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

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

```
setwd(file.path(workDir, "npde"))
system("rm man/*")
cmd<-paste("cp ", file.path(workDir,"latexDoc","userguide_3_0.pdf")," ", file.path(workDir,"userguide_n</pre>
devtools::document()
## Updating npde documentation
## Loading npde
## Loading required package: gridExtra
## Loading required package: ggplot2
## Loading required package: grid
## Writing NAMESPACE
## Writing NAMESPACE
## Writing NpdeSimData-class.Rd
## Writing extract-methods.Rd
## Writing NpdeData-class.Rd
## Writing read.Rd
## Writing show.Rd
## Writing npdeData.Rd
## Writing npdeSimData.Rd
## Writing print.NpdeData.Rd
## Writing showall.Rd
## Writing summary.NpdeData.Rd
## Writing subset.NpdeData.Rd
## Writing NpdeRes-class.Rd
## Writing kurtosis.Rd
## Writing skewness.Rd
## Writing gof.test.Rd
## Writing NpdeObject-class.Rd
## Writing dist.pred.sim.Rd
## Writing computenpde.Rd
## Writing npde.decorr.method.Rd
## Writing computepd.Rd
## Writing compute.ploq.Rd
## Writing autonpde.Rd
## Writing pdemenu.Rd
## Writing npde.main.Rd
## Writing npde.save.Rd
## Writing npde.graphs.Rd
## Writing npde-package.Rd
## Writing theopp.Rd
## Writing simtheopp.Rd
## Writing warfarin.Rd
## Writing virload.Rd
## Writing npde.cens.method.Rd
## Writing npdeControl.Rd
## Writing set.plotoptions.Rd
## Writing replace.plotoptions.Rd
## Writing npde.binning.Rd
## Writing npde.plot.covariate.Rd
## Writing npde.plot.dist.Rd
```

```
## Writing npde.plot.log.Rd
## Writing plot.NpdeData.Rd
## Writing plot.NpdeRes.Rd
## Writing plot.NpdeObject.Rd
## Writing npde.plot.select.Rd
## Writing default.npde.plots.Rd
## Writing npde.plot.splitcov.Rd
## Writing npde.plot.npde.Rd
## Writing npde.plot.data.Rd
## Writing npde.plot.default.Rd
## Writing npde.plot.scatterplot.Rd
roxygenise()
## Loading npde
## Writing NAMESPACE
## Writing NAMESPACE
setwd(workDir)
system("R CMD build npde")
system("R CMD check --as-cran --run-donttest npde_3.0.tar.gz")
```

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!

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)

```
W 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 Rd line widths ...
  checking Rd cross-references ...
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
## Dev mode: ON
install.packages(pkgs=file.path(workDir,"npde_3.0.tar.gz"),repos=NULL)
## Installing package into '/home/eco/R-dev'
## (as 'lib' is unspecified)
library(npde)
library(ggplot2)
library(gridExtra)
library(mclust)
## Package 'mclust' version 5.4.6
## Type 'citation("mclust")' for citing this R package in publications.
library(testthat)
##
## Attaching package: 'testthat'
## The following object is masked from 'package:devtools':
##
##
       test_file
library(grid)
```

Theophylline

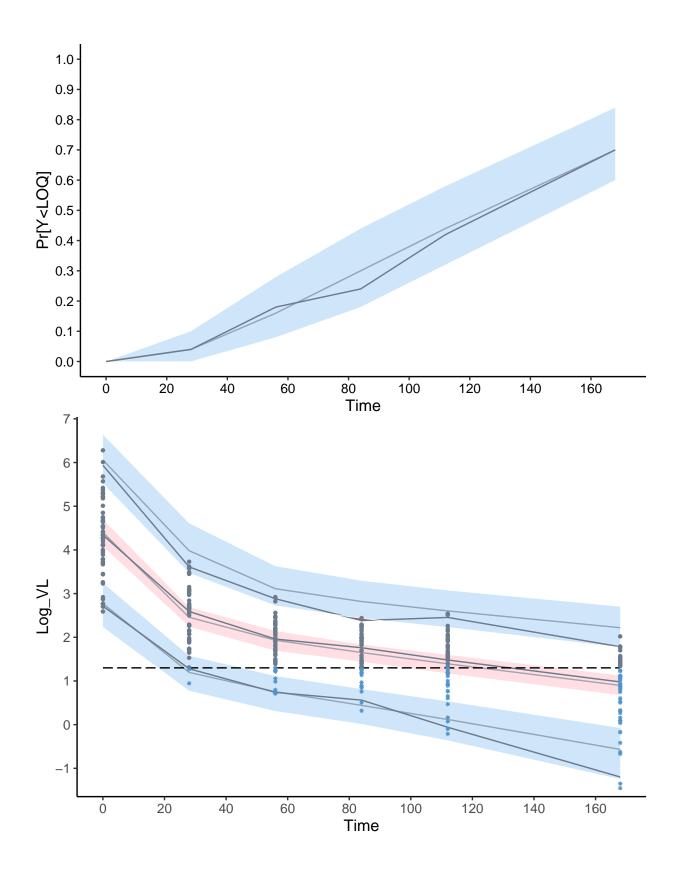
```
## ------
## Distribution of npde :
## nb of obs: 120
## mean= 0.0668 (SE= 0.095 )
```

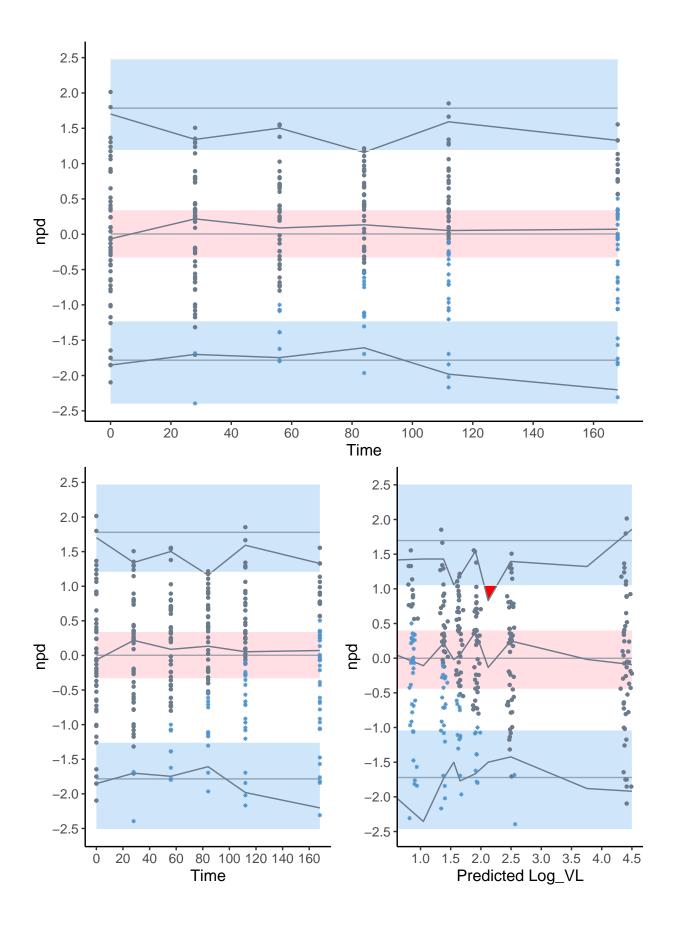
```
variance= 1.074 (SE= 0.14)
##
##
           skewness= 0.511
##
           kurtosis= 0.2912
##
##
   Statistical tests (adjusted p-values):
     t-test
##
     Fisher variance test : 1
##
     SW test of normality : 0.00819 **
##
##
     Global test
                              : 0.00819 **
##
## Signif. codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
                                                      2.5 -
   30
                                                      2.0
                                                 Theoretical npd
   25
                                                      1.0
Counts
   20
                                                      0.5
                                                      0.0
   15
                                                     -0.5
   10
                                                    -1.0
-1.5
    5
                                                     -2.0
                                                     -2.5
      -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
                                                                            0
                                                                                            3
                                                                      Empirical npd
                         npd
    2.5
2.0
1.5
1.0
                                                      2.5
2.0
                                                      1.5
                                                      1.0
    0.5
                                                      0.5
0.5
0.0
0.0
                                                     0.0
   -0.5
-1.0
-1.5
                                                     -0.5
                                                     -1.0
                                                     -1.5
   -2.0
                                                     -2.0
   -2.5·
                                                     -2.5
              4 6 8 10 12 14 16 18 20 22 24
                                                               2
                                                                                              10
                                                            1
                         Time
                                                                     Predicted Conc
##
        ypred ycomp
                       pd
                                  ydobs
                                              npde
                                                         tnpde
          {\tt NaN}
                 NaN NaN
                                     NA
                                                NA
                2.84 0.55 -0.05124648 0.1256613 5.403817
## 2 2.923864
## 3 4.682299 6.57 0.85 1.96398150 2.0537489 11.302178
## 4 6.264357 10.50 0.99
                            2.56602650 2.3263479 12.136107
## 5 6.986255 9.66 0.98 0.41616411 0.5244005 6.623631
## 6 6.511039 8.58 0.93 0.28430866 0.2533471 5.794430
```

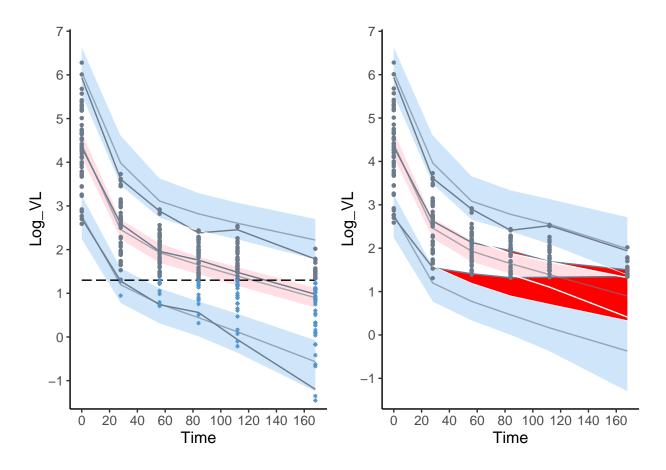
Viral load, base plots

```
## -----
## Distribution of npde :
## nb of obs: 300
## mean= -0.009306 (SE= 0.055 )
## variance= 0.8981 (SE= 0.073 )
## skewness= -0.1034
```

```
kurtosis= -0.1956
## Statistical tests (adjusted p-values):
     t-test : 1
##
##
     Fisher variance test : 0.619
##
     SW test of normality : 1
     Global test : 0.619
## ---
## 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 '**' 0.05 '.' 0.1
   70
                                                   2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
                                                Theoretical npd
  60
20
   10
                                                   -2.0
-2.5
    0
      -3.0-2.5-2.0-1.5-1.0-0.50.0 0.5 1.0 1.5 2.0 2.5
                                                            -3
                                                                           Ò
                                                                    Empirical npd
                        npd
    2.5 -
2.0 -
1.5 -
    1.0-
                                                    1.0
  0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
                                                   0.5
0.0
-0.5
                                                   -1.0
                                                   -1.5
                                                   -2.5
            20 40 60 80 100 120 140 160
                                                          1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5
                                                                  Predicted Log_VL
                        Time
```







End of file, deactivating development mode

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 test that pour veeifier que la fonction et les options passent (use test that for class to generate an object npdeData and plot it)