

Package ‘xpose’

March 21, 2019

Type Package

Title Diagnostics for Pharmacometric Models

Version 0.4.4

Description Diagnostics for non-linear mixed-effects (population) models from 'NONMEM' <<http://www.iconplc.com/innovation/nonmem/>>. 'xpose' facilitates data import, creation of numerical run summary and provide 'ggplot2'-based graphics for data exploration and model diagnostics.

Depends R (>= 3.1.2), ggplot2 (>= 2.2.1)

Imports dplyr (>= 0.7.0), ggforce, grDevices, purrr (>= 0.2.0), readr, rlang (>= 0.1.2), stringr, tibble (>= 1.3.1), tidyr (>= 0.6), utils, stats, vpc (>= 1.0.0)

Suggests gridExtra, rmarkdown, knitr, testthat, plotly, webshot, mvtnorm

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URL <https://github.com/UUPharmacometrics/xpose>

BugReports <https://github.com/UUPharmacometrics/xpose/issues>

Encoding UTF-8

LazyData true

VignetteBuilder knitr

RoxygenNote 6.1.1

NeedsCompilation no

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Date/Publication 2019-03-21 17:10:03 UTC

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xpose-package	<i>xpose: graphical diagnostics for pharmacometric models</i>
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Description

xpose was designed as a ggplot2-based alternative to xpose4. This package aims to reduce the post processing burden and improve diagnostics commonly associated the development of non-linear mixed effect models.

To learn more about xpose, visit our website: <https://UUPharmacometrics.github.io/xpose/>.

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See Also

Useful links:

- <https://github.com/UUPharmacometrics/xpose>
- Report bugs at <https://github.com/UUPharmacometrics/xpose/issues>

amt_vs_idv	<i>Compartment kinetics</i>
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Description

Plot of the change in compartment amounts over the independent variable

Usage

```
amt_vs_idv(xpdb, mapping = NULL, group = "ID", drop_fixed = TRUE,
  type = "l", title = "Compartments amount vs. @x | @run",
  subtitle = "Ofv: @ofv", caption = "@dir", tag = NULL, log = NULL,
  facets, .problem, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
group	Grouping variable to be used for lines.
drop_fixed	Should columns that only have a single unique value (i.e. fixed) be dropped.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on xplot_scatter.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is layer_option where layer is one of the names defined in the list below and option is any option supported by this layer e.g. point_color = 'blue', smooth_method = 'lm', etc.

- point: options to geom_point
- line: options to geom_line
- guide: options to geom_abline
- smooth: options to geom_smooth
- text: options to geom_text
- xscale: options to scale_x_continuous or scale_x_log10
- yscale: options to scale_y_continuous or scale_y_log10

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions [facet_wrap_paginate](#) when the facets argument is a character string (e.g. facets = c('SEX', 'MED1')) or [facet_grid_paginate](#) when facets is a formula (e.g. facets = SEX~MED1). All xpose plot functions accept all the arguments for the [facet_wrap_paginate](#) and [facet_grid_paginate](#) functions e.g. dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...). Faceting options can either be defined in plot functions (e.g. dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')) or assigned globally to an xpdb object via the xp_theme (e.g. xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = ...))). In the latter example all plots generate from this xpdb will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
amt_vs_idv(xpdb_ex_pk)
```

data_opt

Create options for data import

Description

Provide a list of options to the general plotting functions such as `xplot_scatter` in order to create appropriate data input for `ggplot2`.

Usage

```
data_opt(.problem = NULL, .subprob = NULL, .method = NULL,
        .source = "data", simtab = FALSE, filter = NULL, tidy = FALSE,
        index_col = NULL, value_col = NULL, post_processing = NULL)
```

Arguments

<code>.problem</code>	The problem to be used, by default returns the last one.
<code>.subprob</code>	The subproblem to be used, by default returns the last one.
<code>.method</code>	The estimation method to be used, by default returns the last one.
<code>.source</code>	Define the location of the data in the <code>xpdb</code> . Should be either 'data' to use the output tables or the name of an output file attached to the <code>xpdb</code> .
<code>simtab</code>	Only used when 'data' is defined as the source and '.problem' is default. Should the data be coming from an estimation or a simulation table.
<code>filter</code>	A function used to filter the data e.g. <code>filter = function(x) x[x\$TIME > 20,]</code> where <code>x</code> is the data.

tidy	Logical, whether the data should be transformed to tidy data.
index_col	Only used when 'tidy' is defined a TRUE and value_col is NULL. Column names to use as index when tidying the data.
value_col	Only used when 'tidy' is defined a TRUE and index_col is NULL. Column names to be stacked when tidying the data.
post_processing	A function used to modify the data after it has been tidied up e.g. <code>post_processing = function(x) dplyr::mutate(.data = x, variable = as.factor(.\$variable))</code> where x is the tidy data.

See Also

[xplot_distrib](#) [xplot_qq](#) [xplot_scatter](#)

Examples

```
data_opt(.problem = 1, .source = 'data', simtab = TRUE)
```

distrib_plot

Distribution plots of ETA and parameters

Description

Histograms and density plots of the ETA and parameter values.

Usage

```
prm_distrib(xpdb, mapping = NULL, drop_fixed = TRUE, type = "hr",
  title = "Parameter distribution | @run",
  subtitle = "Based on @nind individuals", caption = "@dir",
  tag = NULL, log = NULL, guide = FALSE, facets, .problem, quiet,
  ...)
```

```
eta_distrib(xpdb, mapping = NULL, drop_fixed = TRUE, type = "hr",
  title = "Eta distribution | @run",
  subtitle = "Based on @nind individuals, Eta shrink: @etashk",
  caption = "@dir", tag = NULL, log = NULL, guide = FALSE, facets,
  .problem, quiet, ...)
```

```
res_distrib(xpdb, mapping = NULL, res = "CWRES", type = "hr",
  title = "@x distribution | @run",
  subtitle = "Based on @nobs observations", caption = "@dir",
  tag = NULL, log = NULL, guide = FALSE, facets, .problem, quiet,
  ...)
```

```
cov_distrib(xpdb, mapping = NULL, drop_fixed = TRUE, type = "hr",
```

```

title = "Continuous covariates distribution | @run",
subtitle = "Based on @nind individuals", caption = "@dir",
tag = NULL, log = NULL, guide = FALSE, facets, .problem, quiet,
...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. <code>point_color</code>).
drop_fixed	Should columns that only have a single unique value (i.e. fixed) be dropped.
type	String setting the type of plot to be used. Can be histogram 'h', density 'd', rug 'r' or any combination of the three.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
guide	Should the guide (e.g. reference distribution) be displayed.
facets	Either a character string to use <code>facet_wrap_paginate</code> or a formula to use <code>facet_grid_paginate</code> .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .
res	Only used for <code>res_distrib</code> . Defines the type of residual to be used. Default is "CWRES".

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `histogram_fill = 'blue'`, `rug_sides = 'b'`, etc.

- histogram: options to `geom_histogram`
- density: options to `geom_density`
- rug: options to `geom_rug`
- xscale: options to `scale_x_continuous` or `scale_x_log10`
- yscale: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = list(margins = TRUE)))`). In the latter example all plots generated from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_distrib](#)

Examples

```
# Histogram of parameters
prm_distrib(xpdb_ex_pk, type = 'h')

# Density plot of etas with a rug
eta_distrib(xpdb_ex_pk, type = 'dr')

# Histogram of different residuals
res_distrib(xpdb_ex_pk, type = 'hr', res = c('IWRES', 'CWRES'))

# Density plot of continuous covariates
cov_distrib(xpdb_ex_pk, type = 'd')
```

dv_vs_pred

Observations plotted against model predictions

Description

Plot of observations (DV) vs population predictions (PRED), individual predictions (IPRED) or conditional population predictions (CPRED).

Usage

```
dv_vs_ipred(xpdb, mapping = NULL, group = "ID", type = "pls",
  title = "@y vs. @x | @run",
  subtitle = "Ofv: @ofv, Eps shrink: @epsshk", caption = "@dir",
  tag = NULL, log = NULL, guide = TRUE, facets, .problem, quiet, ...)

dv_vs_pred(xpdb, mapping = NULL, group = "ID", type = "pls",
  title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
  caption = "@dir", tag = NULL, log = NULL, guide = TRUE, facets,
  .problem, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
guide	Enable guide display (e.g. unity line).
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- point: options to `geom_point`
- line: options to `geom_line`
- guide: options to `geom_abline`
- smooth: options to `geom_smooth`
- text: options to `geom_text`
- xscale: options to `scale_x_continuous` or `scale_x_log10`
- yscale: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller =`

Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
dv_vs_pred(xpdb_ex_pk)
```

```
dv_vs_ipred(xpdb_ex_pk)
```

get_code

Access model code

Description

Access model code from an `xpdb` object.

Usage

```
get_code(xpdb, .problem = NULL)
```

Arguments

xpdb	An xpose_data object from which the model code will be extracted.
.problem	The problem to be used, in addition, problem 0 is attributed to general output (e.g. NM-TRAN warnings in NONMEM). By default returns the entire code.

Value

A tibble of the parsed model.

See Also

[xpose_data](#), [read_nm_model](#)

Examples

```
parsed_model <- get_code(xpdb_ex_pk)
parsed_model
```

get_data	<i>Access model output table data</i>
----------	---------------------------------------

Description

Access model output table data from an xpdb object.

Usage

```
get_data(xpdb, table = NULL, .problem = NULL, quiet)
```

Arguments

xpdb	An xpose_data object from which the model output file data will be extracted.
table	Name of the output table to be extracted from the xpdb e.g. 'sdtab001'. Alternative to the '.problem' argument.
.problem	Accesses all tables from the specified problem. Alternative to the 'table' argument.
quiet	Logical, if FALSE messages are printed to the console.

Value

By default returns data from the last estimation problem. If only simulation problems are present then the data from last simulation will be returned instead. Object returned as tibble for single tables/problems or a named list for multiple tables/problems.

See Also

[list_data](#), [xpose_data](#), [read_nm_tables](#)

Examples

```
# By table name
sdtab <- get_data(xpdb_ex_pk, 'sdtab001')
sdtab

# By problem
tables <- get_data(xpdb_ex_pk, .problem = 1)
tables

# Tip to list available tables in the xpdb
print(xpdb_ex_pk)
```

<code>get_file</code>	<i>Access model output file data</i>
-----------------------	--------------------------------------

Description

Access model output file data from an xpdb object.

Usage

```
get_file(xpdb, file = NULL, ext = NULL, .problem = NULL,
         .subprob = NULL, .method = NULL, quiet)
```

Arguments

<code>xpdb</code>	An <code>xpose_data</code> object from which the model output file data will be extracted.
<code>file</code>	Full name of the file to be extracted from the xpdb e.g. 'run001.phi'. Alternative to the 'ext' argument.
<code>ext</code>	Extension of the file to be extracted from the xpdb e.g. 'phi'. Alternative to the 'file' argument.
<code>.problem</code>	The problem to be used, by default returns the last one for each file.
<code>.subprob</code>	The subproblem to be used, by default returns the last one for each file.
<code>.method</code>	The estimation method to be used (e.g. 'foce', 'imp', 'saem'), by default returns the last one for each file.
<code>quiet</code>	Logical, if FALSE messages are printed to the console.

Value

A tibble for single file or a named list for multiple files.

See Also

[list_files](#), [xpose_data](#), [read_nm_files](#)

Examples

```
# Single file (returns a tibble)
ext_file <- get_file(xpdb_ex_pk, file = 'run001.ext')
ext_file

# Multiple files (returns a list)
files <- get_file(xpdb_ex_pk, file = c('run001.ext', 'run001.phi'))
files

# Tip to list available files in the xpdb
print(xpdb_ex_pk)
```

get_prm

Access model parameters

Description

Access model parameter estimates from an xpdb object.

Usage

```
get_prm(xpdb, .problem = NULL, .subprob = NULL, .method = NULL,
        digits = 4, transform = TRUE, show_all = FALSE, quiet)
```

Arguments

xpdb	An xpose_data object from which the model output file data will be extracted.
.problem	The problem to be used, by default returns the last one for each file.
.subprob	The subproblem to be used, by default returns the last one for each file.
.method	The estimation method to be used, by default returns the last one for each file
digits	The number of significant digits to be displayed.
transform	Should diagonal OMEGA and SIGMA elements be transformed to standard deviation and off diagonal elements be transformed to correlations.
show_all	Logical, whether the 0 fixed off-diagonal elements should be removed from the output.
quiet	Logical, if FALSE messages are printed to the console.

Value

A tibble for single problem/subprob or a named list for multiple problems/subprob.

See Also[prm_table](#)**Examples**

```
# Store the parameter table
prm <- get_prm(xpdb_ex_pk, .problem = 1)

# Display parameters to the console
prm_table(xpdb_ex_pk, .problem = 1)
```

get_special	<i>Access special model data</i>
-------------	----------------------------------

Description

Access special model data from an xpdb object.

Usage

```
get_special(xpdb, .problem = NULL, quiet)
```

Arguments

xpdb	An xpose_data object from which the special data will be extracted.
.problem	The problem to be used, by default returns the last one.
quiet	Logical, if FALSE messages are printed to the console.

Value

A list.

See Also[list_special](#), [xpose_data](#)**Examples**

```
special <- get_summary(xpdb_ex_pk)
special
```

get_summary	<i>Access model summary data</i>
-------------	----------------------------------

Description

Access model summary data from an xpdb object.

Usage

```
get_summary(xpdb, .problem = NULL, .subprob = NULL,  
            only_last = FALSE)
```

Arguments

xpdb	An xpose_data object from which the summary data will be extracted.
.problem	The .problem to be used, by default returns the last one for each label.
.subprob	The subproblem to be used, by default returns the last one for each label.
only_last	Logical, if TRUE only the last record for each label is returned in case of multiple problem and/or subproblem. If FALSE all values are returned.

Value

A tibble of model summary.

See Also

[xpose_data](#), [template_titles](#), [summary.xpose_data](#)

Examples

```
run_summary <- get_summary(xpdb_ex_pk)  
run_summary
```

gg_themes	<i>An additional set of themes for ggplot2</i>
-----------	--

Description

An additional set of complete ggplot2 themes intended to make ggplot2 more readable when used in presentation or publications. These themes also bring the legend_position option without having to call the ggplot2 theme() function to modify a complete theme.

- theme_bw2: Black and white theme inspired by a theme from Gunnar Yngman.
- theme_readable: Light grey theme, with dimmed background and grid lines intended to bring the focus on the data.

Usage

```
theme_bw2(base_size = 11, base_family = "",
           legend_position = "right")

theme_readable(base_size = 11, base_family = "",
               legend_position = "right")
```

Arguments

```
base_size      Base font size.
base_family    Base font family.
legend_position
               The position of legends defined as 'none', 'left', 'right', 'bottom', 'top', or a
               two-element numeric vector.
```

Examples

```
# With the gg_theme theme_readable() (default)
dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')

# With the gg_theme theme_bw2()
xpdb_ex_pk %>%
  update_themes(gg_theme = theme_bw2()) %>%
  dv_vs_ipred(facets = 'SEX')
```

ind_plots	<i>Observations, individual predictions and population predictions plotted against the independent variable for every individual</i>
-----------	--

Description

Observations (DV), individual predictions (IPRED) and population predictions (PRED) plotted against the independent variable for every individual

Usage

```
ind_plots(xpdb, mapping = NULL, group = "variable", type = "lp",
          title = "Individual plots | @run",
          subtitle = "Ofv: @ofv, Eps shrink: @epsshk",
          caption = "@dir | Page @page of @lastpage", tag = NULL, log = NULL,
          facets, .problem, quiet, color = c("grey60", "deepskyblue4",
          "deepskyblue3"), point_alpha = c(0.8, 0, 0),
          line_linetype = c("blank", "solid", "55"), ...)
```


Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. <code>point_color</code>).
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
facets	Either a character string to use <code>facet_wrap_paginate</code> or a formula to use <code>facet_grid_paginate</code> .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
color	Changes the <code>**lines, points and text**</code> color. Should be a vector of 3 values (i.e. DV, IPRED, PRED). This color argument is a special case in xpose as it applies to three different layers (<code>geom_line</code> , <code>geom_point</code> and <code>geom_text</code>). This special case is due to the fact that in <code>ggplot2</code> it is not possible to have two different color scales for different layers.
point_alpha	Points alpha, should be a vector of 3 values (i.e. DV, IPRED, PRED).
line_linetype	Lines linetype, should be a vector of 3 values (i.e. DV, IPRED, PRED).
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- point: options to `geom_point`
- line: options to `geom_line`
- guide: options to `geom_abline`
- smooth: options to `geom_smooth`
- text: options to `geom_text`
- xscale: options to `scale_x_continuous` or `scale_x_log10`
- yscale: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = list(facets = 'SEX')))`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
# Basic example
ind_plots(xpdb_ex_pk, page = 1,
          ncol = 3, nrow = 3)
```

irep

Add simulation counter

Description

Add a column containing a simulation counter (irep). A new simulation is counted everytime a value in x is lower than its previous value.

Usage

```
irep(x, quiet = FALSE)
```

Arguments

x The column to be used for computing simulation number, usually the ID column.
quiet Logical, if FALSE messages are printed to the console.

Examples

```
xpdb_ex_pk_2 <- xpdb_ex_pk %>%  
  mutate(sim_id = irep(ID), .problem = 2)
```

list_nm_tables	<i>List NONMEM output tables</i>
----------------	----------------------------------

Description

List NONMEM output tables file names from a `nm_model` object.

Usage

```
list_nm_tables(nm_model = NULL)
```

Arguments

nm_model An xpose `nm_model` object generated with [read_nm_model](#).

See Also

[read_nm_model](#), [read_nm_tables](#)

Examples

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

list_vars *List available variables*

Description

Function listing all available variables in an xpdb object.

Usage

```
list_vars(xpdb, .problem = NULL)
```

Arguments

xpdb An xpose_data object from which the model code will be extracted.
.problem The problem to be used, by lists all available problems.

See Also

[set_var_types](#)

Examples

```
list_vars(xpdb_ex_pk)
```

list_xpdb *List available datasets*

Description

Function providing a detailed listing of all available datasets in an xpdb object.

Usage

```
list_data(xpdb)
```

```
list_files(xpdb)
```

```
list_special(xpdb)
```

Arguments

xpdb An xpose_data object to be evaluated

See Also

[get_data](#), [get_file](#), [get_special](#)

Examples

```
# List output tables data
list_data(xpdb_ex_pk)

# List output files data
list_files(xpdb_ex_pk)

# List special data
xpdb_ex_pk %>%
vpc_data(quiet = TRUE) %>%
list_special()
```

manual_nm_import	<i>Manually define nonmem tables to be imported</i>
------------------	---

Description

Manually provide names of the table files to be imported by xpose_data.

Usage

```
manual_nm_import(tab_names = c("sdtab", "mutab", "patab", "catab",
  "cotab", "mytab", "extra", "xptab", "cwtab"), tab_suffix = "",
  sim_suffix = "sim")
```

Arguments

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

Details

In order to be imported manually, table names must follow the following convention: <tab_names><runno><tab/sim_suffi e.g. sdtab001sim. When the argument 'file' is used in xpose_data, the <runno> part is guessed by taking the portion of the string starting by any digit and ending at the file extension e.g. file = run001a.mod will guess <runno> as '001a'. If no valid <runno> can be guessed, xpose will return an error. In this case it is advised to use the xpose_data argument 'runno' directly rather than 'file' hence preventing xpose from having to guess <runno>.

Note that with manual table import xpose still reads in the NONMEM model file in order to generate the run summary.

See Also[xpose_data](#)**Examples**

```
## Not run:
# Import all names specified by default as in xpose4
xpose_data(runno = '001', manual_import = manual_nm_import())

# Import a specific table name
xpose_data(runno = '001', manual_import = manual_nm_import(tab_names = 'mytab'))

## End(Not run)
```

minimization_plots	<i>Parameter value or gradient vs. iterations</i>
--------------------	---

Description

Change of parameter value or gradient vs. iterations.

Usage

```
prm_vs_iteration(xpdb, mapping = NULL, group = "variable",
  type = "l", title = "Parameter @y vs. @x | @run",
  subtitle = "Method: @method, minimization time: @runtime\nTermination message: @term",
  caption = "@dir", tag = NULL, log = NULL, guide = FALSE, facets,
  .problem, .subprob, .method, quiet, ...)

grd_vs_iteration(xpdb, mapping = NULL, group = "variable",
  type = "l", title = "Gradient @y vs. @x | @run",
  subtitle = "Method: @method, minimization time: @runtime\nTermination message: @term",
  caption = "@dir", tag = NULL, log = NULL, guide = FALSE, facets,
  .problem, .subprob, .method, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.

tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either <code>''</code> , <code>'x'</code> , <code>y</code> or <code>'xy'</code> .
guide	Enable guide display (e.g. unity line).
facets	Either a character string to use <code>facet_wrap_paginate</code> or a formula to use <code>facet_grid_paginate</code> .
.problem	The \$problem number to be used. By default returns the last estimation problem.
.subprob	The sub-problem number to be used. By default returns the last sub-problem associated with the selected problem.
.method	The estimation method to be used, by default returns the last one for each file
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- `point`: options to `geom_point`
- `line`: options to `geom_line`
- `guide`: options to `geom_abline`
- `smooth`: options to `geom_smooth`
- `text`: options to `geom_text`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every `xpose` plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All `xpose` plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller =`

Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generate from this `xpdb` will automatically be stratified by `'SEX'`.

By default, some plot functions use a custom stratifying variable named `'variable'`, e.g. `eta_distrib()`. When using the `facets` argument, `'variable'` needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
prm_vs_iteration(xpdb_ex_pk)
```

```
grd_vs_iteration(xpdb_ex_pk)
```

modify_xpdb

Add, remove or rename variables in an xpdb

Description

`mutate()` adds new variables and preserves existing ones. `select()` keeps only the listed variables; `rename()` keeps all variables.

Usage

```
## S3 method for class 'xpose_data'
mutate(.data, ..., .problem, .source, .where)
```

```
## S3 method for class 'xpose_data'
select(.data, ..., .problem, .source, .where)
```

```
## S3 method for class 'xpose_data'
rename(.data, ..., .problem, .source, .where)
```

Arguments

<code>.data</code>	An xpose database object.
<code>...</code>	Name-value pairs of expressions. Use NULL to drop a variable. These arguments are automatically quoted and evaluated in the context of the data frame. They support unquoting and splicing. See the <code>dplyr</code> vignette("programming") for an introduction to these concepts.
<code>.problem</code>	The problem from which the data will be modified
<code>.source</code>	The source of the data in the xpdb. Can either be 'data' or an output file extension e.g. 'phi'.

`.where` A vector of element names to be edited in special (e.g. `.where = c('vpc_dat', 'aggr_obs')` with `vpc`).

Examples

```
# Mutate columns
xpdb_ex_pk %>%
  mutate(lnDV = log(DV),
         sim_count = irep(ID),
         .problem = 1) %>%
  dv_vs_idv(aes(y = lnDV))

# Rename/select columns
xpdb_ex_pk %>%
  select(ID:TAD, DV, EVID) %>%
  rename(TSLD = TAD) %>%
  dv_vs_idv(aes(x = TSLD))
```

pred_vs_idv	<i>Observations and model predictions plotted against the independent variable</i>
-------------	--

Description

Plot of observations (DV), individual model predictions (IPRED) and/or population predictions (PRED) plotted against the independent variable (IDV).

Usage

```
dv_vs_idv(xpdb, mapping = NULL, group = "ID", type = "pls",
          title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
          caption = "@dir", tag = NULL, log = NULL, facets, .problem, quiet,
          ...)
```

```
ipred_vs_idv(xpdb, mapping = NULL, group = "ID", type = "pls",
             facets, title = "@y vs. @x | @run",
             subtitle = "Ofv: @ofv, Eps shrink: @epsshk", caption = "@dir",
             tag = NULL, log = NULL, .problem, quiet, ...)
```

```
pred_vs_idv(xpdb, mapping = NULL, group = "ID", type = "pls", facets,
            title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
            caption = "@dir", tag = NULL, log = NULL, .problem, quiet, ...)
```

```
dv_preds_vs_idv(xpdb, mapping = NULL, group = "ID", type = "pls",
                 facets,
                 title = "Observations, Individual predictions and Population predictions vs. @x | @run",
                 subtitle = "Ofv: @ofv, Eps shrink: @epsshk", caption = "@dir",
                 tag = NULL, log = NULL, .problem, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- `point`: options to `geom_point`
- `line`: options to `geom_line`
- `guide`: options to `geom_abline`
- `smooth`: options to `geom_smooth`
- `text`: options to `geom_text`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions [facet_wrap_paginate](#) when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or [facet_grid_paginate](#) when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the [facet_wrap_paginate](#) and [facet_grid_paginate](#) functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = list(...)))`). In the latter example all plots generated from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
dv_vs_idv(xpdb_ex_pk)
ipred_vs_idv(xpdb_ex_pk)
pred_vs_idv(xpdb_ex_pk)
dv_preds_vs_idv(xpdb_ex_pk)
```

print.xpose_data	<i>Print an xpose_data object</i>
------------------	-----------------------------------

Description

This function returns to the console a list of the files and options attached to an [xpose_data](#) object.

Usage

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

Arguments

x	An xpose_data object generated with xpose_data .
...	Ignored in this function

Examples

```
# Using the print function
print(xpdb_ex_pk)

# Or simply by writing the xpdb name
xpdb_ex_pk
```

print.xpose_plot	<i>Draw an xpose_plot object</i>
------------------	----------------------------------

Description

This function explicitly draw an xpose_plot and interprets keywords contained in labels.

Usage

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

Arguments

x	An xpose_plot object.
page	The page number to be drawn. Can be specified as vector or range of integer values.
...	Options to be passed on to the ggplot2 print method.

Examples

```
my_plot <- dv_vs_ipred(xpdb_ex_pk) +  
  labs(title = 'A label with keywords: @nind individuals & @nobs observations')  
# Using the print function  
print(my_plot)  
  
# Or simply by writing the plot object name  
my_plot
```

prm_table	<i>Display a parameter estimates to the console</i>
-----------	---

Description

Display parameter estimates from an xpdb object to the console.

Usage

```
prm_table(xpdb, .problem = NULL, .subprob = NULL, .method = NULL,  
  digits = 4, transform = TRUE, show_all = FALSE)
```

Arguments

xpdb	An xpose_data object from which the model output file data will be extracted.
.problem	The problem to be used, by default returns the last one for each file.
.subprob	The subproblem to be used, by default returns the last one for each file.
.method	The estimation method to be used, by default returns the last one for each file
digits	The number of significant digits to be displayed.
transform	Should diagonal OMEGA and SIGMA elements be transformed to standard deviation and off diagonal elements be transformed to correlations.
show_all	Logical, whether the 0 fixed off-diagonal elements should be removed from the output.

See Also

[get_prm](#),

Examples

```
# Store the parameter table
prm <- get_prm(xpdb_ex_pk, .problem = 1)

# Display parameters to the console
prm_table(xpdb_ex_pk, .problem = 1)
```

qq_plot

QQ plots of ETA and residuals

Description

QQ plots of the ETA and model residuals.

Usage

```
prm_qq(xpdb, mapping = NULL, drop_fixed = TRUE, type = "p",
       title = "QQ plot of parameters | @run",
       subtitle = "Based on @nind individuals", caption = "@dir",
       tag = NULL, log = NULL, guide = TRUE, facets, .problem, quiet, ...)

eta_qq(xpdb, mapping = NULL, drop_fixed = TRUE, type = "p",
       title = "QQ plot of etas | @run",
       subtitle = "Based on @nind individuals, Eta shrink: @etashk",
       caption = "@dir", tag = NULL, log = NULL, guide = TRUE, facets,
       .problem, quiet, ...)

res_qq(xpdb, mapping = NULL, res = "CWRES", type = "p",
```

```

title = "QQ plot of @sample | @run",
subtitle = "Based on @nobs observations", caption = "@dir",
tag = NULL, log = NULL, guide = TRUE, facets, .problem, quiet, ...)

cov_qq(xpdb, mapping = NULL, drop_fixed = TRUE, type = "p",
title = "QQ plot of continuous covariates | @run",
subtitle = "Based on @nind individuals", caption = "@dir",
tag = NULL, log = NULL, guide = TRUE, facets, .problem, quiet, ...)

```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. <code>point_color</code>).
drop_fixed	Should columns that only have a single unique value (i.e. fixed) be dropped.
type	String setting the type of plot. Can only be points 'p'.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either <code>"</code> , <code>'x'</code> , <code>y'</code> or <code>'xy'</code> .
guide	Should the guide (e.g. reference line) be displayed.
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on <code>xplot_scatter</code> .
res	Only used for <code>res_qq</code> . Defines the type of residual to be used. Default is "CWRES".

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, etc.

- `point`: options to `geom_point`
- `guide`: options to `geom_abline`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = list(facets = 'SEX')))`). In the latter example all plots generated from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_distrib](#)

Examples

```
# QQ plot of parameters
prm_qq(xpdb_ex_pk)

# QQ plot of eta
eta_qq(xpdb_ex_pk)

# QQ plot of residuals
res_qq(xpdb_ex_pk, res = c('IWRES', 'CWRES'))

# QQ plot of continuous covariates
cov_qq(xpdb_ex_pk)
```

read_nm_files

NONMEM output file import function

Description

Quickly import NONMEM output files into R.

Usage

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

Arguments

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

File path generation

The rules for model file names generation are as follow:

- with runno: the full path is generated as <dir>/<prefix><runno>.<ext> e.g. with dir = 'model/pk', prefix = 'run', runno = '001', ext = '.lst' the resulting path would be model/pk/run001.lst
- with file: the full path is generated as <dir>/<file> e.g. with dir = 'model/pk', file = 'run001.lst' the resulting path would also be model/pk/run001.lst. Note: in this case the file extension should be provided as part of the 'file' argument.

See Also

[xpose_data](#), [read_nm_tables](#)

Examples

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

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

## End(Not run)
```

read_nm_model	<i>NONMEM model file parser</i>
---------------	---------------------------------

Description

Parse NONMEM model files in R format

Usage

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

Arguments

runno	Run number to be used to generate model file name. Used in combination with prefix and ext.
prefix	Prefix to be used to generate model file name. Used in combination with runno and ext.
ext	Extension to be used to generate model file name. Should be one of '.lst' (default), '.out', '.res', '.mod' or '.ctl' for NONMEM.
file	Model file name (preferably a '.lst' file) containing the file extension. Alternative to prefix, runno and ext arguments.
dir	Location of the model files.

Details

A NONMEM model output file (i.e. .lst, .out or .res) should preferably be provided to `read_nm_model` to allow for a more extensive xpose summary. However in some cases these output files may not contain the model code, thus preventing xpose from identifying the associated output tables names. In such cases xpose will attempt to read the associated model file (i.e. .mod or .ctl) instead to find the model code. Note: it is important that between the naming convention between the NONMEM output and the model file remains consistent e.g. run001.lst should be associated with run001.mod.

Value

A [tibble](#) of class `model` containing the following columns:

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

- **comment:** the last comment of a record e.g. '0.5 ; Clearance (L/h) ; TVCL' will return 'TVCL'.

File path generation

The rules for model file names generation are as follow:

- with runno: the full path is generated as <dir>/<prefix><runno>.<ext> e.g. with dir = 'model/pk', prefix = 'run', runno = '001', ext = '.lst' the resulting path would be model/pk/run001.lst
- with file: the full path is generated as <dir>/<file> e.g. with dir = 'model/pk', file = 'run001.lst' the resulting path would also be model/pk/run001.lst. Note: in this case the file extension should be provided as part of the 'file' argument.

See Also

[xpose_data](#), [read_nm_tables](#)

Examples

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

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

## End(Not run)
```

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

Description

Quickly import NONMEM output tables into R. This function automatically detects the optimal settings to import the tables from nonmem.

Usage

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


res_vs_idv

*Residuals plotted against the independent variable***Description**

Model residuals plotted against the independent variable (IDV).

The residuals can be one of:

- RES: model residuals
- WRES: weighted model residuals
- CWRES: conditional weighted model residuals
- EWRES/ECWRES: Monte Carlo based model residuals
- NPDE: Normalized prediction distribution error

Usage

```
res_vs_idv(xpdb, mapping = NULL, res = "CWRES", group = "ID",
  type = "pls", title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
  caption = "@dir", tag = NULL, log = NULL, guide = TRUE, facets,
  .problem, quiet, ...)
```

```
absval_res_vs_idv(xpdb, mapping = NULL, res = "CWRES", group = "ID",
  type = "pls", title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
  caption = "@dir", tag = NULL, log = NULL, guide = FALSE, facets,
  .problem, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
res	Type of residual to be used. Default is "CWRES".
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
guide	Enable guide display (e.g. unity line).
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on xplot_scatter.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- `point`: options to `geom_point`
- `line`: options to `geom_line`
- `guide`: options to `geom_abline`
- `smooth`: options to `geom_smooth`
- `text`: options to `geom_text`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
# Standard residual
res_vs_idv(xpdb_ex_pk, res = c('IWRES', 'CWRES'))

# Absolute value of the residuals
absval_res_vs_idv(xpdb_ex_pk, res = 'CWRES')
```

res_vs_pred

Residuals plotted against population predictions

Description

Model residuals plotted against population predictions (PRED).

The residuals can be one of:

- RES: model residuals
- WRES: weighted model residuals
- CWRES: conditional weighted model residuals
- EWRES/ECWRES: Monte Carlo based model residuals
- NPDE: Normalized prediction distribution error

Usage

```
res_vs_pred(xpdb, mapping = NULL, res = "CWRES", group = "ID",
  type = "pls", title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
  caption = "@dir", tag = NULL, log = NULL, guide = TRUE, facets,
  .problem, quiet, ...)
```

```
absval_res_vs_pred(xpdb, mapping = NULL, res = "CWRES", group = "ID",
  type = "pls", title = "@y vs. @x | @run", subtitle = "Ofv: @ofv",
  caption = "@dir", tag = NULL, log = NULL, guide = FALSE, facets,
  .problem, quiet, ...)
```

Arguments

xpdb	An xpose database object.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
res	Type of residual to be used. Default is "CWRES".
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be points 'p', line 'l', smooth 's' and text 't' or any combination of the four.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
guide	Enable guide display (e.g. unity line).
facets	Either a character string to use facet_wrap_paginate or a formula to use facet_grid_paginate .
.problem	The \$problem number to be used. By default returns the last estimation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics to be passed on xplot_scatter.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is layer_option where layer is one of the names defined in the list below and option is any option supported by this layer e.g. point_color = 'blue', smooth_method = 'lm', etc.

- point: options to geom_point
- line: options to geom_line
- guide: options to geom_abline
- smooth: options to geom_smooth
- text: options to geom_text
- xscale: options to scale_x_continuous or scale_x_log10
- yscale: options to scale_y_continuous or scale_y_log10

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller =`

Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#)

Examples

```
# Standard residual
res_vs_pred(xpdb_ex_pk, res = c('IWRES', 'CWRES'))

# Absolute value of the residuals
absval_res_vs_pred(xpdb_ex_pk, res = 'CWRES')
```

set_vars

Set variable type, label or units

Description

Function designed to change the type, label or unit associated with variables.

Usage

```
set_var_types(xpdb, .problem = NULL, ..., auto_factor = TRUE, quiet)
```

```
set_var_labels(xpdb, .problem = NULL, ..., quiet)
```

```
set_var_units(xpdb, .problem = NULL, ..., quiet)
```

Arguments

xpdb	An xpose_data object.
.problem	The problem number to which the edits will be applied.
...	Specifications of the edits to be made to the xpdb index. Edits are made as type and variable pairs e.g. idv = 'TAD' will assign TAD to the type idv (independent variable).
auto_factor	With set_var_types only. If TRUE new columns assigned to the type 'catcov' will be converted to factor.
quiet	Logical, if FALSE messages are printed to the console.

Value

An xpose_data object

Recognized variable types

- a: Compartments' amount
- amt: Dose amount
- catcov: Categorical covariate
- contcov: Continuous covariate
- dv: Dependent variable
- dvid: DV identifier
- eta: Eta
- evid: Event identifier
- id: Subject identifier
- idv: Independent variable
- ipred: Individual model predictions
- mdv: Missing dependent variable
- na: Not attributed
- occ: Occasion flag
- param: Model parameter
- pred: Typical model predictions
- res: Residuals

See Also[list_vars](#)**Examples**

```
# Change variable type
xpdb_2 <- set_var_types(xpdb_ex_pk, .problem = 1, idv = 'TAD')

# Change labels
xpdb_2 <- set_var_labels(xpdb_2, .problem = 1, ALAG1 = 'Lag time', CL = 'Clearance', V = 'Volume')

# Change units
xpdb_2 <- set_var_units(xpdb_2, .problem = 1, ALAG1 = 'h', CL = 'L/h', V = 'L')
```

subset_xpdb

*Subset datasets in an xpdb***Description**

Use `filter()` to select rows/cases where conditions are true. Unlike base subsetting, rows where the condition evaluates to NA are dropped. Use `slice()` to select row/cases by their position

Usage

```
## S3 method for class 'xpose_data'
filter(.data, ..., .problem, .source, .where)

## S3 method for class 'xpose_data'
slice(.data, ..., .problem, .source, .where)

## S3 method for class 'xpose_data'
distinct(.data, ..., .problem, .source, .where)
```

Arguments

<code>.data</code>	An xpose database object.
<code>...</code>	Name-value pairs of expressions. Use NULL to drop a variable. These arguments are automatically quoted and evaluated in the context of the data frame. They support unquoting and splicing. See the <code>dplyr</code> vignette("programming") for an introduction to these concepts.
<code>.problem</code>	The problem from which the data will be modified
<code>.source</code>	The source of the data in the xpdb. Can either be 'data' or an output file extension e.g. 'phi'.
<code>.where</code>	A vector of element names to be edited in special (e.g. <code>.where = c('vpc_dat', 'aggr_obs')</code> with <code>vpc</code>).

Examples

```

# Subset by condition
xpdb_ex_pk %>%
  filter(DV < 1, .problem = 1) %>%
  dv_vs_ipred()

# Subset by positions
xpdb_ex_pk %>%
  slice(1:100, .problem = 1) %>%
  dv_vs_ipred()

# Deduplicate rows
xpdb_ex_pk %>%
  distinct(TIME, .problem = 1) %>%
  dv_vs_ipred()

```

summarize_xpdb

Group/ungroup and summarize variables in an xpdb

Description

group_by() takes an existing table and converts it into a grouped table where operations are performed "by group". ungroup() removes grouping. summarize() reduces multiple values down to a single value.

Usage

```

## S3 method for class 'xpose_data'
group_by(.data, ..., .problem, .source, .where)

## S3 method for class 'xpose_data'
ungroup(x, ..., .problem, .source, .where)

## S3 method for class 'xpose_data'
summarize(.data, ..., .problem, .source, .where)

## S3 method for class 'xpose_data'
summarise(.data, ..., .problem, .source, .where)

```

Arguments

.data	An xpose database object.
...	Name-value pairs of expressions. Use NULL to drop a variable. These arguments are automatically quoted and evaluated in the context of the data frame. They support unquoting and splicing. See the dplyr vignette("programming") for an introduction to these concepts.
.problem	The problem from which the data will be modified

.source	The source of the data in the xpdb. Can either be 'data' or an output file extension e.g. 'phi'.
.where	A vector of element names to be edited in special (e.g. .where = c('vpc_dat', 'aggr_obs') with vpc).
x	Same as .data (used for consistency with dplyr functions).

Examples

```
# Create a distribution plot of Cmax
xpdb_ex_pk %>%
  group_by(ID, SEX, .problem = 1) %>%
  summarize(CMAX = max(DV), .problem = 1) %>%
  ungroup(.problem = 1) %>%
  plot_distrib(aes(x = CMAX, density_fill = SEX), type = 'dr')
```

summary.xpose_data *Summarizing xpose_data*

Description

This function returns a summary of an [xpose_data](#) to the console.

Usage

```
## S3 method for class 'xpose_data'
summary(object, .problem = NULL, ...)
```

Arguments

object	An xpose_data object generated with xpose_data .
.problem	The problem to be used, by default returns the last one for each label.
...	Ignored in this function

Examples

```
summary(xpdb_ex_pk)
```

template_titles	<i>Template titles</i>
-----------------	------------------------

Description

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and the filename when saving with the `xpose_save` function.

Template titles are defined via a single string containing key variables starting with a `@` (e.g. `@ofv`) which will be replaced by their actual value when rendering the plot. For example `'@run, @nobs observations in @nind subjects'` would become `'run001, 1022 observations in 74 subjects'`

Many key variables are available:

- @condn** Condition number
- @covtime** Covariance matrix runtime
- @data** Model input data used
- @descr** Model description
- @dir** Model directory
- @epsshk** Epsilon shrinkage
- @errors** Run errors (e.g termination error)
- @esampleseed** ESAMPLE seed number (used in NPDE)
- @etashk** Eta shrinkage
- @file** Model file name
- @label** Model label
- @method** Estimation method or sim
- @nesample** Number of ESAMPLE (used in NPDE)
- @nind** Number of individuals
- @nobs** Number of observations
- @nsig** Number of significant digits
- @nsim** Number of simulations
- @ofv** Objective function value
- @page and @lastpage** Are respectively the page number and the number of the last page when faceting on multiple pages
- @probn** Problem number
- @plotfun** Name of the plot function
- @ref** Reference model
- @run** Model run name
- @runtime** Estimation/Sim runtime
- @software** Software used (e.g. NONMEM)

@simseed Simulation seed
@subroutine Differential equation solver
@timestart Run start time
@timestop Run stop time
@timeplot Time of the plot rendering
@term Termination message
@version Software version (e.g. 7.3)
@vpcci VPC confidence interval
@vpkdir VPC data directory
@vpclloq VPC lower limit of quantification
@vpnsim Number of simulations for VPC
@vpcpi VPC prediction interval
@vpculoq VPC upper limit of quantification
@warnings Run warnings (e.g. boundary)
@x @y etc. Name of any ggplot2 variable used for mapping in an aes() type function

See Also

[xpose_save](#)

Examples

```

# Defined when creating a plot
dv_vs_ipred(xpdb_ex_pk,
            title = '@x vs. @y',
            subtitle = '@ofv, @nind subjects, @nobs obs.',
            caption = '@run, @descr')

# Any label can be modified later on
dv_vs_ipred(xpdb_ex_pk, aes(point_color = SEX,
                           line_color = SEX)) +
  labs(title = 'This runs is: @descr',
       color = 'Color scale for @run',
       x = 'IPRED for @nind subjects',
       subtitle = NULL)
  
```

update_themes *Create xpose theme*

Description

Create an xpose theme. This function will update the theme of an xpdb object. All plots generated with this xpdb will automatically use the defined xpose (xp_theme) and ggplot2 (gg_theme) themes.

Usage

```
update_themes(xpdb = NULL, gg_theme = NULL, xp_theme = NULL, quiet)
```

Arguments

xpdb	An xpose_data object generated with xpose_data .
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. <code>c(point_color = 'red', line_linetype = 'dashed')</code>).
quiet	Logical, if FALSE messages are printed to the console.

Examples

```
# Before default theme
dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')

# Updating the gg_theme and xp_theme
xpdb_ex_pk %>%
  update_themes(gg_theme = theme_bw(),
                xp_theme = list(point_color = 'blue',
                                line_color = 'blue')) %>%
  dv_vs_ipred(facets = 'SEX')
```

vpc *Visual predictive checks*

Description

Generate visual predictive checks (VPC)

Usage

```
vpc(xpdb, vpc_type = NULL, mapping = NULL, smooth = TRUE,
    type = "alpr", title = "Visual predictive checks | @run",
    subtitle = "Number of simulations: @vpcnsim, confidence interval: @vpcci%",
    caption = "@vpcdir", tag = NULL, log = NULL, guide = TRUE,
    gg_theme, xp_theme, facets, quiet, area_fill = c("steelblue3",
    "grey60", "steelblue3"), line_linetype = c("93", "solid", "93"), ...)
```

Arguments

xpdb	An xpose database object.
vpc_type	Only used when multiple vpc data are present in the same xpdb. The type of vpc to be created. Can be one of: 'continuous', 'categorical', 'censored' or 'time-to-event'.
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
smooth	Should the bins be smoothed (connect bin midpoints, default) or shown as rectangular boxes.
type	String setting the type of plot to be used. Can be points 'p', line 'l', area 'a', rug 'r' and text 't' or any combination of the five.
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
log	String assigning logarithmic scale to axes, can be either "", 'x', 'y' or 'xy'.
guide	Enable guide display in vpc continuous (e.g. lloq and uloq lines).
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. c(point_color = 'red', line_linetype = 'l', area_fill = 'green')).
facets	Either a character string to use facet_wrap or a formula to use facet_grid .
quiet	Logical, if FALSE messages are printed to the console.
area_fill	Shaded areas filling color, should be a vector of 3 values (i.e. low, med, high).
line_linetype	Lines linetype, should be a vector of 3 values (i.e. low, med, high).
...	any additional aesthetics.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `area_fill = 'green'`, etc.

- point: options to `geom_point`
- line: options to `geom_line`
- area: options to `geom_ribbon` (`smooth = TRUE`) or `geom_rect` (`smooth = FALSE`)
- rug: options to `geom_rug`
- text: options to `geom_text`
- guide: options to `geom_hline`
- xscale: options to `scale_x_continuous` or `scale_x_log10`
- yscale: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(facet_wrap_paginate = list(facets = 'SEX')))`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[vpc_data](#)

Examples

```
xpdb_ex_pk %>%
  vpc_data(opt = vpc_opt(n_bins = 7)) %>%
  vpc()
```

vpc_data

Visual predictive checks data

Description

Generate visual predictive checks (VPC) data

Usage

```
vpc_data(xpdb, opt, stratify, vpc_type = c("continuous", "categorical",
  "censored", "time-to-event"), psn_folder = NULL, psn_bins = FALSE,
  obs_problem = NULL, sim_problem = NULL, quiet)
```


Arguments

xpdb	An xpose database object.
opt	A list of options regarding binning, pi and ci computation. For more information see vpc_opt .
stratify	Either a character string or a formula to stratify the data. For 'categorical' vpcs the stratification fixed to the different categories.
vpc_type	A string specifying the type of VPC to be created, can be one of: 'continuous', 'categorical', 'censored' or 'time-to-event'.
psn_folder	Specify a PsN-generated VPC-folder.
psn_bins	Only used with argument psn_folder. If TRUE bins will be imputed from the PsN vpc_bins.txt file. If FALSE (default) bins will be re-calculated in R. Note that when psn_bins = TRUE only the first bin array will be used and applied to all panels as it is not currently possible to define per panel binning in xpose. In addition when psn_bins = TRUE is used along with vpc(smooth = FALSE) the observations lines may not be centered in the bins. Check the output carefully.
obs_problem	Alternative to the option 'psn_folder'. The \$problem number to be used for observations. By default returns the last estimation problem.
sim_problem	Alternative to the option 'psn_folder'. The \$problem number to be used for simulations. By default returns the last simulation problem.
quiet	Logical, if FALSE messages are printed to the console.
...	any additional aesthetics.

See Also

[vpc vpc_opt](#)

Examples

```
## Not run:
xpdb_ex_pk %>%
  vpc_data() %>%
  vpc()

## End(Not run)
```

vpc_opt

Generate a list of options for VPC data generation

Description

Provide a list of options to vpc_data function.

Usage

```
vpc_opt(bins = "jenks", n_bins = "auto", bin_mid = "mean",
        pred_corr = FALSE, pred_corr_lower_bnd = 0, pi = c(0.025, 0.975),
        ci = c(0.025, 0.975), lloq = NULL, uloq = NULL, rtte = FALSE,
        rtte_calc_diff = TRUE, events = NULL, kmmc = NULL,
        reverse_prob = FALSE, as_percentage = TRUE)
```

Arguments

<code>bins</code>	Binning method, can be one of 'density', 'time', 'data', 'none', or one of the approaches available in <code>classInterval()</code> such as 'jenks' (default), '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>	Specify how to is the mid bin value calculated, can be either 'mean' for the mean of all timepoints (default) or 'middle' to use the average of the bin boundaries.
<code>pred_corr</code>	Option reserved to continuous VPC. Logical, should a prediction correction (pcVPC) of the data be used.
<code>pred_corr_lower_bnd</code>	Option reserved to continuous VPC. Lower bound for the prediction-correction.
<code>pi</code>	Option reserved to continuous VPC. Simulated prediction interval to plot. Default is <code>c(0.05, 0.95)</code> .
<code>ci</code>	Confidence interval around the percentiles to plot. Default is <code>c(0.05, 0.95)</code>
<code>lloq</code>	Number or NULL indicating lower limit of quantification. Default is NULL.
<code>uloq</code>	Number or NULL indicating upper limit of quantification. Default is NULL.
<code>rtte</code>	Option reserved to time-to-event VPC. Is the data repeated time-to-event (RTTE) TRUE or single time-to-event (TTE) FALSE.
<code>rtte_calc_diff</code>	Option reserved to time-to-event VPC. Should the time be recalculated? When simulating in NONMEM, you will probably need to set this to TRUE to recalculate the TIME to the relative time between events (unless you output the time difference between events and specify that as independent variable in the index.
<code>events</code>	Option reserved to time-to-event VPC. 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>kmmc</code>	Option reserved to time-to-event VPC. Either NULL for regular TTE VPC (default), or a variable name for a KMMC plot (e.g. 'WT').
<code>reverse_prob</code>	Option reserved to time-to-event VPC. Should the probability be reversed (i.e. plot 1-probability).
<code>as_percentage</code>	Should the Y-scale be in percent (0-100) TRUE (default), or standard (0-1) FALSE.

See Also

[vpc vpc_data](#)

Examples

```
vpc_opt()
```

xpdb_ex_pk	xpose_data <i>examples</i>
------------	----------------------------

Description

Moxonidine xpose_data example.

Format

An xpose_data object

Source

Moxonidine model: Assumption Testing in Population Pharmacokinetic Models: Illustrated with an Analysis of Moxonidine Data from Congestive Heart Failure Patients. *Journal of Pharmacokinetics and Biopharmaceutics*. 26(2):207–246 (1998).

Examples

```
print(xpdb_ex_pk)
```

xplot_distrib	<i>Default xpose distribution plot function</i>
---------------	---

Description

Manually generate distribution plots from an xpdb object.

Usage

```
xplot_distrib(xpdb, mapping = NULL, type = "hr", guide = FALSE,  
             xscale = "continuous", yscale = "continuous", title = NULL,  
             subtitle = NULL, caption = NULL, tag = NULL,  
             plot_name = "density_plot", gg_theme, xp_theme, opt, quiet, ...)
```

Arguments

xpdb	An xpose_data object generated with xpose_data .
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. <code>point_color</code>).
type	String setting the type of plot to be used. Can be histogram 'h', density 'd', rug 'r' or any combination of the three.
guide	Should the guide (e.g. reference distribution) be displayed.
xscale	Scale type for x axis (e.g. 'continuous', 'discrete', 'log10').
yscale	Scale type for y axis (e.g. 'continuous', 'discrete', 'log10').
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
plot_name	Name to be used by <code>xpose_save()</code> when saving the plot.
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. <code>c(point_color = 'red', line_lin</code>
opt	A list of options in order to create appropriate data input for ggplot2. For more information see data_opt .
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `histogram_fill = 'blue'`, `rug_sides = 'b'`, etc.

- histogram: options to `geom_histogram`
- density: options to `geom_density`
- rug: options to `geom_rug`
- xscale: options to `scale_x_continuous` or `scale_x_log10`
- yscale: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions [facet_wrap_paginate](#) when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or [facet_grid_paginate](#) when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the [facet_wrap_paginate](#) and [facet_grid_paginate](#) functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#) [xplot_qq](#)

Examples

```
# A simple histogram
xplot_distrib(xpdb_ex_pk, aes(x = WT), type = 'hr')

# A simple density plot
xplot_distrib(xpdb_ex_pk, aes(x = CWRES), type = 'dr')
```

xplot_qq	<i>Default xpose QQ plot function</i>
----------	---------------------------------------

Description

Manually generate QQ plots from an `xpdb` object.

Usage

```
xplot_qq(xpdb, mapping = NULL, type = "p", guide = FALSE,
         xscale = "continuous", yscale = "continuous", title = NULL,
         subtitle = NULL, caption = NULL, tag = NULL,
         plot_name = "qq_plot", gg_theme, xp_theme, opt, quiet, ...)
```

Arguments

<code>xpdb</code>	An <code>xpose_data</code> object generated with xpose_data .
<code>mapping</code>	List of aesthetics mappings to be used for the <code>xpose</code> plot (e.g. <code>point_color</code>).
<code>type</code>	String setting the type of plot to be used. Can only be points 'p'.
<code>guide</code>	Should the guide (e.g. reference line) be displayed.
<code>xscale</code>	Scale type for x axis (e.g. 'continuous', 'discrete', 'log10').

yscale	Scale type for y axis (e.g. 'continuous', 'discrete', 'log10').
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
plot_name	Name to be used by xpose_save() when saving the plot.
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. <code>c(point_color = 'red', line_lin</code>
opt	A list of options in order to create appropriate data input for ggplot2. For more information see data_opt .
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, etc.

- `point`: options to `geom_point`
- `guide`: options to `geom_abline`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions [facet_wrap_paginate](#) when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or [facet_grid_paginate](#) when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the [facet_wrap_paginate](#) and [facet_grid_paginate](#) functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller = ...)`. Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generated from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_scatter](#) [xplot_distrib](#)

Examples

```
xplot_qq(xpdb_ex_pk, aes(sample = CWRES), guide = TRUE)
```

xplot_scatter

Default xpose scatter plot function

Description

Manually generate scatter plots from an xpdb object.

Usage

```
xplot_scatter(xpdb, mapping = NULL, group = "ID", type = "pls",
  guide = FALSE, xscale = "continuous", yscale = "continuous",
  title = NULL, subtitle = NULL, caption = NULL, tag = NULL,
  plot_name = "scatter_plot", gg_theme, xp_theme, opt, quiet, ...)
```

Arguments

xpdb	An xpose_data object generated with xpose_data .
mapping	List of aesthetics mappings to be used for the xpose plot (e.g. point_color).
group	Grouping variable to be used for lines.
type	String setting the type of plot to be used. Can be line 'l', point 'p', smooth 's' and text 't' or any combination of the four.
guide	Should the guide (e.g. unity line) be displayed.
xscale	Scale type for x axis (e.g. 'continuous', 'discrete', 'log10').
yscale	Scale type for y axis (e.g. 'continuous', 'discrete', 'log10').
title	Plot title. Use NULL to remove.
subtitle	Plot subtitle. Use NULL to remove.
caption	Page caption. Use NULL to remove.
tag	Plot identification tag. Use NULL to remove.
plot_name	Name to be used by xpose_save() when saving the plot.
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. c(point_color = 'red', line_linewidth = 2)).
opt	A list of options in order to create appropriate data input for ggplot2. For more information see data_opt .
quiet	Logical, if FALSE messages are printed to the console.
...	Any additional aesthetics.

Layers mapping

Plots can be customized by mapping arguments to specific layers. The naming convention is `layer_option` where `layer` is one of the names defined in the list below and `option` is any option supported by this layer e.g. `point_color = 'blue'`, `smooth_method = 'lm'`, etc.

- `point`: options to `geom_point`
- `line`: options to `geom_line`
- `guide`: options to `geom_abline`
- `smooth`: options to `geom_smooth`
- `text`: options to `geom_text`
- `xscale`: options to `scale_x_continuous` or `scale_x_log10`
- `yscale`: options to `scale_y_continuous` or `scale_y_log10`

Faceting

Every xpose plot function has built-in faceting functionalities. Faceting arguments are passed to the functions `facet_wrap_paginate` when the `facets` argument is a character string (e.g. `facets = c('SEX', 'MED1')`) or `facet_grid_paginate` when `facets` is a formula (e.g. `facets = SEX~MED1`). All xpose plot functions accept all the arguments for the `facet_wrap_paginate` and `facet_grid_paginate` functions e.g. `dv_vs_ipred(xpdb_ex_pk, facets = SEX~MED1, ncol = 3, nrow = 3, page = 1, margins = TRUE, labeller =`

Faceting options can either be defined in plot functions (e.g. `dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')`) or assigned globally to an `xpdb` object via the `xp_theme` (e.g. `xpdb <- update_themes(xpdb_ex_pk, xp_theme = list(fa`). In the latter example all plots generate from this `xpdb` will automatically be stratified by 'SEX'.

By default, some plot functions use a custom stratifying variable named 'variable', e.g. `eta_distrib()`. When using the `facets` argument, 'variable' needs to be added manually e.g. `facets = c('SEX', 'variable')` or `facets = c('SEX', 'variable')`, but is optional, when using the `facets` argument in `xp_theme` variable is automatically added whenever needed.

Template titles

Template titles can be used to create highly informative diagnostics plots. They can be applied to any plot title, subtitle, caption and tag. Template titles are defined via a single string containing key variables starting with a '@' (e.g. '@ofv') which will be replaced by their actual value when rendering the plot. For example '@run, @nobs observations in @nind subjects' would become 'run001, 1022 observations in 74 subjects'. The available key variables are listed under [template_titles](#).

See Also

[xplot_distrib](#) [xplot_qq](#)

Examples

```
xplot_scatter(xpdb_ex_pk, aes(x = IPRED, y = DV))
```

xpose_data	<i>Import NONMEM output into R</i>
------------	------------------------------------

Description

Gather model outputs into a R database

Usage

```
xpose_data(runno = NULL, prefix = "run", ext = ".lst", file = NULL,
  dir = NULL, gg_theme = theme_readable(),
  xp_theme = theme_xp_default(), simtab = NULL, manual_import = NULL,
  ignore = NULL, extra_files, quiet, ...)
```

Arguments

runno	Run number to be used to generate model file name. Used in combination with prefix and ext.
prefix	Prefix to be used to generate model file name. Used in combination with runno and ext.
ext	Extension to be used to generate model file name. Should be one of '.lst' (default), '.out', '.res', '.mod' or '.ctl' for NONMEM.
file	Model file name (preferably a '.lst' file) containing the file extension. Alternative to prefix, runno and ext arguments.
dir	Location of the model files.
gg_theme	A ggplot2 theme object (e.g. theme_classic).
xp_theme	An xpose theme or vector of modifications to the xpose theme (e.g. <code>c(point_color = 'red', line_lin</code>
simtab	If TRUE only reads in simulation tables, if FALSE only reads estimation tables. Default NULL reads all tables. Option not compatible with manual_import.
manual_import	If NULL (default) the names of the output tables to import will be obtained from the model file. To manually import files as in previous versions of xpose, the check the function manual_nm_import .
ignore	Character vector be used to ignore the import/generation of: 'data', 'files', 'summary' or any combination of the three.
extra_files	A vector of additional output file extensions to be imported. Default is '.ext', '.cov', '.cor', '.phi', ".grd" for NONMEM.
quiet	Logical, if FALSE messages are printed to the console.
...	Additional arguments to be passed to the read_nm_tables functions.

File path generation

The rules for model file names generation are as follow:

- with runno: the full path is generated as <dir>/<prefix><runno>.<ext> e.g. with dir = 'model/pk', prefix = 'run', runno = '001', ext = '.lst' the resulting path would be model/pk/run001.lst
- with file: the full path is generated as <dir>/<file> e.g. with dir = 'model/pk', file = 'run001.lst' the resulting path would also be model/pk/run001.lst. Note: in this case the file extension should be provided as part of the 'file' argument.

Table format requirement

When importing data, an ID column must be present in at least one table for each problem and for each 'firstonly' category. ID columns are required to properly combine/merge tables and removing NA records. If ID columns are missing xpose will return the following warning: Dropped '<tablenames>' due to missing required 'ID' column..

Examples

```
## Not run:
# Using the `file` argument to point to the model file:
xpdb <- xpose_data(file = 'run001.lst', dir = 'models')

# Using the `runno` argument to point to the model file:
xpdb <- xpose_data(runno = '001', ext = '.lst', dir = 'models')

# Using the `extra_files` argument to import specific output files only:
xpdb <- xpose_data(file = 'run001.lst', dir = 'models', extra_files = c('.ext', '.phi'))

# Using `ignore` to disable import of tables and output files:
xpdb <- xpose_data(file = 'run001.lst', dir = 'models', ignore = c('data', 'files'))

# Using `simtab` to disable import of simulation tables
xpdb <- xpose_data(file = 'run001.lst', dir = 'models', simtab = FALSE)

## End(Not run)
```

xpose_save

Save xpose plot

Description

Inspired by the [ggsave](#), this function facilitates the export of xpose plots.

Usage

```
xpose_save(plot = last_plot(), file = NULL, dir = NULL,
  device = NULL, width = 7, height = 6, units = c("in", "cm",
  "mm"), dpi = 200, ...)
```

Arguments

plot	A xpose plot object.
file	A name with file extension (if device is NULL) to be given to the output file. Template variables such as @run (run number) and @plotfun (plot function) can be used to automatically name files e.g. file = '@run_@plotfun.pdf'.
dir	Directory under which the xpose plots will be saved. Template variables such as @dir can be used to generate template names.
device	Graphical device to use. Can be either be a device function (e.g. png), or one of 'eps', 'ps', 'tex' (pictex), 'pdf' (default), 'jpeg', 'tiff', 'png', 'bmp', 'svg' or 'wmf' (windows only).
width, height	Plot size in units.
units	Units of the plot size ('in', 'cm', or 'mm').
dpi	Plot resolution. Applies only to raster output types.
...	Additional arguments passed on to ggsave or graphics device.

Examples

```
## Not run:
xpdb_ex_pk %>%
  dv_vs_ipred() %>%
  xpose_save(file = file.path(tempdir(), "dv_vs_ipred_example.pdf"))

## End(Not run)
```

xp_themes

A set of xpose themes

Description

xpose themes are used to consistently apply a set of preference for the plot geoms (e.g. color scales, point size, etc.) whereas ggplot2 theme focus on the plot background, axes, titles etc.

- theme_xp_default: The default xp_theme in xpose
- theme_xp_xpose4: An xp_theme that makes xpose look like xpose4.

Usage

```
theme_xp_default()
```

```
theme_xp_xpose4()
```

Examples

```
# With the xp_theme theme_xp_default() (default)
dv_vs_ipred(xpdb_ex_pk, facets = 'SEX')

# With the xp_theme theme_xp_xpose4()
xpdb_ex_pk %>%
  update_themes(xp_theme = theme_xp_xpose4()) %>%
  dv_vs_ipred(facets = 'SEX')
```

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