Open source software from the Uppsala University Pharmacometrics group

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PsN (Perl speaks NONMEM)

https://uupharmacometrics.github.io/PsN

Toolbox for population PK/PD model building using NONMEM. Functionality ranges from results extraction to advanced statistical methods. PsN simplifies the organization of NONMEM output files, helps with starting jobs on different types of clusters (i.e. slurm, torque, sge and lsf) and can perform a cornucopia of statistical and computational task [1][2][3][4].

Example tools

- **bootstrap** – assessing uncertainty of parameter estimates
- **frem** – full random effects modelling
- **qa** – fast and automatic assumption assessment and quality assurance of models
- **scm** – stepwise covariate model
- **simeval** – simulation evaluation diagnostics of outliers
- **sir** - sampling importance resampling for parameter uncertainty assessment
- **sse** – stochastic simulation and estimation
- **vpc** – visual predictive check

piraid

https://github.com/UUPharmacometrics/piraid

An aid for development and diagnostics of pharmacometric IRT and composite score models. It provides assistance for the creation of models as well as the generation of diagnostic plots.

Features

- Generation of NONMEM IRT models for binary and ordered categorical type items
- Estimation of item parameters and calculation of information curves
- Generation of bounded integer and continuous variable total score models as well as support for IRT-informed total score models

ncappc

https://github.com/UUPharmacometrics/ncappc
Available on CRAN

Performs traditional non-compartmental analysis and simulation based posterior predictive checks for PK and PKPD models [5].

bemod

Model-integrated bioequivalence analysis. The goal of bemod is to perform bioequivalence testing. bemod can do this using standard non-comparmental analysis (NCA) methods, or with model-integrated methods that can reduce sample size and/or shorten study duration [6][7].

Pharmpy

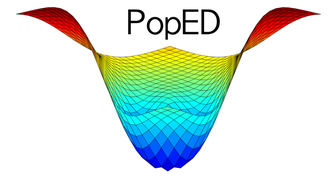
https://pharmpy.github.io/
Available on CRAN (as pharmr)

Library and toolkit for pharmacometrics with R-wrapper pharmr.

See separate PAGE poster.

PopED

https://andrewhooker.github.io/PopED
Available on CRAN



Computes optimal experimental designs for both population and individual studies based on nonlinear mixed-effect models. Often this is based on a computation of the Fisher Information Matrix (FIM) [8][9].

Features

- Flexible and robust model description, which can be done using various R-packages including mrgsolve, RxODE, PKPDsim, deSolve, and Rcpp
- Flexible and robust tools for design evaluation, design visualization and clinical trial simulation
- Flexible and robust design optimization handling complex designs and optimizing of a wide variety of design variables

MBAOD

https://github.com/andrewhooker/MBAOD

The MBAOD package can be used to simulate experiments (often clinical or pre-clinical trials) using predefined adaptation and optimization rules. The package can be used to plan and evaluate the predicted effectiveness of an upcoming trial. In addition the package can be used to optimize any specific cohort of an actual study [10][11].

xpose/xpose4

https://uupharmacometrics.github.io/xpose
https://uupharmacometrics.github.io/xpose4
Available on CRAN

xpose4 is a collection of functions to be used as a model building aid for nonlinear mixed-effects (population) analysis using NONMEM. It facilitates dataset checkout, exploration and visualization, model diagnostics, candidate covariate identification, and model comparison. xpose was designed as a ggplot2-based alternative to xpose4. xpose aims to reduce the post-processing burden and improve diagnostics commonly associated with the development of non-linear mixed effect models [12].

Features

- Tools for data visualization and data checkout
- Basic goodness-of-fit plots
- Structural and residual model diagnostics
- Parameter distribution diagnostics
- Visual predictive checks
- Model evaluation tools – plots and tables created to evaluate all aspects of a pharmacometric model
- Model comparison tools – graphs for comparing various aspects of two models fit to the same data
- Model development tools – used to help the modeler decide what to do next with the model. Most of these functions focus on aspects of covariate inclusion

List of references

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