Package ‘xpose.nlmixr’

April 26, 2021

Type Package
Title Graphical Diagnostics for Pharmacometric Models: Extension to 'nlmixr'
Version 0.2.0
Maintainer Justin Wilkins <justin.wilkins@occams.com>
Description Extension to 'xpose' to support 'nlmixr'. Provides functions to import 'nlmixr' fit data into an 'xpose' data object, allowing the use of 'xpose' for 'nlmixr' model diagnostics.
License GPL (&gt;= 2)
Encoding UTF-8
LazyData true
Depends R (&gt;= 3.2), xpose (&gt;= 0.4.2)
Imports ggplot2 (&gt;= 2.2.1), nlmixr (&gt;= 1.1.0-0), dplyr (&gt;= 0.7.4), tibble (&gt;= 2.0.0), stringr (&gt;= 1.2.0), tidyr (&gt;= 0.7.2), magrittr (&gt;= 1.5), methods (&gt;= 3.4.1), vpc (&gt;= 1.0.2), nlme, crayon, rlang
RoxygenNote 7.1.1
NeedsCompilation no
Author Justin Wilkins [aut, cre, cph],
  Matthew Fidler [aut, cph],
  Benjamin Guiastrennec [aut],
  Andrew C. Hooker [aut],
  Anna Olofsson [aut, cph],
  Sebastian Ueckert [aut],
  Ron Keizer [aut],
  Kajsa Harling [ctb],
  Mike K. Smith [ctb],
  Elodie Plan [ctb],
  Mats O. Karlsson [aut, cph],
  Pharmetheus [ctb],
  Pfizer [ctb],
  Occams [ctb],
  Novartis [ctb]
R topics documented:

- nlmixr_vpc_theme
- summarise_nlmixr_model
- theme_xp_nlmixr
- theo_sd_fit
- xpose_data_nlmixr

---

### nlmixr_vpc_theme

**Default VPC theme for 'xpose.nlmixr'**

**Description**

Default VPC theme for 'xpose.nlmixr'.

**Usage**

```r
nlmixr_vpc_theme
```

**Format**

An object of class vpc_theme of length 23.

**Value**

A list with 'vpc' theme specifiers.

---

### summarise_nlmixr_model

**Data summary function**

**Description**

Convert 'nlmixr' model output into an 'xpose' database

**Usage**

```r
summarise_nlmixr_model(obj, model, software, rounding, runname)
```
theme_xp_nlmixr

Arguments

- **obj**  
  nlmixr fit object to be evaluated

- **model**  
  Model. Can be blank

- **software**  
  Software that generated the model fit

- **rounding**  
  Number of figures to round estimates to

- **runname**  
  Name of the model object being converted

Value

A summary data object used by `xpose_data_nlmixr`.

data("theo_sd_fit")
Format

A tibble with 132 observations and 22 variables, and an additional 13 properties.

ID  Individual identifier, a factor
TIME Time in hours, a numeric vector
DV  Theophylline concentration, a numeric vector
EVID Event identifier, a numeric vector
PRED Population predictions, a numeric vector
RES Residuals, a numeric vector
WRES Weighted residuals, a numeric vector
IPRED Individual predictions, a numeric vector
IRES Individual residuals, a numeric vector
IWRES Individual weighted residuals, a numeric vector
CPRED Conditional predictions, a numeric vector
CRES Conditional residuals, a numeric vector
CWRES Conditional weighted residuals, a numeric vector
eta.ka Interindividual variability in ka, a numeric vector
eta.cl Interindividual variability in CL/F, a numeric vector
eta.v Interindividual variability in V/F, a numeric vector
ka Absorption rate in /h, a numeric vector
c1 Apparent clearance in L/h, a numeric vector
v Apparent volume of distribution in L, a numeric vector
cp Theophylline concentration, a numeric vector
depot Amount of theophylline in the depot compartment, a numeric vector
center Amount of theophylline in the central compartment, a numeric vector
omega Omega matrix
omegaR Omega Correlation matrix
shrink Shrinkage table, includes skewness, kurtosis, and eta p-values
parFixed Fixed Effect Parameter Table
theta Fixed Parameter Estimates
eta Individual Parameter Estimates
seed Seed (if applicable)
coefficients Fixed and random coefficients
meta Model meta information environment
modelName Model name (from R function)
dataName Name of R data input
simInfo RxODE list for simulation
sigma List of sigma components and their values
Details

This dataset is an \texttt{nlmixr} fit object for demonstrating the use of \texttt{xpose.nlmixr}.

Source

NONMEM/nlme.

Examples

```r
data(theo_sd_fit)
str(theo_sd_fit)
```

Description

Convert 'nlmixr' model output into an 'xpose' database.

Usage

```r
xpose_data_nlmixr(
  obj = NULL,
  pred = NULL,
  wres = NULL,
  gg_theme = theme_readable(),
  xp_theme = theme_xp_default(),
  quiet,
  skip = NULL,
  ...
)
```

Arguments

- **obj** \texttt{nlmixr} fit object to be evaluated.
- **pred** Name of the population prediction variable to use for plotting. If unspecified, it will choose either "NPDE", "CWRES", and "RES" (in that order) if the column exists in the data.
- **wres** Name of the weighted residual variable to use for plotting. If unspecified, it will choose either "NPDE", "CWRES", and "RES" (in that order) if the column exists in the data.
- **gg_theme** A ggplot2 theme object.
- **xp_theme** An xpose theme or vector of modifications to the xpose theme (eg. \texttt{c(point_color = 'red', line_linetype = 'dashed')}).
- **quiet** Logical, if FALSE messages are printed to the console.
- **skip** Character vector be used to skip the import/generation of: 'data', 'files', 'summary' or any combination of the three.
- **...** Additional arguments to be passed to the \texttt{read_delim} functions.
Value

An `xpose_data` object suitable for use in 'xpose'.

Examples

```r
xpdb <- xpose_data_nlmixr(obj = theo_sd_fit)
```
Index

* datasets
  nlmixr_vpc_theme, 2
  theo_sd_fit, 3

nlmixr_vpc_theme, 2

read_delim, 5

summarise_nlmixr_model, 2

theme_xp_nlmixr, 3
theo_sd_fit, 3

xpose_data, 6
xpose_data_nlmixr, 3, 5