Package 'xgxr'

March 22, 2023

Title Exploratory Graphics for Pharmacometrics

Version 1.1.2

Description Supports a structured approach
for exploring PKPD data <https://opensource.nibr.com/xgx/>. It also
contains helper functions for enabling the modeler to follow best R
practices (by appending the program name, figure name location, and
draft status to each plot). In addition, it enables the modeler to
follow best graphical practices (by providing a theme that
reduces chart ink, and by providing time-scale, log-scale, and
reverse-log-transform-scale functions for more readable axes).
Finally, it provides some data checking and summarizing functions for
rapidly exploring pharmacokinetics and pharmacodynamics (PKPD) datasets.

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URL https://opensource.nibr.com/xgx/

BugReports https://github.com/Novartis/xgxr/issues

Depends R (>= 3.5.0)

Imports assertthat, binom, Deriv, DescTools, dplyr, ggplot2, glue,
graphics, grDevices, gtable, Hmisc, labeling, magrittr,
minpack.lm, pander, png, RCurl, readr, scales, stats, stringr,
tibble, utils

Suggests caTools, gridExtra, knitr, pkgdown, rmarkdown, testthat,
tidyr

VignetteBuilder knitr

Encoding UTF-8

LazyData true

RoxygenNote 7.1.2

NeedsCompilation no

Author Andrew Stein [aut, cre],
Alison Margolskee [aut],
Fariba Khanshan [aut],
Konstantin Krismer [aut] (<https://orcid.org/0000-0001-8994-3416>),

Matthew Fidler [ctb] (<https://orcid.org/0000-0001-8538-6691>),
Novartis Pharma AG [cph, fnd]

Maintainer Andrew Stein <andy.stein@gmail.com>

Repository CRAN

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R topics documented:

`case1_pkpd` *Case 1 PKPD Data Set*

Description

Case 1 PKPD Data Set

Usage

```
case1_pkpd
```

Format

A data frame with the following 21 columns:

column 1:	`ID`	integer; unique subject ID
column 2:	`TIME`	numeric; time relative to first drug administration
column 3:	`NOMTIME`	numeric; nominal time
column 4:	`TIMEUNIT`	factor; unit of TIME
column 5:	`AMT`	integer; dosing amount (for dosing events) in mg
column 6:	`LIDV`	numeric; observation on a linear scale (observation type determined by CMT), units determined by
column 7:	`CMT`	integer; compartment number (determines observation type): CMT 1 = Dosing event CMT 2 = PK concentration CMT 3 = Continuous response data CMT 4 = Count response data CMT 5 = Ordinal response data CMT 6 = Binary response data
column 8:	`NAME`	factor; description of event
column 9:	`EVENTU`	factor; unit for observation
column 10:	`CENS`	integer; censored values (0 = not censored, 1 = censored)
column 11:	`EVID`	integer; event ID (0 = observation, 1 = dosing event)
column 12:	`WEIGHTB`	numeric; baseline body weight (kg)
column 13:	`eff0`	numeric; efficacy
column 14:	`TRTACT`	factor; treatment group label
column 15:	`DOSE`	integer; Dose in mg
column 16:	`PROFDAY`	integer; day of profile
column 17:	`PROFTIME`	numeric; time within PROFDAY

column 18:	CYCLE	integer; count of drug administrations received
column 19:	PART	integer; part of study
column 20:	STUDY	integer; study
column 21:	IPRED	numeric; individual prediction

`edit_rmd_template_str` *Edit a Rmd Template from xgx*

Description

`edit_rmd_template_str` returns a path to the altered Rmd template

Usage

```
edit_rmd_template_str(
  rmd_str = NULL,
  mapping = NULL,
  rmd_output_path = NULL,
  data_path = NULL,
  multiple_dosing = FALSE,
  pk_cmt = NULL,
  pd_cmt = NULL,
  dose_cmt = NULL,
  steady_state_day = NULL,
  time_between_doses = NULL,
  author_name = NULL,
  add_datetime = TRUE,
  show_explanation = TRUE
)
```

Arguments

`rmd_str`	A character string containing the Rmd template raw characters
`mapping`	A list of column name mappings from the original (template) dataset column names to the corresponding columns in the new dataset
`rmd_output_path`	A custom output path for the generated Rmd file (This is typically left as 'NULL' in order to maintain the hierarchical directory structure of 'xgx_autoexplore_output'))
`data_path`	Path (as a string) to the dataset that is to be analyzed
`multiple_dosing`	if FALSE use single ascending dose template, if TRUE use multiple
`pk_cmt`	An integer denoting the "compartment" containing the PK data. The "CMT" column will typically have these integers, where each row may contain either PK or PD data, potentially of different types (continuous, ordinal, etc.)

pd_cmt An integer denoting the "compartment" containing the PD data, of the desired type (continuous, ordinal, etc.). The "CMT" column will typically have these integers, where each row may contain either PK or PD data

dose_cmt CMT associated with dosing event

steady_state_day For multiple ascending dose, what day is steady state rich profile?

time_between_doses time interval between doses

author_name The name of the author to be displayed on the template

add_datetime Boolean indicating additon of a date stamp to the beginnning of the Rmd file

show_explanation Boolean indicating if the additional explanations (text in between figures) are needed for the user.

Value

A string of the new R markdown template

---

get_rmd_name *Determine the name of a Rmd template*

Description

get_rmd_name returns a name for an Rmd template, based on the desired PKPD parameters

Usage

```
get_rmd_name(
  rmd_template_name = NULL,
  multiple_dosing = FALSE,
  pk_cmt = NULL,
  pd_cmt = NULL,
  pd_data_type = NULL
)
```

Arguments

rmd_template_name A custom output name for the generated Rmd file

multiple_dosing if FALSE use single ascending dose template, if TRUE use multiple

pk_cmt An integer denoting the "compartment" containing the PK data. The "CMT" column will typically have these integers, where each row may contain either PK or PD data, potentially of different types (continuous, ordinal, etc.)

pd_cmt An integer denoting the "compartment" containing the PD data, of the desired type (continuous, ordinal, etc.). The "CMT" column will typically have these integers, where each row may contain either PK or PD data

pd_data_type The type of PD data - acceptable values exist in the following list: ["binary","continuous","count","ordinal

Value

a string for the Rmd template name

`get_rmd_str` *get_rmd_str returns a Rmd template string, based on the desired PKPD parameters*

Description

`get_rmd_str` returns a Rmd template string, based on the desired PKPD parameters

Usage

```
get_rmd_str(
  rmd_template_name = NULL,
  multiple_dosing = FALSE,
  pk_cmt = NULL,
  pd_cmt = NULL,
  pd_data_type = NULL
)
```

Arguments

`rmd_template_name`	A custom output name for the generated Rmd file
`multiple_dosing`	if FALSE use single ascending dose template, if TRUE use multiple
`pk_cmt`	An integer denoting the "compartment" containing the PK data. The "CMT" column will typically have these integers, where each row may contain either PK or PD data, potentially of different types (continuous, ordinal, etc.)
`pd_cmt`	An integer denoting the "compartment" containing the PD data, of the desired type (continuous, ordinal, etc.). The "CMT" column will typically have these integers, where each row may contain either PK or PD data
`pd_data_type`	The type of PD data - acceptable values exist in the following list: ["binary","continuous","count","ordinal

Value

a string for the Rmd template name

mad *Multiple Ascending Dose Data Set*

Description

Model generated PK and PD data to mimic an orally administered small molecule with various endpoints from continuous to ordinal response and count data. Simulated multiple dose administration ranging from 100 mg to 1600 mg, once per day.

Usage

```
mad
```

Format

A data frame with the following 19 columns:

column 1:	ID	numeric; unique subject ID
column 2:	TIME	numeric; time relative to first drug administration
column 3:	NOMTIME	numeric; nominal time
column 4:	TIMEUNIT	character; unit of TIME
column 5:	AMT	numeric; dosing amount (for dosing events) in mg
column 6:	LIDV	numeric; observation on a linear scale (observation type determined by CMT), units determined by
column 7:	MDV	numeric; missing dependent variable
column 8:	CMT	integer; compartment number (determines observation type): CMT 1 = Dosing event CMT 2 = PK concentration CMT 3 = Continuous response data CMT 4 = Count response data CMT 5 = Ordinal response data CMT 6 = Binary response data
column 9:	NAME	character; description of event
column 10:	EVENTU	character; unit for observation
column 11:	CENS	integer; censored values (0 = not censored, 1 = censored)
column 12:	EVID	integer; event ID (0 = observation, 1 = dosing event)
column 13:	WEIGHTB	numeric; baseline body weight (kg)
column 14:	SEX	character; sex
column 15:	TRTACT	factor; treatment group label
column 16:	DOSE	numeric; randomized dose in mg
column 17:	PROFDAY	numeric; day of profile
column 18:	PROFTIME	numeric; time within PROFDAY
column 19:	CYCLE	numeric; count of drug administrations received

mad_missing_duplicates

Multiple Ascending Dose Data Set (Duplicates Removed)

Description

Model generated PK and PD data to mimic an orally administered small molecule with various endpoints from continuous to ordinal response and count data. Simulated multiple dose administration ranging from 100 mg to 1600 mg, once per day.

Usage

```
mad_missing_duplicates
```

Format

A data frame with the following 19 columns:

column 1:	ID	numeric; unique subject ID
column 2:	TIME	numeric; time relative to first drug administration
column 3:	NOMTIME	numeric; nominal time
column 4:	TIMEUNIT	character; unit of TIME
column 5:	AMT	numeric; dosing amount (for dosing events) in mg
column 6:	LIDV	numeric; observation on a linear scale (observation type determined by CMT), units determined by
column 7:	MDV	numeric; missing dependent variable
column 8:	CMT	integer; compartment number (determines observation type): CMT 1 = Dosing event CMT 2 = PK concentration CMT 3 = Continuous response data CMT 4 = Count response data CMT 5 = Ordinal response data CMT 6 = Binary response data
column 9:	NAME	character; description of event
column 10:	EVENTU	character; unit for observation
column 11:	CENS	integer; censored values (0 = not censored, 1 = censored)
column 12:	EVID	integer; event ID (0 = observation, 1 = dosing event)
column 13:	WEIGHTB	numeric; baseline body weight (kg)
column 14:	SEX	character; sex
column 15:	TRTACT	factor; treatment group label
column 16:	DOSE	numeric; randomized dose in mg
column 17:	PROFDAY	numeric; day of profile
column 18:	PROFTIME	numeric; time within PROFDAY
column 19:	CYCLE	numeric; count of drug administrations received

mad_nca

Multiple Ascending Dose Noncompartmental Analysis (NCA) dataset

Description

Multiple Ascending Dose Noncompartmental Analysis (NCA) dataset

Usage

```
mad_nca
```

Format

A data frame with the following 7 columns:

column 1:	ID	numeric; unique subject ID
column 2:	PARAM	character; NCA parameter
column 3:	VALUE	numeric; Value of the NCA parameter
column 4:	DOSE	numeric; randomized dose in mg
column 15:	TRTACT	factor; treatment group label
column 14:	SEX	character; sex
column 13:	WEIGHTB	numeric; baseline body weight (kg)

---

nlmixr_theo_sd *nlmixr Theophylline SD Data Set*

Description

Theophylline dataset, from the nlmixr R package

Usage

```
nlmixr_theo_sd
```

Format

A data frame with the following 7 columns:

column 1:	ID	integer; unique patient identifier
column 2:	TIME	numeric; time relative to first drug administration
column 3:	DV	numeric; dependent variable (drug concentration)
column 4:	AMT	numeric; dose of drug
column 5:	EVID	integer; event ID, 1 if dose, 0 otherwise
column 6:	CMT	integer; compartment number
column 7:	WT	numeric; weight

---

predict.nls *predict.nls*

Description

predict.nls

Usage

```
## S3 method for class 'nls'
predict(
  object,
  newdata = NULL,
  se.fit = FALSE,
  interval = "none",
  level = 0.95,
  ...
)
```

Arguments

object	Object of class inheriting from "nls"
newdata	An optional data frame in which to look for variables with which to predict. If omitted, the fitted values are used.
se.fit	A switch indicating if standard errors are required.
interval	Type of interval calculation, "none" or "confidence"
level	Level of confidence interval to use
...	additional arguments affecting the predictions produced.

Value

predict.nls produces a vector of predictions or a matrix of predictions and bounds with column names fit, lwr, and upr if interval is set.

If se.fit is TRUE, a list with the following components is returned:

fit	vector or matrix as above
se.fit	standard error of predicted means
residual.scale	residual standard deviations
df	degrees of freedom for residual

Examples

```
set.seed(12345)
data_to_plot <- data.frame(x1 = rep(c(0, 25, 50, 100, 200, 400, 600), 10)) %>%
  dplyr::mutate(AUC = x1*rlnorm(length(x1), 0, 0.3),
         x2 = x1*stats::rlnorm(length(x1), 0, 0.3),
         Response = (15 + 50*x2/(20+x2))*stats::rlnorm(length(x2), 0, 0.3))


gg <- ggplot2::ggplot(data = data_to_plot, ggplot2::aes(x = AUC, y = Response)) +
```

```
  ggplot2::geom_point() +
  xgx_geom_smooth(method = "nls",
                  method.args = list(formula = y ~ E0 + Emax* x / (EC50 + x),
                                     start = list(E0 = 15, Emax = 50, EC50 = 20) ),
                  color = "black", size = 0.5, alpha = 0.25)
gg

mod <- stats::nls(formula = Response ~ E0 + Emax * AUC / (EC50 + AUC),
data = data_to_plot,
start = list(E0 = 15, Emax = 50, EC50 = 20))

predict.nls(mod)

predict.nls(mod, se.fit = TRUE)

predict.nls(mod,
            newdata = data.frame(AUC = c(0, 25, 50, 100, 200, 400, 600)),
            se.fit = TRUE)

predict.nls(mod,
            newdata = data.frame(AUC = c(0, 25, 50, 100, 200, 400, 600)),
            se.fit = TRUE, interval = "confidence", level = 0.95)

predict(mod,
            newdata = data.frame(AUC = c(0, 25, 50, 100, 200, 400, 600)),
            se.fit = TRUE, interval = "confidence", level = 0.95)
```

`predictdf` *Prediction data frame from ggplot2 Get predictions with standard errors into data frame*

Description

Prediction data frame from ggplot2 Get predictions with standard errors into data frame

Usage

```
predictdf(model, xseq, se, level)
```

Arguments

`model`	model object
`xseq`	newdata
`se`	Display confidence interval around smooth?
`level`	Level of confidence interval to use

`predictdf.nls` *Prediction data frame for nls*

Description

Get predictions with standard errors into data frame for use with geom_smooth

Usage

```
## S3 method for class 'nls'
predictdf(model, xseq, se, level)
```

Arguments

`model`	nls object
`xseq`	newdata
`se`	Display confidence interval around smooth?
`level`	Level of confidence interval to use

Details

`ggplot2::geom_smooth` produces confidence intervals by silently calling functions of the form predictdf.method, where method is "loess", "lm", "glm" etc. depending on what method is specified in the call to `geom_smooth`. Currently `ggplot2` does not define a `predictdf.nls` function for method of type "nls", and thus confidence intervals cannot be automatically generated by `geom_smooth` for method = "nls". Here we define `predictdf.nls` for calculating the confidence intervals of an object of type nls. `geom_smooth` will silently call this function whenever method = "nls", and produce the appropriate confidence intervals.

`predictdf.nls` calculates CI for a model fit of class nls based on the "delta-method" http://sia.webpopix.org/nonlinearRegres
intervals-and-prediction-intervals)

CI = [f(x0, beta) + qt_(alpha/2, n - d) * se(f(x0, beta)), f(x0, beta) + qt_(1 - alpha/2, n - d) * se(f(x0, beta))]

where: beta = vector of parameter estimates x = independent variable se(f(x0, beta)) = sqrt(delta(f)(x0, beta) * Var(beta) * (delta(f)(x0, beta))') delta(f) is the gradient of f

Value

dataframe with x and y values, if se is TRUE dataframe also includes ymin and ymax

predictdf.polr *Prediction data frame for polr*

Description

Get predictions with standard errors into data frame for use with geom_smooth

Usage

```
## S3 method for class 'polr'
predictdf(model, xseq, se, level)
```

Arguments

model	object returned from polr
xseq	sequence of x values for which to compute the smooth
se	if TRUE then confidence intervals are returned
level	confidence level for confidence intervals

Details

predictdf.polr is used by xgx_geom_smooth when method = "polr" to calculate confidence intervals via bootstraps.

sad *Single Ascending Dose Data Set*

Description

Model generated PK data to mimic an orally administered small molecule. Simulated single dose administration ranging from 100 mg to 1600 mg.

Usage

```
sad
```

Format

A data frame with the following 16 columns:

column 1:	ID	numeric; unique subject ID
column 2:	TIME	numeric; time relative to first drug administration
column 3:	NOMTIME	numeric; nominal time
column 4:	TIMEUNIT	character; unit of TIME
column 5:	AMT	numeric; dosing amount (for dosing events) in mg

column 6:	LIDV	numeric; observation on a linear scale (observation type determined by CMT), units
column 7:	MDV	numeric; missing dependent variable
(1 if missing, 0 otherwise)		
column 8:	CMT	integer; compartment number (determines observation type): CMT 1 = Dosing event CMT 2 = PK concentration
column 9:	NAME	character; description of event
column 10:	EVENTU	character; unit for observation
column 11:	CENS	integer; censored values (0 = not censored, 1 = censored)
column 12:	EVID	integer; event ID (0 = observation, 1 = dosing event)
column 13:	WEIGHTB	numeric; baseline body weight (kg)
column 14:	SEX	character; sex
column 15:	TRTACT	factor; treatment group label
column 16:	DOSE	numeric; randomized dose in mg received

StatSmoothOrdinal *Stat object for producing smooths through ordinal data*

Description

Stat object for producing smooths through ordinal data

Usage

```
StatSmoothOrdinal
```

Format

An object of class `StatSmoothOrdinal` (inherits from `Stat`, `ggproto`, `gg`) of length 8.

StatSummaryBinQuant *Stat ggproto object for binning by quantile for xgx_stat_ci*

Description

Source: https://github.com/tidyverse/ggplot2/blob/351eb41623397dea20ed0059df62a4a5974d88cb/R/stat-summary-bin.R

Usage

```
StatSummaryBinQuant
```

Format

An object of class `StatSummaryBinQuant` (inherits from `Stat`, `ggproto`, `gg`) of length 5.

Details

StatSummaryBinQuant returns a ggproto object for plotting mean +/- confidence bins

Value

ggplot2 ggproto object

StatSummaryOrdinal *Stat ggproto object for creating ggplot layers of binned confidence intervals for probabiliities of classes in ordinal data*

Description

StatSummaryOrdinal returns a ggproto object for plotting mean +/- confidence intervals for ordinal data. It also allows for binning values on the independent axis.

Usage

```
StatSummaryOrdinal
```

Format

An object of class StatSummaryOrdinal (inherits from Stat, ggproto, gg) of length 8.

Value

ggplot2 ggproto object

---

theme_xgx *Calls the standard theme for xGx graphics*

Description

Calls the standard theme for xGx graphics

Usage

```
theme_xgx()
```

Value

xgx ggplot2 compatible theme

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(y = concentration, x = bound_receptor)) +
  ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_y_log10() +
  xgx_scale_x_reverselog10() +
  theme_xgx()
```

---

xgx_annotate_filenames

Append filenames to bottom of the plot

Description

xgx_annotate_filenames appends file details to the bottom of a plot using the plot caption option. File details to append include the parent directory, the path of the R script which generated the plot, and the path of the plot.

Usage

```
xgx_annotate_filenames(dirs, hjust = 0.5, color = "black", size = 11)
```

Arguments

dirs	list containing directories and filenames. It must contain five fields 1. parent_dir = Parent directory containing the Rscript and the Results folder 2. rscript_dir = Subdirectory ofparent_dir that contains the Rscript used to generate the figure 3. rscript_name= Name of the Rscript used to generate the figure 4. results_dir = Subdirectory ofparent_dir where the figure is stored 5. filename = Filename
hjust	horizontal justification of the caption
color	font color for caption, default black
size	font size for caption, default 11

Value

None

Examples

```
dirs <- list(parent_dir = "/your/parent/path/",
             rscript_dir = "./Rscripts/",
             rscript_name = "Example.R",
             results_dir = "./Results/",
             filename = "your_file_name.png")
data <- data.frame(x = 1:1000, y = rnorm(1000))
ggplot2::ggplot(data = data, ggplot2::aes(x = x, y = y)) +
  ggplot2::geom_point() +
  xgx_annotate_filenames(dirs)
```

---

xgx_annotate_status *Create a status (e.g. DRAFT) annotation layer*

Description

xgx_annotate_status adds a status (e.g. DRAFT) annotation layer to a plot. The text of the annotation can be customized, the default is "DRAFT". The color, location, size, fontface, transparency of the annotation can also be customized.

Usage

```
xgx_annotate_status(
  status = "DRAFT",
  x = Inf,
  y = Inf,
  color = "grey",
  hjust = 1.2,
  vjust = 1.2,
  fontsize = 7,
  fontface = "bold",
  alpha = 0.5,
  ...
)
```

Arguments

status	the text to
x	x location, default Inf (right most point)
y	y location, default Inf (up most point)
color	font color, default "grey"
hjust	horizontal justification, default 1.2
vjust	vertical justification, default 1.2
fontsize	font size to use, default 7

fontface	font style to use, default "bold"
alpha	transparency, default is 0.5
...	other arguments passed on to layer

Value

ggplot layer

Examples

```
data <- data.frame(x = 1:1000, y = rnorm(1000))
ggplot2::ggplot(data = data, ggplot2::aes(x = x, y = y)) +
  ggplot2::geom_point() +
  xgx_annotate_status("DRAFT")
```

---

xgx_annotate_status_png

Annotate a png file or directory of png files

Description

These function annotates a single png file or all files within a directory.

Usage

```
xgx_annotate_status_png(
  file_or_dir,
  script = "",
  status = "DRAFT",
  date_format = "%a %b %d %X %Y",
  col = grDevices::grey(0.8, alpha = 0.7),
  font = 2,
  cex_status_mult = 7,
  cex_footnote_mult = 0.8,
  status_angle = 45,
  x11 = FALSE
)
```

Arguments

file_or_dir	The png file to annotate or directory location for annotating png files. Note this will annotate just once, so if you generate multiple png files and then annotate at the end of your script it will have the correct script name on it. Then if you create new images in a different script in the same directory and then annotate with the script name the second script, the PNG files will show the correct script location for each file.

`script`	Script name to add as a footnote; By default this is empty, though it could name the script that
`status`	Draft or other status; If `status="Final"` or `status=""` the status overlay will be removed. By default the status is DRAFT.
`date_format`	Date format for adding the time the png was annotated.
`col`	Color for annotating the draft status
`font`	Font to use for the annotation function
`cex_status_mult`	Multiplication factor for the status annotation. By default 7
`cex_footnote_mult`	Multiplication factor for the footnote annotation. By default 0.8
`status_angle`	Angle to rotate status
`x11`	Display on the X11/Windows device

Details

If a png file has been annotated once, this function will not annotate it again. Therefore, you can run this function on directories with different input script names and it will label each file based on when each file was run.

Based on code from MrFlick on Stack Overflow.

Value

nothing

Author(s)

Matthew Fidler, Alison M, ...

Examples

```
# using the examples from plot()
file.name <- tempfile()
grDevices::png(file.name)
graphics::plot(cars)
graphics::lines(stats::lowess(cars))
grDevices::dev.off()
# annotate one file
xgx_annotate_status_png(file.name, "/tmp/script1.R")
```

xgx_auto_explore	*Produce an xgx-styled report the given dataset using xgx R markdown templates, or a user-provided R markdown template. (Note: The R markdown template provided must be formatted in a similar manner to that of the xgx R markdown templates to work.) The working directory will contain a new directory ('xgx_autoexplore_output') after running this function, which will contain a directory for the dataset, and futher a directory for the type of analysis / R markdown template.*

Description

xgx_auto_explore returns an HTML and PDF document with plots describing the provided dataset

Usage

```
xgx_auto_explore(
  data_path = NULL,
  mapping = list(),
  author_name = NULL,
  multiple_dosing = FALSE,
  pk_cmt = NULL,
  pd_cmt = NULL,
  pd_data_type = NULL,
  dose_cmt = NULL,
  steady_state_day = NULL,
  time_between_doses = NULL,
  rmd_template_name = NULL,
  rmd_template_path = NULL,
  rmd_output_path = NULL,
  pdf_output_path = NULL,
  html_output_path = NULL,
  add_datetime = TRUE,
  show_explanation = TRUE
)
```

Arguments

data_path	Path (as a string) to the dataset that is to be analyzed
mapping	A list of column name mappings from the original (template) dataset column names to the corresponding columns in the new dataset.
author_name	The name of the author to be displayed on the template
multiple_dosing	Whether or not to use a "Multiple" or "Single" Ascending dose template
pk_cmt	An integer denoting the "compartment" containing the PK data. The "CMT" column will typically have these integers, where each row may contain PK, PD, dosing or other events/observations data

pd_cmt
: An integer denoting the "compartment" containing the PD data, of the desired type (continuous, ordinal, etc.). The "CMT" column will typically have these integers, where each row may contain PK, PD, dosing or other events/observations data

pd_data_type
: The type of PD data - acceptable values exist in the following list: ["binary","continuous","count","ordinal

dose_cmt
: Integer denoting the compartment for dosing records

steady_state_day
: used to denote the day of rich sampling of PK at steady state

time_between_doses
: dosing interval, has units to match the time variable of the dataset

rmd_template_name
: A custom output name for the generated Rmd file

rmd_template_path
: A user provided custom template (as a string)

rmd_output_path
: A custom output path for the generated Rmd file (This is typically left as 'NULL' in order to maintain the hierarchical directory structure of 'xgx_autoexplore_output'))

pdf_output_path
: A custom output path for the generated PDF file (This is typically left as 'NULL' in order to maintain the hierarchical directory structure of 'xgx_autoexplore_output'))

html_output_path
: A custom output path for the generated HTML file (This is typically left as 'NULL' in order to maintain the hierarchical directory structure of 'xgx_autoexplore_output'))

add_datetime
: Boolean indicating additon of a date stamp to the beginnning of the Rmd file

show_explanation
: Boolean indicating if the additional explanations (text in between figures) are needed for the user.

Details

This function can be used quickly to explore your data by generating overview plots before constructing non-linear mixed effects models.

Examples

```
author_name = "Your Name Here"
show_explanation = FALSE

## Not run:
# Try out the nonlinear_pkpd dataset with the
# Multiple Ascending Dose PK Rmd template
data_path <- "~/nonlinear_pkpd.csv"

# Specify the mapping of column names
mapping <- list(
  "TIME" = "TIM2",
```

```
  "NOMTIME" = "NT",
  "EVID" = 0,
  "CENS" = 0,
  "DOSE" = "MGKG",
  "TRTACT" = "TRT",
  "LIDV_NORM" = "LIDV/MGKG",
  "LIDV_UNIT" = "UNIT",
  "PROFDAY" = 1,
  "SEX" = 0,
  "WEIGHTB" = 0)


# 5 contains the PK Concentration in this dataset
pk_cmt = 5
# We don't need PD right now
pd_cmt = NULL
pd_data_type = NULL


dose_cmt = 1
steady_state_day = c(0, 6)
time_between_doses = 24
multiple_dosing = TRUE

output_directory = tempdir()

xgx_auto_explore(data_path = data_path,
                 mapping = mapping,
                 author_name = author_name,
                 pk_cmt = pk_cmt,
                 pd_cmt = pd_cmt,
                 dose_cmt = dose_cmt,
                 steady_state_day = steady_state_day,
                 time_between_doses = time_between_doses,
                 multiple_dosing = multiple_dosing,
                 pd_data_type = pd_data_type,
                 rmd_output_path = output_directory,
                 show_explanation = show_explanation)

## End(Not run)
```

`xgx_breaks_log10` *Sets the default breaks for log10*

Description

`xgx_breaks_log10` sets nice breaks for log10 scale. it's better than the default function because it ensures there is at least 2 breaks and also, it will try to go by 3s (i.e. 1,3,10,30,100) if it makes sense

Usage

```
xgx_breaks_log10(data_range)
```

Arguments

data_range	range of the data

Details

for the extended breaks function, weights is a set of 4 weights for

1. simplicity - how early in the Q order are you
2. coverage - labelings that don't extend outside the data: range(data) / range(labels)
3. density (previously granularity) - how close to the number of ticks do you get (default is 5)
4. legibility - has to do with fontsize and formatting to prevent label overlap

Value

numeric vector of breaks

References

Talbot, Justin, Sharon Lin, and Pat Hanrahan. "An extension of Wilkinson's algorithm for positioning tick labels on axes." IEEE Transactions on visualization and computer graphics 16.6 (2010): 1036-1043.

Examples

```
xgx_breaks_log10(c(1, 1000))
xgx_breaks_log10(c(0.001, 100))
xgx_breaks_log10(c(1e-4, 1e4))
xgx_breaks_log10(c(1e-9, 1e9))
xgx_breaks_log10(c(1, 2))
xgx_breaks_log10(c(1, 5))
xgx_breaks_log10(c(1, 10))
xgx_breaks_log10(c(1, 100))
xgx_breaks_log10(c(1, 1.01))
xgx_breaks_log10(c(1, 1.0001))
print(xgx_breaks_log10(c(1, 1.000001)), digits = 10)
```

xgx_breaks_time *Sets the default breaks for a time axis*

Description

xgx_breaks_time sets the default breaks for a time axis, given the units of the data and the units of the plot. It is inspired by scales::extended_breaks

Usage

```
xgx_breaks_time(data_range, units_plot, number_breaks = 5)
```

Arguments

data_range	range of the data
units_plot	units to use in the plot
number_breaks	number of breaks to aim for (default is 5)

Details

for the extended breaks function, weights is a set of 4 weights for

1. simplicity - how early in the Q order are you
2. coverage - labelings that don't extend outside the data: range(data) / range(labels)
3. density (previously granularity) - how close to the number of ticks do you get (default is 5)
4. legibility - has to do with fontsize and formatting to prevent label overlap

Value

numeric vector of breaks

References

Talbot, Justin, Sharon Lin, and Pat Hanrahan. "An extension of Wilkinson's algorithm for positioning tick labels on axes." IEEE Transactions on visualization and computer graphics 16.6 (2010): 1036-1043.

Examples

```
xgx_breaks_time(c(0, 5), "h")
xgx_breaks_time(c(0, 6), "h")
xgx_breaks_time(c(-3, 5), "h")
xgx_breaks_time(c(0, 24), "h")
xgx_breaks_time(c(0, 12), "h")
xgx_breaks_time(c(1, 4), "d")
xgx_breaks_time(c(1, 12), "d")
xgx_breaks_time(c(1, 14), "d")
```

```
xgx_breaks_time(c(1, 50), "d")
xgx_breaks_time(c(1000, 3000), "d")
xgx_breaks_time(c(-21, 100), "d")
xgx_breaks_time(c(-1, 10), "w")
```

`xgx_check_data` *Check data for various issues*

Description

`xgx_check_data` performs a series of checks on a PK or PKPD dataset It was inspired by the dataset preparation table from IntiQuan.

Usage

```
xgx_check_data(data, covariates = NULL)
```

Arguments

`data,`	the dataset to check. Must contain the above columns
`covariates,`	the column names of covariates, to explore

Details

The dataset must have the following columns

- ID = unique subject identifier. USUBJID is another option if ID is not there
- EVID = event ID: 1 for dose, 0 otherwise
- AMT = value of the dose
- TIME = time of the measurement
- DV = dependent value (linear scale). will check if LIDV or LNDV are also there if DV is not
- YTYPE = data measurement for LIDV. will check if CMT is there, if YTYPE is not

The dataset may also have additional columns

- CENS = flag for censoring of the data because it's below the limit of quantification (BLOQ)
- MDV = missing dependent variable - will be counted and then filtered out from the data check

Value

data.frame

Examples

```
covariates <- c("WEIGHTB", "SEX")
check <- xgx_check_data(mad_missing_duplicates, covariates)
```

xgx_conf_int — xgx_conf_int *returns a dataframe with mean +/- confidence intervals*

Description

xgx_conf_int returns a dataframe with mean +/- confidence intervals

Usage

```
xgx_conf_int(y, conf_level = 0.95, distribution = "normal")
```

Arguments

y	data to compute confidence interval of
conf_level	The percentile for the confidence interval (should fall between 0 and 1). The default is 0.95, which corresponds to a 95 percent confidence interval.
distribution	The distribution which the data follow, used for calculating confidence intervals. The options are "normal", "lognormal", and "binomial". The "normal" option will use the Student t Distribution to calculate confidence intervals, the "lognormal" option will transform data to the log space first. The "binomial" option will use the binom.exact function to calculate the confidence intervals. Note: binomial data must be numeric and contain only 1's and 0's.

Value

data.frame

Examples

```
# default settings for normally distributed data, 95% confidence interval,
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = rep(c(1, 2, 3), each = 20) + stats::rnorm(60),
                   group = rep(1:3, 20))
xgx_conf_int(data$y)
```

xgx_dirs2char — *Append filenames to bottom of the plot*

Description

xgx_dirs2char returns a character variable based on the dirs list. The caption gives the filename

Usage

```
xgx_dirs2char(dirs, include_time = TRUE)
```

Arguments

dirs	list containing directories and filenames. It must contain five fields 1. parent_dir = Parent directory containing the Rscript and the Results folder 2. rscript_dir = Subdirectory ofparent_dir that contains the Rscript used to generate the figure 3. rscript_name= Name of the Rscript used to generate the figure 4. results_dir = Subdirectory ofparent_dir where the figure is stored 5. filename = Filename
include_time	is logical with default TRUE. If TRUE, it includes date / time in the output character

Value

character

Examples

```
dirs <- list(parent_dir = "/your/parent/path/",
             rscript_dir = "./Rscripts/",
             rscript_name = "Example.R",
             results_dir = "./Results/",
             filename = "your_file_name.png")
caption <- xgx_dirs2char(dirs)
```

---

xgx_geom_ci *Plot data with mean and confidence intervals*

Description

Plot data with mean and confidence intervals

Usage

```
xgx_geom_ci(
  mapping = NULL,
  data = NULL,
  conf_level = 0.95,
  distribution = "normal",
  bins = NULL,
  breaks = NULL,
  geom = list("point", "line", "errorbar"),
  position = "identity",
  fun.args = list(),
  na.rm = FALSE,
  show.legend = NA,
```

```
  inherit.aes = TRUE,
  ...
)
```

Arguments

mapping	Set of aesthetic mappings created by ‘aes‘ or ‘aes_‘. If specified and ‘inherit.aes = TRUE‘ (the default), it is combined with the default mapping at the top level of the plot. You must supply mapping if there is no plot mapping.
data	The data to be displayed in this layer. There are three options: If NULL, the default, the data is inherited from the plot data as specified in the call to ggplot. A data.frame, or other object, will override the plot data. All objects will be fortified to produce a data frame. See fortify for which variables will be created. A function will be called with a single argument, the plot data. The return value must be a data.frame., and will be used as the layer data.
conf_level	The percentile for the confidence interval (should fall between 0 and 1). The default is 0.95, which corresponds to a 95 percent confidence interval.
distribution	The distribution which the data follow, used for calculating confidence intervals. The options are "normal", "lognormal", and "binomial". The "normal" option will use the Student t Distribution to calculate confidence intervals, the "lognormal" option will transform data to the log space first. The "binomial" option will use the binom.exact function to calculate the confidence intervals. Note: binomial data must be numeric and contain only 1’s and 0’s.
bins	number of bins to cut up the x data, cuts data into quantiles.
breaks	breaks to cut up the x data, if this option is used, bins is ignored
geom	Use to override the default geom. Can be a list of multiple geoms, e.g. list("point","line","errorbar"), which is the default.
position	Position adjustment, either as a string, or the result of a call to a position adjustment function.
fun.args	Optional additional arguments passed on to the functions.
na.rm	If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed.
show.legend	logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes.
inherit.aes	If FALSE, overrides the default aesthetics, rather than combining with them. This is most useful for helper functions that define both data and aesthetics and shouldn’t inherit behaviour from the default plot specification, e.g. borders.
...	other arguments passed on to layer. These are often aesthetics, used to set an aesthetic to a fixed value, like color = "red" or size = 3. They may also be parameters to the paired geom/stat.

Value

ggplot2 plot layer

Examples

```
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = rep(c(1, 2, 3), each = 20) + stats::rnorm(60))
ggplot2::ggplot(data, ggplot2::aes(x = x, y = y)) +
  xgx_geom_ci(conf_level = 0.95)
```

`xgx_geom_pi` *Plot data with median and percent intervals*

Description

Plot data with median and percent intervals

Usage

```
xgx_geom_pi(
  mapping = NULL,
  data = NULL,
  percent_level = 0.95,
  geom = list("line", "ribbon"),
  position = "identity",
  fun.args = list(),
  na.rm = FALSE,
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

`mapping`	Set of aesthetic mappings created by ‘aes‘ or ‘aes_‘. If specified and ‘inherit.aes = TRUE‘ (the default), it is combined with the default mapping at the top level of the plot. You must supply mapping if there is no plot mapping.
`data`	The data to be displayed in this layer. There are three options: If NULL, the default, the data is inherited from the plot data as specified in the call to ggplot. A data.frame, or other object, will override the plot data. All objects will be fortified to produce a data frame. See fortify for which variables will be created. A function will be called with a single argument, the plot data. The return value must be a data.frame., and will be used as the layer data.
`percent_level`	The upper or lower percentile for the percent interval (should fall between 0 and 1). The default is 0.95, which corresponds to (0.05, 0.95) interval. Supplying 0.05 would give the same result
`geom`	Use to override the default geom. Can be a list of multiple geoms, e.g. list("line","ribbon"), which is the default.

position	Position adjustment, either as a string, or the result of a call to a position adjustment function.
fun.args	Optional additional arguments passed on to the functions.
na.rm	If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed.
show.legend	logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes.
inherit.aes	If FALSE, overrides the default aesthetics, rather than combining with them. This is most useful for helper functions that define both data and aesthetics and shouldn't inherit behaviour from the default plot specification, e.g. borders.
...	other arguments passed on to layer. These are often aesthetics, used to set an aesthetic to a fixed value, like color = "red" or size = 3. They may also be parameters to the paired geom/stat.

Value

ggplot2 plot layer

Examples

```
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = rep(c(1, 2, 3), each = 20) + stats::rnorm(60))
ggplot2::ggplot(data, ggplot2::aes(x = x, y = y)) +
  xgx_geom_pi(percent_level = 0.95)
```

---

xgx_labels_log10 *Nice labels for log10.*

Description

Returns a set of labels for ggplot

Usage

```
xgx_labels_log10(breaks)
```

Arguments

breaks,	breaks for the function

Value

either character or expression

Examples

```
print(xgx_labels_log10(c(1e-5, 1, 1e5)))
```

xgx_minor_breaks_log10 *Sets the default minor_breaks for log10 scales*

Description

`xgx_minor_breaks_log10` sets nice minor_breaks for log10 scale.

Usage

```
xgx_minor_breaks_log10(data_range)
```

Arguments

`data_range`	range of the data

Value

numeric vector of breaks

Examples

```
xgx_minor_breaks_log10(c(1, 1000))
xgx_minor_breaks_log10(c(0.001, 100))
xgx_minor_breaks_log10(c(1e-4, 1e4))
xgx_minor_breaks_log10(c(1e-9, 1e9))
xgx_minor_breaks_log10(c(1, 2))
xgx_minor_breaks_log10(c(1, 5))
xgx_minor_breaks_log10(c(1, 10))
xgx_minor_breaks_log10(c(1, 100))
xgx_minor_breaks_log10(c(1, 1.01))
xgx_minor_breaks_log10(c(1, 1.0001))
print(xgx_minor_breaks_log10(c(1, 1.000001)), digits = 10)
```

xgx_plot *Create a new xgx plot*

Description

Create a new xgx plot

Usage

```
xgx_plot(
  data = NULL,
  mapping = ggplot2::aes(),
  ...,
  environment = parent.frame()
)
```

Arguments

data	Default dataset to use for plot. If not already a data.frame, will be converted to one by fortify.
mapping	As in ggplot2; Default list of aesthetic mappings to use for plot. Must define x, y, and group for xgx_spaghetti.
...	Other arguments passed on to methods. Not currently used.
environment	If an variable defined in the aesthetic mapping is not found in the data, ggplot will look for it in this environment. It defaults to using the environment in which ggplot is called.

Value

ggplot2 object

Examples

```
time <- rep(seq(1, 10), 5)
id <- sort(rep(seq(1, 5), 10))
conc <- exp(-time) * sort(rep(stats::rlnorm(5), 10))

data <- data.frame(time = time, concentration = conc, id = id)
xgx_plot(data = data,
         mapping = ggplot2::aes(x = time, y = concentration, group = id)) +
  ggplot2::geom_line() +
  ggplot2::geom_point()
```

---

xgx_save *Saving plot, automatically annotating the status and denoting the filenames*

Description

Saving plot, automatically annotating the status and denoting the filenames

Usage

```
xgx_save(
  width,
  height,
  dirs = NULL,
  filename_main = NULL,
  status = "DRAFT",
  g = ggplot2::last_plot(),
  filetype = "png",
  status_x = Inf,
  status_y = Inf,
  status_fontsize = 7,
  status_fontcolor = "grey",
  filenames_fontsize = 11,
  filenames_fontcolor = "black"
)
```

Arguments

width	width of plot
height	height of plot
dirs	list of directories. If NULL or if directories missing, there is default behavior below 1. parent_dir = Parent directory containing the Rscript and the Results folder, default getwd() 2. rscript_dir = Subdirectory of parent_dir that contains the Rscript used to generate the figure, default "./" 3. rscript_name= Name of the Rscript used to generate the figure, default "Name_Of_Script_Here.R" 4. results_dir = Subdirectory ofparent_dir where the figure is stored, default "./" 5. filename_prefix = prefix of filename to be appended to filename_main
filename_main	main part of the filename, excluding prefix and suffix. no default
status	status to be annotated
g	ggplot plot object, default is ggplot::last_plot()
filetype	file extension (e.g. "pdf","csv" etc.)
status_x	x location of the status in plot
status_y	y location of the status in plot
status_fontsize	font size for status in plot
status_fontcolor	font color for status in plot
filenames_fontsize	font size for filenames info in plot
filenames_fontcolor	font color for filenames info in plot

Value

ggplot2 plot object

Examples

```
directory = tempdir()
dirs <- list(parent_dir  = directory,
             rscript_dir = directory,
             rscript_name = "example.R",
             results_dir = directory,
             filename_prefix = "example_")
data <- data.frame(x = 1:1000, y = stats::rnorm(1000))
ggplot2::ggplot(data = data, ggplot2::aes(x = x, y = y)) +
  ggplot2::geom_point()
xgx_save(4, 4, dirs, "Example", "DRAFT")
```

---

xgx_save_table

Saving table as an image, also labeling the program that created the table and where the table is stored

---

Description

Saving table as an image, also labeling the program that created the table and where the table is stored

Usage

```
xgx_save_table(data, dirs = NULL, filename_main = NULL)
```

Arguments

data	data.frame or table of results
dirs	list of directories. If NULL or if directories missing, there is default behavior below 1. parent_dir = Parent directory containing the Rscript and the Results folder, default getwd() 2. rscript_dir = Subdirectory of parent_dir that contains the Rscript used to generate the figure, default "./" 3. rscript_name= Name of the Rscript used to generate the figure, default "Name_Of_Script_Here.R" 4. results_dir = Subdirectory ofparent_dir where the figure is stored, default "./" 5. filename_prefix = prefix of filename to be appended to filename_main
filename_main	main part of the filename, excluding prefix and extension. no default

Value

ggplot2 plot object

Examples

```
directory = tempdir()
dirs <- list(parent_dir  = directory,
             rscript_dir = directory,
             rscript_name = "example.R",
             results_dir = directory,
             filename_prefix = "example_")
data <- data.frame(x = c(1, 2), y = c(1, 2))
xgx_save_table(data, dirs = dirs, filename_main = "test")
```

---

xgx_scale_x_log10 *log10 scales the x axis with a "pretty" set of breaks*

Description

`xgx_scale_x_log10` is similar to `scale_x_log10`. But it uses what we believe to be a nicer spacing and set of tick marks it can be used the same as `scale_x_log10`

Usage

```
xgx_scale_x_log10(
  breaks = xgx_breaks_log10,
  minor_breaks = NULL,
  labels = xgx_labels_log10,
  ...
)
```

Arguments

`breaks`	major breaks, default is a function defined here
`minor_breaks`	minor breaks, default is a function defined here
`labels`	function for setting the labels, defined here
`...`	other arguments passed to `scale_x_log10`

Value

ggplot2 compatible scale object

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration  = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(x = concentration, y = bound_receptor)) +
ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_x_log10() +
  xgx_scale_y_reverselog10()
```

`xgx_scale_x_reverselog10`

Reverse-log transform for the x scale.

Description

`xgx_scale_x_reverselog10` is designed to be used with data that approaches 100 A common example is receptor occupancy in drug development. It is used when you want even spacing between 90, 99, 99.9, etc.

Usage

```
xgx_scale_x_reverselog10(labels = NULL, accuracy = NULL, ...)
```

Arguments

`labels`	if NULL, then the default is to use scales::percent()
`accuracy`	if NULL, then use the the default as specified by scales::percent() to round to the hundredths place, set accuracy 0.01
`...`	other parameters passed to `scale_x_continuous`

Value

ggplot2 compatible scale object

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(y = concentration, x = bound_receptor)) +
  ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_y_log10() +
```

```
xgx_scale_x_reverselog10()
```

`xgx_scale_x_time_units` *Convert time units for plotting*

Description

`xgx_scale_x_time_units` converts x axis scale from one time unit to another. Supported units include hours, days, weeks, months, and years, which can also be called using just the first letter (h, d, w, m, y).

Usage

```
xgx_scale_x_time_units(
  units_dataset,
  units_plot = NULL,
  breaks = NULL,
  labels = NULL,
  ...
)

xgx_scale_y_time_units(
  units_dataset,
  units_plot = NULL,
  breaks = NULL,
  labels = NULL,
  ...
)
```

Arguments

`units_dataset`	units of the input dataset, must be specified by user as "h", "d", "w", "m", or "y"
`units_plot`	units of the plot, will be units of the dataset if empty
`breaks`	One of: • `NULL` for no breaks • `waiver()` for the default breaks computed by the transformation object • A numeric vector of positions • A function that takes the limits as input and returns breaks as output (e.g., a function returned by `scales::extended_breaks()`). Also accepts rlang lambda function notation.
`labels`	One of: • `NULL` for no labels • `waiver()` for the default labels computed by the transformation object

- A character vector giving labels (must be same length as `breaks`)
- A function that takes the breaks as input and returns labels as output. Also accepts rlang lambda function notation.

`...` other parameters for `scale_x_continuous`

Details

Note: `xgx_scale_x_time_units` only scales the plot axis, all other specifications must be on the original scale of the dataset (e.g. breaks, position, width)

Value

ggplot2 compatible scale object

Examples

```
data <- data.frame(x = 1:1000, y = rnorm(1000))
ggplot2::ggplot(data = data, ggplot2::aes(x = x, y = y)) +
  ggplot2::geom_point() +
  xgx_scale_x_time_units(units_dataset = "hours", units_plot = "weeks")
```

---

xgx_scale_y_log10 *log10 scales the y axis with a "pretty" set of breaks*

Description

`xgx_scale_y_log10` is similar to `scale_y_log10`. But it uses what we believe to be a nicer spacing and set of tick marks it can be used the same as `scale_y_log10`

Usage

```
xgx_scale_y_log10(
  breaks = xgx_breaks_log10,
  minor_breaks = NULL,
  labels = xgx_labels_log10,
  ...
)
```

Arguments

`breaks`	major breaks, default is a function defined here
`minor_breaks`	minor breaks, default is a function defined here
`labels`	function for setting the labels, defined here
`...`	other arguments passed to `scale_y_log10`

Value

ggplot2 compatible scale object

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(y = concentration, x = bound_receptor)) +
  ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_y_log10() +
  xgx_scale_x_reverselog10()
```

---

xgx_scale_y_percentchangelog10

percentchangelog10 transform for the y scale.

Description

xgx_scale_y_percentchangelog10 and xgx_scale_x_percentchangelog10 are designed to be used with percent change (PCHG) from baseline data (on a scale of -1 to +Inf). Common examples include It is used when you have a wide range of data on a percent change scale, especially data close to -100

Usage

```
xgx_scale_y_percentchangelog10(
  breaks = NULL,
  minor_breaks = NULL,
  labels = NULL,
  accuracy = 1,
  n_breaks = 7,
  ...
)

xgx_scale_x_percentchangelog10(
  breaks = NULL,
  minor_breaks = NULL,
  labels = NULL,
  accuracy = 1,
  n_breaks = 7,
  ...
)
```

Arguments

breaks	if NULL, then default is to use a variant of 2^(labeling::extended(log2(PCHG + 1))) - 1, where PCHG represents the range of the data

minor_breaks	if NULL, then default is to use nicely spaced log10(PCHG + 1) minor breaks
labels	if NULL, then the default is to use scales::percent_format()
accuracy	accuracy to use with scales::percent_format(), if NULL, then the default is set to 1
n_breaks	number of desired breaks, if NULL, then the default is set to 7
...	other parameters passed to scale_y_continuous

Value

ggplot2 compatible scale object

Examples

```
dat1 <- data.frame(x = rnorm(100), PCHG = exp(rnorm(100)) - 1)

ggplot2::ggplot(dat1, ggplot2::aes(x = x, y = PCHG)) +
  ggplot2::geom_point() +
  xgx_theme() +
  xgx_scale_y_percentchangelog10()
```

---

xgx_scale_y_reverselog10

Reverselog transform for the y scale.

Description

xgx_scale_y_reverselog10 is designed to be used with data that approaches 100 A common example is receptor occupancy in drug development. It is used when you want even spacing between 90, 99, 99.9, etc.

Usage

```
xgx_scale_y_reverselog10(labels = NULL, accuracy = NULL, ...)
```

Arguments

labels	if NULL, then the default is to use scales::percent()
accuracy	if NULL, then use the the default as specified by scales::percent() to round to the hundredths place, set accuracy 0.01
...	other parameters passed to scale_y_continuous

Value

ggplot2 compatible scale object

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration  = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(x = concentration, y = bound_receptor)) +
ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_x_log10() +
  xgx_scale_y_reverselog10()
```

---

xgx_stat_ci *Plot data with mean and confidence intervals*

Description

xgx_stat_ci returns a ggplot layer plotting mean +/- confidence intervals

Usage

```
xgx_stat_ci(
  mapping = NULL,
  data = NULL,
  conf_level = 0.95,
  distribution = "normal",
  bins = NULL,
  breaks = NULL,
  geom = list("point", "line", "errorbar"),
  position = "identity",
  fun.args = list(),
  fun.data = NULL,
  na.rm = FALSE,
  orientation = "x",
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

mapping	Set of aesthetic mappings created by ‘aes‘ or ‘aes_‘. If specified and ‘inherit.aes = TRUE‘ (the default), it is combined with the default mapping at the top level of the plot. You must supply mapping if there is no plot mapping.

data	The data to be displayed in this layer. There are three options: If NULL, the default, the data is inherited from the plot data as specified in the call to ggplot. A data.frame, or other object, will override the plot data. All objects will be fortified to produce a data frame. See fortify for which variables will be created. A function will be called with a single argument, the plot data. The return value must be a data.frame., and will be used as the layer data.
conf_level	The percentile for the confidence interval (should fall between 0 and 1). The default is 0.95, which corresponds to a 95 percent confidence interval.
distribution	The distribution which the data follow, used for calculating confidence intervals. The options are "normal", "lognormal", and "binomial". The "normal" option will use the Student t Distribution to calculate confidence intervals, the "lognormal" option will transform data to the log space first. The "binomial" option will use the `binom.exact` function to calculate the confidence intervals. Note: binomial data must be numeric and contain only 1's and 0's.
bins	number of bins to cut up the x data, cuts data into quantiles.
breaks	breaks to cut up the x data, if this option is used, bins is ignored
geom	Use to override the default geom. Can be a list of multiple geoms, e.g. list("point","line","errorbar"), which is the default.
position	Position adjustment, either as a string, or the result of a call to a position adjustment function.
fun.args	Optional additional arguments passed on to the functions.
fun.data	A function that is given the complete data and should return a data frame with variables ymin, y, and ymax.
na.rm	If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed.
orientation	The orientation of the layer, passed on to ggplot2::stat_summary. Only implemented for ggplot2 v.3.3.0 and later. The default ("x") summarizes y values over x values (same behavior as ggplot2 v.3.2.1 or earlier). Setting `orientation = "y"` will summarize x values over y values, which may be useful in some situations where you want to flip the axes, e.g. to create forest plots. Setting `orientation = NA` will try to automatically determine the orientation from the aesthetic mapping (this is more stable for ggplot2 v.3.3.2 compared to v.3.3.0). See `stat_summary` (v.3.3.0 or greater) for more information.
show.legend	logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes.
inherit.aes	If FALSE, overrides the default aesthetics, rather than combining with them. This is most useful for helper functions that define both data and aesthetics and shouldn't inherit behaviour from the default plot specification, e.g. borders.
...	other arguments passed on to layer. These are often aesthetics, used to set an aesthetic to a fixed value, like color = "red" or size = 3. They may also be parameters to the paired geom/stat.

Details

This function can be used to generate mean +/- confidence interval plots for different distributions, and multiple geoms with a single function call.

Value

ggplot2 plot layer

Examples

```
# default settings for normally distributed data, 95% confidence interval,
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = rep(c(1, 2, 3), each = 20) + stats::rnorm(60),
                   group = rep(1:3, 20))
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95)

# try different geom
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95, geom = list("ribbon", "point", "line"))

# plotting lognormally distributed data
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = 10^(rep(c(1, 2, 3), each = 20) + stats::rnorm(60)),
                   group = rep(1:3, 20))
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95, distribution = "lognormal")

# note: you DO NOT need to use both distribution = "lognormal"
# and scale_y_log10()
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95) + xgx_scale_y_log10()

# plotting binomial data
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = stats::rbinom(60, 1, rep(c(0.2, 0.6, 0.8),
                   each = 20)),
                   group = rep(1:3, 20))
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95, distribution = "binomial")

# including multiple groups in same plot
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_ci(conf_level = 0.95, distribution = "binomial",
              ggplot2::aes(color = factor(group)),
              position = ggplot2::position_dodge(width = 0.5))

# plotting ordinal or multinomial data
set.seed(12345)
data = data.frame(x = 120*exp(stats::rnorm(100,0,1)),
              response = sample(c("Mild","Moderate","Severe"), 100, replace = TRUE),
              covariate = sample(c("Male","Female"), 100, replace = TRUE))
```

```
xgx_plot(data = data) +
  xgx_stat_ci(mapping = ggplot2::aes(x = x, response = response, colour = covariate),
              distribution = "ordinal", bins = 4) +
 ggplot2::scale_y_continuous(labels = scales::percent_format()) + ggplot2::facet_wrap(~response)

xgx_plot(data = data) +
  xgx_stat_ci(mapping = ggplot2::aes(x = x, response = response, colour = response),
              distribution = "ordinal", bins = 4) +
 ggplot2::scale_y_continuous(labels = scales::percent_format()) + ggplot2::facet_wrap(~covariate)

# Example plotting categorical vs categorical data
set.seed(12345)
data = data.frame(x = 120*exp(stats::rnorm(100,0,1)),
                  response = sample(c("Trt1", "Trt2", "Trt3"), 100, replace = TRUE),
                  covariate = factor(
                    sample(c("White","Black","Asian","Other"), 100, replace = TRUE),
                                   levels = c("White", "Black", "Asian", "Other")))

xgx_plot(data = data) +
  xgx_stat_ci(mapping = ggplot2::aes(x = response, response = covariate),
              distribution = "ordinal") +
  xgx_stat_ci(mapping = ggplot2::aes(x = 1, response = covariate), geom = "hline",
              distribution = "ordinal") +
  ggplot2::scale_y_continuous(labels = scales::percent_format()) +
  ggplot2::facet_wrap(~covariate) +
  ggplot2::xlab("Treatment group") +
  ggplot2::ylab("Percent of subjects by category")

# Same example with orientation flipped (only works for ggplot2 v.3.3.0 or later)
# only run if ggplot2 v.3.3.0 or later
ggplot2_geq_v3.3.0 <- utils::compareVersion(
  as.character(utils::packageVersion("ggplot2")), '3.3.0') >= 0

if(ggplot2_geq_v3.3.0){

xgx_plot(data = data) +
xgx_stat_ci(mapping = ggplot2::aes(y = response, response = covariate), orientation = "y",
            distribution = "ordinal") +
  xgx_stat_ci(mapping = ggplot2::aes(y = 1, response = covariate), orientation = "y",
              geom = "vline", distribution = "ordinal") +
  ggplot2::scale_x_continuous(labels = scales::percent_format()) +
  ggplot2::facet_wrap(~covariate) +
  ggplot2::ylab("Treatment group") +
  ggplot2::xlab("Percent of subjects by category")

}
```

---

xgx_stat_pi *Plot data with median and percent intervals*

Description

xgx_stat_pi returns a ggplot layer plotting median +/- percent intervals

Usage

```
xgx_stat_pi(
  mapping = NULL,
  data = NULL,
  percent_level = 0.95,
  geom = list("line", "ribbon"),
  position = "identity",
  bins = NULL,
  breaks = NULL,
  fun.args = list(),
  na.rm = FALSE,
  show.legend = NA,
  inherit.aes = TRUE,
  ...
)
```

Arguments

mapping	Set of aesthetic mappings created by ‘aes‘ or ‘aes_‘. If specified and ‘inherit.aes = TRUE‘ (the default), it is combined with the default mapping at the top level of the plot. You must supply mapping if there is no plot mapping.
data	The data to be displayed in this layer. There are three options: If NULL, the default, the data is inherited from the plot data as specified in the call to ggplot. A data.frame, or other object, will override the plot data. All objects will be fortified to produce a data frame. See fortify for which variables will be created. A function will be called with a single argument, the plot data. The return value must be a data.frame., and will be used as the layer data.
percent_level	The upper or lower percentile for the percent interval (should fall between 0 and 1). The default is 0.95, which corresponds to (0.05, 0.95) interval. Supplying 0.05 would give the same result
geom	Use to override the default geom. Can be a list of multiple geoms, e.g. list("line","ribbon"), which is the default.
position	Position adjustment, either as a string, or the result of a call to a position adjustment function.
bins	number of bins to cut up the x data, cuts data into quantiles.
breaks	breaks to cut up the x data, if this option is used, bins is ignored
fun.args	Optional additional arguments passed on to the functions.
na.rm	If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed.
show.legend	logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes.

inherit.aes	If FALSE, overrides the default aesthetics, rather than combining with them. This is most useful for helper functions that define both data and aesthetics and shouldn't inherit behaviour from the default plot specification, e.g. borders.
...	other arguments passed on to layer. These are often aesthetics, used to set an aesthetic to a fixed value, like color = "red" or size = 3. They may also be parameters to the paired geom/stat.

Value

ggplot2 plot layer

Examples

```
# default settings for normally distributed data, (5%,95%) interval,
data <- data.frame(x = rep(c(1, 2, 3), each = 20),
                   y = rep(c(1, 2, 3), each = 20) + stats::rnorm(60),
                   group = rep(1:3, 20))
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_pi(percent_level = 0.95)

# try different geom
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_pi(percent_level = 0.95, geom = list("errorbar", "point", "line"))

# including multiple groups in same plot
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_pi(percent_level = 0.95,
              ggplot2::aes(color = factor(group), fill = factor(group)),
              position = ggplot2::position_dodge(width = 0.5))

# including multiple percent intervals in same plot
xgx_plot(data, ggplot2::aes(x = x, y = y)) +
  xgx_stat_pi(percent_level = 0.90) +
  xgx_stat_pi(percent_level = 0.80) +
  xgx_stat_pi(percent_level = 0.70) +
  xgx_stat_pi(percent_level = 0.60)
```

---

xgx_stat_smooth *Wrapper for stat_smooth*

Description

xgx_stat_smooth and xgx_geom_smooth produce smooth fits through continuous or categorical data. For categorical, ordinal, or multinomial data use method = polr. This wrapper also works with nonlinear methods like nls and nlsLM for continuous data.

xgx_geom_smooth_emax uses minpack.lm::nlsLM, predictdf.nls, and stat_smooth to display Emax model fit to data

Usage

```
xgx_stat_smooth(
  mapping = NULL,
  data = NULL,
  geom = "smooth",
  position = "identity",
  ...,
  method = NULL,
  formula = NULL,
  se = TRUE,
  n = 80,
  span = 0.75,
  n_boot = 200,
  fullrange = FALSE,
  level = 0.95,
  method.args = list(),
  na.rm = FALSE,
  orientation = "x",
  show.legend = NA,
  inherit.aes = TRUE
)

xgx_geom_smooth(
  mapping = NULL,
  data = NULL,
  geom = "smooth",
  position = "identity",
  ...,
  method = NULL,
  formula = NULL,
  se = TRUE,
  n = 80,
  span = 0.75,
  fullrange = FALSE,
  level = 0.95,
  method.args = list(),
  na.rm = FALSE,
  orientation = "x",
  show.legend = NA,
  inherit.aes = TRUE
)

xgx_geom_smooth_emax(
  mapping = NULL,
  data = NULL,
  geom = "smooth",
  position = "identity",
  ...,
```

```
  method = "nlsLM",
  formula,
  se = TRUE,
  n = 80,
  span = 0.75,
  fullrange = FALSE,
  level = 0.95,
  method.args = list(),
  na.rm = FALSE,
  orientation = "x",
  show.legend = NA,
  inherit.aes = TRUE
)
```

Arguments

mapping	Set of aesthetic mappings created by ‘aes‘ or ‘aes_‘. If specified and ‘inherit.aes = TRUE‘ (the default), it is combined with the default mapping at the top level of the plot. You must supply mapping if there is no plot mapping. Warning: for ‘method = polr‘, do not define ‘y‘ aesthetic, use ‘response‘ instead.
data	The data to be displayed in this layer. There are three options: If NULL, the default, the data is inherited from the plot data as specified in the call to ggplot. A data.frame, or other object, will override the plot data. All objects will be fortified to produce a data frame. See fortify for which variables will be created. A function will be called with a single argument, the plot data. The return value must be a data.frame., and will be used as the layer data.
geom	Use to override the default geom. Can be a list of multiple geoms, e.g. list("point","line","errorbar"), which is the default.
position	Position adjustment, either as a string, or the result of a call to a position adjustment function.
...	other arguments passed on to layer. These are often aesthetics, used to set an aesthetic to a fixed value, like color = "red" or size = 3. They may also be parameters to the paired geom/stat.
method	method (function) to use, eg. lm, glm, gam, loess, rlm. Example: ‘"polr"‘ for ordinal data. ‘"nlsLM"‘ for nonlinear least squares. If method is left as ‘NULL‘, then a typical ‘StatSmooth‘ is applied, with the corresponding defaults, i.e. For datasets with n < 1000 default is loess. For datasets with 1000 or more observations defaults to gam.
formula	formula to use in smoothing function, eg. y ~ x, y ~ poly(x, 2), y ~ log(x)
se	display confidence interval around smooth? (TRUE by default, see level to control)
n	number of points to evaluate smoother at
span	Controls the amount of smoothing for the default loess smoother. Smaller numbers produce wigglier lines, larger numbers produce smoother lines.

n_boot	number of bootstraps to perform to compute confidence interval, currently only used for method = "polr", default is 200
fullrange	should the fit span the full range of the plot, or just the data
level	The percentile for the confidence interval (should fall between 0 and 1). The default is 0.95, which corresponds to a 95 percent confidence interval.
method.args	Optional additional arguments passed on to the method.
na.rm	If FALSE, the default, missing values are removed with a warning. If TRUE, missing values are silently removed.
orientation	The orientation of the layer, passed on to ggplot2::stat_summary. Only implemented for ggplot2 v.3.3.0 and later. The default ("x") summarizes y values over x values (same behavior as ggplot2 v.3.2.1 or earlier). Setting orientation = "y" will summarize x values over y values, which may be useful in some situations where you want to flip the axes, e.g. to create forest plots. Setting orientation = NA will try to automatically determine the orientation from the aesthetic mapping (this is more stable for ggplot2 v.3.3.2 compared to v.3.3.0).
show.legend	logical. Should this layer be included in the legends? NA, the default, includes if any aesthetics are mapped. FALSE never includes, and TRUE always includes.
inherit.aes	If FALSE, overrides the default aesthetics, rather than combining with them. This is most useful for helper functions that define both data and aesthetics and shouldn't inherit behaviour from the default plot specification, e.g. borders.

Value

ggplot2 plot layer

Warning

nlsLM uses nls.lm which implements the Levenberg-Marquardt algorithm for fitting a nonlinear model, and may fail to converge for a number of reasons. See ?nls.lm for more information.

nls uses Gauss-Newton method for estimating parameters, and could fail if the parameters are not identifiable. If this happens you will see the following warning message: Warning message: Computation failed in 'stat_smooth()': singular gradient

nls will also fail if used on artificial "zero-residual" data, use nlsLM instead.

See Also

predictdf.nls for information on how nls confidence intervals are calculated.

Examples

```
# Example with nonlinear least squares (method = "nlsLM")
Nsubj <- 10
Doses <- c(0, 25, 50, 100, 200)
Ntot <- Nsubj*length(Doses)
times <- c(0,14,30,60,90)
```

```
dat1 <- data.frame(ID = 1:(Ntot),
                   DOSE = rep(Doses, Nsubj),
                   PD0 = stats::rlnorm(Ntot, log(100), 1),
                   Kout = exp(stats::rnorm(Ntot,-2, 0.3)),
                   Imax = 1,
                   ED50 = 25) %>%
 dplyr::mutate(PDSS = PD0*(1 - Imax*DOSE/(DOSE + ED50))*exp(stats::rnorm(Ntot, 0.05, 0.3))) %>%
 merge(data.frame(ID = rep(1:(Ntot), each = length(times)), Time = times), by = "ID") %>%
  dplyr::mutate(PD = ((PD0 - PDSS)*(exp(-Kout*Time)) + PDSS),
                PCHG = (PD - PD0)/PD0)

gg <- ggplot2::ggplot(dat1 %>% subset(Time == 90),
                      ggplot2::aes(x = DOSE, y = PCHG)) +
  ggplot2::geom_boxplot(ggplot2::aes(group = DOSE)) +
  xgx_theme() +
  xgx_scale_y_percentchangelog10() +
  ggplot2::ylab("Percent Change from Baseline") +
  ggplot2::xlab("Dose (mg)")

gg +
  xgx_stat_smooth(method = "nlsLM", formula = y ~ E0 + Emax*x/(ED50 + x),
                  method.args = list(
                    start = list(Emax = -0.50, ED50 = 25, E0 = 0),
                    lower = c(-Inf, 0, -Inf)
                  ),
                  se = TRUE)

gg +
  xgx_geom_smooth_emax()

## Not run:
# example with ordinal data (method = "polr")
set.seed(12345)
data = data.frame(x = 120*exp(stats::rnorm(100,0,1)),
                  response = sample(c("Mild","Moderate","Severe"), 100, replace = TRUE),
                  covariate = sample(c("Male","Female"), 100, replace = TRUE)) %>%
  dplyr::mutate(y = (50 + 20*x/(200 + x))*exp(stats::rnorm(100, 0, 0.3)))

# example coloring by the response categories
xgx_plot(data = data) +
  xgx_stat_smooth(mapping = ggplot2::aes(x = x, response = response,
                                         colour = response, fill = response),
                  method = "polr") +
  ggplot2::scale_y_continuous(labels = scales::percent_format())


# example faceting by the response categories, coloring by a different covariate
xgx_plot(data = data) +
xgx_stat_smooth(mapping = ggplot2::aes(x = x, response = response,
                                       colour = covariate, fill = covariate),
                method = "polr", level = 0.80) +
                ggplot2::facet_wrap(~response) +
                ggplot2::scale_y_continuous(labels = scales::percent_format())
```

```
## End(Not run)
```

---

xgx_summarize_covariates *Summarize Covariate information in a dataset*

Description

xgx_summarize_covariates

Usage

```
xgx_summarize_covariates(data, covariates = NULL, n_cts = 8)
```

Arguments

data,	the dataset to check. must contain a USUBJID or ID column for subject id
covariates,	the column names of covariates, to explore
n_cts,	the number of unique values for a covariate to be treated as continuous, default is 8

Value

list

Examples

```
data <- data.frame(ID = 1:10, WT0 = rnorm(10, 70, 10),
                   SEX = round(runif(10)))
x <- xgx_summarize_covariates(data, c("WT0", "SEX"))
```

---

xgx_summarize_data *Check data for various issues*

Description

Calls xgx_check_data

Usage

```
xgx_summarize_data(data, covariates = NULL)
```

Arguments

data	the dataset to check. Must contain the above columns
covariates	the column names of covariates, to explore

Value

data.frame

Examples

```
covariates <- c("WEIGHTB", "SEX")
check <- xgx_summarize_data(mad_missing_duplicates, covariates)
```

---

xgx_theme *Calls the standard theme for xGx graphics*

Description

Calls the standard theme for xGx graphics

Usage

```
xgx_theme()
```

Value

xgx ggplot2 compatible theme

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
ggplot2::ggplot(data, ggplot2::aes(y = concentration, x = bound_receptor)) +
  ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_y_log10() +
  xgx_scale_x_reverselog10() +
  xgx_theme()
```

`xgx_theme_set` *Sets the standard theme for xGx graphics*

Description

xgx_theme_set

Usage

```
xgx_theme_set()
```

Value

xgx ggplot2 compatible theme

Examples

```
conc <- 10^(seq(-3, 3, by = 0.1))
ec50 <- 1
data <- data.frame(concentration = conc,
                   bound_receptor = 1 * conc / (conc + ec50))
xgx_theme_set()
ggplot2::ggplot(data, ggplot2::aes(y = concentration, x = bound_receptor)) +
  ggplot2::geom_point() +
  ggplot2::geom_line() +
  xgx_scale_y_log10() +
  xgx_scale_x_reverselog10()
```

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