

Open source software from the Uppsala University Pharmacometrics group

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<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]

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>

Aids the development of pharmacometric IRT and composite score models. It provides assistance for the creation of the models as well as for 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

Flexible tool in R to:

- Perform non-compartmental analysis (NCA)
- Perform simulation-based posterior predictive checks (PPC) for population models using NCA metrics [2]

bemod

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

assemblerr

<https://uupharmacometrics.github.io/assemblerr>

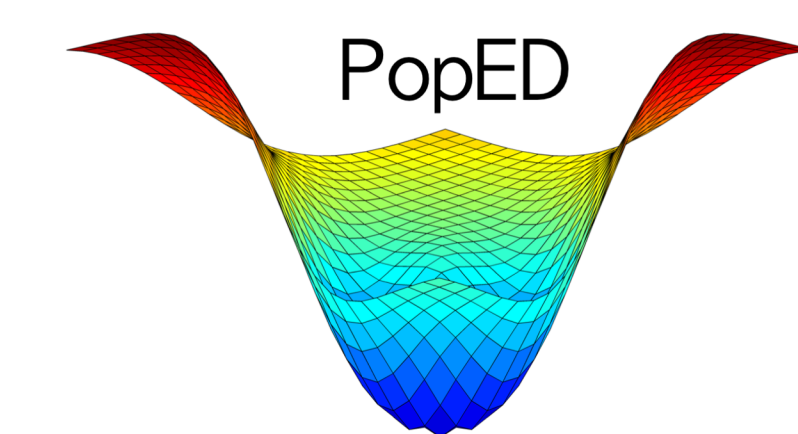
Construction of pharmacometric models by combining pre-defined model components.

List of references

- [1] Karlsson MO, Nordgren R et al., PsN: An open source toolkit for non-linear mixed effects modelling, 2004-, <https://uupharmacometrics.github.io/PsN/> [Online; accessed 2024-05-16]
[2] Acharya C, Hooker AC, Turkyilmaz GY, Jonsson S, Karlsson MO (2016), A diagnostic tool for population models using non-compartmental analysis: The ncappc functionality for R, Computer Methods and Programs in Biomedicine, 127, 83-93.
[3] Nyberg J, Ueckert S, Stroemberg EA, Hennig S, Karlsson MO, Hooker AC (2012), PopED: An extended, parallelized, nonlinear mixed effects models optimal design tool. Computer Methods and Programs in Biomedicine, 108.
[4] Foracchia M, Hooker AC, Vicini P, Ruggeri A (2004), POPED, a software for optimal experiment design in population kinetics. Computer Methods and Programs in Biomedicine, 74.
[5] Jonsson EN, Karlsson MO. Xpose--an S-PLUS based population pharmacokinetic/pharmacodynamic model building aid for NONMEM. Computer Methods and Programs in Biomedicine. 58(1):51-64.
[6] Nordgren R, Belin S, Chen X, Borg J, Hufnagl A, Shi K, Hooker AC, Karlsson MO. PharmPy: a versatile open-source software package for pharmacometrics, PAGE 2024.

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). [3][4]

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 using MBAOD.

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 data set 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 the development of non-linear mixed effect models. [5]

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

PharmPy

<https://pharmPy.github.io/>
Available on CRAN (as pharmr)



Library and toolkit for pharmacometrics with R-wrapper pharmr. See separate PAGE poster. [6]



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