

Package ‘tidyvpc’

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Type Package

Title VPC Percentiles and Prediction Intervals

Version 1.6.0

Description Perform a Visual Predictive Check (VPC), while accounting for stratification, censoring, and prediction correction. Using piping from 'magrittr', the intuitive syntax gives users a flexible and powerful method to generate VPCs using both traditional binning and a new binless approach Jansen et al. (2018) <[doi:10.1002/psp4.12319](https://doi.org/10.1002/psp4.12319)> with Additive Quantile Regression (AQR) and Locally Estimated Scatterplot Smoothing (LOESS) prediction correction.

URL <https://github.com/certara/tidyvpc>

BugReports <https://github.com/certara/tidyvpc/issues>

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bininfo	<i>Obtain information about the bins from a tidyvpcobj</i>
---------	--

Description

Obtain information about the bins from a tidyvpcobj

Usage

```
bininfo(o, ...)

## S3 method for class 'tidyvpcobj'
bininfo(o, by.strata = o$bin.by.strata, ...)
```

Arguments

<code>o</code>	An object.
<code>...</code>	Additional arguments.
<code>by.strata</code>	Should the calculations be done by strata? Defaults to what was specified when the binning was done.

Value

A ‘data.table’ containing the following columns:

- `nobs`: Number of observed data points in the bin
- `xmedian`: Median x-value of the observed data points in the bin
- `xmean`: Mean x-value of the observed data points in the bin
- `xmax`: Maximum x-value of the observed data points in the bin
- `xmin`: Minimum x-value of the observed data points in the bin
- `xmid`: Value halfway between ‘`xmin`’ and ‘`xmax`’. x-value of the observed data points in the bin
- `xleft`: Value halfway between the minimum x-value of the current bin and the maximum x-value of the previous bin to the left (for the left-most bin, it is the minimum x-value).
- `xright`: Value halfway between the maximum x-value of the current bin and the minimum x-value of the next bin to the right (for the right-most bin, it is the maximum x-value).
- `xcenter`: Value halfway between ‘`xleft`’ and ‘`xright`’.

In addition, if stratification was performed, the stratification columns will be included as well.

Methods (by class)

- `bininfo(tidyvpcobj)`: Method for `tidyvpcobj`.

binless

Perform binless Visual Predictive Check (VPC)

Description

Use this function in place of traditional binning methods to derive VPC. For continuous VPC, this is obtained using additive quantile regression (`quantreg::rqss()`) and LOESS for pcVPC. While for categorical VPC, this is obtained using a generalized additive model (`gam(family = "binomial")`).

Usage

```
binless(o, ...)

## S3 method for class 'tidyvcobj'
binless(
  o,
  optimize = TRUE,
  optimization.interval = c(0, 7),
  loess.ypc = NULL,
  lambda = NULL,
  span = NULL,
  sp = NULL,
  ...
)
```

Arguments

<code>o</code>	A <code>tidyvcobj</code> .
<code>...</code>	Other arguments to include will be ignored.
<code>optimize</code>	Logical indicating whether smoothing parameters should be optimized using AIC.
<code>optimization.interval</code>	Numeric vector of length 2 specifying the min/max range of smoothing parameter for optimization. Only applicable if <code>optimize = TRUE</code> .
<code>loess.ypc</code>	(Deprecated) Argument is ignored. For a LOESS pcVPC using the ‘binless’ method, usage of predcorrect will automatically perform LOESS prediction correction.
<code>lambda</code>	Numeric vector of length 3 specifying lambda values for each quantile. If stratified, specify a <code>data.frame</code> with given strata represented the column name, and value specified as a numeric vector of length 3. See below examples. Only applicable to continuous VPC with <code>optimize = FALSE</code> .
<code>span</code>	Numeric between 0,1 specifying smoothing parameter for LOESS prediction correction. Only applicable for continuous VPC with <code>optimize = FALSE</code> and usage of predcorrect .
<code>sp</code>	List of smoothing parameters applied to <code>mgcv::gam()</code> . Elements of list must be in the same order as unique values of DV. If one or more stratification variables present, the order of <code>sp</code> should be specified as unique combination of strata + DV, in ascending order. See below examples. Only applicable for categorical VPC, if <code>optimize = FALSE</code> .

Value

For continuous VPC, updates `tidyvcobj` with additive quantile regression fits for observed and simulated data for quantiles specified in the `qpred` argument of `vcstats()`. If the `optimize = TRUE` argument is specified, the resulting `tidyvcobj` will contain optimized lambda values according to AIC. For prediction corrected VPC (pcVPC), specifying `loess.ypc = TRUE` will return optimized span value for LOESS smoothing. For categorical VPC, updates `tidyvcobj` with fits

obtained by `gam(family="binomial")` for observed and simulated data for each category of DV (in each stratum if `stratify` defined). If `optimize = TRUE` argument is specified, the resulting `tidyvpcojb` will contain optimized `sp` values according to AIC.

See Also

[observed](#) [simulated](#) [censoring](#) [predcorrect](#) [stratify](#) [binning](#) [vpcstats](#)

Examples

```
require(magrittr)
require(data.table)

obs_data <- obs_data[MDV == 0]
sim_data <- sim_data[MDV == 0]

vpc <- observed(obs_data, y = DV, x = TIME) %>%
  simulated(sim_data, y = DV) %>%
  binless() %>%
  vpcstats()

# Binless example with LOESS prediction correction
obs_data$PRED <- sim_data[REP == 1, PRED]

vpc <- observed(obs_data, y = DV, x = TIME) %>%
  simulated(sim_data, y = DV) %>%
  binless(optimize = TRUE) %>%
  predcorrect(pred = PRED) %>%
  vpcstats()

# Binless example with user specified lambda values stratified on
# "GENDER" with 2 levels ("M", "F"), 10%, 50%, 90% quantiles.

lambda_strat <- data.table(
  GENDER_M = c(3,5,2),
  GENDER_F = c(1,3,4)
)

vpc <- observed(obs_data, y = DV, x = TIME) %>%
  simulated(sim_data, y = DV) %>%
  stratify(~ GENDER) %>%
  binless(optimize = FALSE, lambda = lambda_strat) %>%
  vpcstats(qpred = c(0.1, 0.5, 0.9))

# Binless example for categorical DV with optimized smoothing
vpc <- observed(obs_cat_data, x = agemoths, yobs = zlencat) %>%
  simulated(sim_cat_data, ysim = DV) %>%
  stratify(~ Country_ID_code) %>%
  binless() %>%
```

```

vpcstats(vpc.type = "cat", quantile.type = 6)

# Binless example for categorical DV with user specified sp values
user_sp <- list(
Country1_prob0 = 100,
Country1_prob1 = 3,
Country1_prob2 = 4,
Country2_prob0 = 90,
Country2_prob1 = 3,
Country2_prob2 = 4,
Country3_prob0 = 55,
Country3_prob1 = 3,
Country3_prob2 = 200)

vpc <- observed(obs_cat_data, x = agemoths, yobs = zlencat) %>%
  simulated(sim_cat_data, ysim = DV) %>%
  stratify(~ Country_ID_code) %>%
  binless(optimize = FALSE, sp = user_sp) %>%
  vpcstats(vpc.type = "categorical", conf.level = 0.9, quantile.type = 6)

```

binning

Binning methods for Visual Predictive Check (VPC)

Description

This function executes binning methods available in `classInt` e.g., "jenks", "kmeans", "sd", "pretty", "pam", "kmeans", "hclust", "bclust", "fisher", "dpih", "box", "headtails", and "maximum". You may also bin directly on x-variable or alternatively specify "centers" or "breaks". For explanation of binning methods see [classIntervals](#).

Usage

```

binning(o, ...)

## S3 method for class 'tidyvpcobj'
binning(
  o,
  bin,
  data = o$data,
  xbin = "xmedian",
  centers,
  breaks,
  nbins,
  altx,
  stratum = NULL,
  by.strata = TRUE,
  ...
)

```

Arguments

<code>o</code>	A tidyvpcobj.
<code>...</code>	Other arguments to include for <code>classIntervals</code> . See <code>...</code> usage for style in <code>?classIntervals</code> .
<code>bin</code>	Character string indicating binning method or unquoted variable name if binning on x-variable.
<code>data</code>	Observed data supplied in <code>observed()</code> function.
<code>xbin</code>	Character string indicating midpoint type for binning.
<code>centers</code>	Numeric vector of centers for binning. Use <code>bin = "centers"</code> , if supplying centers.
<code>breaks</code>	Numeric vector of breaks for binning. Use <code>bin = "breaks"</code> , if supplying breaks.
<code>nbins</code>	Numeric number indicating the number of bins to use.
<code>altx</code>	Unquoted variable name in observed data for alternative x-variable binning.
<code>stratum</code>	List indicating the name of stratification variable and level, if using different binning methods by strata.
<code>by.strata</code>	Logical indicating whether binning should be performed by strata.

Value

Updates `tidyvpcobj` with `data.frame` containing bin information including left/right boundaries and midpoint, as specified in `xbin` argument.

See Also

[observed](#) [simulated](#) [censoring](#) [predcorrect](#) [stratify](#) [binless](#) [vpcstats](#)

Examples

```
require(magrittr)

# Binning on x-variable NTIME
vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  binning(bin = NTIME) %>%
  vpcstats()

# Binning using ntile and xmean for midpoint
vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  binning(bin = "ntile", nbins = 8, xbin = "xmean") %>%
  vpcstats()

# Binning using centers
vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  binning(bin = "centers", centers = c(1,3,5,7)) %>%
  vpcstats()
```

```

# Different Binning for each level of Strata
vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  stratify(~ GENDER) %>%
  binning(stratum = list(GENDER = "M"), bin = "jenks", nbins = 5, by.strata = TRUE) %>%
  binning(stratum = list(GENDER = "F"), bin = "kmeans", nbins = 4, by.strata = TRUE) %>%
  vpcstats()

# Binning Categorical DV using rounded time variable

vpc <- observed(obs_cat_data, x = agemoths, y = zlencat ) %>%
  simulated(sim_cat_data, y = DV) %>%
  binning(bin = round(agemoths, 0)) %>%
  vpcstats(vpc.type = "categorical")

```

binningfunctions *Different functions that perform binning.*

Description

Different functions that perform binning.

Usage

```

cut_at(breaks)

nearest(centers)

bin_by_ntile(nbins)

bin_by_eqcut(nbins)

bin_by_pam(nbins)

bin_by_classInt(style, nbins = NULL)

```

Arguments

breaks	A numeric vector of values that designate cut points between bins.
centers	A numeric vector of values that designate the center of each bin.
nbins	The number of bins to split the data into.
style	a binning style (see classIntervals for details).

Value

Each of these functions returns a function of a single numeric vector 'x' that assigns each value of 'x' to a bin.

Examples

```
x <- c(rnorm(10, 1, 1), rnorm(10, 3, 2), rnorm(20, 5, 3))
centers <- c(1, 3, 5)
nearest(centers)(x)
```

```
breaks <- c(2, 4)
cut_at(breaks)(x)
```

```
bin_by_eqcut(nbins=4)(x)
bin_by_ntile(nbins=4)(x)
```

```
bin_by_pam(nbins=4)(x)
bin_by_classInt("pretty", nbins=4)(x)
```

censoring

Censoring observed data for Visual Predictive Check (VPC)

Description

Specify censoring variable or censoring value for VPC.

Usage

```
censoring(o, ...)
```

```
## S3 method for class 'tidyvpobj'
censoring(o, blq, lloq, alq, uloq, data = o$data, ...)
```

Arguments

o	A tidyvpobj.
...	Other arguments to include.
blq	blq variable if present in observed data.
lloq	Numeric value or numeric variable in data indicating the upper limit of quantification.
alq	Logical variable indicating above limit of quantification.
uloq	Numeric value or numeric variable in data indicating the upper limit of quantification.
data	Observed data supplied in observed() function.

Value

Updates obs data.frame in tidypcobj with censored values for observed data which includes lloq and uloq specified values for lower/upper limit of quantification. Logicals for blq and alq are returned that indicate whether the DV value lies below/above limit of quantification.

See Also

[observed](#) [simulated](#) [stratify](#) [predcorrect](#) [binning](#) [binless](#) [vpcstats](#)

Examples

```
require(magrittr)

vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  censoring(blq=(DV < 50), lloq=50) %>%
  binning(bin = "pam", nbins = 5) %>%
  vpcstats()

#Using LLOQ variable in data with different values of LLOQ by Study:

obs_data$LLOQ <- obs_data[, ifelse(STUDY == "Study A", 50, 25)]

vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  censoring(blq=(DV < LLOQ), lloq=LLOQ) %>%
  stratify(~ STUDY) %>%
  binning(bin = "kmeans", nbins = 4) %>%
  vpcstats()
```

check_order

Perform a consistency check on observed and simulated data

Description

This function performs a simple consistency check on an observed and simulated dataset to make sure they are consistent with respect to ordering as required by the other functions used in the VPC calculation.

Usage

```
check_order(obs, sim, tol = 1e-05)
```

Arguments

obs, sim	A 'data.frame' with 2 columns (see Details).
tol	A tolerance for comparing time values.

Details

The consistency check is performed by comparing a combination of unique subject identifier (ID) and time. Both data.frame objects must be given with those in positions 1 and 2, respectively.

Value

The number of replicates contained in 'sim'.

See Also

[observed](#), [simulated](#).

Examples

```
require(data.table)

check_order(obs_data[, .(ID, TIME)], sim_data[, .(ID, TIME)])
```

<code>generics</code>	<i>Perform a Visual Predictive Check (VPC) computation</i>
-----------------------	--

Description

These functions work together to calculate the statistics that are plotted in a VPC. They would typically be chained together using the "pipe" operator (see Examples).

Arguments

- `o` A tidyvpcobj.
- `...` Additional arguments.

<code>nopredcorrect</code>	<i>Remove prediction correction for Visual Predictive Check (VPC)</i>
----------------------------	---

Description

Optional function to use indicating no pred correction for VPC.

Usage

```
nopredcorrect(o, ...)

## S3 method for class 'tidyvpcobj'
nopredcorrect(o, ...)
```

Arguments

o A tidyvpcobj.
 ... Other arguments to include.

 npde

Normalized Prediction Distribution Errors

Description

Normalized Prediction Distribution Errors

Usage

```
npde(o, ...)
```

```
## S3 method for class 'tidyvpcobj'
```

```
npde(o, id, data = o$data, smooth = FALSE, ...)
```

Arguments

o A tidyvpcobj.
 ... Additional arguments.
 id A vector of IDs. Used to associate observations (y) that originate from the same individual. Evaluated in the data.frame data.
 data A data.frame.
 smooth Should a uniform random perturbation be used to smooth the pd/pde values?

References

Brendel, K., Comets, E., Laffont, C., Laveille, C. & Mentrée, F. Metrics for external model evaluation with an application to the population pharmacokinetics of gliclazide. *Pharm. Res.* (2006) 23(9), 2036–2049.

Nguyen, T.H.T., et al. Model evaluation of continuous data pharmacometric models: metrics and graphics. *CPT Pharmacometrics Syst. Pharmacol.* (2017) 6(2), 87–109; doi:10.1002/psp4.12161.

Examples

```
require(magrittr)
require(ggplot2)
```

```
obs <- obs_data[MDV==0]
sim <- sim_data[MDV==0]
```

```
npde <- observed(obs, x=NULL, y=DV) %>%
  simulated(sim, y=DV) %>%
  npde(id=ID)
```

```

vpc <- observed(npde$npdeobs, x=epred, y=npde) %>%
  simulated(npde$npdesim, y=npde) %>%
  binning("eqcut", nbins=10) %>%
  vpcstats()

plot(vpc) +
  labs(x="Simulation-based Population Prediction", y="Normalized Prediction Distribution Error")

```

observed

Specify observed dataset and variables for VPC

Description

The `observed` function is the first function in the `vpc` piping chain and is used for specifying observed data and variables for VPC. Note: Observed data must not contain missing DV and may require filtering `MDV == 0` before generating VPC. Also observed data must be ordered by: Subject (ID), IVAR (Time)

Usage

```

observed(o, ...)

## S3 method for class 'data.frame'
observed(
  o,
  x,
  yobs,
  pred = NULL,
  blq = NULL,
  lloq = -Inf,
  alq = NULL,
  uloq = Inf,
  ...
)

```

Arguments

<code>o</code>	A <code>data.frame</code> of observation data.
<code>...</code>	Other arguments.
<code>x</code>	Numeric x-variable, typically named <code>TIME</code> .
<code>yobs</code>	Numeric y-variable, typically named <code>DV</code> .
<code>pred</code>	Population prediction variable, typically named <code>PRED</code> .
<code>blq</code>	Logical variable indicating below limit of quantification.

lloq	Number or numeric variable in data indicating the lower limit of quantification.
alq	Logical variable indicating above limit of quantification .
uloq	Number or numeric variable in data indicating the upper limit of quantification.

Value

A tidyvpcobj containing both original data and observed data formatted with x and y variables as specified in function. Resulting data is of class data.frame and data.table.

See Also

[simulated censoring stratify predcorrect binning binless vpcstats](#)

Examples

```
obs_data <- obs_data[MDV == 0]
sim_data <- sim_data[MDV == 0]

vpc <- observed(obs_data, x=TIME, y=DV)
```

obs_cat_data

Example observed data with categorical DV

Description

An observed dataset with 3 levels of categorical DV.

Usage

```
obs_cat_data
```

Format

A data frame with 4014 rows and 4 variables:

PID_code Subject identifier

agemonths Time

zlencat Categorical DV with the 3 levels

Country_ID_code Country code for stratification

Source

Certara University

`obs_data`*Example observed data with continuous DV*

Description

An observed dataset from a hypothetical PK model, altered to include NTIME, GROUP, GENDER.

Usage`obs_data`**Format**

A data.table with 600 rows and 7 variables:

ID Subject identifier

TIME Time

DV Concentration of drug

AMT Amount of dosage initially administered at DV = 0, TIME = 0

DOSE Dosage amount

MDV Dummy indicating missing dependent variable value

NTIME Nominal Time

GENDER Character variable indicating subject's gender ("M", "F")

STUDY Character variable indicating study type ("Study A", "Study B")

Source

[simple_data](#)

`plot.tidyvpcobj`*Plot a tidyvpcobj*

Description

Use ggplot2 graphics to plot and customize the appearance of VPC.

Usage

```
## S3 method for class 'tidyvpcobj'
plot(
  x,
  facet = FALSE,
  show.points = TRUE,
  show.boundaries = TRUE,
  show.stats = !is.null(x$stats),
  show.binning = isFALSE(show.stats),
  xlab = NULL,
  ylab = NULL,
  color = c("red", "blue", "red"),
  linetype = c("dotted", "solid", "dashed"),
  point.alpha = 0.4,
  point.size = 1,
  point.shape = "circle-fill",
  point.stroke = 1,
  ribbon.alpha = 0.1,
  legend.position = "top",
  facet.scales = "free",
  custom.theme = NULL,
  censoring.type = c("none", "both", "blq", "alq"),
  censoring.output = c("grid", "list"),
  censoring.color = c(observed = "black", simulated = "red"),
  censoring.fill = "red",
  ...
)
```

Arguments

x	A tidyvpcobj.
facet	Set to TRUE to facet plot by quantile (continuous VPC) or category (categorical VPC).
show.points	Should the observed data points be plotted?
show.boundaries	Should the bin boundary be displayed?
show.stats	Should the VPC stats be displayed?
show.binning	Should the binning be displayed by coloring the observed data points by bin?
xlab	A character label for the x-axis.
ylab	A character label for the y-axis.
color	A character vector of colors for the percentiles, from low to high.
linetype	A character vector of line type for the percentiles, from low to high.
point.alpha	Numeric value specifying transparency of points.
point.size	Numeric value specifying size of point.

point.shape	Character one of "circle", "circle-fill", "diamond", "diamond-fill", "square", "square-fill", "triangle-fill", "triangle"). Defaults to "circle-fill".
point.stroke	Numeric value specifying size of point stroke.
ribbon.alpha	Numeric value specifying transparency of ribbon.
legend.position	A character string specifying the position of the legend. Options are "top", "bottom", "left", "right".
facet.scales	A character string specifying the scales argument to use for faceting. Options are "free", "fixed".
custom.theme	A custom ggplot2 theme supplied either as a character string, function, or object of class "theme".
censoring.type	A character string specifying additional blq/alq plots to include. Only applicable if censoring was performed.
censoring.output	A character string specifying whether to return percentage of blq/alq plots as an arranged "grid" or as elements in a "list". Only applicable if censoring.type != "none".
censoring.color	A named character vector of colors for the censoring plot lines. Names must include "observed" and "simulated". Default is c(observed = "black", simulated = "red"). Only applicable if censoring.type != "none".
censoring.fill	A character string specifying the fill color for the censoring plot ribbon. Default is "red". Only applicable if censoring.type != "none".
...	Additional arguments for ggarrange e.g., ncol and nrow. Only used if censoring.type != "none" and censoring.output == "grid".

Value

A ggplot object.

See Also

[ggplot](#)

predcorrect

Prediction corrected Visual Predictive Check (pcVPC)

Description

Specify prediction variable for pcVPC.

Usage

```
predcorrect(o, ...)
```

```
## S3 method for class 'tidyvpobj'
```

```
predcorrect(o, pred, data = o$data, ..., log = FALSE, varcorr = FALSE)
```

Arguments

o	A 'tidyvpobj'.
...	Other arguments to include.
pred	Prediction variable in observed data.
data	Observed data supplied in 'observed()' function.
log	Logical indicating whether DV was modeled in logarithmic scale.
varcorr	Logical indicating whether variability correction should be applied for prediction corrected dependent variable

Value

Updates 'tidyvpobj' with required information to perform prediction correction, which includes the 'predcor' logical indicating whether prediction corrected VPC is to be performed, the 'predcor.log' logical indicating whether the DV is on a log-scale, the 'varcorr' logical indicating whether variability correction for prediction corrected dependent variable is applied and the 'pred' prediction column from the original data. Both 'obs' and 'sim' data tables in the returned 'tidyvpobj' object have additional 'ypc' column with the results of prediction correction and 'ypcvc' column if variability correction is requested.

See Also

[observed simulated censoring stratify binning binless vpcstats](#)

Examples

```
require(magrittr)

obs_data <- obs_data[MDV == 0]
sim_data <- sim_data[MDV == 0]

# Add PRED variable to observed data from first replicate of
# simulated data

obs_data$PRED <- sim_data[REP == 1, PRED]

vpc <- observed(obs_data, x=TIME, yobs=DV) %>%
  simulated(sim_data, ysim=DV) %>%
  binning(bin = NTIME) %>%
  predcorrect(pred=PRED, varcorr = TRUE) %>%
  vpcstats()

# For binless loess prediction corrected, use predcorrect() before
# binless() and set loess.ypc = TRUE

vpc <- observed(obs_data, x=TIME, yobs=DV) %>%
  simulated(sim_data, ysim=DV) %>%
  predcorrect(pred=PRED) %>%
  binless() %>%
  vpcstats()
```

```
print.tidyvpcobj      Print a tidyvpcobj
```

Description

Print generic used to return information about VPC.

Usage

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

Arguments

`x` An tidyvpcobj.
`...` Further arguments can be specified but are ignored.

Value

Returns `x` invisibly.

```
qpcstats      Compute Quantitative Predictive Check (QPC) statistics
```

Description

Compute quantitative predictive quality metrics that summarize agreement between observed and simulated data in a VPC. QPC statistics numerically encode features typically assessed visually (coverage, deviation, trend, and sharpness), and include a composite `qpc_score` (lower is better) suitable for automated model comparison and optimization.

Usage

```
qpcstats(
  o,
  alpha = 0.05,
  w = c(med_cov = 0.35, tail_cov = 0.2, mae = 0.15, drift = 0.1, sharp = 0.1, interval =
    0.1),
  sharp_ref = NULL,
  interval_ref = NULL,
  ...
)
```

Arguments

<code>o</code>	A <code>tidyvcobj</code> produced by <code>vcstats</code> (typically using <code>binless</code> VPC summaries).
<code>alpha</code>	Numeric. Miscoverage level for interval scoring (default <code>0.05</code> corresponds to a 95% prediction interval).
<code>w</code>	Named numeric vector of weights used to combine component penalties into <code>qpc_score</code> . Names must include: <code>med_cov</code> , <code>tail_cov</code> , <code>mae</code> , <code>drift</code> , <code>sharp</code> , <code>interval</code> . Lower <code>qpc_score</code> is better.
<code>sharp_ref</code>	Numeric or <code>NULL</code> . Reference value used to scale the sharpness (interval width) penalty. If <code>NULL</code> (default), a self-normalizing bounded transform is used so that a single VPC can be scored without external calibration. Set <code>sharp_ref</code> when you need scores to be comparable across a population of models (e.g., Darwin searches, benchmarking across multiple datasets/runs).
<code>interval_ref</code>	Numeric or <code>NULL</code> . Reference value used to scale the interval-score penalty. If <code>NULL</code> (default), a self-normalizing bounded transform is used. Set <code>interval_ref</code> for cross-model or cross-run comparability (e.g., Darwin optimization or evaluation studies).
<code>...</code>	Additional arguments (reserved for future extensions).

Details**When should I set `sharp_ref` / `interval_ref`?**

- *Single-model / single-VPC scoring (default)*: leave both as `NULL`. This produces stable, bounded penalties without requiring any prior run for calibration.
- *Population scoring / optimization*: provide references when comparing many models (e.g., Darwin search) where you want the sharpness and interval-score penalties to be on a consistent scale across models/runs. A common choice is to compute `sharp_ref` and `interval_ref` from a representative run (e.g., median or 75th percentile values across all evaluated models).

Value

Returns `tidyvcobj` with an additional `qpc.stats` data table containing QPC summary metrics and `qpc_score`.

See Also

[vcstats](#), [binless](#), [predcorrect](#)

Examples

```
## Not run:
vpc <- observed(obs_data, y = DV, x = TIME) %>%
  simulated(sim_data, y = DV) %>%
  binless(optimize = TRUE) %>%
  predcorrect(pred = PRED) %>%
  vcstats()
```

```

# Default: single-model scoring (no calibration required)
vpc <- qpcstats(vpc)

# Population scoring (e.g., Darwin run): anchor penalties for comparability
vpc <- qpcstats(
  vpc,
  sharp_ref = 0.15,
  interval_ref = 2.5
)

vpc$qpc.stats

## End(Not run)

```

simulated

Specify simulated dataset and variables for VPC

Description

The simulated function is used for specifying simulated input data and variables for VPC. Note: Simulated data must not contain missing DV and may require filtering MDV == 0 before generating VPC. Simulated data must be ordered by: Replicate, Subject (ID), IVAR (Time).

Usage

```

simulated(o, ...)

## S3 method for class 'tidyvpcobj'
simulated(o, data, ysim, xsim, repl, ...)

```

Arguments

o	A tidyvpcobj.
...	Other arguments.
data	A data.frame of simulated data.
ysim	Numeric y-variable, typically named DV.
xsim	Numeric x-variable, typically named TIME. This argument is not required, see details below.
repl	Numeric replicate variable, typically named REPL. This argument is not required, see details below.

Value

A tidyvpcobj containing simulated dataset sim formatted with columns x, y, and repl, which indicates the replicate number. The column x is used from the observed() function. Resulting dataset is of class data.frame and data.table.

See Also

[observed](#) [censoring](#) [stratify](#) [predcorrect](#) [binning](#) [binless](#) [vpcstats](#)

Examples

```
require(magrittr)

vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV)
```

sim_cat_data

Example simulated data with categorical DV

Description

A simulated dataset with the 3 levels of categorical DV across 100 replicates.

Usage

```
sim_cat_data
```

Format

A data frame with 401400 rows and 4 variables:

PID_code Subject identifier

IVAR Time

DV Categorical DV with 3 levels

Replicate Replicate num for simulation

Source

Certara University

sim_data	<i>Example simulated data with continuous DV</i>
----------	--

Description

A simulated dataset from a hypothetical PK model with 100 replicates.

Usage

```
sim_data
```

Format

A data.table with 60000 rows and 10 variables:

ID Subject identifier

REP Replicate num for simulation

TIME Time

DV Concentration of drug

IPRED Individual prediction variable

PRED Population prediction variable

AMT Amount of dosage initially administered at DV = 0, TIME = 0

DOSE Dosage amount

MDV Dummy indicating missing dependent variable value

NTIME Nominal Time

Source

[simple_data](#)

stratify	<i>Stratification for Visual Predictive Check (VPC)</i>
----------	---

Description

Use to specify stratification variables for VPC.

Usage

```
stratify(o, ...)
```

```
## S3 method for class 'tidyvpobj'
```

```
stratify(o, formula, data = o$data, data.sim = NULL, ...)
```

Arguments

<code>o</code>	A <code>tidyvpcobj</code> .
<code>...</code>	Other arguments to include.
<code>formula</code>	Formula for stratification.
<code>data</code>	Observed data supplied in <code>observed()</code> function.
<code>data.sim</code>	Simulated data supplied in <code>simulated()</code> function.

Value

Returns updated `tidyvpcobj` with stratification formula, stratification column(s), and `strat.split` datasets, which is `obs` split by unique levels of stratification variable(s). Resulting datasets are of class object `data.frame` and `data.table`.

See Also

[observed](#) [simulated](#) [censoring](#) [predcorrect](#) [binning](#) [binless](#) [vpcstats](#)

Examples

```
require(magrittr)

vpc <- observed(obs_data, x=TIME, y=DV) %>%
  simulated(sim_data, y=DV) %>%
  stratify(~ GENDER) %>%
  binning(NTIME) %>%
  vpcstats()

# Example with 2-way stratification by GENDER and STUDY.

vpc <- vpc %>%
  stratify(~ GENDER + STUDY) %>%
  binning(bin = "centers", centers = c(1,3,5,7,10)) %>%
  vpcstats()
```

vpcstats

Compute VPC statistics

Description

Compute prediction interval statistics for VPC.

Usage

```
vpcstats(o, ...)

## S3 method for class 'tidyvpcobj'
vpcstats(
  o,
  vpc.type = c("continuous", "categorical"),
  qpred = c(0.05, 0.5, 0.95),
  ...,
  conf.level = 0.95,
  quantile.type = 7
)
```

Arguments

<code>o</code>	A <code>tidyvpcobj</code> .
<code>...</code>	Other arguments to include.
<code>vpc.type</code>	Character specifying type of VPC (e.g., "continuous" (Default) or "categorical").
<code>qpred</code>	Numeric vector of length 3 specifying quantile prediction interval. Only applicable for <code>vpc.type = "continuous"</code> .
<code>conf.level</code>	Numeric specifying confidence level.
<code>quantile.type</code>	Numeric indicating quantile type. See quantile .

Value

Updates `tidyvpcobj` with `stats` data.table object, which contains the following columns:

- `bin`: Resulting bin value as specified in `binning()` function
- `xbin`: Midpoint x-value of the observed data points in the bin as specified in `xbin` argument of `binning()` function
- `qname`: Quantiles specified in `qpred`. Only returned if `vpc.type = "continuous"`
- `pname`: Categorical probability names. Only returned if `vpc.type = "categorical"`
- `y`: Observed y value for the specified quantile
- `lo`: Lower bound of specified confidence interval for y value in simulated data
- `md`: Median y value in simulated data
- `hi`: Upper bound of specified confidence interval for y value in simulated data

See Also

[observed](#) [simulated](#) [censoring](#) [stratify](#) [binning](#) [binless](#) [predcorrect](#)

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