

User Guide for PKgraph Package

Xiaoyong Sun^{†‡*}

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[†]Biinformatics and Computational Biology Program, [‡]Department of Statistics
Iowa State University, Ames, Iowa 50010, USA

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1 Introduction

Population pharmacokinetic (PopPK) modeling has become increasingly important in drug development because it allows unbalanced design, sparse data and the study of individual variation. However, this complexity of the model makes it a challenge to diagnose the fit. Graphics can play an important and unique role in PopPK model diagnostics. The software described in this paper, PKgraph, provides a graphical user interface for PopPK model diagnosis with interactive graphics. It also provides an integrated and comprehensive platform for analysis of pharmacokinetic data including exploratory data analysis, goodness of model fit, model validation and model comparison. It can be used with a variety of modeling fitting software, including NONMEM, Monolix, SAS and R. PKgraph is programmed in R, and uses the R packages lattice, ggplot2 for static graphics, and rggobi for interactive graphics. This R package is supported with a user-friendly graphical user interface so that users can easily control diagnosing with simple clicks. The PKgraph software serves as a supplement to the existing packages: NONMEM, Xpose and PsN for diagnosing models.

PKgraph is an R package built on the following R packages: RGtk2, gWidgets, gWidgetsRGtk2, lattice, and ggplot2. It requires R (> 2.0) and GTK+, and runs under Windows, Linux and Mac.

*johnsunx1@gmail.com

2 Installation

PKgraph needs to install the following programs and R packages:

1. install GTK

For Windows, you can download the GTK Developer's Pack from <http://gladewin32.sourceforge.net/>

For Unix, you can fetch the source files for the different libraries from <ftp://ftp.gtk.org/pub/gtk/v2.8/>

2. Install RGtk2 (Please see RGtk2 Installation notes if you have problems)

install.packages("RGtk2")

3. install rggobi

a. Download and install ggobi (www.ggobi.org)

b. Install rggobi: *install.packages("rggobi")*

4. Install gWidgets

install.packages("gWidgets")

5. Install cairoDevice

install.packages("cairoDevice")

6. Install gWidgetsRGtk2

install.packages("gWidgetsRGtk2")

7. Install lattice

install.packages("lattice")

8. Install ggplot2

install.packages("ggplot2")

3 User Guide

Please see the user guide at <https://sourceforge.net/projects/pkgraph/files/>