

Package: Certara.ModelResults (via r-universe)

March 4, 2025

Title Generate Diagnostics for Pharmacometric Models Using 'shiny'

Version 3.0.1

Description Utilize the 'shiny' interface to generate Goodness of Fit (GOF) plots and tables for Non-Linear Mixed Effects (NLME / NONMEM) pharmacometric models. From the interface, users can customize model diagnostics and generate the underlying R code to reproduce the diagnostic plots and tables outside of the 'shiny' session. Model diagnostics can be included in a 'rmarkdown' document and rendered to desired output format.

Depends R (>= 4.0)

License LGPL-3

URL <https://certara.github.io/R-model-results/>

Encoding UTF-8

LazyData true

RoxygenNote 7.3.2

Suggests knitr, rmarkdown, testthat (>= 3.0.0), Certara.RsNLME

Imports colourpicker, shinyAce, shinymeta, Certara.Xpose.NLME, xpose, dplyr, flextable, shinyjqui, grDevices, ggplot2, plotly, magrittr, scales, shiny (>= 1.7.0), shinyjs, shinyWidgets, shinyTree (>= 0.3.1), sortable, tidyr, rlang, bslib (>= 0.7.0)

Config/testthat/edition 3

NeedsCompilation no

Author James Craig [aut, cre], Shuhua Hu [ctb], Mike Talley [aut], Certara USA, Inc [cph, fnd]

Maintainer James Craig <james.craig@certara.com>

Date/Publication 2025-03-03 11:50:24 UTC

Config/pak/sysreqs libcairo2-dev libfontconfig1-dev libfreetype6-dev libfribidi-dev make libharfbuzz-dev libicu-dev libjpeg-dev libpng-dev libtiff-dev libxml2-dev libssl-dev libx11-dev zlib1g-dev

Repository <https://certara-jcraig.r-universe.dev>

RemoteUrl <https://github.com/cran/Certara.ModelResults>

RemoteRef HEAD

RemoteSha e29bdbb72d51eadc900937e04e2a7d3dce433464

Contents

get_eps_shk	2
get_eta_shk	3
resultsUI	3
theme_certara	5
write_code	6
xpdb_NLME	6
xpdb_NONMEM	7
Index	8

get_eps_shk	<i>Get eps shrinkage values xpdb</i>
-------------	--------------------------------------

Description

This function returns eps shrinkage values from xpdb object as a data.frame.

Usage

```
get_eps_shk(xpdb)
```

Arguments

xpdb Object of class xpose_data.

Value

Returns an object of class data.frame.

Examples

```
get_eps_shk(xpdb_NLME$TwCpt_IVBo1us_FOCE_ELS)
```

get_eta_shk	<i>Get eta shrinkage values xpdb</i>
-------------	--------------------------------------

Description

This function returns eta shrinkage values from xpdb object as a data.frame.

Usage

```
get_eta_shk(xpdb)
```

Arguments

xpdb Object of class xpose_data.

Value

Returns an object of class data.frame.

Examples

```
get_eta_shk(xpdb_NLME$TwCpt_IVBolus_FOCE_ELS)
```

resultsUI	<i>Generate and Report Model Diagnostics from NLME or NONMEM runs</i>
-----------	---

Description

Shiny application to generate, customize, and report diagnostic plots and tables from NLME or NONMEM output files. Create an Rmarkdown file of tagged model diagnostics and render into submission ready report.

Usage

```
resultsUI(model, xpdb = NULL, tagged = NULL, settings = NULL, ...)
```

Arguments

model A single object, vector, or list of objects of class NlmePmlModel.
 xpdb A single object or list of objects of class xpose_data.
 tagged List of tagged objects returned from previous tagged <- resultsUI() session.
 settings List of settings (e.g., settings.Rds) returned from previous Shiny session.
 ... Additional arguments for Pirana integration.

Value

If `interactive()`, returns a list of tagged diagnostics from the Shiny application, otherwise returns `TRUE`.

Examples

```
if (interactive()) {

# RsNLME
library(Certara.RsNLME)
library(Certara.ModelResults)

model1 <- pkmodel(numCompartments = 1,
                  data = pkData,
                  ID = "Subject",
                  Time = "Act_Time",
                  A1 = "Amount",
                  CObs = "Conc",
                  modelName = "OneCpt_IVBolus_FOCE-ELS")

baseFitJob1 <- fitmodel(model1)

model2 <- pkmodel(numCompartments = 2,
                  data = pkData,
                  ID = "Subject",
                  Time = "Act_Time",
                  A1 = "Amount",
                  CObs = "Conc",
                  modelName = "TwCpt_IVBolus_FOCE-ELS")

baseFitJob2 <- fitmodel(model2)

# Run Model Results
resultsUI(model = c(model1, model2))

# NONMEM via xpose

library(Certara.ModelResults)
library(xpose)

xpdb <- xpose_data(
  runno = "1",
  prefix = "run",
  ext = ".lst",
  dir = "./NONMEM/Hands_onB/")

resultsUI(xpdb = xpdb)

# Multiple models
```

```
xpdb_multiple <- list(  
  run1 = xpose_data(file = "run1.lst"),  
  run2 = xpose_data(file = "run2.lst"),  
  run3 = xpose_data(file = "run3.lst"),  
  run4 = xpose_data(file = "run4.lst")  
)  
}
```

theme_certara	<i>A ggplot2 theme for Certara.</i>
---------------	-------------------------------------

Description

A ggplot2 theme for Certara.

Usage

```
theme_certara(  
  base_size = 11,  
  base_family = "",  
  base_line_size = base_size/22,  
  base_rect_size = base_size/22,  
  grid = c("none", "horizontal", "both")  
)
```

Arguments

base_size	base font size, given in pts.
base_family	base font family
base_line_size	base size for line elements
base_rect_size	base size for rect elements
grid	Which grid lines should appear? Horizontal only, both horizontal and vertical, or none (default). continuous_scale() .

Details

There are 3 variants of the theme: no grid `theme_certara()`, full grid `theme_certara(grid = "both")`, and horizontal grid lines only `theme_certara(grid = "horizontal")`.

Value

An object of class `theme()`.

write_code	<i>Write code to R script from tagged diagnostics</i>
------------	---

Description

Use this function to write code to R script from diagnostics tagged in Certara's Model Results Shiny Application.

Usage

```
write_code(tagged, file)
```

Arguments

tagged	List of tagged objects from returned from resultsUI().
file	Character specifying path of output file. If missing, it will be saved as code.R in working directory.

Value

Returns NULL after writing to file.

Examples

```
if (interactive()) {
  tagged_diagnostics <- resultsUI(xpdb = xpdb_NLME)

  write_code(tagged_diagnostics, "tagged_results.R")
}
```

xpdb_NLME	<i>List of xpose data objects from RsNLME example tutorials</i>
-----------	---

Description

The following object contains a list of 2 xpose_data objects generated in the RsNLME example script TwoCptIVBolus_FitBaseModel_CovariateSearch_VPC_BootStrapping.R.

Usage

```
xpdb_NLME
```

Format

List of 2 xpose_data objects constructed from NLME model output.

Details

- `xpdb_NLME$`TwCpt_IVBolus_FOCE-ELS`` is an `xpose_data` object created from the base model in `RsNLME` example script. The model can be used as a reference to compare model diagnostics in final model.
- `xpdb_NLME$`TwCpt_IVBolus_SelectedCovariateModel_FOCE-ELS`` is an `xpose_data` object created from the final model in the `RsNLME` example script. The final model includes selected covariate `BodyWeight` added from the results of stepwise covariate search.

Source

Certara

xpdb_NONMEM

List of xpose data objects from NONMEM model output

Description

The following object contains of list of 2 `xpose_data` objects:

Usage

`xpdb_NONMEM`

Format

List of 2 `xpose_data` objects constructed from `NONMEM` model output.

Details

- `xpdb_NONMEM$ex_pk` is an `xpose_data` object from `xpose::xpdb_ex_pk`. The model contains multiple covariates and can be used to explore covariate model diagnostics.
- `xpdb_NONMEM$mult_obs` is an `xpose_data` object created from `NONMEM` model with multiple observed variables. Users will see that appropriate model diagnostic plots are automatically faceted by `DVID` in the Shiny GUI.

Source

Certara

Index

* datasets

xpdb_NLME, [6](#)

xpdb_NONMEM, [7](#)

continuous_scale, [5](#)

get_eps_shk, [2](#)

get_eta_shk, [3](#)

resultsUI, [3](#)

theme, [5](#)

theme_certara, [5](#)

write_code, [6](#)

xpdb_NLME, [6](#)

xpdb_NONMEM, [7](#)