

Package ‘xpose.nlmixr’

June 6, 2022

Type Package

Title Graphical Diagnostics for Pharmacometric Models: Extension to 'nlmixr'

Version 0.3.0

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 (>= 2)

Encoding UTF-8

LazyData true

Depends R (>= 3.2), xpose (>= 0.4.2)

Imports ggplot2 (>= 2.2.1), nlmixr (>= 1.1.0-0), dplyr (>= 0.7.4),
tibble (>= 2.0.0), stringr (>= 1.2.0), tidyr (>= 0.7.2),
magrittr (>= 1.5), methods (>= 3.4.1), vpc (>= 1.0.2), nlme,
crayon, rlang

RoxygenNote 7.1.2

NeedsCompilation no

Author Justin Wilkins [aut, cre, cph],
Matthew Fidler [aut, cph],
Benjamin Guiastronnet [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]

Repository CRAN

Date/Publication 2022-06-06 18:40:02 UTC

R topics documented:

nlmixr_vpc_theme	2
summarise_nlmixr_model	2
theme_xp_nlmixr	3
theo_sd_fit	3
xpose_data_nlmixr	5

Index [7](#)

nlmixr_vpc_theme	<i>Default VPC theme for 'xpose.nlmixr'</i>
------------------	---

Description

Default VPC theme for 'xpose.nlmixr'.

Usage

```
nlmixr_vpc_theme
```

Format

An object of class vpc_theme of length 23.

Value

A list with 'vpc' theme specifiers.

summarise_nlmixr_model	<i>Data summary function</i>
------------------------	------------------------------

Description

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

Usage

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

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](#).

theme_xp_nlmixr	<i>Default 'nlmixr' theme for 'xpose'</i>
-----------------	---

Description

Default 'nlmixr' theme for 'xpose'.

Usage

```
theme_xp_nlmixr()
```

Value

A list with 'xpose' theme specifiers.

theo_sd_fit	<i>Single-dose theophylline PK data fit</i>
-------------	---

Description

Single-dose theophylline PK data fit using the first-order conditional estimation method with interaction (FOCEI) in 'nlmixr', a modified tibble.

Usage

```
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 k_a , 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
 cl 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 `nlmixr` fit object for demonstrating the use of `xpose.nlmixr`.

Source

NONMEM/nlme.

Examples

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

```
xpose_data_nlmixr      Import nlmixr output into xpose
```

Description

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

Usage

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

Arguments

<code>obj</code>	nlmixr fit object to be evaluated.
<code>pred</code>	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.
<code>wres</code>	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.
<code>gg_theme</code>	A <code>ggplot2</code> theme object.
<code>xp_theme</code>	An <code>xpose</code> theme or vector of modifications to the <code>xpose</code> theme (eg. <code>c(point_color = 'red', line_linetype = 'dashed')</code>).
<code>quiet</code>	Logical, if <code>FALSE</code> messages are printed to the console.
<code>skip</code>	Character vector be used to skip the import/generation of: 'data', 'files', 'summary' or any combination of the three.
<code>...</code>	Additional arguments to be passed to the <code>read_delim</code> functions.

Value

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

Examples

```
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

tibble, 4

xpose_data, 6

xpose_data_nlmixr, 3, 5