# Package 'xgxr'

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Title Exploratory Graphics for Pharmacometrics

Version 1.1.1

**Description** Supports a structured approach

for exploring PKPD data <a href="https://opensource.nibr.com/xgx/">https://opensource.nibr.com/xgx/</a>. 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.

License MIT + file LICENSE

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

**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

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NeedsCompilation no

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# **R** topics documented:

case1_pkpd
edit_rmd_template_str
get_rmd_name
get_rmd_str
mad
mad_missing_duplicates
mad_nca
nlmixr_theo_sd
predict.nls
predictdf
predictdf.nls
predictdf.polr
sad
StatSmoothOrdinal
StatSummaryBinQuant
StatSummaryOrdinal
theme_xgx
xgx_annotate_filenames
xgx_annotate_status
xgx_annotate_status_png
xgx_auto_explore
xgx_breaks_log10
xgx_breaks_time
xgx_check_data
xgx_conf_int
xgx_dirs2char
xgx_geom_ci
xgx_geom_pi
xgx_labels_log10
xgx_minor_breaks_log10
xgx_plot
xgx_save
xgx_save_table
xgx_scale_x_log10
xgx_scale_x_reverselog10
xgx_scale_x_time_units
xgx_scale_y_log10
xgx_scale_y_percentchangelog10
xgx_scale_y_reverselog10
xgx_stat_ci
xgx_stat_pi

case I_pkpd	3

Index																55
	xgx_theme_set			٠			•						 •		 •	. 54
	xgx_theme															. 53
	xgx_summarize_	data														. 52
	xgx_summarize_	covariates														. 52
	xgx_stat_smooth		 													. 47

# **Description**

Case 1 PKPD Data Set

# Usage

case1\_pkpd

column 18:

column 19:

**CYCLE** 

**PART** 

#### **Format**

A data frame with the following 21 columns:

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

integer; count of drug administrations received

integer; part of study

```
column 20: STUDY integer; study
```

column 21: IPRED numeric; individual prediction

# **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

5 get\_rmd\_name

```
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 addition of a date stamp to the beginning 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

An integer denoting the "compartment" containing the PK data. The "CMT" pk\_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

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

get\_rmd\_str

#### 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
             NOMTIME
                          numeric; nominal time
 column 3:
 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
             MDV
 column 7:
                          numeric; missing dependent variable
                          integer; compartment number (determines observation type):
 column 8:
             CMT
                          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 = \text{not censored}, 1 = \text{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
```

8 mad\_nca

```
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:
                          character; unit of TIME
             TIMEUNIT
 column 5:
                          numeric; dosing amount (for dosing events) in mg
             AMT
 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:
                          character; description of event
             NAME
column 10:
             EVENTU
                          character; unit for observation
column 11:
             CENS
                          integer; censored values (0 = \text{not censored}, 1 = \text{censored})
column 12:
             EVID
                          integer; event ID (0 = observation, 1 = dosing event)
column 13:
             WEIGHTB
                          numeric; baseline body weight (kg)
column 14:
                          character; sex
             SEX
column 15:
                          factor; treatment group label
             TRTACT
column 16:
             DOSE
                          numeric; randomized dose in mg
column 17:
             PROFDAY
                          numeric; day of profile
```

numeric; time within PROFDAY

numeric; count of drug administrations received

column 18:

column 19:

**PROFTIME** 

CYCLE

predict.nls 9

## **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
                       numeric; baseline body weight (kg)
column 13:
            WEIGHTB
```

 $nlmixr\_theo\_sd$ 

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
                    numeric; weight
column 7:
            WT
```

predict.nls

predict.nls

10 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
```

predictdf 11

```
ggplot2::geom_point() +
  xgx_geom_smooth(method = "nls",
                  method.args = list(formula = y \sim 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),</pre>
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

12 predictdf.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 13

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,
   data,
   method,
   formula,
   method.args,
   weight,
   n_boot = 200
)
```

200

# **Arguments**

model object returned from polr sequence of x values for which to compute the smooth xseq if TRUE then confidence intervals are returned se level confidence level for confidence intervals data data to fit method only works for method MASS::polr formula formula to fit method.args arguments to pass to method weights to use for method weight number of bootstraps to perform for confidence interval calculation, default is n\_boot

# **Details**

predictdf.polr is used by  $xgx\_geom\_smooth$  when method = "polr" to calculate confidence intervals via bootstraps.

14 StatSmoothOrdinal

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:
                                        character; unit of TIME
                           TIMEUNIT
               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 = \text{not censored}, 1 = \text{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
```

Stat object for producing smooths through ordinal data

# Description

Stat object for producing smooths through ordinal data

## Usage

StatSmoothOrdinal

StatSmoothOrdinal

StatSummaryBinQuant 15

#### **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 probabilities 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**

```
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)
```

xgx\_annotate\_status 17

#### **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 of parent\_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**

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

```
the text to
status
                   x location, default Inf (right most point)
                   y location, default Inf (up most point)
У
                   font color, default "grey"
color
hjust
                   horizontal justification, default 1.2
                   vertical justification, default 1.2
vjust
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")</pre>
```

```
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.

19

#### 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

20 xgx\_auto\_explore

## 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")</pre>
```

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
)
```

xgx\_auto\_explore 21

#### **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 addition of a date stamp to the beginning 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.

22 xgx\_auto\_explore

```
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"</pre>
# Specify the mapping of column names
mapping <- list(</pre>
 "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)
```

xgx\_breaks\_log10 23

```
## 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.

```
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))
```

24 xgx\_breaks\_time

```
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.

xgx\_check\_data 25

## **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

26 xgx\_conf\_int

#### Value

data.frame

## **Examples**

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

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

xgx\_dirs2char 27

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 of parent\_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

28 xgx\_geom\_ci

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.

xgx\_geom\_pi 29

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 Use to override the default geom. Can be a list of multiple geoms, e.g. list("point", "line", "errorbar"), geom 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. If FALSE, the default, missing values are removed with a warning. If TRUE, na.rm missing values are silently removed. logical. Should this layer be included in the legends? NA, the default, includes if show.legend 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**

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",
```

30 xgx\_geom\_pi

```
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 adjust-

ment 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

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

xgx\_labels\_log10 31

```
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

32 xgx\_plot

#### **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, 1.00))
xgx_minor_breaks_log10(c(1, 1.000))
print(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

xgx\_save 33

## **Examples**

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

 parent\_dir = Parent directory containing the Rscript and the Results folder, default getwd() 34 xgx\_save

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()

file type 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

xgx\_save\_table 35

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

36 xgx\_scale\_x\_log10

```
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

```
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 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

```
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\_plot

units of the input dataset, must be specified by user as "h", "d", "w", "m", or "y" 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())

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

.. other parameters for scale\_x\_continuous

xgx\_scale\_y\_log10 39

# **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")</pre>
```

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**

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()</pre>
```

```
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

42 xgx\_stat\_ci

## **Examples**

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.

xgx\_stat\_ci 43

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.

distribution

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.

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 adjust-

ment 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 imple-

mented 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.

44 xgx\_stat\_ci

#### **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

```
# 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_v_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 \times \exp(\text{stats}::\text{rnorm}(100,0,1)),
              response = sample(c("Mild","Moderate","Severe"), 100, replace = TRUE),
              covariate = sample(c("Male","Female"), 100, replace = TRUE))
```

xgx\_stat\_pi 45

```
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 \times \exp(\text{stats}::\text{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(</pre>
 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")
}
```

46 xgx\_stat\_pi

#### **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 adjust-

ment 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.  $y \sim x$ ,  $y \sim poly(x, 2)$ ,  $y \sim log(x)$ 

se

display confidence interval around smooth? (TRUE by default, see level to con-

trol)

n

number of points to evaluate smoother at

span

Controls the amount of smoothing for the default loess smoother. Smaller num-

bers 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 imple-

mented 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.

```
# 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),</pre>
                   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)")
 xgx_stat_smooth(method = "nlsLM", formula = y \sim 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 \times \exp(\text{stats}::\text{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())
```

52 xgx\_summarize\_data

```
## 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**

xgx\_summarize\_data

Check data for various issues

# Description

```
Calls xgx_check_data
```

# Usage

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

xgx\_theme 53

# **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)</pre>
```

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

54 xgx\_theme\_set

xgx\_theme\_set

Sets the standard theme for xGx graphics

# Description

```
xgx\_theme\_set
```

# Usage

```
xgx_theme_set()
```

#### Value

xgx ggplot2 compatible theme

# **Index**

* datasets	StatSmoothOrdinal, 14
case1_pkpd, 3	StatSummaryBinQuant, 15
mad, 7	StatSummaryOrdinal, 15
<pre>mad_missing_duplicates, 8</pre>	
mad_nca, 8	theme_xgx, 16
<pre>nlmixr_theo_sd, 9</pre>	transformation object, $38$
sad, 14	
StatSmoothOrdinal, 14	xgx_annotate_filenames, 16
StatSummaryBinQuant, 15	xgx_annotate_status, 17
StatSummaryOrdinal, 15	xgx_annotate_status_png, 18
	xgx_auto_explore, 20
binom.exact, 26, 28, 43	xgx_breaks_log10, 23
	xgx_breaks_time,24
case1_pkpd, 3	xgx_check_data, 25, 52
	xgx_conf_int, 26
edit_rmd_template_str,4	xgx_dirs2char, 27
and and area 5	xgx_geom_ci, 28
get_rmd_name, 5	xgx_geom_pi, 29
get_rmd_str, 6	xgx_geom_smooth(xgx_stat_smooth), 47
ggplot, <i>32</i>	<pre>xgx_geom_smooth_emax (xgx_stat_smooth),</pre>
layer, <i>18</i>	47
	xgx_labels_log10, 31
mad, 7	xgx_minor_breaks_log10,31
mad_missing_duplicates, 7	xgx_plot, 32
mad_nca, 8	xgx_save, 33
	xgx_save_table, 35
nlmixr_theo_sd,9	xgx_scale_x_log10,36
	xgx_scale_x_percentchangelog10
predict.nls,9	<pre>(xgx_scale_y_percentchangelog10),</pre>
predictdf, 11	40
predictdf.nls, 12,50	xgx_scale_x_reverselog10,37
predictdf.polr,13	xgx_scale_x_time_units, 38
	xgx_scale_y_log10,39
sad, 14	$xgx\_scale\_y\_percentchangelog10,40$
scale_x_continuous, 37, 38	xgx_scale_y_reverselog10,41
scale_x_log10, 36	xgx_scale_y_time_units
scale_y_continuous, 41	<pre>(xgx_scale_x_time_units), 38</pre>
scale_y_log10, 39	xgx_stat_ci,42
scales::extended_breaks(), 38	xgx_stat_pi,45
stat_summary, 43	xgx_stat_smooth, 47

56 INDEX

```
xgx_summarize_covariates, 52
xgx_summarize_data, 52
xgx_theme, 53
xgx_theme_set, 54
```