSE,
  verbose = FALSE
)
```

Arguments

sim	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
obs	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
psn_folder	instead of specifying "sim" and "obs", specify a PsN-generated VPC-folder
bins	either "density", "time", or "data", "none", or one of the approaches available in <code>classInterval()</code> such as "jenks" (default) or "pretty", or a numeric vector specifying the bin separators.

n_bins	when using the "auto" binning method, what number of bins to aim for
bin_mid	either "mean" for the mean of all timepoints (default) or "middle" to use the average of the bin boundaries.
obs_cols	observation dataset column names (list elements: "dv", "idv", "id", "pred")
sim_cols	simulation dataset column names (list elements: "dv", "idv", "id", "pred")
software	name of software platform using (e.g. nonmem, phoenix)
show	what to show in VPC (obs_ci, pi, pi_as_area, pi_ci, obs_median, sim_median, sim_median_ci)
ci	confidence interval to plot. Default is (0.05, 0.95)
uloq	Number or NULL indicating upper limit of quantification. Default is NULL.
lloq	Number or NULL indicating lower limit of quantification. Default is NULL.
xlab	label for x-axis
ylab	label for y-axis
title	title
smooth	"smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.
vpc_theme	theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()
facet	either "wrap", "columns", or "rows"
labeller	ggplot2 labeller function to be passed to underlying ggplot object
plot	Boolean indicting whether to plot the ggplot2 object after creation. Default is FALSE.
vpcdb	boolean whether to return the underlying vpcdb rather than the plot
verbose	show debugging information (TRUE or FALSE)

Value

a list containing calculated VPC information (when vpcdb=TRUE), or a ggplot2 object (default)

See Also

[sim_data](#), [vpc](#), [vpc_tte](#), [vpc_cens](#)

Examples

```
## See vpc.ronkeizer.com for more documentation and examples
library(vpc)

# simple function to simulate categorical data for single individual
sim_id <- function(id = 1) {
  n <- 10
  logit <- function(x) exp(x) / (1+exp(x))
  data.frame(id = id, time = seq(1, n, length.out = n),
             dv = round(logit((1:n) - n/2 + rnorm(n, 0, 1.5))) )
}
```

```

}
## simple function to simulate categorical data for a trial
sim_trial <- function(i = 1, n = 20) { # function to simulate categorical data for a trial
  data.frame(sim = i, do.call("rbind", lapply(1:n, sim_id)))
}

## simulate single trial for 20 individuals
obs <- sim_trial(n = 20)

## simulate 200 trials of 20 individuals
sim <- do.call("rbind", lapply(1:200, sim_trial, n = 20))

## Plot categorical VPC
vpc_cat(sim = sim, obs = obs)

```

vpc_cens

VPC function for left- or right-censored data (e.g. BLOQ data)

Description

Creates a VPC plot from observed and simulation data for censored data. Function can handle both left- (below lower limit of quantification) and right-censored (above upper limit of quantification) data.

Usage

```

vpc_cens(
  sim = NULL,
  obs = NULL,
  psn_folder = NULL,
  bins = "jenks",
  n_bins = 8,
  bin_mid = "mean",
  obs_cols = NULL,
  sim_cols = NULL,
  software = "auto",
  show = NULL,
  stratify = NULL,
  stratify_color = NULL,
  ci = c(0.05, 0.95),
  uloq = NULL,
  lloq = NULL,
  plot = FALSE,
  xlab = "Time",
  ylab = "Probability of <LOQ",
  title = NULL,
  smooth = TRUE,
  vpc_theme = NULL,

```

```

    facet = "wrap",
    labeller = NULL,
    vpcdb = FALSE,
    verbose = FALSE
  )

```

Arguments

sim	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
obs	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
psn_folder	instead of specifying "sim" and "obs", specify a PsN-generated VPC-folder
bins	either "density", "time", or "data", or a numeric vector specifying the bin separators.
n_bins	number of bins
bin_mid	either "mean" for the mean of all timepoints (default) or "middle" to use the average of the bin boundaries.
obs_cols	observation dataset column names (list elements: "dv", "idv", "id", "pred")
sim_cols	simulation dataset column names (list elements: "dv", "idv", "id", "pred")
software	name of software platform using (e.g. nonmem, phoenix)
show	what to show in VPC (obs_ci, pi, pi_as_area, pi_ci, obs_median, sim_median, sim_median_ci)
stratify	character vector of stratification variables. Only 1 or 2 stratification variables can be supplied.
stratify_color	variable to stratify and color lines for observed data. Only 1 stratification variables can be supplied.
ci	confidence interval to plot. Default is (0.05, 0.95)
uloq	Number or NULL indicating upper limit of quantification. Default is NULL.
lloq	Number or NULL indicating lower limit of quantification. Default is NULL.
plot	Boolean indicating whether to plot the ggplot2 object after creation. Default is FALSE.
xlab	ylab as numeric vector of size 2
ylab	ylab as numeric vector of size 2
title	title
smooth	"smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.
vpc_theme	theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()
facet	either "wrap", "columns", or "rows"
labeller	ggplot2 labeller function to be passed to underlying ggplot object
vpcdb	boolean whether to return the underlying vpcdb rather than the plot
verbose	show debugging information (TRUE or FALSE)

Value

a list containing calculated VPC information, and a ggplot2 object

See Also

[sim_data](#), [vpc](#), [vpc_tte](#), [vpc_cat](#)

Examples

```
## See vpc.ronkeizer.com for more documentation and examples
library(vpc)

vpc_cens(sim = simple_data$sim, obs = simple_data$obs, lloq = 30)
vpc_cens(sim = simple_data$sim, obs = simple_data$obs, uloq = 120)
```

vpc_tte

VPC function for time-to-event (survival) data

Description

This function can be used for either single time-to-event (TTE) or repeated time-to-event (RTTE) data.

Usage

```
vpc_tte(
  sim = NULL,
  obs = NULL,
  psn_folder = NULL,
  rtte = FALSE,
  rtte_calc_diff = TRUE,
  rtte_conditional = TRUE,
  events = NULL,
  bins = FALSE,
  n_bins = 10,
  software = "auto",
  obs_cols = NULL,
  sim_cols = NULL,
  kmmc = NULL,
  reverse_prob = FALSE,
  stratify = NULL,
  stratify_color = NULL,
  ci = c(0.05, 0.95),
  plot = FALSE,
  xlab = "Time",
  ylab = "Survival (%)",
```

```

    show = NULL,
    as_percentage = TRUE,
    title = NULL,
    smooth = FALSE,
    vpc_theme = NULL,
    facet = "wrap",
    labeller = NULL,
    verbose = FALSE,
    vpcdb = FALSE
  )

```

Arguments

<code>sim</code>	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
<code>obs</code>	a data.frame with observed data, containing the independent and dependent variable, a column indicating the individual, and possibly covariates. E.g. load in from NONMEM using read_table_nm
<code>psn_folder</code>	instead of specifying "sim" and "obs", specify a PsN-generated VPC-folder
<code>rtte</code>	repeated time-to-event data? Default is FALSE (treat as single-event TTE)
<code>rtte_calc_diff</code>	recalculate time (T/F)? When simulating in NONMEM, you will probably need to set this to TRUE to recalculate the TIME to relative times between events (unless you output the time difference between events and specify that as independent variable to the <code>vpc_tte()</code> function.
<code>rtte_conditional</code>	'TRUE' (default) or 'FALSE'. Compute the probability for each event newly ('TRUE'), or calculate the absolute probability ('FALSE', i.e. the "probability of a 1st, 2nd, 3rd event etc" rather than the "probability of an event happening").
<code>events</code>	numeric vector describing which events to show a VPC for when repeated TTE data, e.g. <code>c(1:4)</code> . Default is NULL, which shows all events.
<code>bins</code>	either "density", "time", or "data", or a numeric vector specifying the bin separators.
<code>n_bins</code>	number of bins
<code>software</code>	name of software platform using (e.g. nonmem, phoenix)
<code>obs_cols</code>	observation dataset column names (list elements: "dv", "idv", "id", "pred")
<code>sim_cols</code>	simulation dataset column names (list elements: "dv", "idv", "id", "pred", "sim")
<code>kmmc</code>	either NULL (for regular TTE vpc, default), or a variable name for a KMMC plot (e.g. "WT")
<code>reverse_prob</code>	reverse the probability scale (i.e. plot 1-probability)
<code>stratify</code>	character vector of stratification variables. Only 1 or 2 stratification variables can be supplied.
<code>stratify_color</code>	character vector of stratification variables. Only 1 stratification variable can be supplied, cannot be used in conjunction with 'stratify'.

ci	confidence interval to plot. Default is (0.05, 0.95)
plot	Boolean indicating whether to plot the ggplot2 object after creation. Default is FALSE.
xlab	label for x-axis
ylab	label for y-axis
show	what to show in VPC (obs_ci, obs_median, sim_median, sim_median_ci)
as_percentage	Show y-scale from 0-100 percent? TRUE by default, if FALSE then scale from 0-1.
title	title
smooth	"smooth" the VPC (connect bin midpoints) or show bins as rectangular boxes. Default is TRUE.
vpc_theme	theme to be used in VPC. Expects list of class vpc_theme created with function vpc_theme()
facet	either "wrap", "columns", or "rows"
labeller	ggplot2 labeller function to be passed to underlying ggplot object
verbose	TRUE or FALSE (default)
vpcdb	Boolean whether to return the underlying vpcdb rather than the plot

Details

Creates a VPC plot from observed and simulation survival data

Value

a list containing calculated VPC information, and a ggplot2 object

See Also

[sim_data](#), [vpc](#), [vpc_tte](#), [vpc_cens](#)

Examples

```
## See vpc-docs.ronkeizer.com for more documentation and examples.

## Example for repeated) time-to-event data
## with NONMEM-like data (e.g. simulated using a dense grid)

data(rtte_obs_nm)
data(rtte_sim_nm)

# treat RTTE as TTE, no stratification
vpc_tte(sim = rtte_sim_nm[rtte_sim_nm$sim <= 20,],
        obs = rtte_obs_nm,
        rtte = FALSE,
        sim_cols=list(dv = "dv", idv = "t"), obs_cols=list(idv = "t"))
```

Index

- * **aggregate functions**
 - sim_data, [17](#)
- * **datasets**
 - rtte_obs_nm, [15](#)
 - rtte_sim_nm, [15](#)
 - show_default, [16](#)
 - show_default_tte, [16](#)
 - simple_data, [16](#)
- add_noise, [3](#)
- add_sim_index_number, [3](#)
- add_stratification, [4](#)
- auto_bin, [4](#)
- bin_data, [5](#)
- check_stratification_columns_available,
[5](#)
- compute_kaplan, [6](#)
- compute_kmmc, [6](#)
- create_vpc_theme, [7](#)
- define_data_columns, [7](#)
- draw_params_mvr, [8](#)
- loq_perc, [8](#)
- new_vpc_theme, [9](#)
- pk_iv_1cmt, [10](#)
- pk_oral_1cmt, [11](#)
- plot_vpc, [12](#)
- quantile_cens, [13](#)
- read_table_nm, [13](#), [20](#), [22](#), [25](#), [27](#)
- replace_list_elements, [14](#)
- rtte_obs_nm, [15](#)
- rtte_sim_nm, [15](#)
- show_default, [16](#)
- show_default_tte, [16](#)
- sim_data, [12](#), [17](#), [21](#), [23](#), [26](#), [28](#)
- simple_data, [16](#)
- theme_empty, [18](#)
- theme_plain, [18](#)
- triangle_to_full, [19](#)
- vpc, [18](#), [19](#), [23](#), [26](#), [28](#)
- vpc-package, [2](#)
- vpc_cat, [12](#), [21](#), [22](#), [26](#)
- vpc_cens, [12](#), [21](#), [23](#), [24](#), [28](#)
- vpc_tte, [12](#), [21](#), [23](#), [26](#), [26](#), [28](#)
- vpc_vpc (vpc), [19](#)