Model Diagnostics with xpose : : CHEAT SHEET

The **xpose** package facilitates the creation of model diagnostics from NONMEM output. Inspired by **xpose4**, this new version is actively being redesigned around the popular **tidyverse** packages **ggplot2**, **dplyr** and **readr**.

Getting started

INSTALLATION
- **From CRAN**
  install.packages('xpose')
- **From github** *(development version)*
  library(devtools)
  install_github('UUPharmacometrics/xpose')

GETTING HELP
- Comprehensive documentation and examples are available at:
  uupharmacometrics.github.io/xpose/
- Use **?<function_name>** in R to access functions' help (e.g. ?xpose_data).

PLOT TYPE
Plot **type** is specified via a single string, where values: **a** (area), **d** (density), **h** (histogram), **l** (line), **p** (point), **r** (rug), **s** (smooth) and **t** (text) can be combined depending on the plot function.
  dv_vs_ipred(xpdb_ex_pk, **type = 'pls'**)
  eta_distrib(xpdb_ex_pk, **type = 'hdr'**)

PLOT LAYERS
All **ggplot2** functions can be used to add or modify **xpose** plot layers, mapping, labels, scales, annotations, etc.
  plot <- dv_vs_ipred(xpdb_ex_pk)
  plot + geom_hline(yintercept = 1)

PIPES
All **xpose** functions can be used with pipes (%>%)
  xpdb_ex_pk %>%
  filter(OCC == 3) %>%
  dv_vs_ipred()

Plot functions

The **xpdb** (xpose database) is a structured object containing the NONMEM output tables, output files, the parsed model code, general options and plot themes.

BASIC GOF
Accepted plot types: l, p, s, t
Layer names: guide, line, point, smooth, text, xscale, yscale

dv_vs_ipred(xpdb, guide = TRUE)
dv_vs_pred(xpdb, guide = TRUE)

res_vs_idv(xpdb, res = 'CWRES', guide = TRUE)
res_vs_pred(xpdb, res = 'CWRES', guide = TRUE)

absval_res_vs_idv(xpdb, res = 'CWRES')
absval_res_vs_pred(xpdb, res = 'CWRES')

dv_vs_idv(xpdb, group = 'ID')
ipred_vs_idv(xpdb, group = 'ID')
pred_vs_idv(xpdb, group = 'ID')

dv_preds_vs_idv(xpdb, group = 'ID')
display of DV, IPRED and PRED side by side

INDIVIDUAL PLOTS
Accepted plot types: l, p, s, t
Layer names: line, point, smooth, text, xscale, yscale

ind_plots(xpdb)

COMPARTMENT KINETICS
Accepted plot types: l, p, s, t
Layer names: line, point, smooth, text, xscale, yscale

amt_vs_idv(xpdb, group = ID)
uses A1, A2, …, columns by default

VISUAL PREDICTIVE CHECKS
Accepted plot types: a, l, p, r, t
Layer names: area, line, point, rug, text, xscale, yscale

compute vpc data in R
advanced options (e.g. bins, lloq, pi, ci, etc.)

vpc_data(xpdb, opt = **vpc_opt**(…), vpc_type, stratify, psn_folder) %>%
vpc(smooth)   **plot** the vpc

DISTRIBUTIONS
Accepted plot types: d, h, r
Layer names: density, histogram, rug, xscale, yscale

prm_distrib(xpdb)
eta_distrib(xpdb)
cov_distrib(xpdb)
res_distrib(xpdb, res = 'CWRES')

QQ PLOTS
Accepted plot types: p
Layer names: guide, point

prm_qq(xpdb, guide = TRUE)
eta_qq(xpdb, guide = TRUE)
cov_qq(xpdb, guide = TRUE)
res_qq(xpdb, res = 'CWRES', guide =TRUE)

MINIMIZATION DIAGNOSTICS
Accepted plot types: l, p, s, t
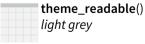*Layer names: line, point, smooth, text, xscale, yscale*

grd_vs_iteration(xpdb) *(.grd file required)*
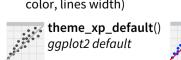**prm_vs_iteration**(xpdb) *(.ext file required)*

Customize plots
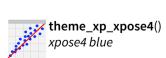
THEMES
The xpdb objects contain two types of themes :
- **gg_theme**: sets plot background and text properties

  theme_readable()
  light grey
  theme_bw2()
  black and white

- **xp_theme**: sets default aesthetics values (e.g. points color, lines width)

  theme_xp_default()
  ggplot2 default
  theme_xp_xpose4()
  xpose4 blue

New themes can be applied globally:
  xpdb <- update_themes(xpdb, gg_theme, xp_theme)
Or locally in each plot function:
  dv_vs_ipred(xpdb, gg_theme, xp_theme)

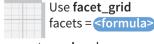### PLOTS AESTHETICS
Arguments for aesthetics are composed of the target layer name (e.g. point, line) and the name of the argument in the format **<layer>_<argument>** (e.g. point_color = 'red', line_linetype = 'dashed', smooth_method = 'lm').

FACETING & PAGINATION
All **xpose** plot functions accept arguments for **facet_wrap** and **facet_grid** (e.g. facets, ncol, nrow, scales)

Use **facet_wrap** facets = **<string>**
Use **facet_grid** facets = **<formula>**

Pagination is enabled when the arguments **ncol** and **nrow** are both set. The argument **page** can then be used to output specific pages or a range of pages:
  xpdb_ex_pk %>%
  dv_vs_ipred(facets=MED1~OCC, **ncol=2**, **nrow=1**, **page=1:2**)

Data

The **xpdb** (xpose database) is a structured object containing the NONMEM output tables, output files, the parsed model code, general options and plot themes.

IMPORT
Data import in **xpose** is structured as follows:
1. Read NONMEM **control stream** (.mod/.lst) to list table filenames for each $PROBLEM
2. Import and index tables (compatible with FIRSTONLY option, .csv and compressed (.zip) files)
3. Import NONMEM output files (.ext, .phi, .cov, etc.)
4. Summarize control stream

Runs can automatically be imported either by using the **file** or the **prefix**, **runno** and **ext** arguments.
xpdb <- xpose_data(dir, file, prefix, runno, ext)

EDIT
Data in the xpdb can be edited using **dplyr** functionalities
- **filter**(xpdb, …, .problem, .source)
  subset data based on logical condition(s)
- **mutate**(xpdb, …, .problem, .source)
  add, modify and remove columns
- **set_var_type**(xpdb, …, .problem)
  assign or modify output tables' index

xpdb_ex_pk %>%   *built-in xpdb example*
mutate(TAD = TIME %% 24) %>%   *e.g. generate and*
dv_vs_idv(aes(x = TAD))   *plot time after dose*

ACCESS
Access and extract data from an xpdb.
- **get_code**(xpdb, .problem) *(parsed control stream)*
- **get_prm**(xpdb, .problem) *(table of parameter estimates)*
- **get_file**(xpdb, ext, .problem) *(parsed output files)*
- **get_data**(xpdb, .problem) *(combined dataset)*
- **get_summary**(xpdb, .problem) *(table of run summary)*

SUMMARY
- **print**(xpdb) or xpdb
  display xpdb structure
- **list_vars**(xpdb)
  display data variables
- **summary**(xpdb)
  display run summary
- **prm_table**(xpdb)
  display parameter table

Template titles

Special **@<keywords>** can be used in plot labels. They are automatically replaced by their actual value in the run summary when plotting (e.g. title = 'ofv: @ofv' can give 'ofv: -1518.108'). Check **?template_titles** in R for a full list.

Save plots

The file and dir argument can contain template title keywords. Also handles plots with multiple pages.
xpose_save(plot, file = '@run_@plotfun', dir, width, height)