Package compilation and basic run - current version 3.4

Emmanuelle Comets

15/06/2023

Compilation

First creation date: 02/02/2021

- structure
 - tests: removed all other folders and files except testthat from the package otherwise warnings about RDS files
 - data : removed remifentanil example from data folder
- roxygen documentation
 - warnings for ggplot (no visible global function definition)
 - added import command for pnorm (found in distribution plot) and median (found nowhere, so suspect it's the name median used in the ggplot plots, but added it all the same)
- package size: still 5.9 Mb so much too large for CRAN
 - the 3 simulated data files for warfarin and viral load data are all around 5Mb, consider making them available only on bookdown/website
- · necessary files
 - added a DESCRIPTION file
 - added a CHANGES file
- for compilation:
 - removed NAMESPACE
 - removed man pages
- Compilation steps from Build menu
 - Document => create NAMESPACE, DESCRIPTION (update collate directive), create man pages
 - Check => update documentation, create NAMESPACE

FINAL COMPILATION FOR CRAN

- removed documentation (too large)
- removed simwarfarineBase
- still over 5Mo but seems to be ok
- CRAN pre-test doesn't pass :-/
 - added importFrom for ggplot functions, also for gridExtra (grid.arrange) and grid
 - 'solved' problem by adding a dependency on rlang
 - * partially fixed with rlang
 - * workaround by defining global variables so check won't complain about them, but we need to use the .data systematically in ggplot aes() => Romain TODO
- March 2021
 - mail Fu (15/03): added again the option to save the output in autonpde (probably removed by Romain :-/)
- June 2023
 - fixed scatterplot when only one X-value (removed interpolation in this case as was causing the plot to fail)
 - note: the case when this happens within covsplit is **not fixed**

```
# Reduce size of viral load simulation data (to 500 simulations) for CRAN
if(FALSE) {
    cmd<-paste("mv ", file.path(workDir, "npde", "data", "simvirload.tab"), " ", file.path(workDir, "keep", "data", "keep", "keep", "data", "keep", "data", "keep", "data", "keep", "keep
    system(cmd)
    tab<-read.table(file.path(workDir, "npde", "data", "simvirload.tab"), header=TRUE)
    tab1<-tab[1:(dim(tab)[1]/2),]
    write.table(tab1, file.path(workDir, "npde", "data", "simvirload.tab"), quote=FALSE, row.names=FALSE, co
cmd<-paste("rm -r ",file.path(compilDir,"*"),sep="")</pre>
system(cmd)
dir.create(compilDir)
## Warning in dir.create(compilDir): '/home/eco/work/npde/compileNpde' existe déjà
dir.create(file.path(compilDir, "npde"))
dir.create(file.path(compilDir, "npde", "inst"))
# File too large
if(FALSE) {
    cmd<-paste("cp ", file.path(workDir,"latexDoc","userguide_3_3.pdf")," ", file.path(compilDir,"inst","</pre>
    system(cmd)
}
cmd<-paste("cp -rp ",file.path(workDir,"npde","R")," ", file.path(compilDir,"npde"),sep="")</pre>
system(cmd)
cmd<-paste("cp -rp ",file.path(workDir,"data")," ", file.path(compilDir,"npde"),sep="")</pre>
system(cmd)
for(ifile in c("CHANGES","DESCRIPTION")) {
    cmd<-paste("cp ",file.path(workDir,"keep",ifile)," ", file.path(compilDir,"npde"),sep="")</pre>
    system(cmd)
}
for(ifile in c("CITATION")) {
    cmd<-paste("cp ",file.path(workDir,"keep",ifile)," ", file.path(compilDir,"npde","inst"),sep="")</pre>
    system(cmd)
# cmd<-paste("cp ",file.path(workDir,"LICENSE")," ", file.path(compilDir,"inst"),sep="")
# system(cmd)
setwd(compilDir)
system("R CMD build npde")
system("R CMD check --as-cran --run-donttest npde_3.4.tar.gz")
```

npde 3.1 Apres correction, la compilation du package passe sans erreurs et avec 2 notes restantes.

- notes
 - previous version archived
 - package size too large (recommended size less than 5Mb): reduce nb of simulations for warfarin?
 - ggplot variables (rien a faire pour ça)
- warnings corriges
 - jeux de donnees non documentes: removed remifentanil, added virload documentation (used to be a specific man page, reintegrated them into roxygen format in npde.R like warfarin)
 - duplicated alias: fixed!

npde 3.2, 3.3

notes

- time to run examples Examples with CPU or elapsed time $>5 \mathrm{s}$ user system elapsed npde.cens.method 7.51 0.019 7.605

Warnings

- ggplot warnings
 - solved in npde 3.0 by adding global variables (horrible)
 - * in 3.3, tried to add .data\$ to all the ggplot functions
 - can't remove the .x because of scales

Undefined global functions or variables:

.x X2.5. X50. X97.5. Y0.025 Y0.025.1 Y0.5 Y0.5.1 Y0.975 Y0.975.1 aes annotation_logticks category coord_cartesian coord_flip element_blank element_line element_rect element_text expand_limits facet_wrap geom_bar geom_boxplot geom_crossbar geom_hline geom_line geom_point geom_ribbon ggplot ggtitle gpar grid.arrange group grp guides labs lower name obs.inf obs.median obs.sup pinf.lower pinf.median pinf.upper pmid.lower pmid.median pmid.upper psup.lower psup.median psup.upper scale_fill_manual scale_x_continuous scale_x_discrete scale_x_log10 scale_y_continuous scale_y_log10 textGrob theme upper value x x1 x2 x_area_0.25 x_area_0.5 x_area_0.975 xcent y y1 y2 y_area_0.25 y_area_0.5 y_area_0.975

• Warnings in first compilation (solved)

```
checking Rd metadata ...
 Rd files with duplicated alias 'aux.npdeplot.computepi':
   'npde.plot.default.Rd' 'npde.plot.scatterplot.Rd'
 Rd files with duplicated alias 'compute.bands':
   'npde.plot.default.Rd' 'npde.plot.scatterplot.Rd'
 Rd files with duplicated alias 'compute.bands.true':
   'npde.plot.default.Rd' 'npde.plot.scatterplot.Rd'
 Rd files with duplicated alias 'npde':
   'npde-package.Rd' 'npde.Rd'
checking for missing documentation entries (346ms)
 Undocumented code objects:
   'remifent' 'simremifent' 'simremifent_base' 'simvirload' 'virload'
   'virload20' 'virload50' 'virloadMDV20'
 Undocumented data sets:
   'remifent' 'simremifent' 'simremifent base' 'simvirload' 'virload'
   'virload20', 'virload50', 'virloadMDV20',
 All user-level objects in a package should have documentation entries.
 See chapter 'Writing R documentation files' in the 'Writing R
 Extensions' manual.
```

Install package in development mode

```
dev_mode() # development mode

## v Dev mode: ON
install.packages(pkgs=file.path(compilDir,"npde_3.4.tar.gz"),repos=NULL)

## Installation du package dans '/home/eco/R-dev'
## (car 'lib' n'est pas spécifié)
```

```
library(npde)
library(ggplot2)
library(gridExtra)
library(mclust)

## Package 'mclust' version 6.0.0

## Type 'citation("mclust")' for citing this R package in publications.
library(testthat)

##

## Attachement du package : 'testthat'

##

## L'objet suivant est masqué depuis 'package:devtools':

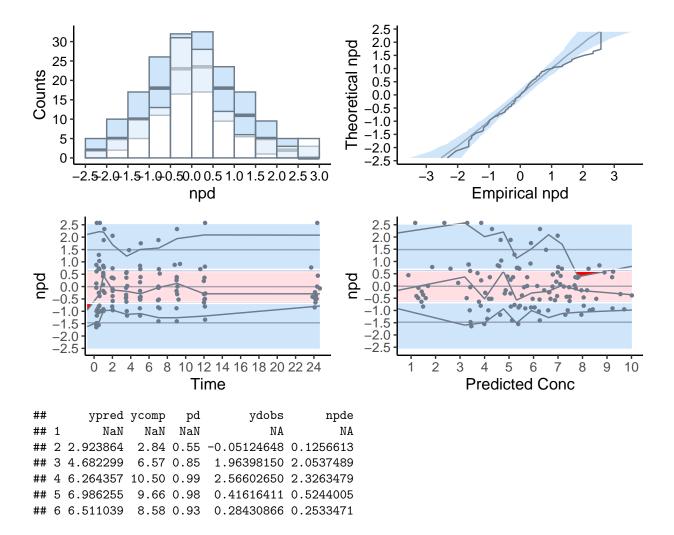
##

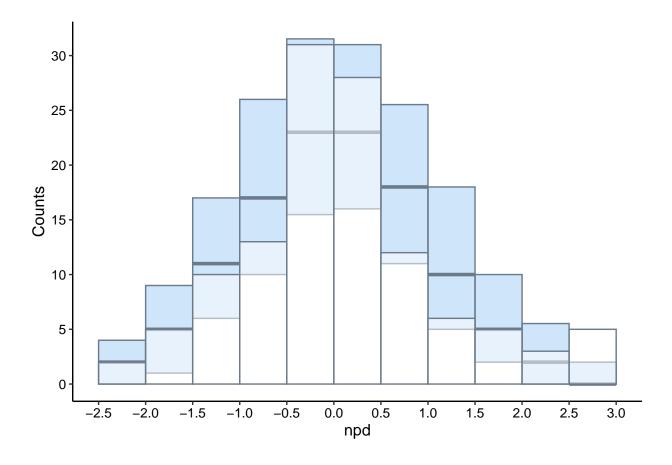
## test_file
library(grid)
```

Theophylline

- computation of npde and npd
- default plots

```
## -----
## Distribution of npde :
## nb of obs: 120
          mean= 0.0668 (SE= 0.095)
##
      variance= 1.074 (SE= 0.14)
##
##
      skewness= 0.511
      kurtosis= 0.2912
## Statistical tests (adjusted p-values):
## t-test : 1
## Fisher variance test : 1
  SW test of normality : 0.00819 **
##
##
   Global test
               : 0.00819 **
## ---
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
```



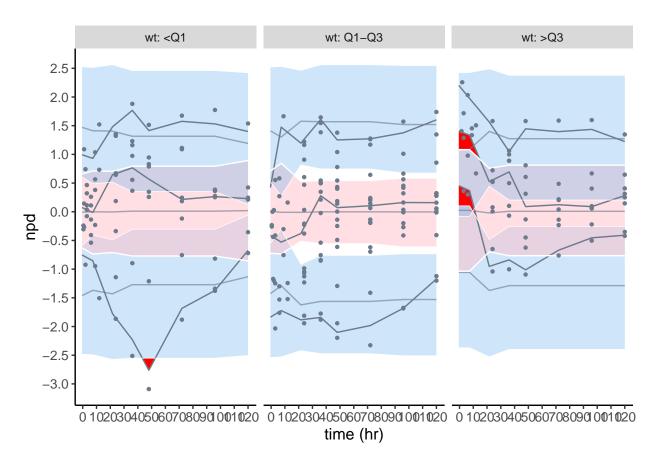


Warfarin

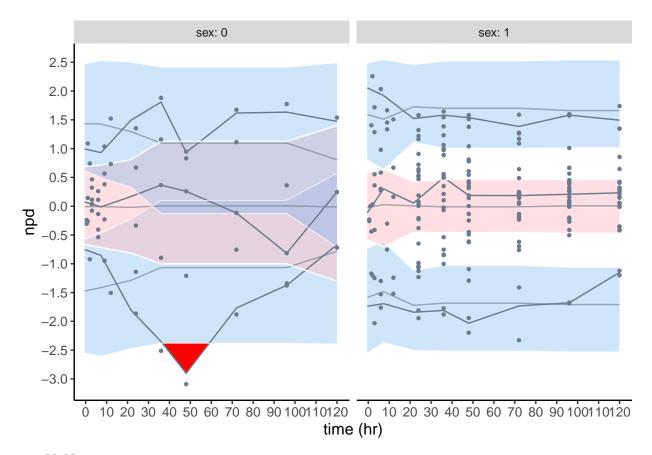
```
• covariate plots
```

```
\bullet reference profiles
```

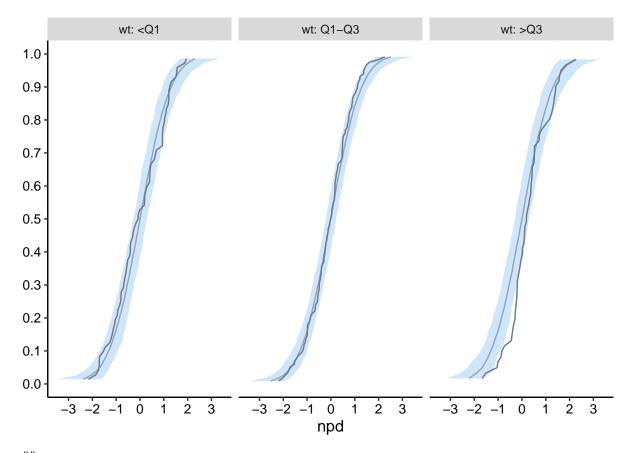
```
## Distribution of npde :
##
        nb of obs: 247
                             (SE= 0.059)
##
             mean = 0.02928
##
         variance= 0.8549
                            (SE= 0.077)
##
         skewness= -0.07211
##
         kurtosis= -0.4172
## Statistical tests (adjusted p-values):
    t-test
##
##
    Fisher variance test : 0.288
##
    SW test of normality : 1
##
    Global test
                          : 0.288
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
## [[1]]
```



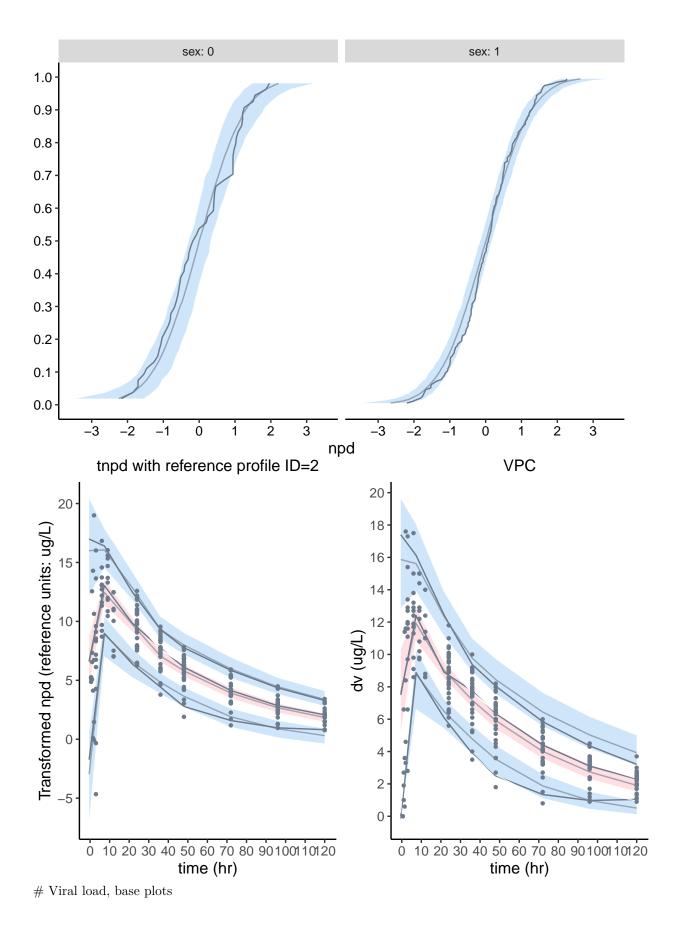
[[2]]



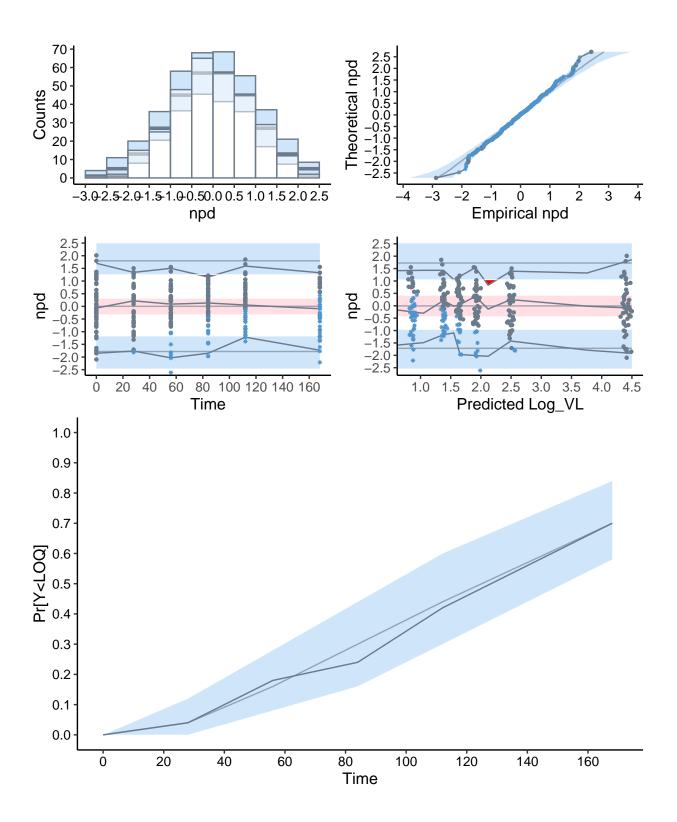
[[1]]

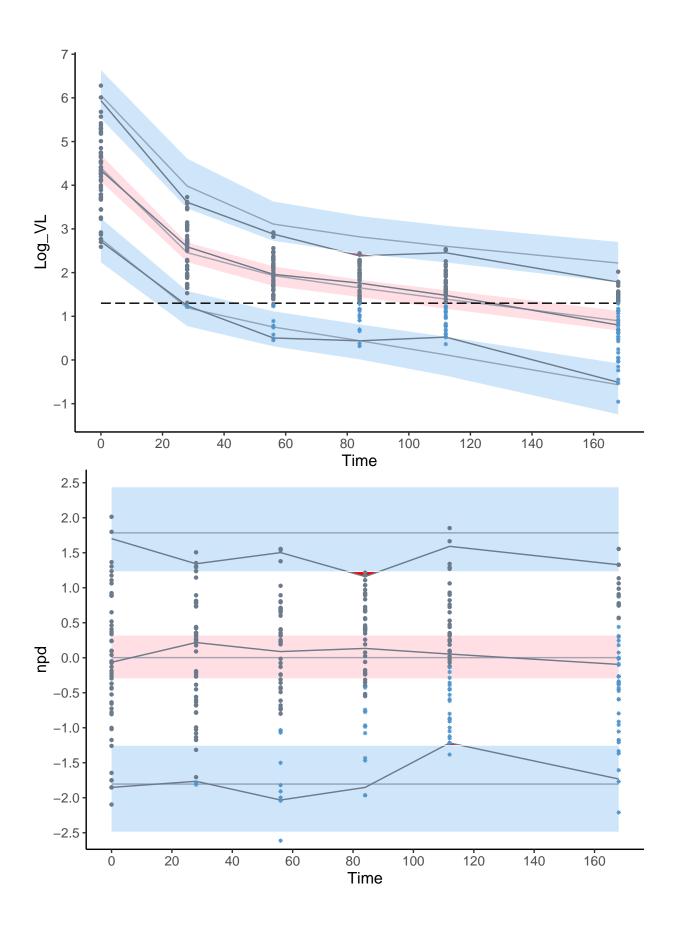


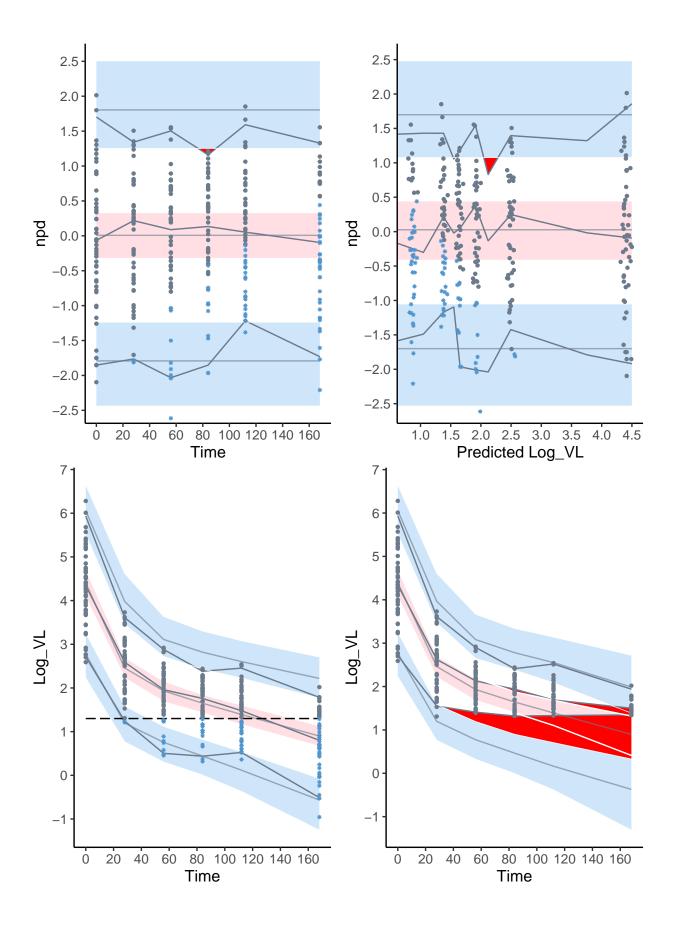
[[2]]



```
## Distribution of npde :
  nb of obs: 300
##
        mean= -0.008692 (SE= 0.052)
##
      variance= 0.824 (SE= 0.067)
##
      skewness= -0.04594
      kurtosis= -0.244
## -----
## Statistical tests (adjusted p-values):
## t-test
           : 1
## Fisher variance test : 0.0704 .
## SW test of normality : 1
## Global test
            : 0.0704 .
## ---
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
## -----
## -----
## Distribution of npde :
     nb of obs: 221
##
##
         mean= 0.09917 (SE= 0.062)
##
     variance= 0.8611 (SE= 0.082)
      skewness= -0.1174
##
      kurtosis= -0.1955
## -----
## Statistical tests (adjusted p-values):
## t-test
                   : 0.341
  Fisher variance test : 0.402
##
  SW test of normality : 1
##
## Global test
             : 0.341
## ---
## Signif. codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
## -----
```







End of file, deactivating development mode

v Dev mode: OFF

Bugs to sort

Sort out covariate plots

There were two functions with almost the same name - npde.plot.covariates: regular plots split by covariates, only for x, pred, ecdf => renamed to npde.plot.splitcov and added options hist and qqplot - do we need those subplots, or maybe just simplify call to function (use covsplit and capture arguments instead of using which.plot) - npde.plot.covariate: covariate plots as in Brendel => kept as is

plot.NpdeRes (dans plotNpde-methods.R)

- Romain TODO: la fonction devrait prendre un objet NpdeRes et pas un objet NpdeObject (NpdeRes n'a pas d'element data, c'est juste le slot res d'un element NpdeObject !!!)
 - il faut lui donner des defauts pour xlab, ylab (et la possiblite de passer outre en passant des arguments en ...)
 - normalement il doit y avoir l'equivalent de xobs dans le dataframe res de l'objet
 - pas sure qu'on ait not.miss mais dans ce cas le reconstruire (a tester +++)
 - il n'y a pas de liste plot.opt donc prendre des defauts dans set.default.options()
- faire un test that pour verifier que cette fonction marche par elle-meme (use test that for class to generate an object npdeData and plot it)

plot.NpdeData (dans plotNpde-methods.R)

• Romain TODO: faire un testthat pour veeifier que la fonction et les options passent (use testthat for class to generate an object npdeData and plot it)