PKtools

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The following is the additional setup for the interfaces from PKtools to NONMEM and WinBUGS.

1 Setup to run NONMEM through R

- NONMEM must be purchased from Globomax http://www.globomax.net/products/nonmem_software.cfm and setup following the included directions. To use the additional subroutines required to read the fixed and random population parameters you will need to use Visual Fortran as the Fortran compiler.
- Additional Required Subroutines and the NONMEM control file used in the examples are included in the `\nonmemAdd` directory in the package PKtools.
  - infnx5u.for
  - wrtab5msb.for
  - control.model3
  - control.model5
  - control.model6
- Place above subroutines and control files in the `C:\nmv\run` directory.
- The NMdata file as well as the tex or html files will be saved in this directory.

2 Setup to run WinBUGS through R

- `C:\Program Files\WinBUGS14\System\Rsrc`
  - copy the Registry.odc file and name the copy Registry_default.odc
- Create the directory `C:\bugsR`.
  - Place the txt file (theosw.txt) used in the examples in the `C:\bugsR` directory. theosw.txt is stored in `\bugsAdd` in the package PKtools.
  - The tex and html files will be saved in this directory.

3 Testing the NONMEM and WinBUGS

3.1 Testing the R to NONMEM interface

- Start R, at the command line type library(PKtools); example(RunNM)
- > library(PKtools); example(RunNM)
- R should return the following results.

```
Attaching package: 'PKtools'


        The following object(s) are masked from package:stats :

         cov


RunNM> if (.Platform$OS.type == "windows") {
    setwd("C:/nmv/run")
    data(Theoph)
    Theoph <- Theoph[Theoph$Time != 0, ]
    id <- as.numeric(as.character(Theoph$Subject))
    dose <- Theoph$Dose
    time <- Theoph$Time
    concblq <- round(sqrt(Theop .... [TRUNCATED]
object of class NONMEM
the objective function is:
[1] -237.92
the population parameters are:
          Estimate Standard Error
log(Ka)  0.3594780     0.40571700
log(V)  -0.7795500     0.10409500
log(Cl) -3.1984400     0.22354300
D[1,1]   0.4261940     0.74846700
D[1,2]  -0.0133228     0.04634360
D[2,2]   0.0140928     0.04371580
D[1,3]  -0.0195110     0.15941900
D[2,3]   0.0294696     0.05444040
D[3,3]   0.0617928     0.05697050
sigma^2  0.0285694     0.00423325
```

3.2 Testing the R to WinBUGS interface

- Start R, at the command line type library(PKtools); example(RunWB)
- > library(PKtools); example(RunWB)
- when WinBUGS is done, the WinBUGS Window.
- R should return the following results.

```
Attaching package: 'PKtools'


        The following object(s) are masked from package:stats :

         cov


RunWB> if (.Platform$OS.type == "windows") {
    setwd("C:/bugsR")
    library(nlme)
    data(Theoph)
    Theoph <- Theoph[Theoph$Time != 0, ]
    id <- as.numeric(as.character(Theoph$Subject))
    dose <- Theoph$Dose
    time  .... [TRUNCATED]
the population parameters are:

mu
[1]  0.3742185 -0.7791072 -3.2214135

D
             [,1]        [,2]        [,3]
[1,]  0.50127061 -0.01006574 -0.02083169
[2,] -0.01006574  0.03502918  0.03115066
[3,] -0.02083169  0.03115066  0.08390756

sigma2
[1] 0.02991828
>
```