ddsPLS Exploration

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```
library(ddsPLS2)
library(MASS)
library(spls)
ddsPLS2::ddsPLS2_App()
```

This code chunk opens an applet that can be used to build models using ddsPLS. Note that it requires the X and Y variables as separate csv files.

Code copied from the simulation ssdpls2 repository created by Hadrien Lorenzo.

The get_toy_example() function simulates a data frame with n observations of where 50 of p predictors are associated with the single response variable.

```
# Creates a toy data set for the ddsPLS function
toy_ex <- get_toy_example()

# Creates model from the toy data
toy_mod <- ddsPLS(toy_ex$X, toy_ex$Y)

toy_results <- toy_mod$results</pre>
```

Recreate Toy Example

This is a recreation of the toy example created by Hadrien Lorenzo, the original example can be found here.

doBoot = FALSE,

```
criterion = "Q2",
  lambdas = lambdas,
  n_B = n_B,
  verbose = T # whether trace during process
)
```

Design 1

Generates n samples of p observations with q response variables. Projects 5 latent variables onto p components.

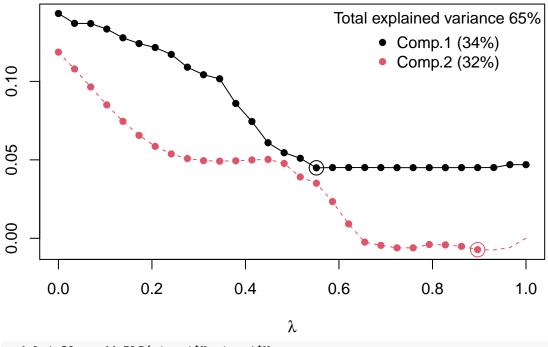
```
simu_1 \leftarrow get_design_1(n=50, sqrt_1_minus_sig2 = 0.99, p = 1000, q = 3)
```

What does the NCORES argument do? Setting it to integers greater than 1 gives an error.

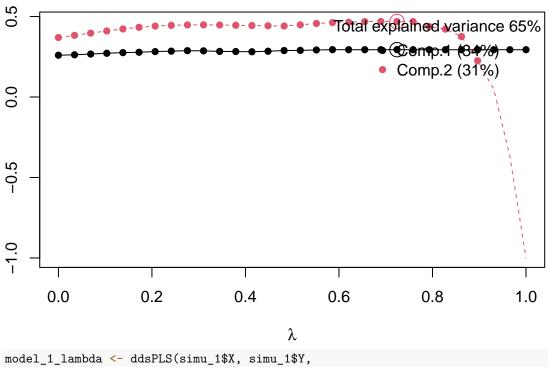
Is there a way to include more components in the model?

```
##
##
                           ddsPLS
##
  Should we build component 1 ? Bootstrap pending...
##
       lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
         0.55 0.35 0.35 0.3 0.3
                                  34%
##
                                     ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
       lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.9 0.4 0.12 0.41 0.27
##
                                   32%
##
                                     ...component 2 built!
## Should we build component 3 ? Bootstrap pending...
                                 ...component 3 not built!
                                     ===========
##
  ##
                      ==========
```

$\overline{R}_B^2\!-\!\overline{Q}_B^2$

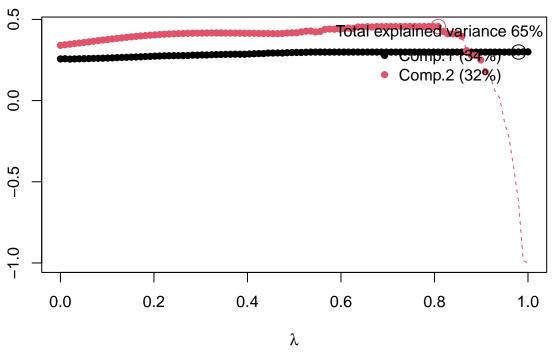


```
##
##
                             {\tt ddsPLS}
##
   Should we build component 1 ? Bootstrap pending...
##
                 R2 R2h
                           Q2 Q2h VarExpl VarExpl.Tot
##
          0.72 0.34 0.34 0.29 0.29
                                        34%
##
                                         ...component 1 built!
   Should we build component 2 ? Bootstrap pending...
##
##
        lambda R2 R2h
                          Q2 Q2h VarExpl VarExpl.Tot
          0.72 0.63 0.29 0.63 0.47
##
                                        31%
                                                    65%
##
                                         ...component 2 built!
   Should we build component 3 ? Bootstrap pending...
                                     ...component 3 not built!
##
```



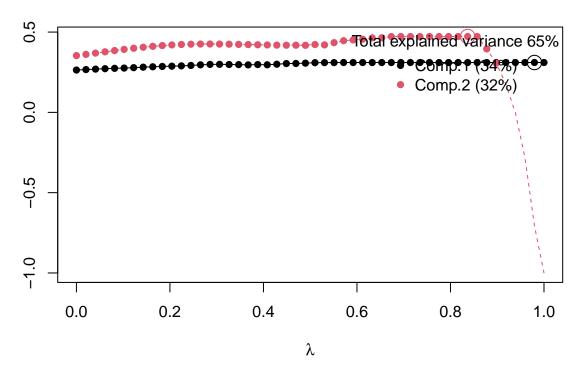
```
##
##
                             ddsPLS
  Should we build component 1 ? Bootstrap pending...
##
##
               R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.98 0.34 0.34 0.3 0.3
                                     34%
##
                                        ...component 1 built!
##
   Should we build component 2 ? Bootstrap pending...
##
        lambda R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
          0.81 0.64 0.3 0.62 0.46
                                      32%
##
                                                  65%
##
                                        ...component 2 built!
   Should we build component 3 ? Bootstrap pending...
##
                                    ...component 3 not built!
##
##
```





```
##
##
                             ddsPLS
##
  Should we build component 1 ? Bootstrap pending...
##
               R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
##
          0.98 0.33 0.33 0.31 0.31
                                       34%
                                                   34%
##
                                        ...component 1 built!
##
   Should we build component 2 ? Bootstrap pending...
##
        lambda R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
          0.84 0.63 0.29 0.63 0.47
##
                                       32%
                                                   65%
##
                                        ...component 2 built!
   Should we build component 3 ? Bootstrap pending...
                                    ...component 3 not built!
##
```



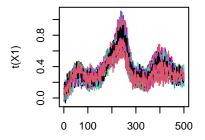


Different Simulations of Design 1 Data

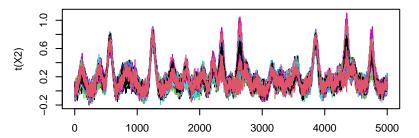
There is a problem with get_design_1, q cannot take values other than 5.

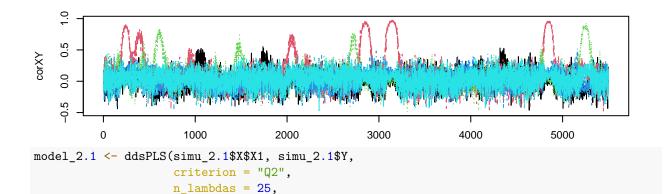
Design 2

```
simu_2.1 <- get_design_2(plot = T)
```



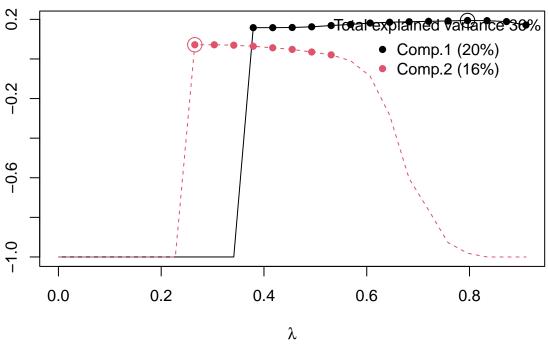
##





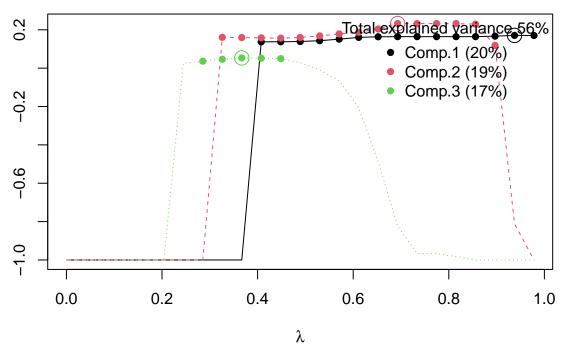
```
##
##
                            ddsPLS
##
##
  Should we build component 1 ? Bootstrap pending...
                          Q2 Q2h VarExpl VarExpl.Tot
                R2 R2h
##
##
          0.8 0.19 0.19 0.19 0.19
                                     20%
##
                                       ...component 1 built!
##
  Should we build component 2 ? Bootstrap pending...
       lambda R2 R2h
                        Q2 Q2h VarExpl VarExpl.Tot
##
         0.27 0.4 0.2 0.24 0.07
##
                                    16%
                                               36%
##
                                       ...component 2 built!
##
  Should we build component 3 ? Bootstrap pending...
                                   ...component 3 not built!
##
```

verbose = TRUE)

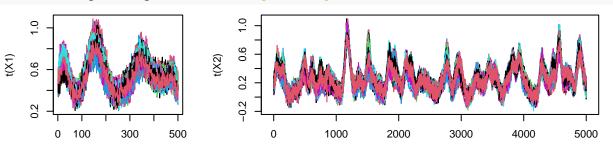


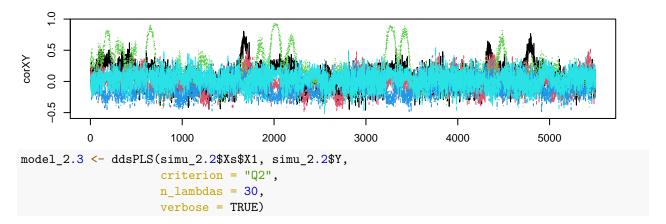
```
##
##
                             ddsPLS
   Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
##
          0.94 0.2 0.2 0.17 0.17
                                                  20%
##
                                        ...component 1 built!
   Should we build component 2 ? Bootstrap pending...
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
##
          0.69 0.38 0.19 0.38 0.23
                                       19%
##
                                         ...component 2 built!
##
   Should we build component 3 ? Bootstrap pending...
        lambda
                 R2 R2h
                           Q2 Q2h VarExpl VarExpl.Tot
##
##
          0.37 0.57 0.19 0.39 0.05
                                       17%
##
                                        ...component 3 built!
  Should we build component 4 ? Bootstrap pending...
##
                                    ...component 4 not built!
##
##
```





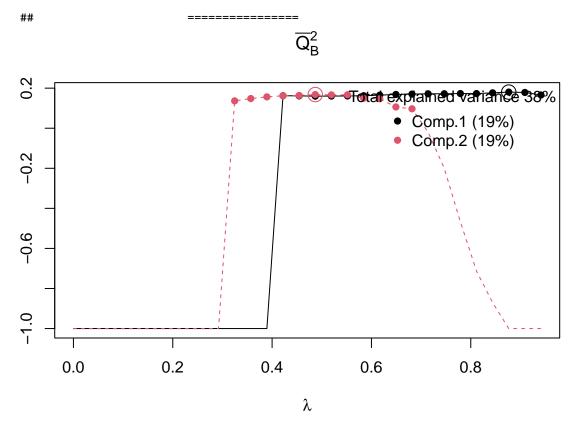
simu_2.2 <- get_design_2(seed = 2, ncpX = 20, plot = T)</pre>





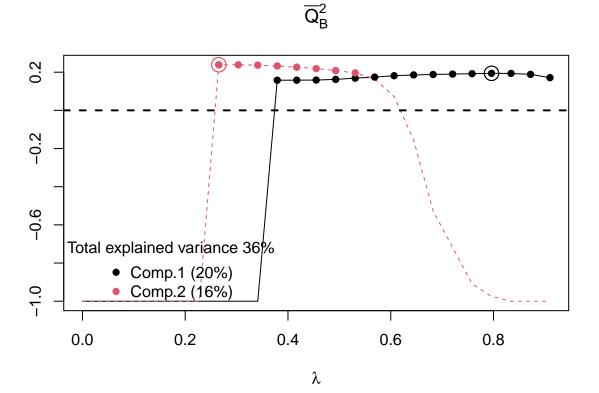
##

```
ddsPLS
##
  Should we build component 1 ? Bootstrap pending...
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
##
          0.52 0.22 0.22 0.16 0.16
                                      19%
##
                                       ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                                    ...component 2 not built!
   _____
                                       ##
                                       \overline{Q}_{B}^{2}
0.2
                                              পঞ্জির explained variance ৭৩%
                                                     • Comp.1 (19%)
                     0.2
      0.0
                                     0.4
                                                     0.6
                                                                     8.0
                                        λ
model_2.4 <- ddsPLS(simu_2.2$Xs$X2, simu_2.2$Y,</pre>
                   criterion = "Q2",
                   n_{\text{lambdas}} = 30,
                   verbose = TRUE)
##
                            ddsPLS
  Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.88 0.2 0.2 0.18 0.18
                                    19%
                                                19%
##
                                       ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.49 0.39 0.2 0.32 0.17
                                     19%
##
                                       ...component 2 built!
## Should we build component 3 ? Bootstrap pending...
##
                                   ...component 3 not built!
  _____
```



Model results can also be plotted using the plot function.

plot(model_2.1,type="Q2",legend.position = "bottomleft")

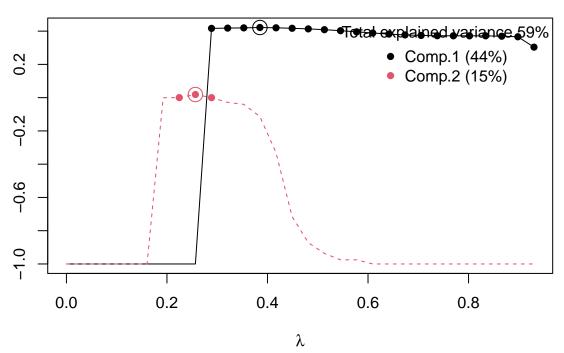


Get Data Simulation

The following get_data function is from the vignette for the ddsPLS package

The variable eps seems to relate the predictors and response, as well as phi. The dimension of phi specifies the number of latent variables.

```
##
##
                             ddsPLS
##
   Should we build component 1 ? Bootstrap pending...
##
        lambda
                R2 R2h
                           Q2 Q2h VarExpl VarExpl.Tot
##
          0.38 0.43 0.43 0.42 0.42
                                       44%
##
                                        ...component 1 built!
  Should we build component 2 ? Bootstrap pending...
##
##
        lambda
                R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
          0.26 0.63 0.2 0.43 0.02
##
##
                                        ...component 2 built!
##
  Should we build component 3 ? Bootstrap pending...
##
                                    ...component 3 not built!
##
                                        -----
##
```



```
data_3.2 \leftarrow get_data(p1 = 50, p2 = 50, p3 = 50, p = 250)
```

```
model_3.2 <- ddsPLS(data_3.2$X, data_3.2$Y,</pre>
                     criterion = "Q2",
                     n_{\text{lambdas}} = 30,
                     verbose = TRUE)
##
##
                              ddsPLS
## Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
          0.29 0.41 0.41 0.39 0.39
##
                                          ...component 1 built!
##
## Should we build component 2 ? Bootstrap pending...
##
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.16 0.62 0.2 0.55 0.3
                                          ...component 2 built!
##
  Should we build component 3 ? Bootstrap pending...
##
                                     ...component 3 not built!
##

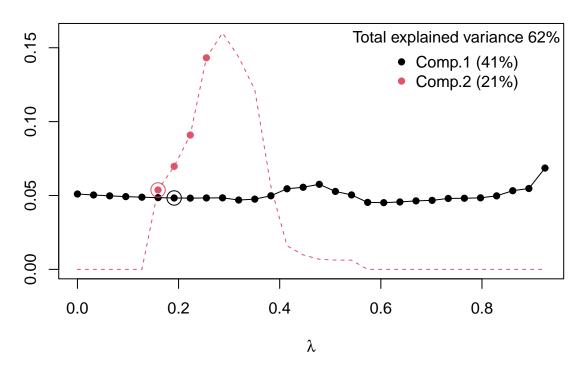
    Total explained variance 61%

                                                        • Comp.1 (40%)
                                                        • Comp.2 (21%)
      0.0
                     0.2
                                    0.4
                                                   0.6
                                                                   8.0
                                          λ
model_3.3 <- ddsPLS(data_3.2$X, data_3.2$Y,</pre>
                     criterion = "Q2",
                     n_{\text{lambdas}} = 30,
                     verbose = TRUE,
                     LD = TRUE)
##
                           ddsPLS |
##
```

```
## Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h
                         Q2 Q2h VarExpl VarExpl.Tot
           0.1 0.4 0.4 0.39 0.39
##
                                     41%
##
                                         ...component 1 built!
##
  Should we build component 2 ? Bootstrap pending...
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
##
          0.16 0.62 0.21 0.57 0.31
##
                                         ...component 2 built!
  Should we build component 3 ? Bootstrap pending...
                                     ...component 3 not built!
##

    Total explained variance 62%

                                                      • Comp.1 (41%)
                                                      Comp.2 (21%)
      0.0
                     0.2
                                   0.4
                                                  0.6
                                                                 8.0
model_3.4 <- ddsPLS(data_3.2$X, data_3.2$Y,</pre>
                    criterion = "diffR2Q2",
                    n_{\text{lambdas}} = 30,
                    verbose = TRUE,
                    LD = TRUE)
##
##
                             ddsPLS
   Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h
                           Q2 Q2h VarExpl VarExpl.Tot
##
          0.19 0.42 0.42 0.37 0.37
                                       41%
##
                                         ...component 1 built!
   Should we build component 2 ? Bootstrap pending...
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
                                       21%
##
          0.16 0.62 0.21 0.57 0.29
                                                    62%
##
                                         ...component 2 built!
```



Novel Simulations

The following code simulates a data set with 100 uncorrelated predictors and 1 response variable all sampled from a normal distribution.

```
Sigma <- diag(100)
sim_pred <- mvrnorm(n = 1000, mu = rep(0, 100), Sigma = Sigma)
sim_resp <- matrix(rnorm(1000), 1000, 1)</pre>
ddsPLS(sim_pred, sim_resp, verbose = TRUE)
##
##
                              ddsPLS
##
##
   Should we build component 1 ? Bootstrap pending...
##
                                      ...component 1 not built!
##
                 ...no Q2r large enough for tested lambda.
##
##
##
## Call:
## NULL
```

```
##
## No ddsPLS model built.
```

##

As expected no model is built as performance is awful. Interestingly message "no Q2r large enough for tested lambda" is given for justification, seems to suggest it checks just Q^2 . Perhaps this just means that mean estimation performs better.

```
Sigma <- matrix(c(1,.75,.75,1),2,2)

n <- 20
p <- 5
p <- p - 2

sim_preds <- cbind(mvrnorm(n = n, rep(0, 2), Sigma), matrix(rep(0,n*p),n, p))

sim_resp <- as.matrix(apply(sim_preds,1,function(x) 5*x[1]+x[2]))

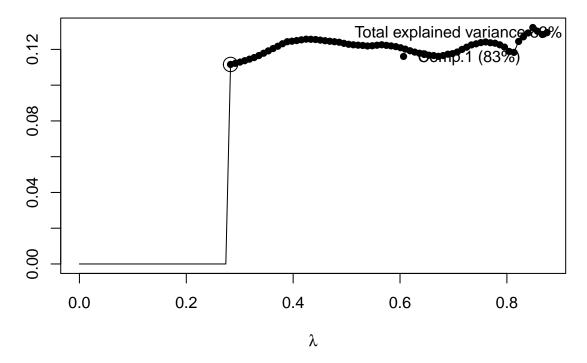
sim_preds <- sim_preds + matrix(rnorm(n*(p+2), sd = 0.6), n,(p+2))

sim_resp <- sim_resp + matrix(rnorm(n, sd = 0.8), n,1)</pre>
```

The above code simulates data with n observations of p predictors and 1 response variable. There are two predictors from which responses are linearly generated. Random noise is then added to the predictors and the response. As expected, the ddsPLS model performs very well.

```
pls_model <- ddsPLS(sim_preds, sim_resp, verbose = TRUE)</pre>
##
##
                        ddsPLS
##
  ______
##
  Should we build component 1 ? Bootstrap pending...
##
             R2 R2h
                     Q2 Q2h VarExpl VarExpl.Tot
##
        0.28 0.79 0.79 0.67 0.67
                                83%
                                          83%
##
                                 ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
##
                              ...component 2 not built!
##
                                 ==============
```





Complex Simulated Data

The general structure of simulated data is $\mathbf{X} = \mathbf{A}^T \phi + \epsilon_X$ and $\mathbf{Y} = \mathbf{D}^T \phi + \epsilon_Y$. Note that ϕ provides the structure between the two. Code structures it as $\mathbf{X} = \phi \mathbf{A} + \epsilon_X$ and similarly for \mathbf{Y} . ϵ is added random error. $\text{Cov}(\mathbf{X}, \mathbf{Y}) = \mathbf{D}^T \mathbf{A}$.

```
sim_data <- function(n = 5, p = 10, q = 2, R = 5, x = 3, noise_weight = 1, D_method = "new") {
  # Ensures x \le R, if x > R the dimension of A is incompatible with phi
  if(x > R){
    x = R
  }
  # Creates A and D matrices
  A <- matrix(c(rep(rep(1,p),x), rep(rep(0,p),R-x)), ncol = p)
  if(D_method == "new") {
     D \leftarrow matrix(rep(1, R*q), nrow = R)
  } else {
    D \leftarrow diag(max(q, R))[1:R, 1:q]
  d <- ncol(A)+nrow(A)+ncol(D)</pre>
  psi <- MASS::mvrnorm(n = n,mu = rep(0,d),Sigma = diag(d))
  phi <- psi[,1:nrow(A)]</pre>
  epsilon_X <- mvrnorm(n = dim(phi)[1],</pre>
                        rep(0, dim(A)[2]),
                         Sigma = noise_weight*diag(dim(A)[2]))
```

```
epsilon_Y <- mvrnorm(n = dim(phi)[1],</pre>
                      rep(0, dim(D)[2]),
                      Sigma = noise_weight*diag(dim(D)[2]))
 X <- phi %*% A + epsilon_X
 Y <- phi %*% D + epsilon_Y
 list(X=X, Y=Y)
# This chunk isn't running, my guess is that setting a seed causes
# problems for the bootstrapping done to run ddsPLS
set.seed(1999)
sim_1 <- sim_data()</pre>
sim1_pls <- ddsPLS(sim_1$X, sim_1$Y,</pre>
                  n_B = 30,
                  n_{\text{lambdas}} = 25,
                  verbose = TRUE)
ddsPLS is not an appropriate method when working with a small sample size as
set.seed(1999)
sim_1 <- sim_data()</pre>
sim1_pls <- ddsPLS(sim_1$X, sim_1$Y,</pre>
                  verbose = TRUE)
set.seed(1894)
sim_2 < -sim_data(n = 100, p = 150, q = 5, R = 5, x = 4, D_method = "old")
sim2_pls <- ddsPLS(sim_2$X, sim_2$Y,</pre>
              verbose = TRUE)
##
##
                          ddsPLS
## Should we build component 1 ? Bootstrap pending...
##
       lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
         0.23 0.14 0.14 0.09 0.09
                                       ...component 1 built!
##
## Should we build component 2 ? Bootstrap pending...
##
                                   ...component 2 not built!
##
```

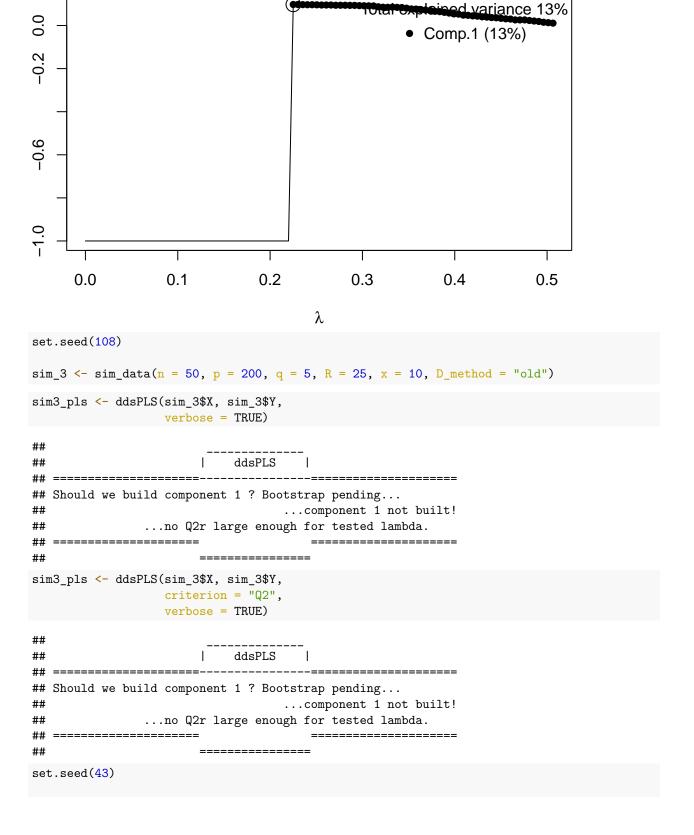
 $\overline{R}_B^2\!-\!\overline{Q}_B^2$

```
Total explained variance 13%
• Conip.1 (13%)
• Conip.1 (13%)

0.0 0.1 0.2 0.3 0.4 0.5
```

```
##
##
                          ddsPLS
  Should we build component 1 ? Bootstrap pending...
       lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
##
         0.23 0.14 0.14 0.1 0.1
                                 13%
##
                                    ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                                ...component 2 not built!
                                    _____
##
  _____
##
```





```
sim_4 \leftarrow sim_data(n = 250, p = 1000, q = 10, R = 100, x = 95, D_method = "old")
sim4_pls <- ddsPLS(sim_4$X, sim_4$Y,</pre>
      verbose = TRUE)
##
##
                    | ddsPLS |
## Should we build component 1 ? Bootstrap pending...
                               ...component 1 not built!
##
             ...no Q2r large enough for tested lambda.
##
sim4_pls <- ddsPLS(sim_4$X, sim_4$Y,</pre>
                criterion = "Q2",
                verbose = TRUE)
##
                    | ddsPLS |
##
## Should we build component 1 ? Bootstrap pending...
                              ...component 1 not built!
##
             ...no Q2r large enough for tested lambda.
## =========
##
                     ===========
set.seed(99)
sim_5 < -sim_data(n = 500, p = 500, q = 10, R = 100, x = 95, D_method = "old")
sim5_pls <- ddsPLS(sim_5$X, sim_5$Y,</pre>
          verbose = TRUE)
##
##
                    | ddsPLS |
## Should we build component 1 ? Bootstrap pending...
##
      lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
        0.11 0.01 0.01 0 0
                               1%
##
                                  ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                               ...component 2 not built!
## =========
```

$\overline{R}_B^2\!-\!\overline{Q}_B^2$

```
Total explained variance 1%
900.0
0.004
0.002
0.000
      0.00
                                0.05
                                                         0.10
                                                                                  0.15
                                               λ
sim5_pls <- ddsPLS(sim_5$X, sim_5$Y,</pre>
                      criterion = "Q2",
```

```
verbose = TRUE)
```

```
##
##
                         ddsPLS
  Should we build component 1 ? Bootstrap pending...
       lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
##
        0.11 0.01 0.01 0
                                   ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                               ...component 2 not built!
                                   ##
  _____
##
```

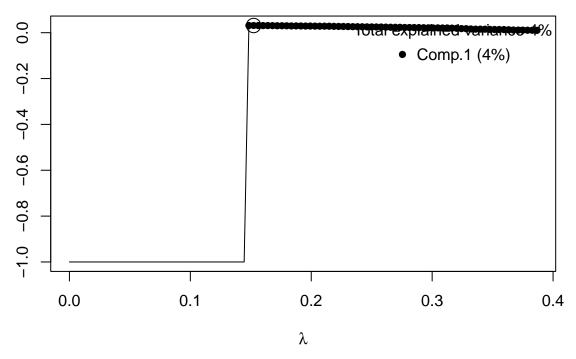
```
0.0
                                                  Total explained variance 1%
                                                           Comp.1 (1%)
-0.4
9.0-
-0.8
-1.0
     0.00
                            0.05
                                                  0.10
                                                                         0.15
                                          λ
set.seed(99)
sim_6 \leftarrow sim_data(n = 250, p = 200, q = 10, R = 8, x = 7, D_method = "old")
sim6_pls <- ddsPLS(sim_6$X, sim_6$Y,</pre>
                   verbose = TRUE)
##
##
                              ddsPLS
##
   Should we build component 1 ? Bootstrap pending...
##
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
##
          0.34 0.03 0.03 0.02 0.02
##
##
                                          ...component 1 built!
\mbox{\tt \#\#} Should we build component 2 ? Bootstrap pending...
##
                                      ...component 2 not built!
                                          -----
##
                         ===========
```



```
100 0000 Comp.1 (3%)
000 0000 0.1 0.2 0.3 0.4 λ
```

```
##
##
                         ddsPLS
  Should we build component 1 ? Bootstrap pending...
                       Q2 Q2h VarExpl VarExpl.Tot
       lambda R2 R2h
##
##
        0.15 0.05 0.05 0.03 0.03
##
                                   ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
                                ...component 2 not built!
                                   ##
  _____
##
```





It looks like there is a problem with the way I am simulating the data. All of the simulations have only explained a low amount of the variation in the data, perhaps due to the relation between R and x.

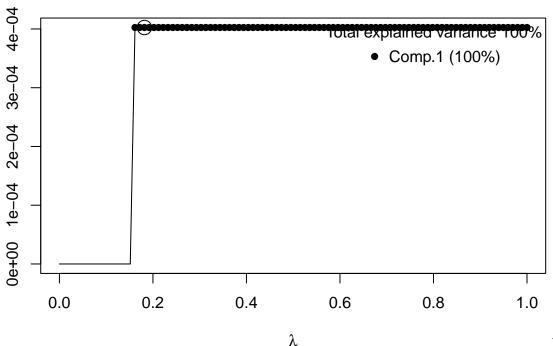
I changed A from a subset of a diagonal matrix to a matrix of all 1s and the function starts to work well. Running the code with different values of q and noise_weight = 0 returns a model that perfectly explains the data.

```
set.seed(12)
sim_7 \leftarrow sim_data(n = 100, p = 200, q = 5, noise_weight = 0.5)
sim7_pls <- ddsPLS(sim_7$X, sim_7$Y,</pre>
                    verbose = TRUE)
##
##
                               ddsPLS
##
   Should we build component 1 ? Bootstrap pending...
##
##
        lambda R2 R2h Q2 Q2h VarExpl VarExpl.Tot
          0.27 0.9 0.9 0.9 0.9
##
##
                                           ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
##
                                       ...component 2 not built!
##
##
```

$\overline{R}_B^2\!-\!\overline{Q}_B^2$

```
Total explained variance 92%
                                                      • Comp.1 (92%)
0.015
0.010
0.005
      0.0
                    0.2
                                   0.4
                                                 0.6
                                                               8.0
                                         λ
set.seed(12)
sim_8 \leftarrow sim_data(n = 100, p = 200, q = 150, noise_weight = 0)
sim8_pls <- ddsPLS(sim_8$X, sim_8$Y,</pre>
                   verbose = TRUE)
##
##
                             ddsPLS
##
##
   Should we build component 1 ? Bootstrap pending...
                           Q2 Q2h VarExpl VarExpl.Tot
##
        lambda R2 R2h
          0.18 0.99 0.99 0.99 0.99
##
##
                                         ...component 1 built!
## Should we build component 2 ? Bootstrap pending...
##
                                     ...component 2 not built!
##
                                         -----
##
                        ===========
```



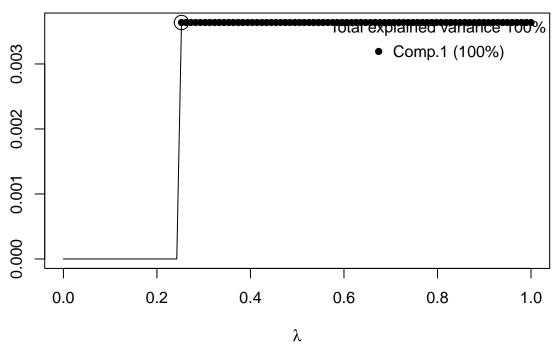


If q > n, then

the model is still able to perfectly explain the variance.

```
##
##
                            ddsPLS
  Should we build component 1 ? Bootstrap pending...
##
##
                R2 R2h
                          Q2 Q2h VarExpl VarExpl.Tot
##
         0.25 0.97 0.97 0.97 0.97
                                       ...component 1 built!
##
## Should we build component 2 ? Bootstrap pending...
                                   ...component 2 not built!
                                       ===========
##
   ================
##
```





Still works

when n < q and p < q.