Package compilation and basic run

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Compilation

- 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 :-/)

```
# 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 system(cmd)
   tab<-read.table(file.path(workDir,"npde","data","simvirload.tab"), header=TRUE)
   tabl<-tab[1:(dim(tab)[1]/2),]
   write.table(tab1, file.path(workDir,"npde","data","simvirload.tab"), quote=FALSE, row.names=FALSE, co</pre>
```

```
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","
  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_3.3.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 $>5 \rm s$ user system elapsed npde.cens.method 7.51 0.019 7.605

Warnings

• ggplot warnings

```
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'
W 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_3.3.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)

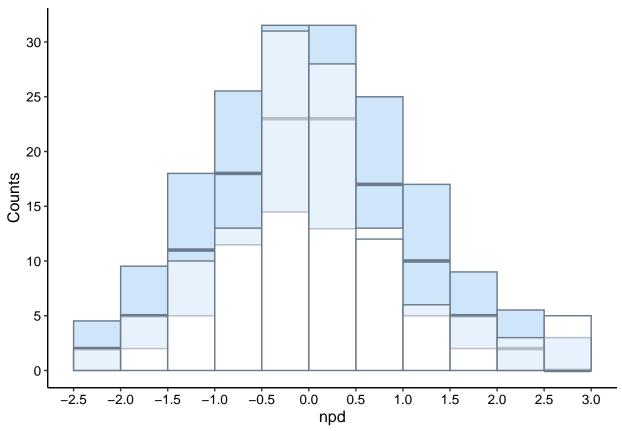
```
## Attachement du package : 'testthat'
##
## L'objet suivant est masqué depuis 'package:devtools':
##
## test_file
library(grid)
```

Theophylline

- computation of npde and npd
- default plots

```
## Distribution of npde :
##
          nb of obs: 120
##
                 mean = 0.0668
                                    (SE= 0.095)
                                  (SE= 0.14)
##
            variance= 1.074
##
            skewness= 0.511
##
            kurtosis= 0.2912
##
##
   Statistical tests (adjusted p-values):
##
##
      Fisher variance test : 1
##
      SW test of normality : 0.00819 **
      Global test
                                 : 0.00819 **
##
##
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
                                                            2.5
   30
                                                            2.0
                                                       Theoretical npd
   25
                                                            1.0
Counts
   20
                                                           0.5
                                                           0.0
   15
                                                           -0.5
                                                          -1.0
-1.5
-2.0
   10
    5
                                                           -2.5
                                                                                     ò
       -2.5-2.0-1.5-1.0-0.50.0 0.5 1.0 1.5 2.0 2.5 3.0
                                                                    -3
                                                                                                2
                                                                                                      3
                                                                              Empirical npd
                           npd
                                                            2.5
2.0
1.5
   2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
                                                            1.0
                                                          0.5
0.0
-0.5
                                                          -1.0
-1.5
                                                          -2.0
-2.5
                   6 8 10 12 14 16 18 20 22 24
                                                                      2
                                                                                                8
             2
                4
                                                                           3
                                                                                    5
                                                                                        6
                                                                                                     9
                                                                                                        10
                            Time
                                                                            Predicted Conc
##
         ypred ycomp
                           pd
                                      ydobs
                                                   npde
```

```
## 1 NaN NaN NaN NA NA
## 2 2.923864 2.84 0.55 -0.05124648 0.1256613
## 3 4.682299 6.57 0.85 1.96398150 2.0537489
## 4 6.264357 10.50 0.99 2.56602650 2.3263479
## 5 6.986255 9.66 0.98 0.41616411 0.5244005
## 6 6.511039 8.58 0.93 0.28430866 0.2533471
```



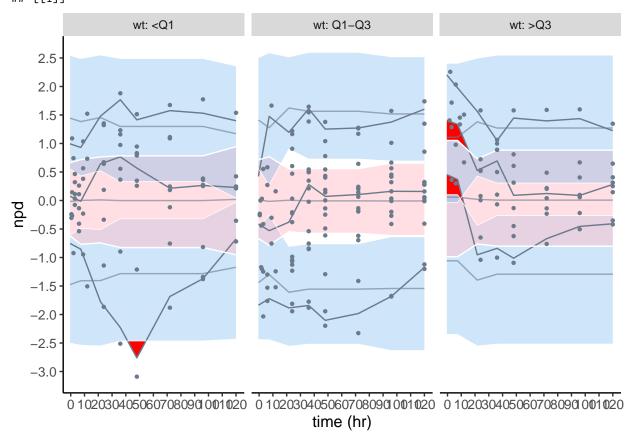
Warfarin

```
• covariate plots
```

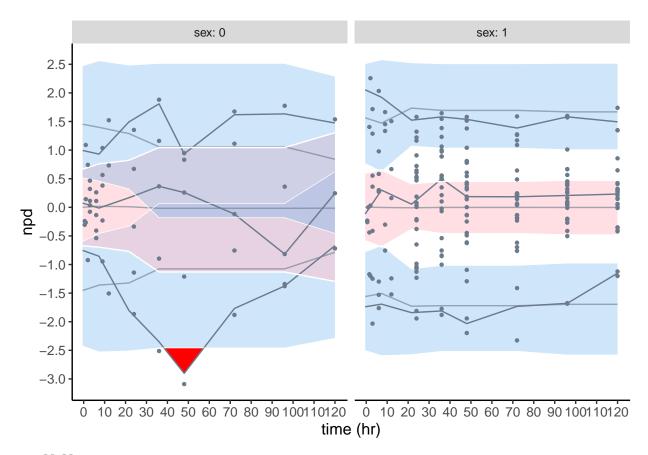
• reference profiles

```
## Distribution of npde :
        nb of obs: 247
##
##
              mean = 0.02928
                              (SE = 0.059)
##
          variance= 0.8549
                             (SE= 0.077)
##
          skewness= -0.07211
##
         kurtosis = -0.4172
##
## Statistical tests (adjusted p-values):
                           : 1
##
     Fisher variance test : 0.288
     SW test of normality : 1
##
     Global test
                           : 0.288
## ---
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
```

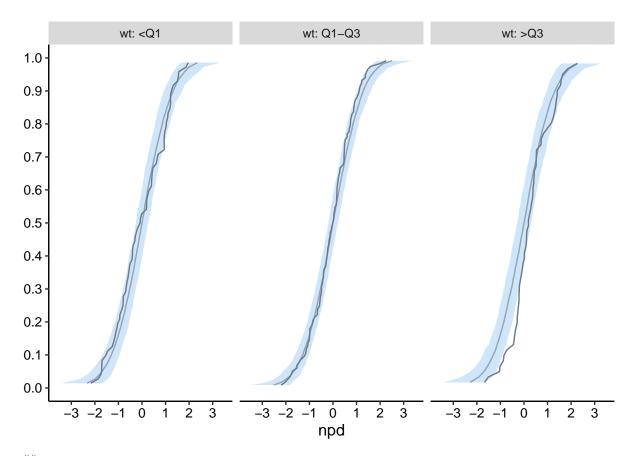
[[1]]



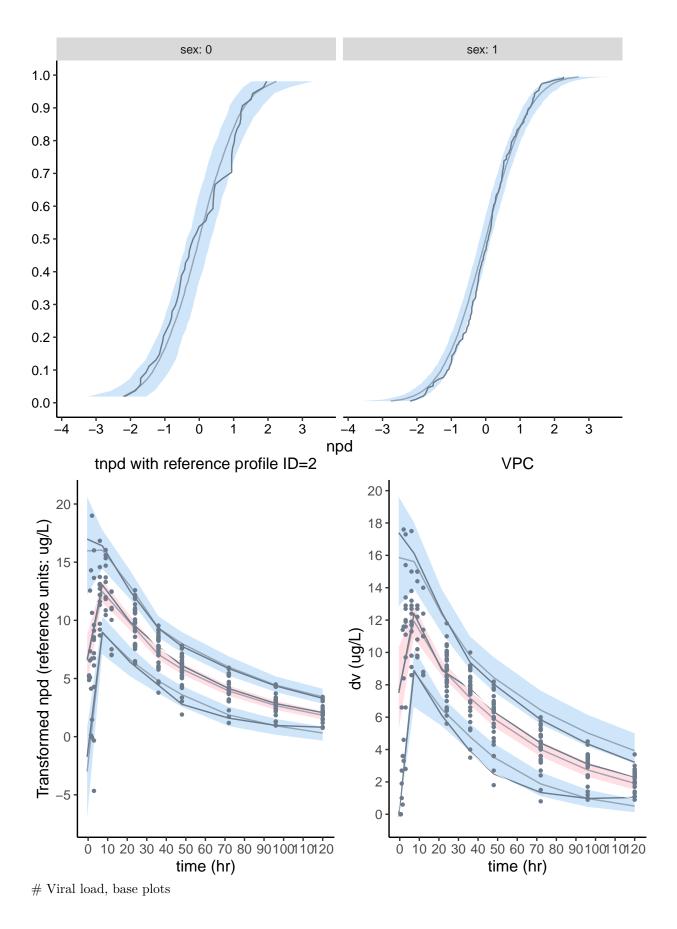
[[2]]



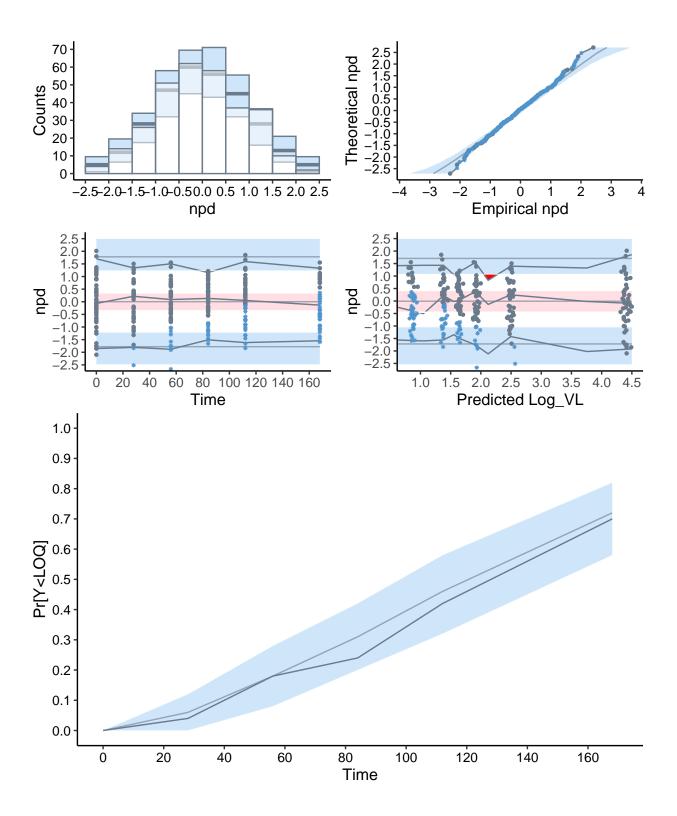
[[1]]

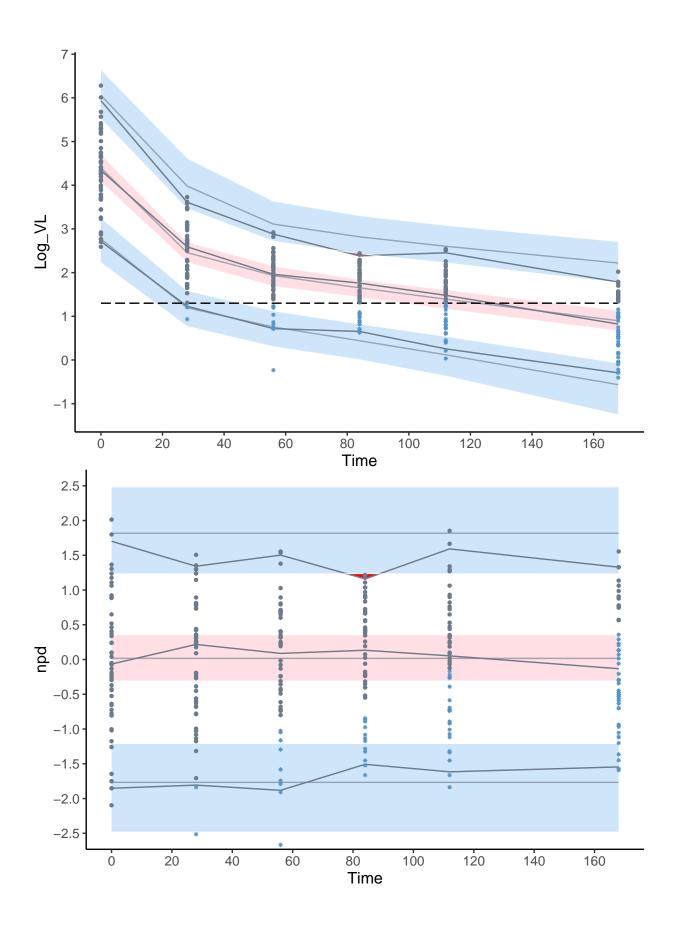


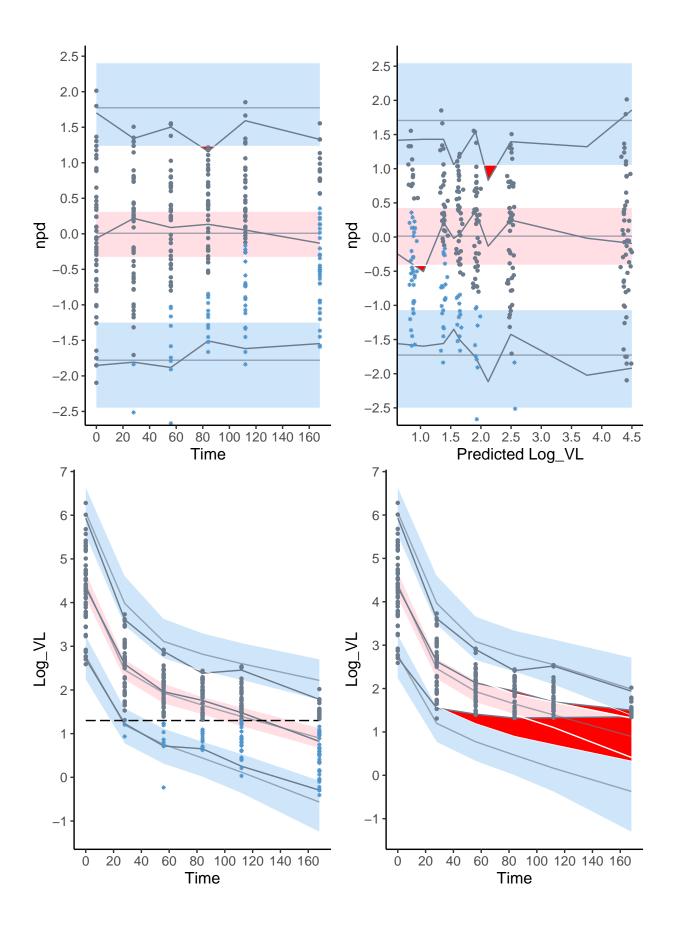
[[2]]



```
## Distribution of npde :
  nb of obs: 300
##
       mean= -0.02569 (SE= 0.053)
      variance= 0.8335 (SE= 0.068)
##
##
      skewness= 0.01504
      kurtosis= -0.4413
## -----
## Statistical tests (adjusted p-values):
## t-test
           : 1
## Fisher variance test : 0.0986 .
## SW test of normality : 1
## Global test
            : 0.0986 .
## ---
## 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)