

PLSR for corn V2 PDF Markdown

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```
library(R.matlab)
```

```
## R.matlab v3.6.2 (2018-09-26) successfully loaded. See ?R.matlab for help.
```

```
##
```

```
## Attaching package: 'R.matlab'
```

```
## The following objects are masked from 'package:base':
```

```
##
```

```
##      getOption, isOpen
```

```
library(pls)
```

```
## Warning: package 'pls' was built under R version 3.5.2
```

```
##
```

```
## Attaching package: 'pls'
```

```
## The following object is masked from 'package:stats':
```

```
##
```

```
##      loadings
```

```
library(lars)
```

```
## Loaded lars 1.2
```

```
library(ggplot2)
```

```
rawdata <- readMat("/Users/hongwei/Downloads/corn.mat")
```

```
m5data <- rawdata$m5spec$data
```

```
mp5data <- rawdata$mp5spec$data
```

```
mp6data <- rawdata$mp6spec$data
```

```
propvals <- rawdata$propvals$data
```

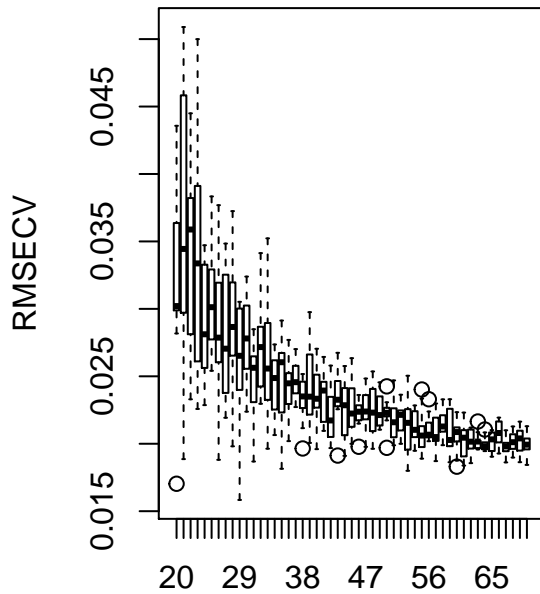
```
corn_PLS=function(n){  
  NV <- 10                                #n is the number of calibration  
  sample <- sample(1:80)                  #number of variables  
  DF <- data.frame(NIR = I(m5data),        #set random order; the begin of reset order  
                   y=propvals[,1])        #input data  
  class(DF$NIR) <- "matrix"               # just to be certain, it was "AsIs"  
  #str(DF)                                #check point  
  DF$train <- rep(FALSE, 80)  
  DF$train[sample<=n] <- TRUE              #chose calibration  
  corn.pls <- pls(y ~ NIR, data = DF, ncomp = NV, validation="LOO", jackknife = TRUE, subset = train)  
  #summary(corn.pls,what="all")            #check point  
  RMSECV <- RMSEP(corn.pls)$val[1,1,NV]  
  #print(RMSECV)                           #check point  
  predict <- predict(corn.pls, ncomp = NV, newdata = DF[!DF$train,])  
  RMSEP <- sqrt(sum((predict-DF[!DF$train,]$y)^2)/(80-n))  
  #print(RMSEP)                             #check point  
  #plot(R2(corn.pls))                       #check point  
  return(cbind(RMSECV,RMSEP))              #return 1x2matrix
```

```

}
#corn_PLS(n)
n <- as.matrix(rep(20:70,10))
PlsResult <- apply(n,1,corn_PLS)
PlotData <- as.data.frame(cbind(n,t(PlsResult)))
par(mfrow=c(1,2))
boxplot(V2~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSECV",main="PLS 1~m5data Loop=10")
boxplot(V3~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSEP",main="PLS 1~m5data Loop=10")

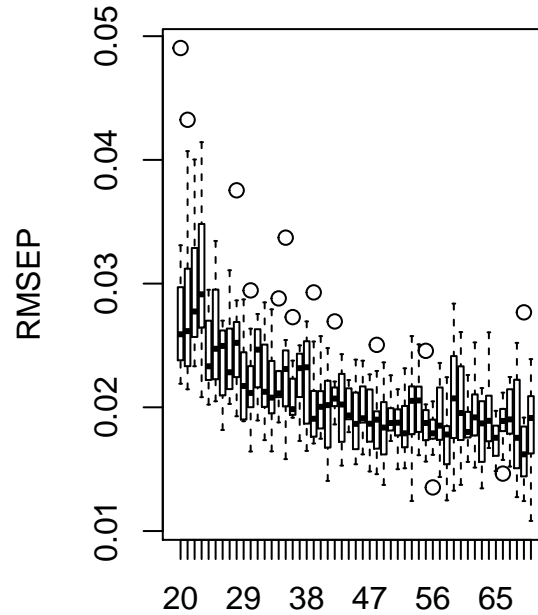
```

PLS 1~m5data Loop=10



Number of Calibration

PLS 1~m5data Loop=10



Number of Calibration

```

library(R.matlab)
library(pls)
library(lars)
library(ggplot2)
rawdata <- readMat("/Users/hongwei/Downloads/corn.mat")
m5data <- rawdata$m5spec$data
mp5data <- rawdata$mp5spec$data
mp6data <- rawdata$mp6spec$data
propvals <- rawdata$propvals$data

corn_PLS=function(n){
  NV <- 10
  sample <- sample(1:80)
  DF <- data.frame(NIR = I(m5data),
                   y=propvals[,2])
  class(DF$NIR) <- "matrix"
  #str(DF)
  DF$train <- rep(FALSE, 80)
  DF$train[sample<=n] <- TRUE
  corn.pls <- pls(y ~ NIR, data = DF, ncomp = NV, validation="LOO", jackknife = TRUE, subset = train)

```

#n is the number of calibration
#number of variables
#set random order; the begin of reset order
#input data

just to be certain, it was "AsIs"
#check point

#chose calibration

```

#summary(corn.pls,what="all")
RMSECV <- RMSEP(corn.pls)$val[1,1,NV]
#print(RMSECV)
predict <- predict(corn.pls, ncomp = NV, newdata = DF[!DF$train,])
RMSEP <- sqrt(sum((predict-DF[!DF$train,]$y)^2)/(80-n))
#print(RMSEP)
#plot(R2(corn.pls))
return(cbind(RMSECV,RMSEP))
}

#corn_PLS(n)
n <- as.matrix(rep(20:70,10))
PlsResult <- apply(n,1,corn_PLS)
PlotData <- as.data.frame(cbind(n,t(PlsResult)))
par(mfrow=c(1,2))
boxplot(V2~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSECV",main="PLS 2~m5data Loop=10")
boxplot(V3~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSEP",main="PLS 2~m5data Loop=10")

```

#check point

#check point

#check point

#check point

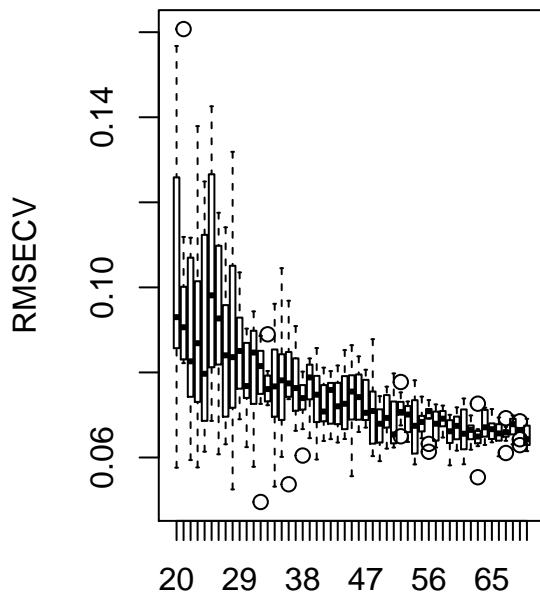
#return 1x2matrix

#the number of calibration, rep(a:b,c): from a to b, c times

#loop

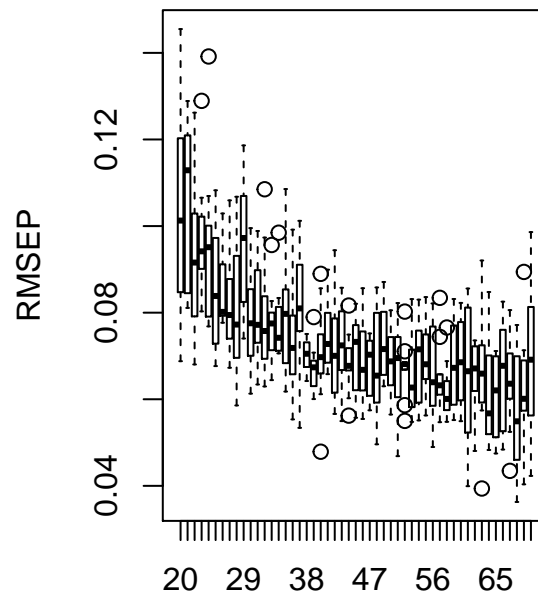
#combine the results

PLS 2~m5data Loop=10



Number of Calibration

PLS 2~m5data Loop=10



Number of Calibration

```

library(R.matlab)
library(pls)
library(lars)
library(ggplot2)
rawdata <- readMat("/Users/hongwei/Downloads/corn.mat")
m5data <- rawdata$m5spec$data
mp5data <- rawdata$mp5spec$data
mp6data <- rawdata$mp6spec$data
propvals <- rawdata$propvals$data

corn_PLS=function(n){
  NV <- 10

```

#n is the number of calibration

#number of variables

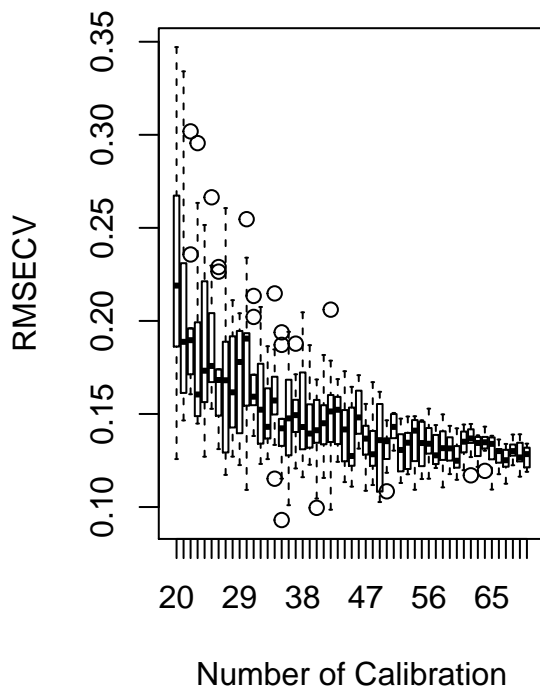
```

sample <- sample(1:80)
DF <- data.frame(NIR = I(m5data),
                 y=propvals[,3])
class(DF$NIR) <- "matrix"
#str(DF)
DF$train <- rep(FALSE, 80)
DF$train[sample<=n] <- TRUE
corn.pls <- plsr(y ~ NIR, data = DF, ncomp = NV, validation="LOO", jackknife = TRUE, subset = train)
#summary(corn.pls,what="all")
RMSECV <- RMSEP(corn.pls)$val[1,1,NV]
#print(RMSECV)
predict <- predict(corn.pls, ncomp = NV, newdata = DF[!DF$train,])
RMSEP <- sqrt(sum((predict-DF[!DF$train,]$y)^2)/(80-n))
#print(RMSEP)
#plot(R2(corn.pls))
return(cbind(RMSECV, RMSEP))
}

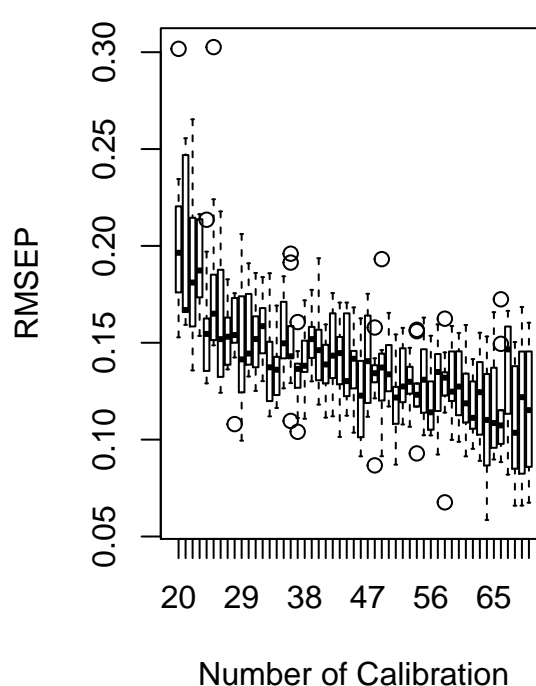
#corn_PLS(n)
n <- as.matrix(rep(20:70,10))
PlsResult <- apply(n,1,corn_PLS)
PlotData <- as.data.frame(cbind(n,t(PlsResult)))
par(mfrow=c(1,2))
boxplot(V2~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSECV",main="PLS 3~m5data Loop=10")
boxplot(V3~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSEP",main="PLS 3~m5data Loop=10")

```

PLS 3~m5data Loop=10



PLS 3~m5data Loop=10



```

library(R.matlab)
library(pls)
library(lars)
library(ggplot2)

```

```

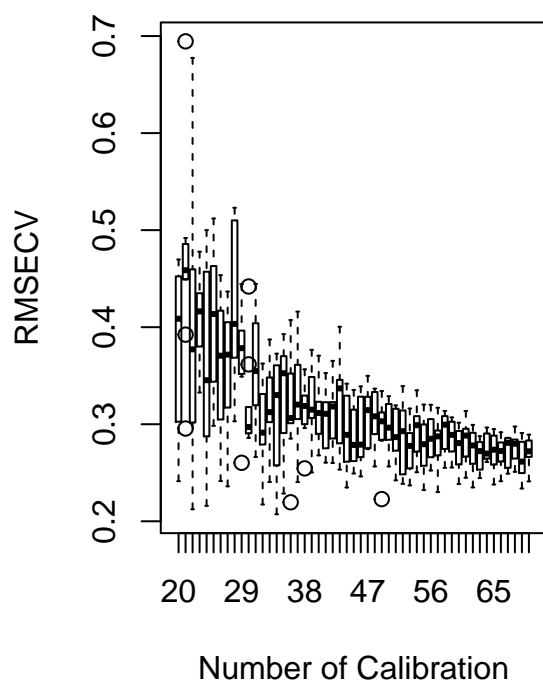
rawdata <- readMat("/Users/hongwei/Downloads/corn.mat")
m5data <- rawdata$m5spec$data
mp5data <- rawdata$mp5spec$data
mp6data <- rawdata$mp6spec$data
propvals <- rawdata$propvals$data

corn_PLS=function(n){
  NV <- 10                                     #n is the number of calibration
  sample <- sample(1:80)                       #number of variables
  DF <- data.frame(NIR = I(m5data),             #set random order; the begin of reset order
                  y=propvals[,4])             #input data
  class(DF$NIR) <- "matrix"                    # just to be certain, it was "AsIs"
  #str(DF)                                     #check point
  DF$train <- rep(FALSE, 80)
  DF$train[sample<=n] <- TRUE                  #chose calibration
  corn.pls <- plsr(y ~ NIR, data = DF, ncomp = NV, validation="LOO", jackknife = TRUE, subset = train)
  #summary(corn.pls,what="all")                #check point
  RMSECV <- RMSEP(corn.pls)$val[1,1,NV]
  #print(RMSECV)                              #check point
  predict <- predict(corn.pls, ncomp = NV, newdata = DF[!DF$train,])
  RMSEP <- sqrt(sum((predict-DF[!DF$train,]$y)^2)/(80-n))
  #print(RMSEP)                               #check point
  #plot(R2(corn.pls))                          #check point
  return(cbind(RMSECV, RMSEP))                 #return 1x2matrix
}

#corn_PLS(n)
n <- as.matrix(rep(20:70,10))                 #the number of calibration, rep(a:b,c): from a to
PlsResult <- apply(n,1,corn_PLS)                #loop
PlotData <- as.data.frame(cbind(n,t(PlsResult))) #combine the results
par(mfrow=c(1,2))
boxplot(V2~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSECV",main="PLS 4~m5data Loop=10")
boxplot(V3~V1,data=PlotData,xlab="Number of Calibration", ylab="RMSEP",main="PLS 4~m5data Loop=10")

```

PLS 4~m5data Loop=10



PLS 4~m5data Loop=10

