# SImulations 4

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```
library(ddsPLS2)
library(MASS)
library(pls)
library(mixOmics)
library(glmnet)
library(ggplot2)
```

#### New Data Simulation Method

```
sim_data <- function(n = 25, p = 50, q = 5, R = 5, noise_weight = 1, D_method = "newest", noise_type =
  # Creates A and D matrices
  if(D_method == "complex") {
    R = 13
  Row1 \leftarrow c(rep(1, 5), rep(0, p - 5))
  Row2 \leftarrow c(rep(0, 5), rep(1, 10), rep(0, p - 15))
  reps1 <- round(3*R/5)
  reps2 <- R - reps1
  A1 <- do.call("rbind", replicate(reps1, Row1, simplify = FALSE))
  A2 <- do.call("rbind", replicate(reps2, Row2, simplify = FALSE))
  A \leftarrow rbind(A1, A2)
  if(struc == "complex") {
    R = 13
    Row1 \leftarrow c(rep(1, 5), rep(0, p - 5))
    Row2 \leftarrow c(rep(0, 5), rep(1, 10), rep(0, p - 15))
    Row3 \leftarrow c(rep(0, 15), rep(1, 5), rep(0, p - 20))
    Row4 \leftarrow c(rep(0, 20), 1, rep(0, p - 21))
    Row5 \leftarrow c(rep(0, 21), rep(1, 2), rep(0, p - 23))
    A1 <- do.call("rbind", replicate(3, Row1, simplify = FALSE))
    A2 <- do.call("rbind", replicate(2, Row2, simplify = FALSE))
    A3 <- do.call("rbind", replicate(3, Row3, simplify = FALSE))
    A4 <- do.call("rbind", replicate(2, Row4, simplify = FALSE))
```

```
A5 <- do.call("rbind", replicate(3, Row5, simplify = FALSE))
  A <- rbind(A1, A2, A3, A4, A5)
}
if(D method == "new") {
  D \leftarrow matrix(rep(1, R*q), nrow = R)
} else if(D_method == "diag") {
  D \leftarrow diag(max(q, R))[1:R, 1:q]
} else if(D_method == "simple") {
  D <- cbind(rep(1, R), matrix(rep(0, R*(q-1)), \frac{1}{2} R))
} else if(D_method == "complex") {
  D1 \leftarrow c(rep(1, 3), rep(0, 10))
  D2 \leftarrow c(rep(0, 3), rep(1, 3), rep(0, 7))
  D3 \leftarrow c(rep(0, 6), rep(1, 3), rep(0, 4))
  D4 \leftarrow c(rep(0, 9), rep(1, 3), rep(0, 1))
  D5 \leftarrow matrix(rep(0, R*(q-4)), nrow = R)
  D <- cbind(D1, D2, D3, D4, D5)
} else {
   q_s \leftarrow round(q/4)
   if(q_s == 0) {
     q_s = 1
   Row1D \leftarrow c(rep(1, q_s), rep(0, q - q_s))
   Row2D \leftarrow c(rep(0, q_s), rep(1, q_s), rep(0, q - 2*q_s))
   reps1D <- round(3*R/5)
   reps2D <- R - reps1D
   D1 <- do.call("rbind", replicate(reps1D, Row1D, simplify = FALSE))
   D2 <- do.call("rbind", replicate(reps2D, Row2D, simplify = FALSE))
   D <- rbind(D1, D2)
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>
```

```
phi <- matrix(rnorm(n*R), nrow = n)</pre>
  # If `rnorm` is used to generate noise a lower noise weight should be used as
  # the function is more sensitive since we directly weight results and not the
  # covariance matrix.
  if(noise type == "mvrnorm") {
    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]))
  } else {
   epsilon_X <- matrix(noise_weight*rnorm(n = n*p), nrow = n)</pre>
   epsilon_Y <- matrix(noise_weight*rnorm(n = n*q), nrow = n)</pre>
 X <- phi %*% A + epsilon_X
 Y <- phi %*% D + epsilon_Y
  #X <- scale(X)
  #Y <- scale(Y)
 list(X=X, Y=Y)
}
```

## PLS Test Function

```
pls_test <- function(n, sim, func, passed_arg, criterion = "diffR2Q2") {
    # Splits into training and test
    in_train <- round(n/3)
    in_test <- round(2*n/3)

split <- sample(c(rep(0, in_train), rep(1, in_test)))

sim_train_X <- sim$X[split == 0, ]
    sim_train_Y <- sim$Y[split == 0, ]

sim_test_X <- sim$X[split == 1, ]
    sim_test_Y <- sim$Y[split == 1, ]

# Generates model using the training set and predicts RMSE
if(func == "ddsPLS") {
    mod <- ddsPLS(sim_train_X, sim_train_Y, criterion = criterion)

    preds <- predict(mod, sim_test_X)
    preds_ib <- predict(mod, sim_train_X)

    rmse <- sqrt(sum((preds$y_est - sim_test_Y)^2)/nrow(sim_test_Y))</pre>
```

```
pred_mean_tr <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
  R2 <- 1 - (sum((preds_ib$y_est - sim_train_Y)^2)/sum((sim_train_Y - pred_mean_tr)^2))
  pred_mean_ts <- t(replicate(nrow(sim_test_Y)), colMeans(sim_test_Y)))</pre>
  Q2 \leftarrow 1 - (sum((preds\$y_est - sim_test_Y)^2)/sum((sim_test_Y - pred_mean_ts)^2))
 ncomp <- mod$R
  } else if(func == "pls") {
  df <- data.frame(X = I(sim_train_X), Y = I(sim_train_Y))</pre>
  mod <- plsr(Y~X, data = df, ncomp = 10, method = "oscorespls", validation = "CV", scale = TRUE)
  R2 \leftarrow R2 \pmod{1}
  Q2 \leftarrow colSums(R2$val, dims = 2)
 ncomp \leftarrow which(Q2 == max(Q2)) - 1
 ncomp <- unname(ncomp)</pre>
  if(ncomp == 0){
    preds <- t(replicate(nrow(sim_test_Y), colMeans(sim_train_Y)))</pre>
    preds_ib <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
  } else {
    preds <- predict(mod, sim_test_X)[,,ncomp]</pre>
    preds_ib <- predict(mod, sim_train_X)[,,ncomp]</pre>
     }
  rmse <- sqrt(sum((preds - sim_test_Y)^2)/nrow(sim_test_Y))</pre>
 pred_mean_tr <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
 R2 <- 1 - (sum((preds_ib - sim_train_Y)^2)/sum((sim_train_Y - pred_mean_tr)^2))
  pred_mean_ts <- t(replicate(nrow(sim_test_Y), colMeans(sim_test_Y)))</pre>
  Q2 <- 1 - (sum((preds - sim_test_Y)^2)/sum((sim_test_Y - pred_mean_ts)^2))
} else if(func == "lasso") {
  mod <- cv.glmnet(sim_train_X, sim_train_Y, family = "mgaussian")</pre>
  preds <- predict(mod, sim_test_X)[,,1]</pre>
  preds_ib <- predict(mod, sim_train_X)[,,1]</pre>
 rmse <- sqrt(sum((preds - sim_test_Y)^2)/nrow(sim_test_Y))</pre>
  pred_mean_tr <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
 R2 <- 1 - (sum((preds_ib - sim_train_Y)^2)/sum((sim_train_Y - pred_mean_tr)^2))
  pred_mean_ts <- t(replicate(nrow(sim_test_Y), colMeans(sim_test_Y)))</pre>
  Q2 <- 1 - (sum((preds - sim_test_Y)^2)/sum((sim_test_Y - pred_mean_ts)^2))
 ncomp <- NA
} else {
  colnames(sim_train_X) <- c(1:ncol(sim_train_X))</pre>
```

```
colnames(sim_test_X) <- c(1:ncol(sim_train_X))</pre>
  colnames(sim_test_Y) <- c(1:ncol(sim_test_Y))</pre>
  colnames(sim_train_Y) <- c(1:ncol(sim_test_Y))</pre>
  tune <- tune.spls(sim_train_X, sim_train_Y,</pre>
                      validation = "Mfold",
                      folds = 10,
                      ncomp = 10,
                      mode = "regression")
  ncomp <- tune$choice.ncomp</pre>
  mod <- spls(sim_train_X, sim_train_Y, ncomp = ncomp, mode = "regression")</pre>
  if(ncomp == 0){
    preds <- t(replicate(nrow(sim_test_Y), colMeans(sim_train_Y)))</pre>
    preds_ib <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
    } else {
      preds <- predict(mod, sim_test_X)</pre>
      preds <- preds$predict[,,ncomp]</pre>
      preds_ib <- predict(mod, sim_train_X)</pre>
      preds_ib <- preds_ib$predict[,,ncomp]</pre>
  rmse <- sqrt(sum((preds - sim_test_Y)^2)/nrow(sim_test_Y))</pre>
  pred_mean_tr <- t(replicate(nrow(sim_train_Y), colMeans(sim_train_Y)))</pre>
  R2 <- 1 - (sum((preds_ib - sim_train_Y)^2)/sum((sim_train_Y - pred_mean_tr)^2))</pre>
  pred_mean_ts <- t(replicate(nrow(sim_test_Y), colMeans(sim_test_Y)))</pre>
  Q2 <- 1 - (sum((preds - sim_test_Y)^2)/sum((sim_test_Y - pred_mean_ts)^2))
out <- c(passed_arg, ncomp, rmse, R2, Q2, R2-Q2)
return(out)
```

#### **Noise Test Function**

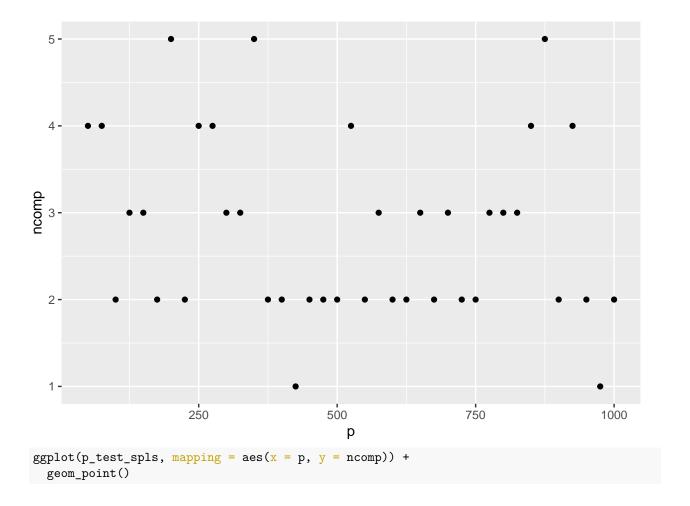
```
noise_eval <- function(noise_weight, func = "ddsPLS", n = 300, p = 100, q = 5){
    sim <- sim_data(n = n, p = p, q = q, noise_weight = noise_weight, noise_type = "rnorm", struc = "completest(n = n, sim = sim, func = func, passed_arg = noise_weight)
}</pre>
```

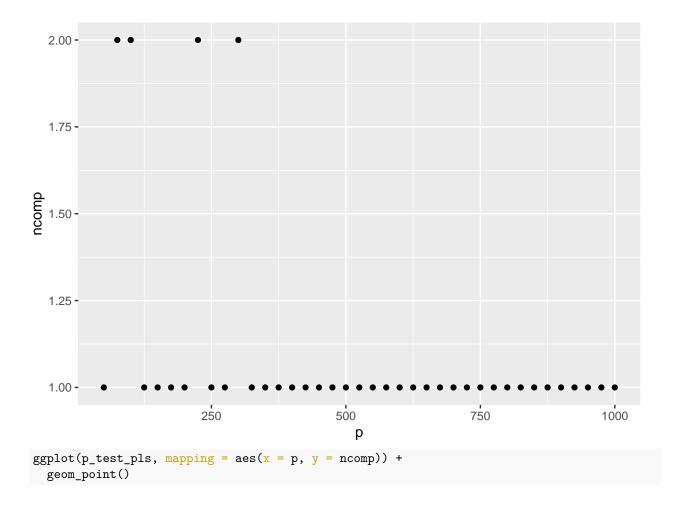
### **Predictors Tests**

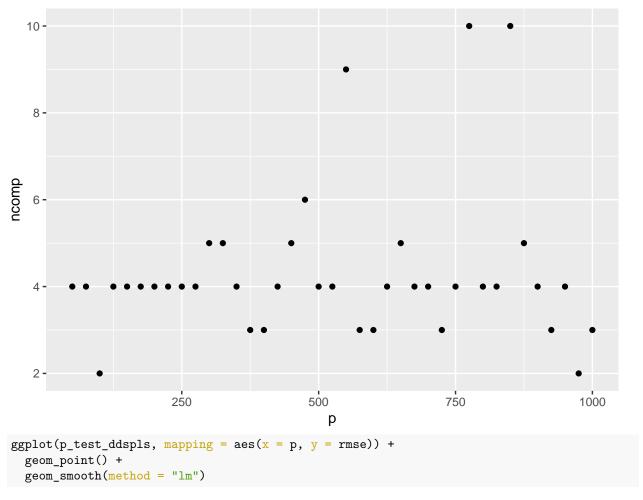
```
p_eval <- function(p, noise_weight = 1, n = 150, q = 5,func = "ddsPLS", struc = "complex", D_method = ":
# Randomly simulates data</pre>
```

```
sim <- sim_data(n = n, p = p, q = q, noise_weight = noise_weight, noise_type = "rnorm", struc = stru</pre>
   # Passes Data to test function
   pls_test(n = n, sim = sim, func = func, passed_arg = p, criterion = criterion)
p_test_ddspls <- apply(matrix(seq(from = 50, to = 1000, by = 25),
                             nrow = 1),
                    MARGIN = 2.
                   p_eval,
                    D_method = "complex")
p_test_spls <- apply(matrix(seq(from = 50, to = 1000, by = 25),</pre>
                             nrow = 1),
                   MARGIN = 2.
                   p_eval,
                   func = "spls",
                    D_method = "complex")
p_test_pls <- apply(matrix(seq(from = 50, to = 1000, by = 25),</pre>
                             nrow = 1),
                   MARGIN = 2,
                   p_eval,
                   func = "pls",
                   D_method = "complex")
p_test_ddspls_Q2 <- apply(matrix(seq(from = 50, to = 1000, by = 25),
                             nrow = 1),
                   MARGIN = 2,
                   p_eval,
                   D_method = "complex",
                   criterion = "Q2")
p_test_ddspls <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/p_test_ddspls.csv")</pre>
p_test_spls <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/p_test_spls.csv")</pre>
p_test_pls <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/p_test_pls.csv")</pre>
p_test_ddspls_Q2 <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/p_test_ddspls_Q2.csv"
ggplot(p_test_ddspls, mapping = aes(x = p, y = ncomp)) +
```

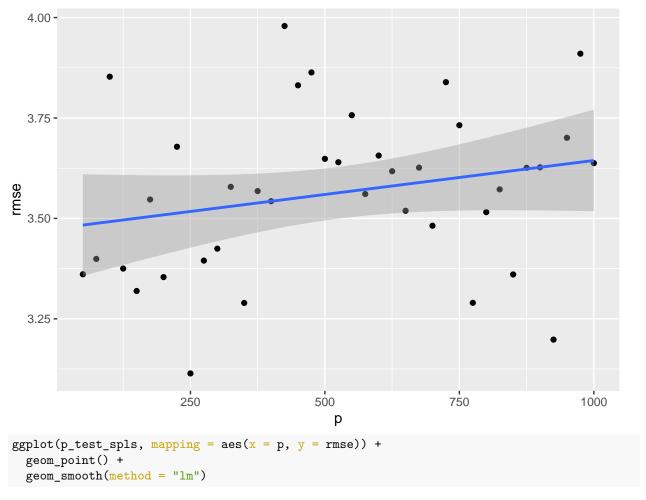
geom\_point()



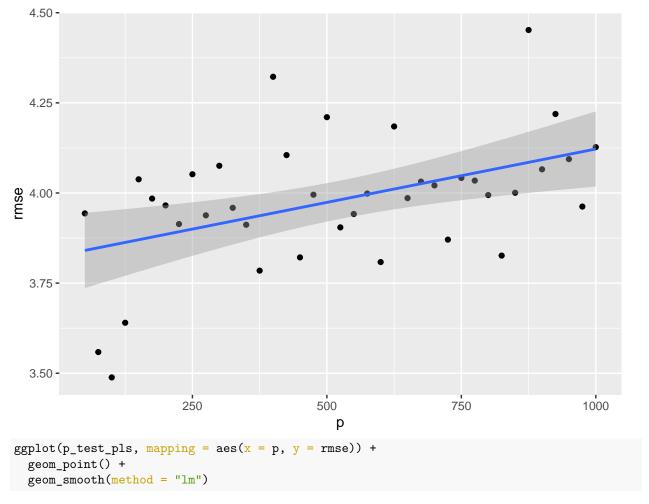




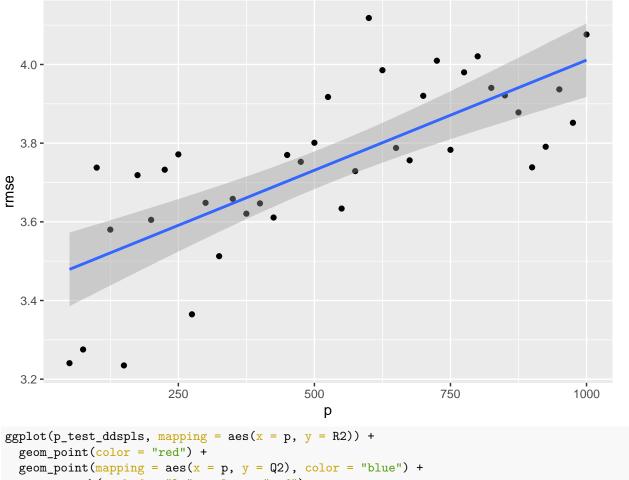
##  $geom_smooth()$  using formula 'y ~ x'



##  $geom_smooth()$  using formula 'y ~ x'

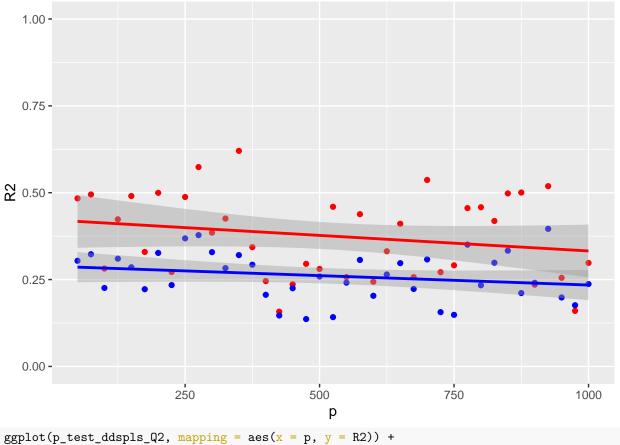


##  $geom_smooth()$  using formula 'y ~ x'



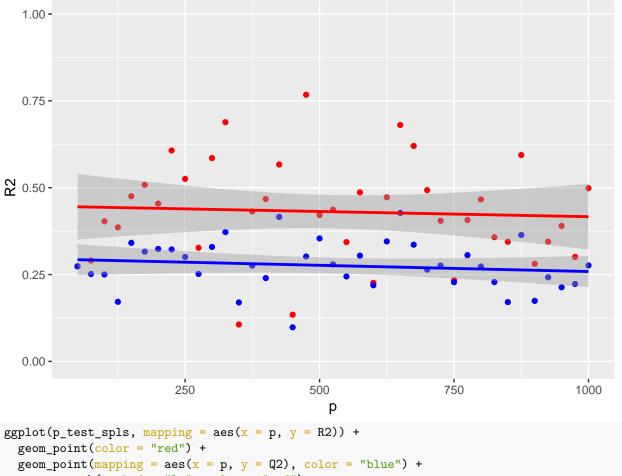
```
geom_smooth(method = "lm", color = "red") +
geom\_smooth(mapping = aes(x = p, y = Q2), method = "lm", color = "blue") +
ylim(c(0, 1))
```

```
## geom_smooth() using formula 'y ~ x'
## geom_smooth() using formula 'y ~ x'
```



```
ggplot(p_test_ddspls_Q2, mapping = aes(x = p, y = R2)) +
geom_point(color = "red") +
geom_point(mapping = aes(x = p, y = Q2), color = "blue") +
geom_smooth(method = "lm", color = "red") +
geom_smooth(mapping = aes(x = p, y = Q2), method = "lm", color = "blue") +
ylim(c(0, 1))
```

```
## `geom_smooth()` using formula 'y ~ x'
## `geom_smooth()` using formula 'y ~ x'
```



```
geom_smooth(method = "lm", color = "red") +
geom\_smooth(mapping = aes(x = p, y = Q2), method = "lm", color = "blue") +
ylim(c(0, 1))
```

```
## `geom_smooth()` using formula 'y ~ x'
## `geom_smooth()` using formula 'y ~ x'
```

<sup>##</sup> Warning: Removed 7 rows containing non-finite values (stat\_smooth).

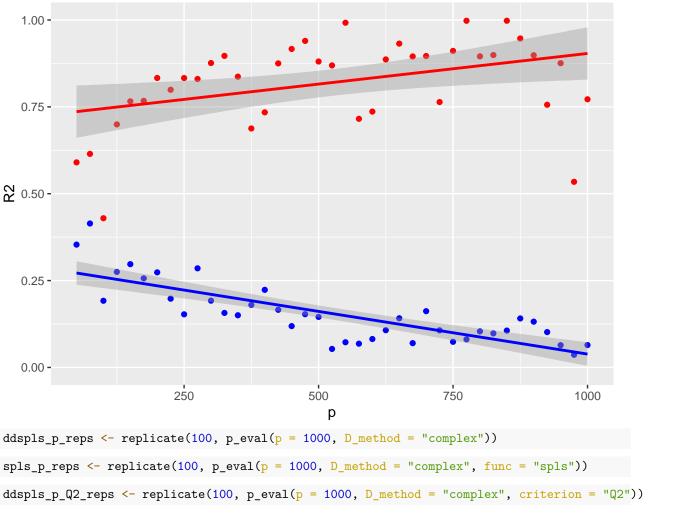
<sup>##</sup> Warning: Removed 7 rows containing missing values (geom\_point).

<sup>##</sup> Warning: Removed 4 rows containing missing values (geom\_smooth).

```
1.00 -
  0.75 -
2 0.50 -
  0.25 -
  0.00 -
                                                                   750
                          250
                                              500
                                                                                       1000
                                                  р
ggplot(p_test_pls, mapping = aes(x = p, y = R2)) +
  geom_point(color = "red") +
  geom\_point(mapping = aes(x = p, y = Q2), color = "blue") +
```

```
geom_smooth(method = "lm", color = "red") +
geom\_smooth(mapping = aes(x = p, y = Q2), method = "lm", color = "blue") +
ylim(c(0, 1))
```

```
## geom_smooth() using formula 'y ~ x'
## geom_smooth() using formula 'y ~ x'
```



```
spls_p_reps <- replicate(100, p_eval(p = 1000, D_method = "complex", func = "spls"))

ddspls_p_Q2_reps <- replicate(100, p_eval(p = 1000, D_method = "complex", criterion = "Q2"))

pls_p_reps <- replicate(100, p_eval(p = 1000, D_method = "complex", func = "pls"))

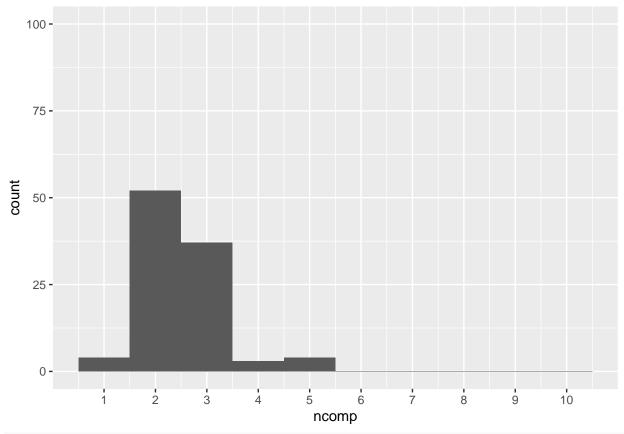
ddspls_1000_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/ddspls_p_1000.csv")

spls_1000_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/spls_p_1000.csv")

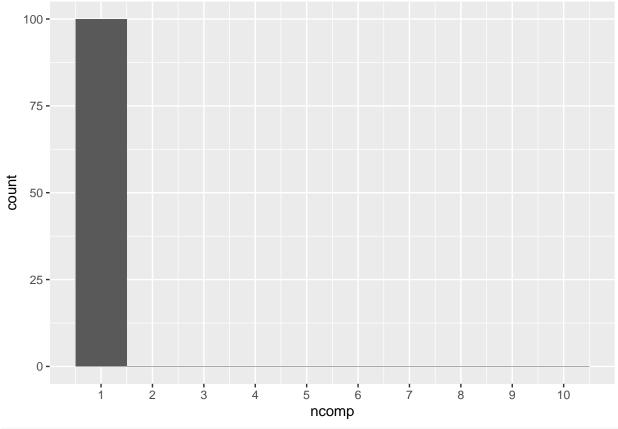
pls_1000_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/pls_p_1000.csv")

ddspls_1000_reps_Q2 <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/ddspls_p_1000_Q2.c</pre>
```

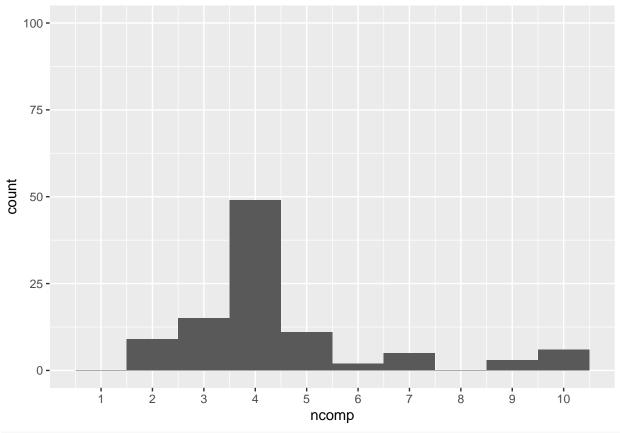
```
ggplot(ddspls_1000_reps, aes(x = ncomp)) +
  geom_histogram(binwidth = 1) +
  scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
  ylim(c(0, 100))
```



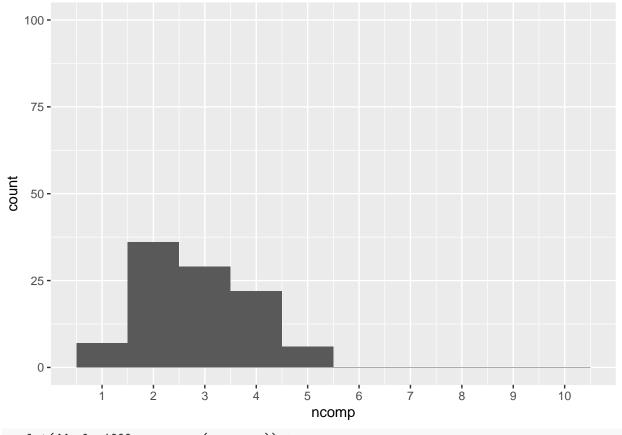
```
ggplot(spls_1000_reps, aes(x = ncomp)) +
  geom_histogram(binwidth = 1) +
  scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
  ylim(c(0, 100))
```



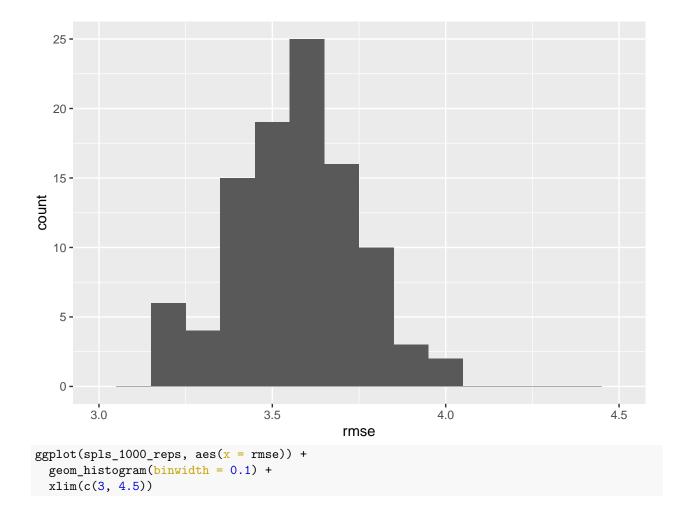
```
ggplot(pls_1000_reps, aes(x = ncomp)) +
geom_histogram(binwidth = 1) +
scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
ylim(c(0, 100))
```

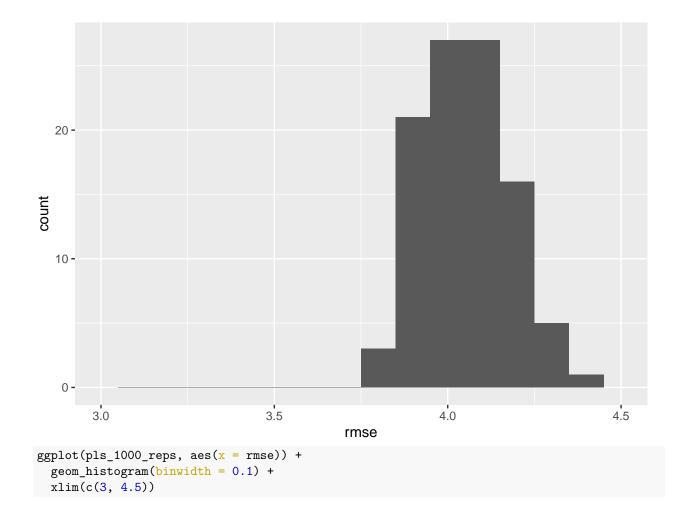


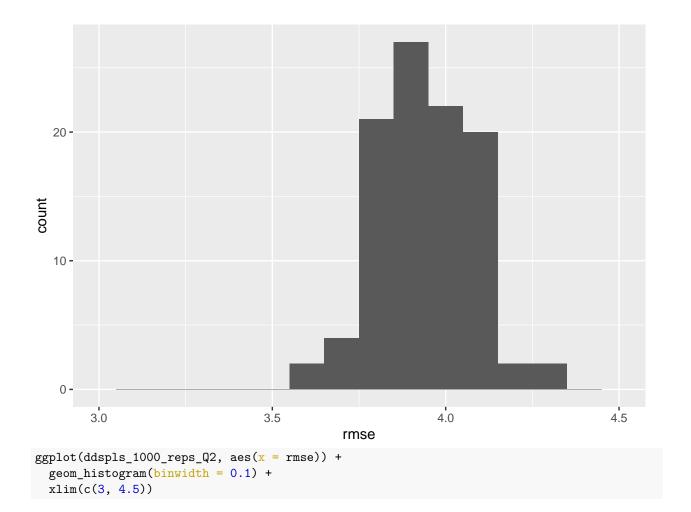
```
ggplot(ddspls_1000_reps_Q2, aes(x = ncomp)) +
  geom_histogram(binwidth = 1) +
  scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
  ylim(c(0, 100))
```

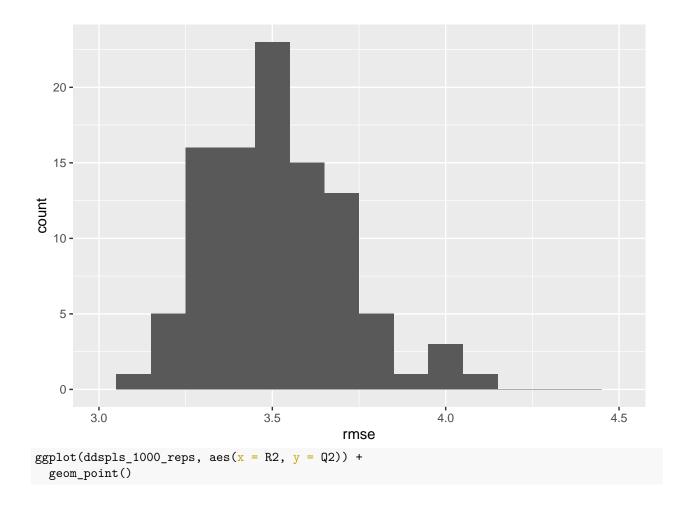


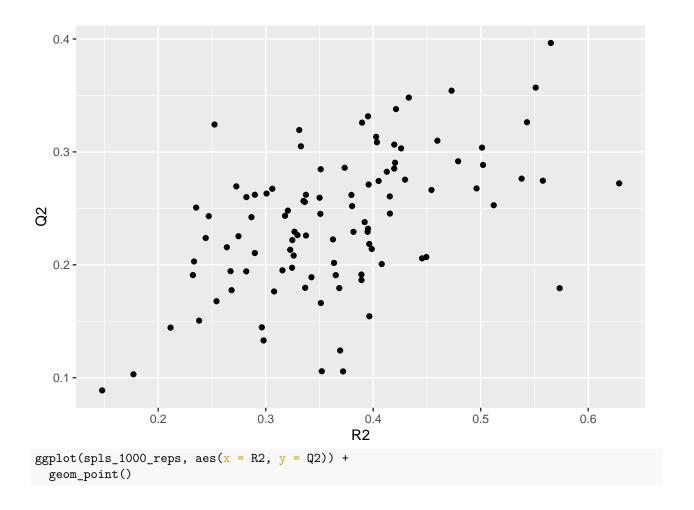
ggplot(ddspls\_1000\_reps, aes(x = rmse)) +
 geom\_histogram(binwidth = 0.1) +
 xlim(c(3, 4.5))

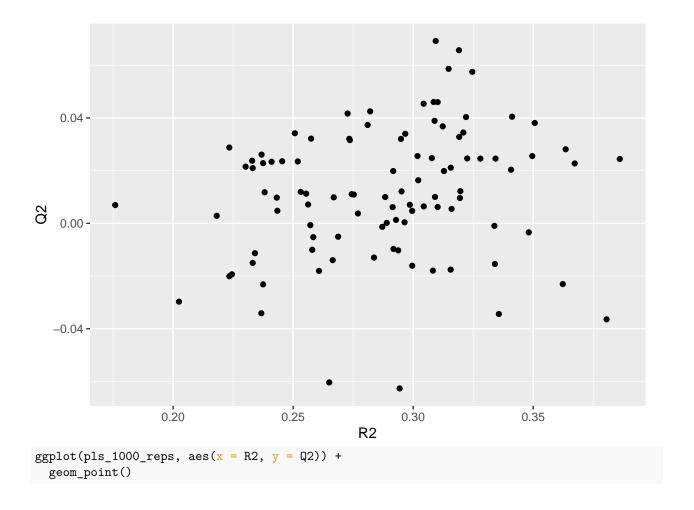


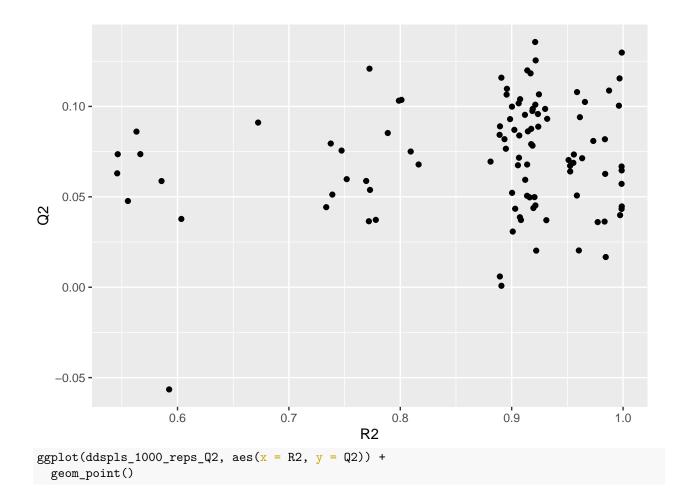


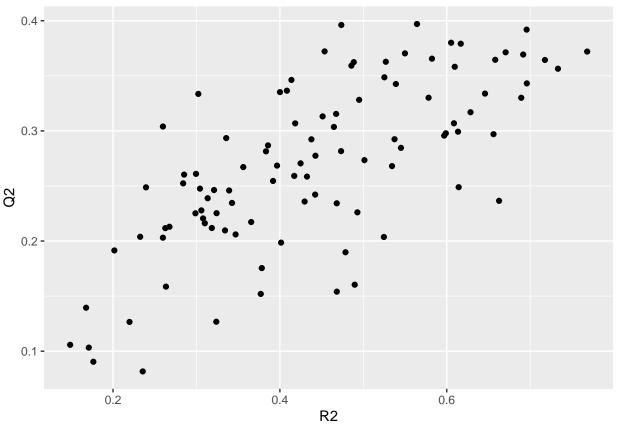








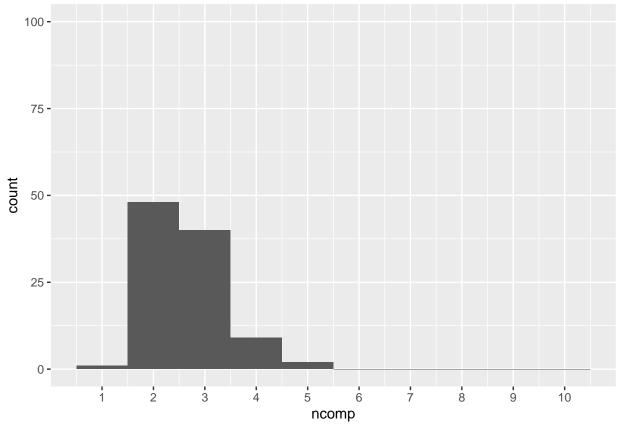




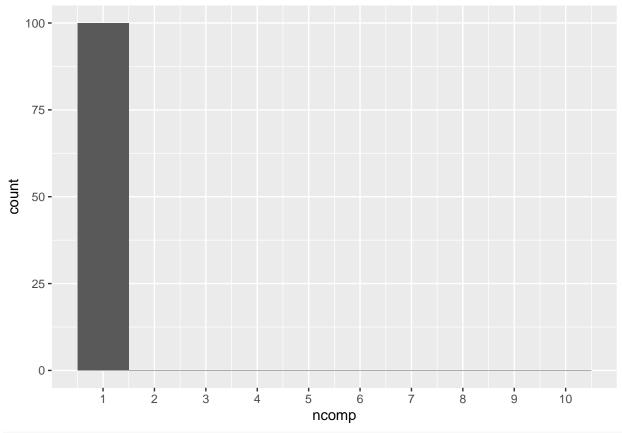
```
reps_df <- data.frame(c(mean(ddspls_1000_reps$rmse), median(ddspls_1000_reps$rmse), var(ddspls_1000_rep
   c(mean(spls_1000_reps$rmse), median(spls_1000_reps$rmse), var(spls_1000_reps$rmse)),
   c(mean(pls_1000_reps$rmse), median(pls_1000_reps$rmse), var(pls_1000_reps$rmse)),
   c(mean(ddspls_1000_reps_Q2$rmse), median(ddspls_1000_reps_Q2$rmse), var(ddspls_1000_reps_Q2$rmse)))
reps_df <- as.data.frame(t(as.matrix(reps_df)))</pre>
colnames(reps_df) <- c("mean", "median", "var")</pre>
row.names(reps_df) <- c("ddsPLS", "sPLS", "PLS", "ddsPLS_Q2")</pre>
reps_df
##
                        median
                 mean
## ddsPLS
             3.569282 3.565361 0.02974532
## sPLS
             4.052281 4.041317 0.01489767
## PLS
             3.944839 3.942986 0.01851942
## ddsPLS_Q2 3.508364 3.492494 0.03847528
ddspls_p_reps <- replicate(100, p_eval(p = 500, D_method = "complex"))
spls_p_reps <- replicate(100, p_eval(p = 500, D_method = "complex", func = "spls"))</pre>
ddspls_p_Q2_reps <- replicate(100, p_eval(p = 500, D_method = "complex", criterion = "Q2"))
pls_p_reps <- replicate(100, p_eval(p = 500, D_method = "complex", func = "pls"))
ddspls_500_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/ddspls_p_500.csv")
spls_500_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/spls_p_500.csv")</pre>
pls_500_reps <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/pls_p_500.csv")
```

ddspls\_500\_reps\_Q2 <- read.csv2("/Users/johnlee/R Files/thesis-lee/Simulations/data/ddspls\_p\_500\_Q2.csv

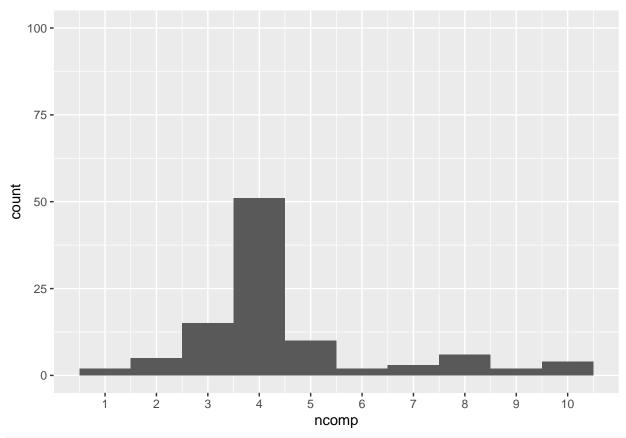
```
ggplot(ddspls_500_reps, aes(x = ncomp)) +
geom_histogram(binwidth = 1) +
scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
ylim(c(0, 100))
```



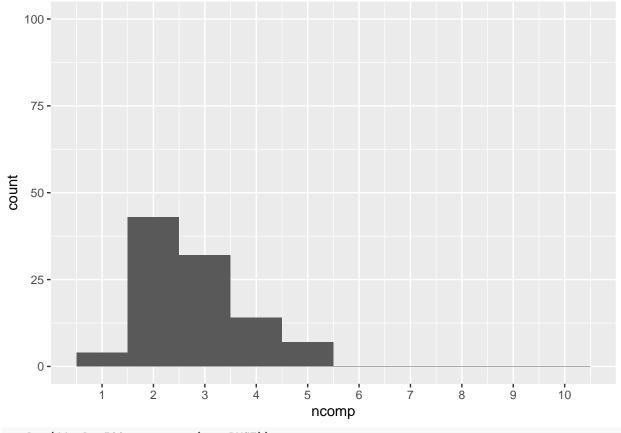
```
ggplot(spls_500_reps, aes(x = ncomp)) +
  geom_histogram(binwidth = 1) +
  scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
  ylim(c(0, 100))
```



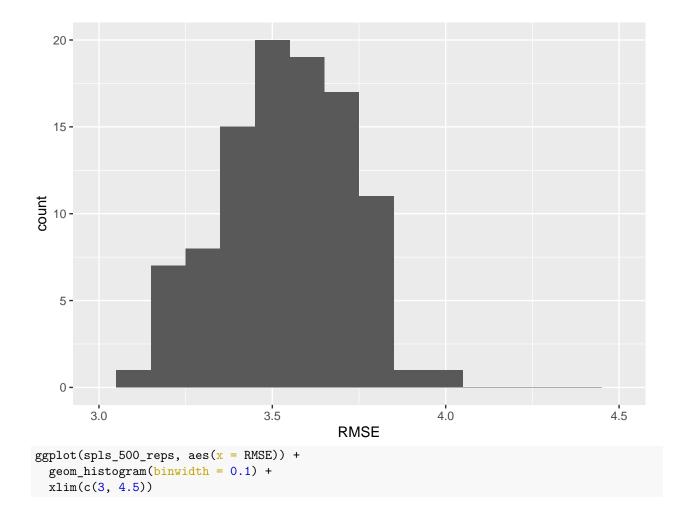
```
ggplot(pls_500_reps, aes(x = ncomp)) +
  geom_histogram(binwidth = 1) +
  scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
  ylim(c(0, 100))
```

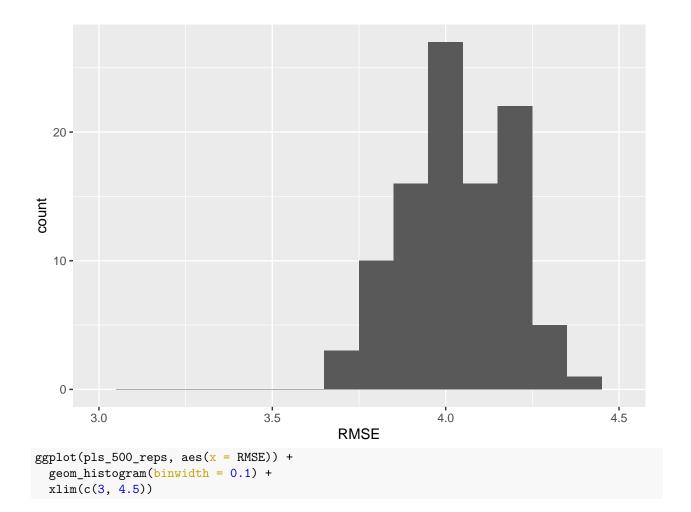


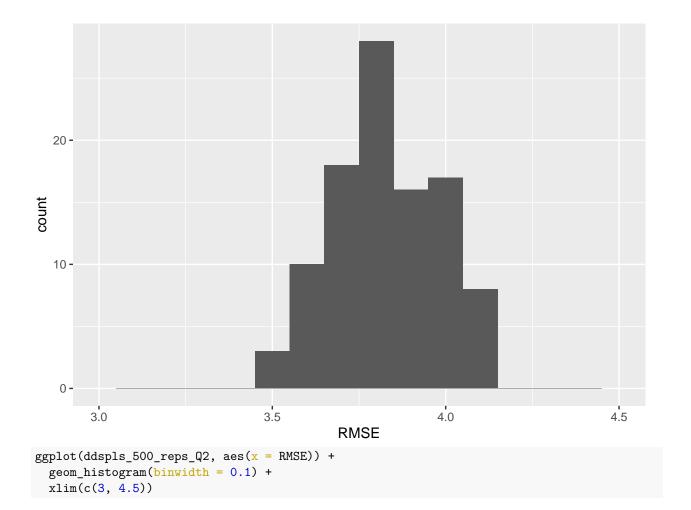
```
ggplot(ddspls_500_reps_Q2, aes(x = ncomp)) +
geom_histogram(binwidth = 1) +
scale_x_continuous(breaks = 1:10, limits = c(0.5,10.5)) +
ylim(c(0, 100))
```

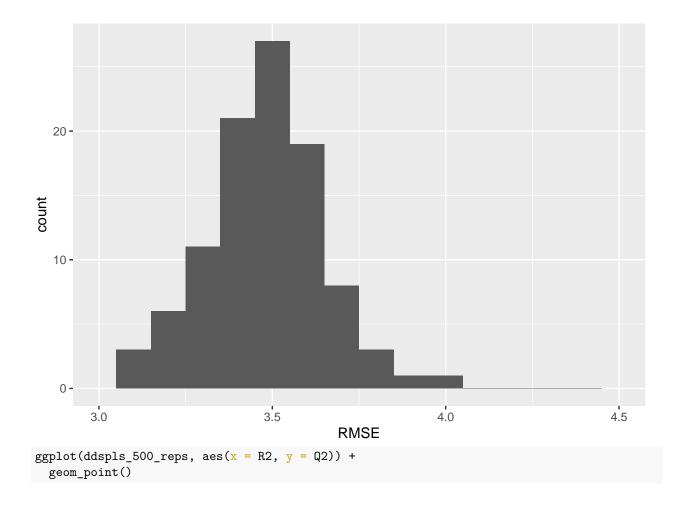


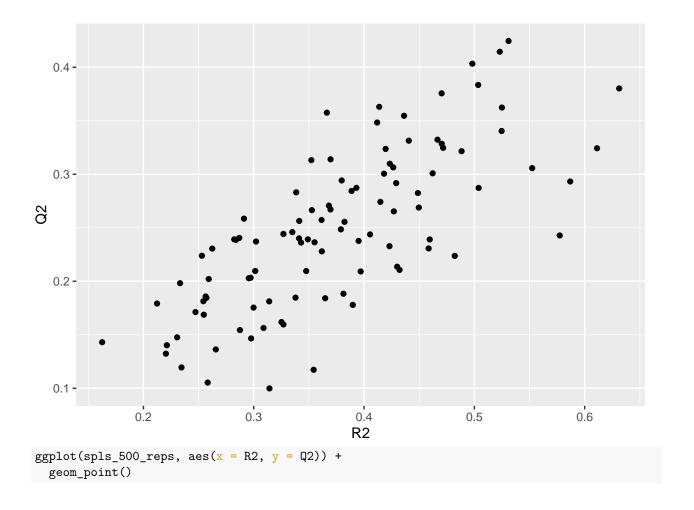
```
ggplot(ddspls_500_reps, aes(x = RMSE)) +
geom_histogram(binwidth = 0.1) +
xlim(c(3, 4.5))
```

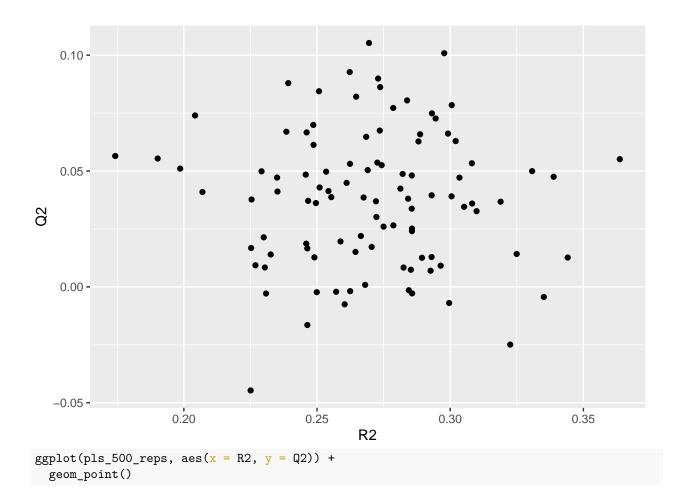


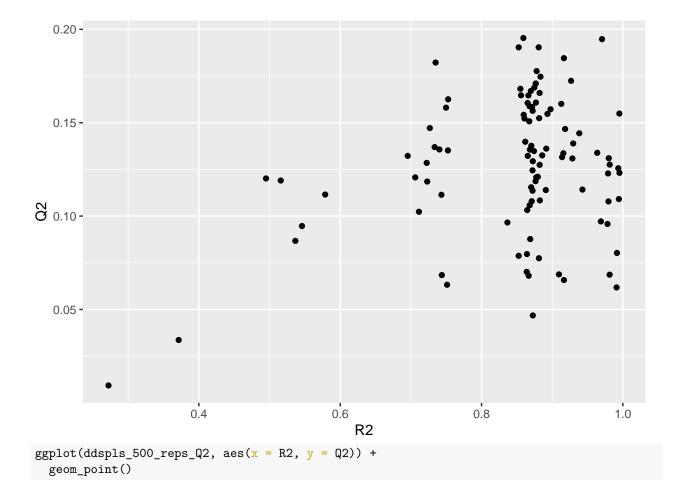


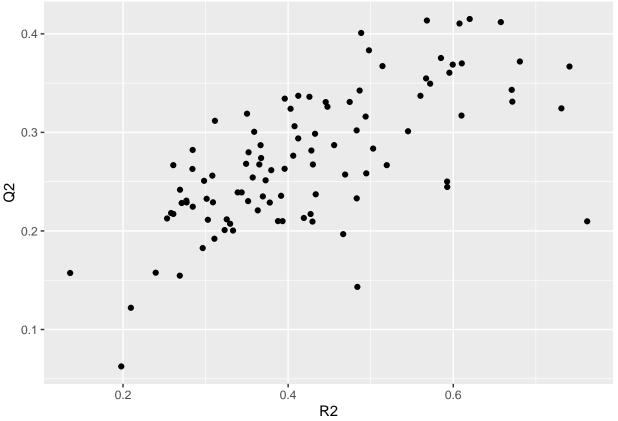












```
reps_df <- data.frame(c(mean(ddspls_500_reps$RMSE), median(ddspls_500_reps$RMSE), var(ddspls_500_reps$R
   c(mean(spls_500_reps$RMSE), median(spls_500_reps$RMSE), var(spls_500_reps$RMSE)),
   c(mean(pls_500_reps$RMSE), median(pls_500_reps$RMSE), var(pls_500_reps$RMSE)),
   c(mean(ddspls_500_reps_Q2$RMSE), median(ddspls_500_reps_Q2$RMSE), var(ddspls_500_reps_Q2$RMSE)))
reps_df <- as.data.frame(t(as.matrix(reps_df)))</pre>
colnames(reps_df) <- c("mean", "median", "var")</pre>
row.names(reps_df) <- c("ddsPLS", "sPLS", "PLS", "ddsPLS_Q2")</pre>
reps_df
##
                 mean
                        median
## ddsPLS
             3.538211 3.534172 0.03526031
## sPLS
             4.035095 4.024334 0.02223995
## PLS
             3.829996 3.826565 0.02289107
## ddsPLS_Q2 3.474859 3.483749 0.02864078
t.test(ddspls_1000_reps$rmse, ddspls_1000_reps_Q2$rmse)
## Welch Two Sample t-test
## data: ddspls_1000_reps$rmse and ddspls_1000_reps_Q2$rmse
## t = 2.3323, df = 194.81, p-value = 0.02071
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
```

## 0.009405659 0.112430572

```
## sample estimates:
## mean of x mean of y
## 3.569282 3.508364

t.test(ddspls_500_reps$RMSE, ddspls_500_reps_Q2$RMSE)

##
## Welch Two Sample t-test
##
## data: ddspls_500_reps$RMSE and ddspls_500_reps_Q2$RMSE
## t = 2.5061, df = 195.9, p-value = 0.01302
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## 0.01349816 0.11320468
## sample estimates:
## mean of x mean of y
## 3.538211 3.474859
```