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)
  tab1<-tab[1:(dim(tab)[1]/2),]</pre>
```

```
write.table(tab1, file.path(workDir, "npde", "data", "simvirload.tab"), quote=FALSE, row.names=FALSE, co
}
setwd(file.path(workDir, "npde"))
system("rm man/*")
cmd<-paste("cp ", file.path(workDir,"latexDoc","userguide_3_1.pdf")," ", file.path(workDir,"userguide_n</pre>
system(cmd)
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.loq.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_3.1.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_3.1.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)
```

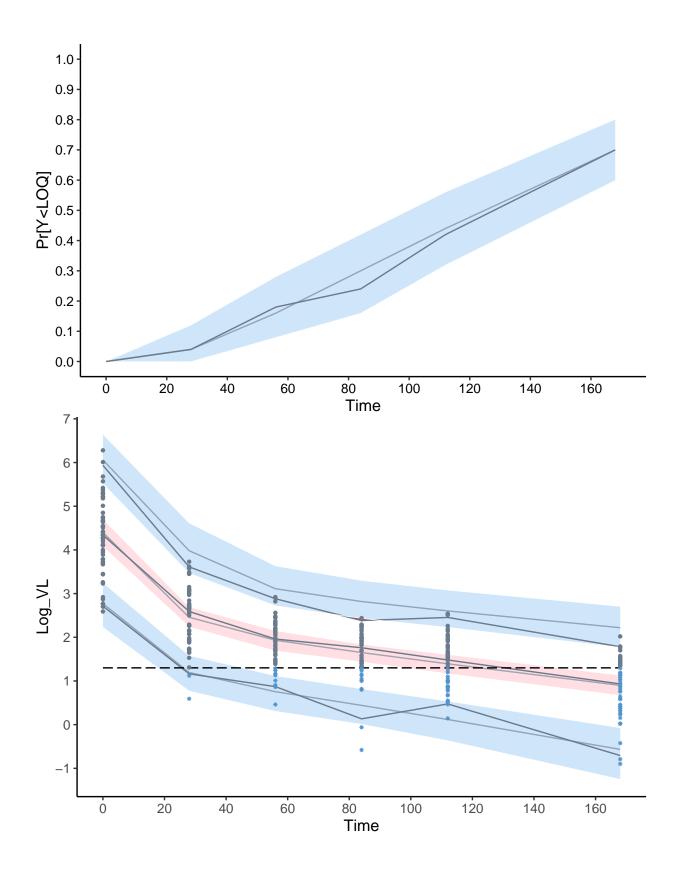
Theophylline

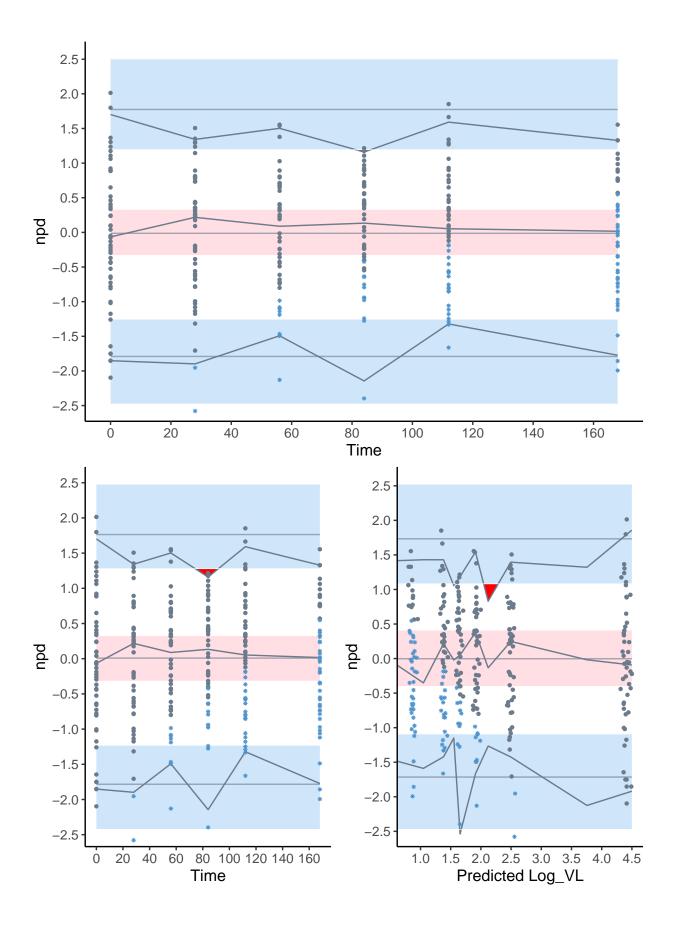
```
## Distribution of npde :
##
          nb of obs: 120
##
               mean = 0.0668
                                (SE = 0.095)
                               (SE= 0.14)
##
           variance= 1.074
##
           skewness= 0.511
##
           kurtosis= 0.2912
   Statistical tests (adjusted p-values):
##
     t-test
                              : 1
     Fisher variance test : 1
##
     SW test of normality : 0.00819 **
##
     Global test
                              : 0.00819 **
##
## Signif. codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
                                                       2.5 -
   30
                                                       2.0
                                                  Theoretical npd
                                                       1.5
   25
                                                       1.0
Counts 15 10
                                                       0.5
                                                       0.0
                                                      -0.5
   10
                                                      -1.0
-1.5
    5
                                                      -2.0
    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
                                                                              Ò
                                                                       Empirical npd
                         npd
    2.5
                                                       2.5
2.0
1.5
    1.5
1.0
                                                       1.0
                                                      0.5
0.0
-0.5
-1.0
    0.5
   0.0
-0.5
   -1.0
   -1.5
                                                      -1.5
   -2.0
-2.5
                                                      -2.0
-2.5
                    8 10 12 14 16 18 20 22 24
                  6
                                                                 2
                                                                     3
                                                                                               10
                                                                                            9
                         Time
                                                                      Predicted Conc
##
        ypred ycomp
                        pd
                                   ydobs
                                               npde
                 NaN NaN
## 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
```

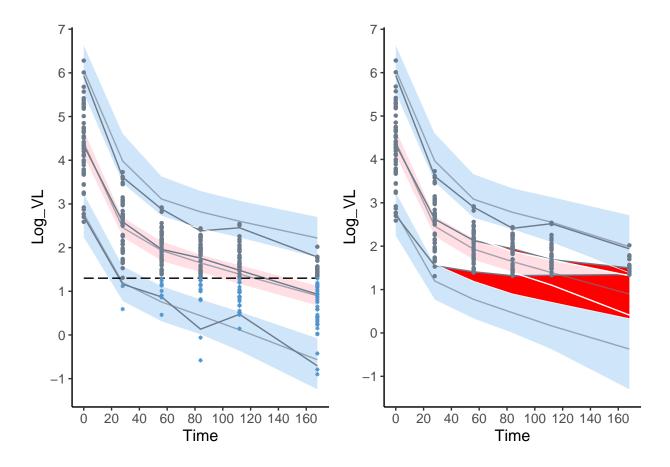
Viral load, base plots

```
## ------
## Distribution of npde :
## nb of obs: 300
```

```
##
                mean = -0.01476 (SE= 0.053)
##
           variance= 0.8387 (SE= 0.069)
##
           skewness = -0.04585
           kurtosis= 0.2535
##
   Statistical tests (adjusted p-values):
                 : 1
     t-test
     Fisher variance test : 0.118
##
     SW test of normality : 1
##
     Global test
##
                              : 0.118
## Signif. codes: '***' 0.001 '**' 0.05 '.' 0.1
##
   Distribution of npde :
          nb of obs: 221
##
                                 (SE= 0.062 )
##
                mean = 0.09917
           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
   70
                                                     2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
                                                  Theoretical npd
   60
   50
Counts
   40
   30
   20
   10
             .
–2
                                                                   <u>-2</u>
                                                                            Ö
                                                                                       2
                               1
                                                              -3
                                                                        -1
                   -1
                         0
                         npd
                                                                       Empirical npd
                                                       2.5
2.0
1.5
   2.5
2.0
1.5
1.0
0.5
-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
                                                                       2.0 2.5 3.0 3.5 4.0 4.5
             20
                40 60 80 100 120 140 160
                                                             1.0 1.5
                                                                    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)