

Package ‘nonmem2R’

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Type Package

Title Loading NONMEM Output Files with Functions for Visual Predictive Checks (VPC) and Goodness of Fit (GOF) Plots

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Description Loading NONMEM (NONlinear Mixed-Effect Modeling, <<https://www.iconplc.com/solutions/technologies/nonmem/>>) and PSN (Perlspeaks-NONMEM, <<https://uupharmacometrics.github.io/PsN/>>) output files to extract parameter estimates, provide visual predictive check (VPC) and goodness of fit (GOF) plots, and simulate with parameter uncertainty.

License Unlimited

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Imports mvtnorm, lattice, latticeExtra, MASS, splines2, reshape2

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| | |
|-------------|-------------------------------------|
| add.caption | <i>Add caption to ggplot object</i> |
|-------------|-------------------------------------|

Description

Adds caption text as returned by `get.caption` to a ggplot object

Usage

```
add.caption(p, control = GOF.control())
```

Arguments

| | |
|----------------------|---|
| <code>p</code> | ggplot object |
| <code>control</code> | an optional list of control settings. See <code>GOF.control</code> for the names of the settable control values and their effect. |

`basic.eta.GOF`*Histogram and/or QQ-norm GOF for ETA's*

Description

Provides histogram and/or QQ-norm GOF for all ETA's included in the input data.frame with caption added as returned by `get.caption`

Usage

```
basic.eta.GOF(  
  data,  
  title = "",  
  global.ggplot.options = NULL,  
  type = c("both", "qqnorm", "hist"),  
  ETA.subset = NULL,  
  refline = TRUE,  
  drop.fixed = TRUE,  
  id.column = "ID",  
  standardize = TRUE,  
  bins = NA,  
  control = GOF.control()  
)
```

```
eta.hist.GOF(  
  data,  
  title = "",  
  drop.fixed = TRUE,  
  refline = TRUE,  
  id.column = "ID",  
  standardize = TRUE,  
  bins = NA,  
  control = GOF.control()  
)
```

```
eta.qqnorm.GOF(  
  data,  
  title = "",  
  drop.fixed = TRUE,  
  refline = TRUE,  
  id.column = "ID",  
  standardize = TRUE,  
  control = GOF.control()  
)
```

Arguments

`data` data.frame to plot

| | |
|-----------------------|--|
| title | title |
| global.ggplot.options | ggplot option added to each ggplot before plotting/returning object |
| type | do only qq-norm plots (qqnorm), only histograms (hist), or do both (both) |
| ETA.subset | index for subset of ETA's to plot. If NULL (default) all ETA's are plotted. |
| refline | add reference line (default =TRUE) or not (FALSE) |
| drop.fixed | drop ETA's that are fixed, i.e. any ETA with the same value in all subjects |
| id.column | column name that indicate subject identifier |
| standardize | Standardize all ETA's (e.g. scale to unit variance) |
| bins | number of histogram bins, if NA, bins are set using Sturges' formula |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
basic.eta.GOF(sdtab)
```

basic.GOF4

Basic 4- and 6-panel GOF

Description

basic.GOF4 provides a 4-panel GOF plot showing

- i) Observations (DV) vs population predictions (PRED)
- ii) Observations (DV) vs individual predictions (IPRED)
- iii) $\sqrt{\text{abs}(\text{CWRES})}$ vs individual predictions (IPRED), and
- iv) CWRES vs TIME or other columns as set by idv

basic.GOF6 provides 2 additional GOF's showing histogram and qqnorm GOF's for CWRES.

Caption is added as returned by get.caption

Usage

```
basic.GOF4(
  data,
  residual = "CWRES",
  idv1 = "IPRED",
  idv2 = "TIME",
  title = "",
  color = "",
```

```

    log.scale = FALSE,
    global.ggplot.options = NULL,
    refline = TRUE,
    add.loess = TRUE,
    control = GOF.control()
  )

basic.GOF6(
  data,
  residual = "CWRES",
  idv1 = "IPRED",
  idv2 = "TIME",
  title = "",
  color = "",
  log.scale = FALSE,
  global.ggplot.options = NULL,
  refline = TRUE,
  add.loess = TRUE,
  bins = NA,
  control = GOF.control()
)

```

Arguments

| | |
|-----------------------|--|
| data | data.frame to plot |
| residual | column name for residuals, default="CWRES" |
| idv1 | independent variable for plot of sqrt of absolute CWRES |
| idv2 | independent variable for plot of CWRES |
| title | title |
| color | data columns to set different colors in plot, interpreted as factor |
| log.scale | use log scale for DV, IPRED and PRED (TRUE) or normal scale (FALSE) |
| global.ggplot.options | ggplot option added to each ggplot before plotting/returning object |
| refline | add reference line (default =TRUE) or not (FALSE) |
| add.loess | add loess smoother to plot (TRUE), or not (FALSE) |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |
| bins | number of histogram bins, if NA, bins are set using Sturges' formula |

Examples

```

# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
## Example 4 panel basic GOF

```

```
basic.GOF4(subset(sdtab,DV>0),idv2="TAPD")
## Example 6 panel basic GOF
basic.GOF6(subset(sdtab,DV>0),idv1="TAPD",idv2="PRED")
```

 covload

Load the covariance matrix from a nonmem .cov output file.

Description

Load the covariance matrix from a nonmem .cov output file. Either the covariance matrix of all THETA parameters (default) or the covariance matrix of all parameters, THETA, OMEGA and SIGMA.

For cov-files with multiple table results either only the last table result is loaded (`last.table.only=TRUE`, default) or all table results are loaded (`last.table.only=FALSE`). The result is then a named list of covariance matrix's, `LastTable` is the last table in the cov-files.

Usage

```
covload(
  model,
  use.model.path = TRUE,
  last.table.only = TRUE,
  theta.only = TRUE
)
```

Arguments

| | |
|------------------------------|--|
| <code>model</code> | name of the cov file with or without the .cov extension. <code>model</code> may include full or relative path to the cov file. See examples. |
| <code>use.model.path</code> | Load file from a global defined model library (<code>TRUE</code> =default). If so will look for a global character vector named <code>model.path</code> |
| <code>last.table.only</code> | Include only the last table result for cov files with multiple table results |
| <code>theta.only</code> | return covariance matrix of theta's only (default) |

Value

The covariance matrix or a named list of covariance matrix's

Examples

```
##### Load the .cov file "run001.cov"
# 1) Get path to the example file included in nonmem2R package
file1 <- system.file("extdata", "run001.cov", package = "nonmem2R")
# 2) Load the file using the covload function
covload(file1)
```

do.cat.GOF

*Y vs categorical X GOF-plot***Description**

GOF plot with boxplots of Y grouped by categorical data in X, with refine and with caption added as returned by get.caption

Usage

```
do.cat.GOF(
  data,
  x,
  y,
  color = "",
  add.points = TRUE,
  refine = c("abline", "href0", "hrefmean", "hrefmedian", "none"),
  title = "",
  lines.by.id = FALSE,
  id.column = "ID",
  fx = NULL,
  fy = NULL,
  control = GOF.control()
)
```

Arguments

| | |
|-------------|--|
| data | data.frame to plot |
| x | character string with name of column for x |
| y | character string with name of column for y |
| color | data columns to set different colors in plot, interpreted as factor |
| add.points | add jittered points of data (TRUE), or not (FALSE) |
| refline | add reference line with intercept=0, slope=1 (abline), horizontal at y=0(href0), horizontal at y=mean of y(hrefmean), horizontal at y=median of y(hrefmedian), or don't add reference line (none) |
| title | title |
| lines.by.id | connect subjects by lines (TRUE), or don't (FALSE) |
| id.column | column name that indicate subject identifier |
| fx | function for transformation of x before plotting |
| fy | function for transformation of y before plotting |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

do.individual.GOF *Individual GOF-plots*

Description

DV, IPRED and PRED (default) individual GOF plots with one panel per subject. Caption added as returned by get.caption

Usage

```
do.individual.GOF(
  data,
  x = "TIME",
  y = c("DV", "IPRED", "PRED"),
  type = c("point", "line", "line"),
  title = "",
  per.page = 20,
  fx = NULL,
  fy = NULL,
  ylab = "Observations/Predictions",
  equal.lims = TRUE,
  global.ggplot.options = NULL,
  control = GOF.control()
)
```

Arguments

| | |
|-----------------------|--|
| data | data.frame to plot |
| x | character string with name of column for x |
| y | character string vector with names of columns for y, default = c(DV, IPRED , PRED) |
| type | plot symbol or line for each y variable, length of type must match length of y |
| title | title |
| per.page | number of subjects/panels on each page |
| fx | function for transformation of x before plotting |
| fy | function for transformation of y before plotting |
| ylab | y axis label |
| equal.lims | use same x- and y-limits on all pages and panels (TRUE), or use allow to vary across pages (FALSE) |
| global.ggplot.options | ggplot option added to each ggplot before plotting/returning object |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
do.individual.GOF(subset(sdtab,DV>0 & ID<13))
```

do.multi.GOF *Multiple Y vs single X GOF-plot*

Description

X-Y GOF plots for multiple Y's and shared X with refines and data smoother and with caption added as returned by get.caption

Usage

```
do.multi.GOF(
  data,
  x,
  y,
  color = "",
  add.loess = TRUE,
  refline = c("none", "abline", "href0", "hrefmean", "hrefmedian"),
  title = "",
  lines.by.id = FALSE,
  id.column = "ID",
  fx = NULL,
  fy = NULL,
  ylab = "Observations/Predictions",
  control = GOF.control()
)
```

Arguments

| | |
|-------------|--|
| data | data.frame to plot |
| x | character string with name of column for x |
| y | character string with name of column for y |
| color | data columns to set different colors in plot, interpreted as factor |
| add.loess | add loess smoother to plot (TRUE), or not (FALSE) |
| refline | add reference line with intercept=0, slope=1 (abline), horizontal at y=0(href0), horizontal at y=mean of y(hrefmean), horizontal at y=median of y(hrefmedian), or don't add reference line (none) |
| title | title |
| lines.by.id | connect subjects by lines (TRUE), or don't (FALSE) |

| | |
|-----------|--|
| id.column | column name that indicate subject identifier |
| fx | function for transformation of x before plotting |
| fy | function for transformation of y before plotting |
| ylab | y axis label |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

do.one.GOF

X-Y GOF-plot

Description

X-Y GOF plot with refines and data smoother and with caption added as returned by get.caption

Usage

```
do.one.GOF(
  data,
  x,
  y,
  color = "",
  add.loess = TRUE,
  refline = c("abline", "href0", "hrefmean", "hrefmedian", "none"),
  title = "",
  lines.by.id = FALSE,
  id.column = "ID",
  fx = NULL,
  fy = NULL,
  control = GOF.control()
)
```

Arguments

| | |
|-------------|--|
| data | data.frame to plot |
| x | character string with name of column for x |
| y | character string with name of column for y |
| color | data columns to set different colors in plot, interpreted as factor |
| add.loess | add loess smoother to plot (TRUE), or not (FALSE) |
| refline | add reference line with intercept=0, slope=1 (abline), horizontal at y=0(href0), horizontal at y=mean of y(hrefmean), horizontal at y=median of y(hrefmedian), or don't add reference line (none) |
| title | title |
| lines.by.id | connect subjects by lines (TRUE), or don't (FALSE) |

| | |
|-----------|--|
| id.column | column name that indicate subject identifier |
| fx | function for transformation of x before plotting |
| fy | function for transformation of y before plotting |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
do.one.GOF(subset(sdtab,DV>0),"IPRED","DV")
```

eta.cov.GOF

Covariate and pairs ETA GOFs

Description

ETA's vs numerical covariates (eta.cov.GOF) and ETA's vs categorical covariates GOF plots on multiple or single pages with refines, data smoother, and caption added as returned by get.caption.

eta.pairs.GOF provides a pairs plot of all ETA's.

Usage

```
eta.cov.GOF(
  data,
  covariates = c("AGE", "BWT"),
  ETA.subset = NULL,
  exclude.zero.ETA = FALSE,
  title = "",
  drop.fixed = TRUE,
  id.column = "ID",
  standardize = TRUE,
  refline = TRUE,
  type = c("all-in-one", "covariate-by-page", "eta-by-page"),
  layout = c("ETAbbyROW", "ETAbbyCOL"),
  add.loess = TRUE,
  control = GOF.control()
)
```

```
eta.cat.GOF(
  data,
  covariates = c("SEX"),
  ETA.subset = NULL,
  exclude.zero.ETA = FALSE,
```

```

title = "",
drop.fixed = TRUE,
id.column = "ID",
standardize = TRUE,
refline = TRUE,
type = c("all-in-one", "covariate-by-page", "eta-by-page"),
layout = c("ETAbYROW", "ETAbYCOL"),
add.points = TRUE,
control = GOF.control()
)

eta.pairs.GOF(
  data,
  ETA.subset = NULL,
  title = "",
  drop.fixed = TRUE,
  id.column = "ID",
  density2D = c("none", "upper", "lower"),
  standardize = TRUE,
  control = GOF.control()
)

```

Arguments

| | |
|-------------------------------|---|
| <code>data</code> | data.frame to plot |
| <code>covariates</code> | covariates, list of character strings |
| <code>ETA.subset</code> | index for subset of ETA's to plot. If NULL (default) all ETA's are plotted. |
| <code>exclude.zero.ETA</code> | If set to TRUE any $ETA==0$ is excluded before plotting. This option is useful if the model have full shrinkage for subset of individuals e.g. for ETA on ED50 in patents on placebo or on dose==0. |
| <code>title</code> | title |
| <code>drop.fixed</code> | drop ETA's that are fixed, i.e. any ETA with the same value in all subjects |
| <code>id.column</code> | column name that indicate subject identifier |
| <code>standardize</code> | Standardize all ETA's (e.g. scale to unit variance) |
| <code>refline</code> | add reference line (default =TRUE) or not (FALSE) |
| <code>type</code> | do all ETA's and covariates on one page (all-in-one), one page for each covariate (covariate-by-page), or one page for each ETA (eta-by-page) |
| <code>layout</code> | Layout for ETA's and covariates |
| <code>add.loess</code> | add loess smoother to plot (TRUE), or not (FALSE) |
| <code>control</code> | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |
| <code>add.points</code> | add jittered points of data (TRUE), or not (FALSE) |
| <code>density2D</code> | add 2D-density above (upper) or below (lower), or don't add (none) |

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
eta.cov.GOF(sdtab,covariates=c("AGE","BWT"))
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
eta.cat.GOF(sdtab,covariates=c("SEX"))
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab999", package = "nonmem2R")
sdtab<-read.table(file=file1,skip=1,header=TRUE)
set.script.name("MyScript.R")
eta.pairs.GOF(sdtab)
```

extload

Load final parameter values from a nonmem .ext output file.

Description

Load parameter values from a nonmem .ext output file. For output files from FO, FOCE and IMP only the final parameter values are loaded. For output tables of MCMC and SAEM all parameter values from ITERATIONS>0 will be loaded unless positive.iterations=FALSE in case all the output from all iterations are loaded.

For ext-files with multiple table results either only the last table result is loaded (last.table.only=TRUE, default) or all table result are loaded (last.table.only=FALSE). All but the last table results are then returned as sub-lists to the last table result.

Usage

```
extload(
  model,
  use.model.path = TRUE,
  positive.iterations.only = TRUE,
  last.table.only = TRUE
)
```

Arguments

| | |
|--------------------------|---|
| model | name of the ext file with or without the .ext extension. model may include full or relative path to the ext file. See examples. |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| positive.iterations.only | Include only rows with ITERATIONS>0 from MCMC and SEAM table results (default=TRUE) |

```
last.table.only
```

Include only the last table result for ext files with multiple table results

Value

Named list including theta, theta.sd, omega, omega.sd, sigma, sigma.sd, and ofv. Here .sd is the vector(matrix) with standard errors estimated parameter values in theta(omega & sigma).

For MCMC output files each object are matrixes.

Examples

```
##### Load the .ext file "run001.ext"
# 1) Get path to the example file included in nonmem2R package
file1 <- system.file("extdata", "run001.ext", package = "nonmem2R")
# 2) Load the file using the extload function
extload(file1)
```

extToTable

Compile parameter table suitable for reports

Description

Load parameter values from a nonmem .ext output file and compile to table suitable for reports. Format can be "wide" (wide=TRUE, default) with a similar look as from sumoR, or similar a 3 column layout (wide=FALSE).

Usage

```
extToTable(
  model,
  use.model.path = TRUE,
  tableType = 2,
  wide = TRUE,
  format.estimate = "% -#6.4g",
  format.rse = "%#6.3g"
)
```

Arguments

| | |
|----------------|--|
| model | name of the ext file with or without the .ext extension. model may include full or relative path to the ext file. See examples. |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| tableType | Table type for THETA's, OMEGA's and SIGMA's tableType=0: Present OMEGA and SIGMA as variance and covariances and display SE for THETA, OMEGA, SIGMA |

tableType=1: Present OMEGA and SIGMA as variance and covariances and display RSE for THETA, OMEGA, SIGMA
 tableType=2: Present OMEGA and SIGMA as standard-deviation and correlations and display RSE for THETA, OMEGA, SIGMA
 tableType=3: Present OMEGA and SIGMA as standard-deviation and correlations and display SE for THETA, OMEGA, SIGMA
 wide produce a wide 9-column table (wide=TRUE, default) or a thin 3-column table(wide=FALSE)
 format.estimate format for estimated value, passed to sprintf
 format.rse format for rse, passed to sprintf

Value

a character-matrix

Examples

```
##### Load the .ext file "run001.ext"
# 1) Get path to the example file included in nonmem2R package
file1 <- system.file("extdata", "run001.ext", package = "nonmem2R")
# 2) Load the file using the extload function
extToTable(file1)
```

get.GOF.dictionary *Get, set, and modify the global (or local) GOF parameters and GOF dictionary for labels*

Description

The current global GOF parameters and dictionary is automatically applied to every plot you draw. Use 'get.GOF.params' to get the current GOF parameters, and 'set.GOF.params' to change one or several parameters. To change settings for one GOF only you can use GOF.control as input to the GOF function. See details below for complete list of GOF parameters.

Similarly use 'get.GOF.dictionary' and 'set.GOF.dictionary' for the dictionary of labels. 'set.GOF.dictionary' also allows for adding new items to the dictionary.

Use 'set.ETA.labels' to set labels for ETA's in all plots

Usage

```
get.GOF.dictionary()

set.GOF.dictionary(...)

default.GOF.dictionary()
```

```

set.GOF.params(...)
get.GOF.params()
default.GOF.params()
set.ETA.labels(labels)
set.script.name(script.name)
GOF.control(...)

```

Arguments

```

...          named list of GOF parameter or GOF dictionary for labels
labels       vector of character strings with the labels
script.name  character strings for script name to put at end of caption

```

Details

Table below describe each of the global GOF parameters that can be modified by 'set.GOF.params'

| Parameter | Default | Description |
|--------------------|---------------|---|
| col.data | "gray20" | color for points in all GOFs |
| cex.data | 1.5 | cex for points in all GOFs |
| pch.data | 19 | pch for points in all GOFs |
| alpha.data | 0.5 | alpha for points in all GOFs |
| col.smooth | "#3366FF" | color for smoothers |
| lty.smooth | 1 | lty for smoothers |
| lwd.smooth | 1 | lwd for smoothers |
| se.smooth | TRUE | show confidence interval for loess smoother (TRUE) or not (FALSE) |
| span.smooth | 0.6666667 | span parameter for loess smothers |
| degree.smooth | 1 | degree parameter for loess smothers |
| family.smooth | "symmetric" | family parameter for loess smothers |
| col.refline | "red" | color for reference lines in all GOFs |
| lty.refline | 2 | lty for reference lines in all GOFs |
| lwd.refline | 1 | lwd for reference lines in all GOFs |
| fill.hist | "gray30" | color for filling of histograms |
| col.hist | "transparent" | color for border of histograms |
| alpha.hist | 0.5 | alpha for fill area in histograms |
| fill.box | "steelblue" | color for filling of box-plots |
| col.box | "black" | color for border and whisker of box-plots |
| alpha.box | 0.6 | alpha for fill area in box-plots |
| axis.labels | TRUE | use dictionary for labels (TRUE) or just use column names for axis labels (FALSE) |
| add.caption | TRUE | add caption to GOF plots (true) or not (FALSE) |
| size.caption | 8 | size for caption text |
| col.caption | 1 | color for caption text |
| caption.path.depth | 99 | number of folders levels to include in caption |

| | | |
|---------------|------|--|
| corr.fontface | 4 | font face for correlation in eta.pairs.GOF |
| eta.labels | NULL | vector of labels for ETA's |
| script.name | "" | script name for caption |

Examples

```
### Example setting ETA labels
set.ETA.labels(c("Ka", "CL", "V"))
### Example setting script name
set.script.name("MyScript.R")
```

| | |
|-----------|--|
| get.label | <i>Labels for known NONMEM variables</i> |
|-----------|--|

Description

get.label match known NONMEM variables to the GOF-dictionary and returns the matched label. Unless trans is NULL, the label is modified to 'f(matched label)'

Usage

```
get.label(x, trans = NULL)
```

Arguments

| | |
|-------|-------------------------|
| x | column to get label for |
| trans | transformation |

See Also

[get.GOF.dictionary()], [set.GOF.dictionary()], and [default.GOF.dictionary()].

| | |
|----------------|-------------------------------|
| get.model.path | <i>Get and set model.path</i> |
|----------------|-------------------------------|

Description

The model.path in the nonmem2R set of global variables is used by functions loading NONMEM or PSN generated output file. The model.path can be retrieved by get.model.path and can be set using set-model.path. When loading nonmem2R the model-path is set to "", e.g. the current working directory. The model.path can be set absolute or relative, see examples.

Usage

```
get.model.path()

set.model.path(model.path)
```

Arguments

model.path character string for path to model files

Examples

```
## Not run:
## Example for setting absolute path
set.model.path("c:/NONMEM")
## Example for setting relative path,
set.model.path("../NONMEM")

## End(Not run)
```

grid.sim

Combine fix grid and simulated grid based on multivariate normal distribution

Description

grid.sim produce comparable output to mvnorm, however for methods 2 to 4 grid.sim make use of center and scaling, and or use a fix grid of values for one column of the output. The intended use of grid.sim is for computing confidence intervals (CI) for model predictions. Method 1 is the same as rmvnorm, however can handle cases of zero variances in sigma. Method 2 is method 1 followed by centering and scaling of the simulated matrix. Thus output when using method 2 always have sample mean and covariance equal to input parameters means and sigma. Method 3 is the same as method 1 however with one column having a fixed range of values rather than a simulated range of values. Method 4 is method 3 followed by centering and scaling of the simulated matrix. Thus output when using method 4 always have sample mean and covariance equal to input parameters means and sigma.

As the number of simulations (n) goes to infinity all methods in grid.sim are identical to mvnorm in that the sample covariance (mean) of the output will converge to the input covariance matrix sigma (vector means).

The advantage with methods 2 to 4 (over method 1 and rmvnorm) is that they provides more stable results, hence number of simulations can be reduced and still have equally stable results when used to represent parameter uncertainty and or population variability in model predictions.

Usage

```
grid.sim(n, means = NULL, sigma, grid.param = NULL, method = 4)
```

Arguments

| | |
|------------|---|
| n | Number of simulations |
| means | vector of mean values |
| sigma | covariance matrix |
| grid.param | the index of the parameter for which a fix grid (from qnorm) is used instead of a simulated grid (rnorm). If grid.param=NULL (default) the fix grid will be used for the parameter with largest variance. |
| method | simulation method, default=4 |

Value

row-matrix of parameters

Examples

```
sigma<-matrix(c(1,0.5,0.5,2),ncol=2)
sim1<-grid.sim(1000,sigma=sigma)
pairs(sim1)
cov(sim1)
```

histGOF

Histogram GOF

Description

Histogram GOF showing histogram, smooth density, and normal density as reference line and caption added as returned by get.caption

Usage

```
histGOF(
  data,
  x,
  title = "",
  color = "",
  fx = NULL,
  bins = NA,
  refline = TRUE,
  control = GOF.control()
)
```

Arguments

| | |
|---------|--|
| data | data.frame to plot |
| x | character string with name of column for x |
| title | title |
| color | data columns to set different colors in plot, interpreted as factor |
| fx | function for transformation of x before plotting |
| bins | number of histogram bins, if NA, bins are set using Sturges' formula |
| refline | add reference line (default =TRUE) or not (FALSE) |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

Examples

```
dd<-data.frame(CWRES=rnorm(100),gr=rep(LETTERS[1:5],20))
histGOF(dd,"CWRES",color="gr")
```

merge2GOF

Merging 2, 4, or 6 GOF's into one graph

Description

Merging multiple GOFs (ggplot objects) into one graph with caption added as returned by get.caption. Any legend present in first GOF is added to the combined graph.

Usage

```
merge2GOF(p1, p2, byrow = TRUE)
```

```
merge4GOF(p1, p2, p3, p4)
```

```
merge6GOF(p1, p2, p3, p4, p5, p6)
```

Arguments

| | |
|-------|--|
| p1 | first ggplot object |
| p2 | second ggplot object |
| byrow | combine plots side by side (TRUE) or one above the other (FALSE) |
| p3 | third ggplot object |
| p4 | 4th ggplot object |
| p5 | 5th ggplot object |
| p6 | 6th ggplot object |

| | |
|---------|------------------------|
| modload | <i>Show model file</i> |
|---------|------------------------|

Description

Load and dump model file in the consol.

Usage

```
modload(model, use.model.path = TRUE)
```

Arguments

| | |
|----------------|---|
| model | name of the mod file with or without the .mod extension. model may include full or relative path to the mod file. See examples. |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |

Value

data.frame

Examples

```
##### Load the .ext file "run001.mod"
# 1) Get path to the example file included in nonmem2R package
file1 <- system.file("extdata", "run001.mod", package = "nonmem2R")
# 2) Load the file using the extload function
modload(file1)
```

| | |
|----------------|-------------------------------|
| position_scale | <i>Position for scaling y</i> |
|----------------|-------------------------------|

Description

Position for scaling y

Usage

```
position_scale(y = 1)
```

Arguments

| | |
|---|-------------|
| y | scale value |
|---|-------------|

Details

Position for scaling y

 qqnormGOF

QQ-norm GOF

Description

QQ-norm GOF qqnorm plots with reference line and caption added as returned by get.caption

Usage

```
qqnormGOF(
  data,
  sample,
  title = "",
  color = "",
  fx = NULL,
  refline = TRUE,
  control = GOF.control()
)
```

Arguments

| | |
|---------|--|
| data | data.frame to plot |
| sample | character string with name of column for x |
| title | title |
| color | data columns to set different colors in plot, interpreted as factor |
| fx | function for transformation of x before plotting |
| refline | add reference line (default =TRUE) or not (FALSE) |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |

Examples

```
dd<-data.frame(CWRES=rnorm(100))
qqnormGOF(dd, "CWRES")
```

| | |
|-----------|--|
| stat_corr | <i>Adding correlation to x-y plots</i> |
|-----------|--|

Description

Correlation to x-y plots. This stat is intended for providing correlations e.g. above the diagonal of a pairs plot

Usage

```
stat_corr(
  mapping = NULL,
  data = NULL,
  geom = "text",
  position = "identity",
  na.rm = FALSE,
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

| | |
|-------------|--|
| mapping | Set of aesthetic mappings created by aes or aes_. |
| data | The data to be displayed in this layer. |
| geom | Use to override the default geom |
| position | Position adjustment, either as a string, or the result of a call to a position adjustment function. |
| na.rm | If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed. |
| show.legend | logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes. |
| inherit.aes | If FALSE, overrides the default aesthetics, rather than combining with them. |
| ... | other arguments passed on to layer. |

Details

Provide normal QQplot

| | |
|-----------|----------------------------------|
| stat_denx | <i>Density for x in x-y plot</i> |
|-----------|----------------------------------|

Description

Density for x in x-y plot. This stat is intended for providing the a density on the diagonal of a pairs plot

Usage

```
stat_denx(
  mapping = NULL,
  data = NULL,
  geom = "polygon",
  position = "identity",
  na.rm = FALSE,
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

| | |
|-------------|--|
| mapping | Set of aesthetic mappings created by aes or aes_. |
| data | The data to be displayed in this layer. |
| geom | Use to override the default geom |
| position | Position adjustment, either as a string, or the result of a call to a position adjustment function. |
| na.rm | If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed. |
| show.legend | logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes. |
| inherit.aes | If FALSE, overrides the default aesthetics, rather than combining with them. |
| ... | other arguments passed on to layer. |

Details

Provide normal QQplot

| | |
|------------|-----------------------|
| stat_dnorm | <i>Normal density</i> |
|------------|-----------------------|

Description

Normal density with ggplot2

Usage

```
stat_dnorm(  
  mapping = NULL,  
  data = NULL,  
  geom = "line",  
  position = "identity",  
  na.rm = FALSE,  
  show.legend = NA,  
  inherit.aes = TRUE,  
  ...  
)
```

Arguments

| | |
|-------------|--|
| mapping | Set of aesthetic mappings created by aes or aes_. |
| data | The data to be displayed in this layer. |
| geom | Use to override the default geom |
| position | Position adjustment, either as a string, or the result of a call to a position adjustment function. |
| na.rm | If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed. |
| show.legend | logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes. |
| inherit.aes | If FALSE, overrides the default aesthetics, rather than combining with them. |
| ... | other arguments passed on to layer. |

Details

Provide normal QQplot

| | |
|------------|-------------------------------------|
| stat_hmean | <i>Horizontal reference at mean</i> |
|------------|-------------------------------------|

Description

Horizontal reference at mean with ggplot2

Usage

```
stat_hmean(  
  mapping = NULL,  
  data = NULL,  
  geom = "hline",  
  position = "identity",  
  na.rm = FALSE,  
  show.legend = NA,  
  inherit.aes = TRUE,  
  ...  
)
```

Arguments

| | |
|-------------|--|
| mapping | Set of aesthetic mappings created by aes or aes_. |
| data | The data to be displayed in this layer. |
| geom | Use to override the default geom |
| position | Position adjustment, either as a string, or the result of a call to a position adjustment function. |
| na.rm | If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed. |
| show.legend | logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes. |
| inherit.aes | If FALSE, overrides the default aesthetics, rather than combining with them. |
| ... | other arguments passed on to layer. |

Details

Provide normal QQplot

| | |
|--------------|---------------------------------------|
| stat_hmedian | <i>Horizontal reference at median</i> |
|--------------|---------------------------------------|

Description

Horizontal reference at median with ggplot2

Usage

```
stat_hmedian(
  mapping = NULL,
  data = NULL,
  geom = "hline",
  position = "identity",
  na.rm = FALSE,
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

| | |
|-------------|--|
| mapping | Set of aesthetic mappings created by aes or aes_. |
| data | The data to be displayed in this layer. |
| geom | Use to override the default geom |
| position | Position adjustment, either as a string, or the result of a call to a position adjustment function. |
| na.rm | If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed. |
| show.legend | logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes. |
| inherit.aes | If FALSE, overrides the default aesthetics, rather than combining with them. |
| ... | other arguments passed on to layer. |

Details

Provide normal QQplot

Aesthetics

geom_smooth understands the following aesthetics (required aesthetics are in bold):
x, alpha, colour, fill, group, shape, size, stroke

| | |
|-------|--|
| sumoR | <i>Compile summary information for NONMEM model based on the lst file, ext file, and the cov file.</i> |
|-------|--|

Description

Compile summary information similar to that of the sumo PSN function, based on the NONMEM output files lst, ext, and if covariance setp was run, the cov file.

Usage

```
sumoR(
  model,
  use.model.path = TRUE,
  tableType = 2,
  format.estimate = "% -#6.4g",
  format.rse = "%#6.3g"
)
```

Arguments

| | |
|-----------------|---|
| model | name of the lst file with or without the .lst extension. model may include full or relative path to the lst file. |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| tableType | Table type for THETA's, OMEGA's and SIGMA's tableType=0: Present OMEGA and SIGMA as variance and covariances and display SE for THETA, OMEGA, SIGMA tableType=1: Present OMEGA and SIGMA as variance and covariances and display RSE for THETA, OMEGA, SIGMA tableType=2: Present OMEGA and SIGMA as standard-deviation and correlations and display RSE for THETA, OMEGA, SIGMA tableType=3: Present OMEGA and SIGMA as standard-deviation and correlations and display SE for THETA, OMEGA, SIGMA |
| format.estimate | format for estimated value, passed to sprintf |
| format.rse | format for RSE or SE, passed to sprintf |

Value

named list of class sumoR

Examples

```
##### Compile summary information from the .lst file "run001.lst"
# 1) Get path to the example file included in nonmem2R package
file1 <- system.file("extdata", "run001.lst", package = "nonmem2R")
# 2) Compile summary information from "run001.lst"
sumoR(file1)
```

test.grid.sim

*Function for testing grid.sim and compare with rmvnorm***Description**

Test grid.sim

Usage

```
test.grid.sim(n = 1000, k = 1:4)
```

Arguments

| | |
|---|--|
| n | number of simulations |
| k | subset of parameters from a 4X4 sigma to use |

Value

graphics

Examples

```
## Not run:
require(lattice)
test.grid.sim(n=1000)

## End(Not run)
```

vpcfig

*Visual Predictive Check (VPC) based on Perl-speaks-NONMEM (PsN) generated VPC files (lattice version).***Description**

This function creates VPC using output files from the vpc command in Pearl Speaks NONMEM (PsN). Graphs are generated using the lattice package with many arguments for plot settings are passed directly to the xyplot function and have the same flexibility as when used in xyplot.

Usage

```

vpcfig(
  vpcdir = NULL,
  vpctab = NULL,
  vpcresult = NULL,
  use.model.path = TRUE,
  strata.names = NULL,
  strata.subset = NULL,
  percentile = 10,
  fy = function(y) { y },
  fx = function(x) { x },
  xlab = NULL,
  ylab = NULL,
  col.data = 8,
  cex.data = 0.3,
  pch.data = 3,
  col.line = c("blue", "red", "blue"),
  lwd.line = c(1, 2, 1),
  lty.line = c(1, 1, 1),
  col.segm = c("lightblue", "pink", "lightblue"),
  alpha.segm = c(0.5, 0.5, 0.5),
  type = 3,
  ...
)

```

Arguments

| | |
|----------------|--|
| vpcdir | Path of directory of the VPC files |
| vpctab | Path to the vpctab-file |
| vpcresult | Path to the vpcresult file |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| strata.names | Character vector for strata names. Must have length equal to number of strata's in vpc files, otherwise ignored. |
| strata.subset | Vector specifying subset of strata to use. Either a vector of index, e.g. strata.subset=c(1,3), or a character vector naming which strata to use. See details. |
| percentile | percentile to use, default=10 will display 10 Percentile argument must match columns included in the vpcresult file. |
| fy | transformation function for y-axis, default to identity function (f(y)=y). |
| fx | transformation function for x-axis, default to identity function (f(x)=x) |
| xlab | label for x-axis, default is IDV as found in vpcresultfile, passed to xyplot. |
| ylab | label for y-axis, default is DV as found in vpcresultfile, passed to xyplot. |
| col.data | color for data points, passed to xyplot, default=8 |
| cex.data | cex for data points, passed to xyplot, default=0.3 |

| | |
|------------|--|
| pch.data | plot symbol (pch) for data points, passed to xyplot, default=3 |
| col.line | line color for low quartile, median, and high quartile of data, passed to xyplot, default=c("blue","red","blue") |
| lwd.line | line width (lwd) for low quartile, median, and high quartile of data, passed to xyplot, default=c(1,2,1) |
| lty.line | line type (lty) for low quartile, median, and high quartile of data, passed to xyplot, default=c(1,1,1) |
| col.segm | Color of CI regions (low, median and high) for model, passed to xyplot, default=c("lightblue","pink","lightblue") |
| alpha.segm | alpha of CI regions (low, median and high) for model, passed to xyplot, default=c(0.5,0.5,0.5) |
| type | type of VPC plot, 1=display model regions only, 2=as 1 + lines (low, median and high) of data, 3= as 2 + points for data. type=0 can also be used and then no graph is produced but instead a list with 2 dataframes is returned. one for the vpcresult and on for the observed data in the vpctab file. |
| ... | Further arguments, passed to xyplot, e.g xlim and ylim axis limits, main for title of plot, abline for adding reference lines, or scales for formatting axes, see help files for xyplot. Note: col, cex, pch, lty, lwd, and alpha should not be used. Instead use the corresponding arguments defined above. |

Details

The lattice package is used for creating the VPC and vpctfig have functionality for e.g. modify names of strata, change layout of panels, use log-scale.

The data used is either specified by the directory of the PsN generated files, or by specifying the file names of both the vpctab-file and the vpcresult file. See examples 1 and 2 below.

Names of strata can be changed with the strata.names argument, if strata.names is NULL the names as specified in the vpcresult file are used.

strata.subset can be used to select a subset of strata, and or to change the order of stratas. See example 3. NOTE: strata.subset is matched with strata.names unless strata.names=NULL. If strata.names=NULL then strata.subset is matched to names as specified in vpcresult file. Default is to use all strata's (strata.subset=NULL).

The fy and fx arguments can be used to alter the scale of data plotted. For example, using `fy=function(y)(log(y+1))` is a convenient way to get log-scale for y-axis but with an off-set to show any values==0. Proper y tick marks can then be set by using the xyplot argument scales.

Value

lattice object of VPC plot

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "vpctab004.dat", package = "nonmem2R")
file2 <- system.file("extdata", "vpc_results.csv", package = "nonmem2R")
```

```

# Ex 1, produce VPC with default setting, here specifying both vpctab and vpcresult
vpcfig(vpctab=file1,vpcresult=file2)

## Not run:
# Ex 2, produce VPC with default setting, here specifying only directory of vpc files
path1<-gsub("vpctab004.dat","",file1)
vpcfig(vpcdir=path1)

## End(Not run)

# Ex 3, produce VPC with i) modifies strata names, ii) strata in reverse order, and
#      iii) labels
strata.names<-c("Group A","Group B")
xlab<-"Time after dose (hrs)"
ylab<-"Plasma Conc(mmol/L)"
vpcfig(vpctab=file1,vpcresult=file2,strata.names=strata.names,strata.subset=2:1,
       xlab=xlab,ylab=ylab)

```

vpcfig2

Visual Predictive Check (VPC) based on Perl-speaks-NONMEM (PsN) generated VPC files (ggplot2-version).

Description

This function creates VPC using output files from the vpc command in Pearl Speaks NONMEM (PsN). Graphs are generated using the ggplot2 package and the return object is an ggplot class and can be further modified, see details below and documentation for ggplot2 for further details.

Usage

```

vpcfig2(
  vpcdir = NULL,
  vpctab = NULL,
  vpcresult = NULL,
  use.model.path = TRUE,
  strata.names = NULL,
  strata.subset = NULL,
  median.only = FALSE,
  bin.idv = c("median", "midpoint"),
  percentile = 10,
  fy = function(y) { y },
  fx = function(x) { x },
  xlab = NULL,
  ylab = NULL,
  col.data = "gray20",
  cex.data = 1,

```



```

pch.data = 19,
alpha.data = 0.5,
col.line = "grey20",
lwd.line = 1,
lty.line = c(2, 1, 2),
col.segm = c("steelblue", "gray50", "steelblue"),
alpha.segm = 0.6,
type = 3,
panel.height.censored = 0.25,
censoring.labels = c("ALQ", "BLQ"),
ignore.censoring = FALSE,
control = GOF.control()
)

```

Arguments

| | |
|----------------|---|
| vpcdir | Path of directory of the VPC files |
| vpctab | Path to the vpctab-file |
| vpcresult | Path to the vpcresult file |
| use.model.path | Load file from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| strata.names | Character vector for strata names. Must have length equal to number of strata's in vpc files, otherwise ignored. |
| strata.subset | Vector specifying subset of strata to use. Either a vector of index, e.g. strata.subset=c(1,3), or a character vector naming which strata to use. See details. |
| median.only | Logical to plot only median and no quantiles for model and data (FALSE=default) |
| bin.idv | Method for computed idv value for plotting bin summary values. Set to "median" to use median of independent variable in each bin on x-axis (default), or set to "midpoint" to use midpoint of bins on x-axis. |
| percentile | percentile to use, default=10 will display 10 Percentile argument must match columns included in the vpcresult file. |
| fy | transformation function for y-axis, default to identity function (f(y)=y). |
| fx | transformation function for x-axis, default to identity function (f(x)=x) |
| xlab | label for x-axis, default is IDV as found in vpcresultfile, passed to labs. |
| ylab | label for y-axis, default is DV as found in vpcresultfile, passed to labs. |
| col.data | color for data points, passed to geom_point, default="gray20" |
| cex.data | cex for data points, passed to geom_point, default=1 |
| pch.data | plot symbol (pch) for data points, passed to geom_point, default=19 |
| alpha.data | alpha for plotting of data points, passed to geom_point, default=0.5 |
| col.line | line color for low quartile, median, and high quartile of data, passed to geom_line, default="gray20" |
| lwd.line | line width (lwd) for low quartile, median, and high quartile of data, passed to geom_line, default=1 |

| | |
|------------------------------------|---|
| <code>lty.line</code> | line type (lty) for low quartile, median, and high quartile of data, passed to <code>geom_line</code> , should be vector of length 3, default= <code>c(2,1,2)</code> |
| <code>col.segm</code> | Color of CI regions (low, median and high) for model, passed to <code>geom_polygon</code> , should be vector of length 3, default= <code>c("steelblue", "gray50", "steelblue")</code> |
| <code>alpha.segm</code> | alpha of CI regions (low, median and high) for model, passed to <code>geom_polygon</code> , default=0.6 |
| <code>type</code> | type of VPC plot: 1=display model regions only, 2=as 1 + lines (low, median and high) of data, 3= as 2 + points for data. type=0 can also be used and then no graph is produced but instead a list with 2 dataframes is returned. one for the <code>vpcresult</code> and one for the observed data in the <code>vpctab</code> file. |
| <code>panel.height.censored</code> | Height for BLQ ALQ panels. Height is relative to height of Un-censored panel, default=0.25 |
| <code>censoring.labels</code> | Character vector used as labels for panels when VPC have either BLQ or ALQ data Default set to <code>c("ALQ","BLQ")</code> . NOTE: must be character vector of length 2 |
| <code>ignore.censoring</code> | Ignore any censoring results in VPC result file (BLQ and ALQ), default=FALSE |
| <code>control</code> | an optional list of control settings. See <code>GOF.control</code> for the names of the settable control values and their effect. |

Details

The `ggplot2` package is used for creating the VPC and `vpcfig2` have functionality for e.g. modify names of strata, order of and subset of strata's, and transform the x- and or y-axis before plotting.

The data used is either specified by the directory of the PsN generated files, or by specifying the file names of both the `vpctab`-file and the `vpcresult` file. See examples 1 and 2 below.

Names of strata can be changed with the `strata.names` argument, if `strata.names` is NULL the names as specified in the `vpcresult` file are used.

`strata.subset` can be used to select a subset of strata, and or to change the order of stratas. See example 3.

Strata.subset is matched with `strata.names` unless `strata.names=NULL`. If `strata.names=NULL` then `strata.subset` is matched to names as specified in `vpcresult` file. Default is to use all strata's (`strata.subset=NULL`).

The `fy` and `fx` arguments can be used to alter the scale of data plotted. For example, using `fy=function(y){log(y+1)}` is a convenient way to get log-scale for y-axis but with an off-set to show any values==0. Proper y tick marks can then be set using the `scale_y_continuous` `ggplot2` function.

Since the returned object is a `ggplot`-class object it can be further modified to e.g. to log-scale for y-axis;

```
vpcfig2(...)+scale_y_log10(),
```

adding/changing labels & titles;

```
vpcfig2(...)+labs(y="Modified y-label", title="New title").
```

Axis-limits are preferably set using the ggplot2 function `coord_cartesian(...)`. This way data points outside the axis-limit are only hidden when plotting.

Stratified VPC's are created with `facet_wrap(~strata)` as default but can be modified to use `facet_grid` for setting the panel grid.

However faceting must be done with `~strata`.

See examples below and documentation for ggplot2 for further details.

Value

ggplot object of VPC plot

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "vpctab004.dat", package = "nonmem2R")
file2 <- system.file("extdata", "vpc_results.csv", package = "nonmem2R")

# Ex 1, produce VPC with default setting, here specifying both vpctab and vpcresult
vpcfig2(vpctab=file1,vpcresult=file2)

## Not run:
# Ex 2, produce VPC with default setting, here specifying only directory of vpc files
path1<-gsub("vpctab004.dat","",file1)
vpcfig2(vpcdir=path1)

## End(Not run)

# Ex 3, produce VPC with i) modifies strata names, ii) strata in reverse order, and
#      iii) labels
strata.names<-c("Group A","Group B")
xlab<-"Time after dose (hrs)"
ylab<-"Plasma Conc(mmol/L)"
vpcfig2(vpctab=file1,vpcresult=file2,strata.names=strata.names,strata.subset=2:1,
        xlab=xlab,ylab=ylab)

# Example using the fy argument to transform y-axis setting y-ticks using scale_y_continuous(...)
tmp<-c(1,2,3,4,6)
yticks<-c(0.1,tmp,tmp*10,tmp*100,tmp*1000)
vpcfig2(vpctab=file1,vpcresult=file2,fy=function(y){log(y+1)})+
  scale_y_continuous(breaks=log(yticks+1),labels=yticks,minor_breaks=NULL)

## Not run:
# Example changing to slog-scale using the ggplot2 function scale_y_log10
vpcfig2(vpctab=file1,vpcresult=file2)+scale_y_log10()
```

```
## End(Not run)
# Example changing y-axis label and adding figure title using ggplot2 function labs(...).
vpcfig2(vpctab=file1,vpcresult=file2)+labs(y="Modified y-label", title="New title")
```

| | |
|---------|---|
| vpcfig3 | <i>Visual Predictive Check (VPC) based on raw Perl-speaks-NONMEM (PsN) generated VPC files.</i> |
|---------|---|

Description

This function compile VPC simulated data from the vpc command in Pearl Speaks NONMEM (PsN). The compiled data is then plotted (unless type=0) and returned (ggplot-object) and can then be further modified.

Usage

```
vpcfig3(
  sdtab,
  vpcdir,
  use.model.path = TRUE,
  dv = "DV",
  idvs = "TIME",
  numerical = rep(TRUE, length(idvs)),
  strata = NULL,
  method = c("loess", "spline"),
  pred.corr = c("none", "pred-corr-pro p", "pred-corr-add"),
  maxNsim = NULL,
  knots = 5,
  minobs = 8,
  col.data = "gray20",
  cex.data = 1,
  pch.data = 19,
  alpha.data = 0.5,
  col.line = "grey20",
  lwd.line = 1,
  lty.line = 1,
  col.segm = "steelblue",
  alpha.segm = 0.6,
  type = 3,
  control = GOF.control(),
  ...
)
```

Arguments

| | |
|----------------|--|
| sdtab | file path to sdtab output from model, ALTERNATIVELY a data.frame of the loaded sdtab file. See details. |
| vpcdir | Path of directory of the VPC files, ALTERNATIVELY a data.frame of the loaded matrix file. See details. |
| use.model.path | Load files from a global defined model library (TRUE=default). If so will look for a global character vector named model.path |
| dv | Dependent variable (y-axis) |
| idvs | Independent variable (x-axis) |
| numerical | Logical indicator if idvs is numerical variable(TRUE) or categorical (FALSE), default=TRUE NOTE: must be of same length as idvs |
| strata | Stratification column of sdtab, NOTE must be a column in the sdtab |
| method | either "loess" (default) or "spline" for continuous IDV's |
| pred.corr | Set to "pred-corr-prop" or "pred-corr-add" to perform prediction corrected VPC or set to "none" (default) otherwise. With "pred-corr-prop" correction is recommended for strictly positive data, use "pred-corr-add" if some data points are negative, |
| maxNsim | maximum number of simulations used to use for computing VPC. Default=NULL, meaning all simulations in the input datafile/data.frame will be used. |
| knots | number of knots (bins) for method spline. See details. |
| minobs | minimum number of observations per number of knots(bins) for method spline. See details. |
| col.data | color for data points, passed to geom_point, default="gray20" |
| cex.data | cex for data points, passed to geom_point, default=1 |
| pch.data | plot symbol (pch) for data points, passed to geom_point, default=19 |
| alpha.data | alpha for plotting of data points, passed to geom_point, default=0.5 |
| col.line | line color for mean of data, passed to geom_line, default="gray20" |
| lwd.line | line width (lwd) for mean of data, passed to geom_line, default=1 |
| lty.line | line type (lty) for mean of data, passed to geom_line, default=1 |
| col.segm | Color of CI region for model, passed to geom_ribbon, default="steelblue" |
| alpha.segm | alpha of CI region for model, passed to geom_polygon, default=0.6 |
| type | type of VPC plot: 1=display model regions only, 2=as 1 + mean of data, 3= as 2 + points for data. type=0 can also be used and then no graph is produced but instead a list with 2 dataframes is returned. one for the vpcresult and one for the observed data in the vptab file. |
| control | an optional list of control settings. See GOF.control for the names of the settable control values and their effect. |
| ... | Additional named arguments (e.g. span and degree) are passed to loess.smooth. |

Details

The sdtab and vpcdir can either be file name of the sdtab file and the folder name of the psn generated VPC, or can be data.frames of sdtab and simulation data loaded outside vpcfig3, see example below for the latter case.

Loading the sdtab and matrix file outside vpcfig2 is convenient when dosing multiple VPC plots or for VPC using new strata (or idv) variables not included in the sdtab file, see example.

If vpcdir is given as a folder names, then a matrix.csv file is loaded from the /m1 subfolder of vpcdir.

The raw simulated results from the matrix file is loaded to compute mean of data with confidence intervals For numerical idv variables loess-smooth or linear spline is used on observed actual data and on simulated data. For categorical idv mean is computed for each unique value if idv

For method=spline, the actual number of knots(bins) is set as $\min(\text{knots}, N/\text{minobs})$ where N is the number of observations.

Value

A ggplot object if type>0, or if type==0 a list of 3 data.frames, D1=individual data, D3=mean data, D5=mean model with confidence intervals

Examples

```
# Get path to the example files included in nonmem2R package
file1 <- system.file("extdata", "sdtab", package = "nonmem2R")
file2 <- system.file("extdata", "DV_matrix.csv", package = "nonmem2R")

#load sdtab and matrix file
sdtab<-read.table(file=file1,skip=1,header=TRUE)
vpc<-read.table(file=file2,header=FALSE,sep=",")

# VPC stratified by gender
vpcfig3(sdtab,vpc,dv="DV",idvs="TAD",strata="SEX")

# create new strata variable and do VPC
sdtab$age.group<-cut(sdtab$AGE,c(22,30,50))
vpcfig3(sdtab,vpc,dv="DV",idvs="TAD",strata="age.group")
```

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