Compulsory exercise 2: Group 13

TMA4268 Statistical Learning V2020

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```r
# install.packages('knitr') #probably already installed
# install.packages('rmarkdown') #probably already installed
# install.packages('ggplot2') #plotting with ggplot install.packages('ggfortify')
# install.packages('MASS') install.packages('dplyr')
library(knitr)
library(rmarkdown)
library(ggplot2)
library(ggfortify)
library(GGally)
library(MASS)
library(dplyr)
library(ISLR)
library(leaps)
library(glmnet)
library(tree)
library(randomForest)
library(e1071)
```

Problem 1

a)

The ridge regression coefficients β_{Ridge} are the ones that minimize

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2 \tag{1}$$

with $\lambda > 0$ being a tuning parameter. The residual sum of squares is defined as

$$RSS = \sum_{i=1}^{n} \left(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} \hat{\beta}_j x_{ij} \right)^2 \tag{2}$$

Equation 1 can be rewritten in terms of matrices and vectors as

$$(y - X\hat{\beta}_{Ridge})^\top (y - X\hat{\beta}_{Ridge}) + \lambda \hat{\beta}_{Ridge}^\top \hat{\beta}_{Ridge} \tag{3}$$

Differentiating this with respect to $\hat{\beta}_{Ridge}$ and setting equal to 0 gives

$$-2X^\top(y - X\hat{\beta}_{Ridge}) + 2\lambda\hat{\beta}_{Ridge} = 0 \tag{4a}$$
$$X^\top X\hat{\beta}_{Ridge} + \lambda\hat{\beta}_{Ridge} = X^\top y \tag{4b}$$
$$\hat{\beta}_{Ridge} = (X^\top X + \lambda I)^{-1}X^\top y \tag{4c}$$

Where I is the identity matrix. This is done assuming that X has been centered such that the mean is zero, i.e $\beta_0 \approx 0$. It is also smart to standardize the predictors before using ridge regression, as ridge regression is not scale invariant.

b)

The expectation value of $y = X\beta + \epsilon$ is $\mathrm{E}[y] = X\beta$, as $\mathrm{E}[\epsilon] = 0$. The expectation value of β_{Ridge} is then

$$\mathrm{E}[\hat{\beta}_{Ridge}] = (X^\top X + \lambda I)^{-1}X^\top \mathrm{E}[y] \tag{5a}$$
$$= (X^\top X + \lambda I)^{-1}X^\top X\beta \tag{5b}$$

This is a biased estimator as long as $\lambda \neq 0$.

The variance covariance matrix of y is $\mathrm{Var}[y] = \mathrm{Var}[X\beta] + \mathrm{Var}[\epsilon] = \sigma^2$.

$$\mathrm{Var}[\hat{\beta}_{Ridge}] = \mathrm{Var}[(X^\top X + \lambda I)^{-1}X^\top y] \tag{6a}$$
$$= (X^\top X + \lambda I)^{-1}X^\top \mathrm{Var}[y][(X^\top X + \lambda I)^{-1}X^\top]^\top \tag{6b}$$
$$= \sigma^2(X^\top X + \lambda I)^{-1}X^\top X[(X^\top X + \lambda I)^{-1}]^\top \tag{6c}$$

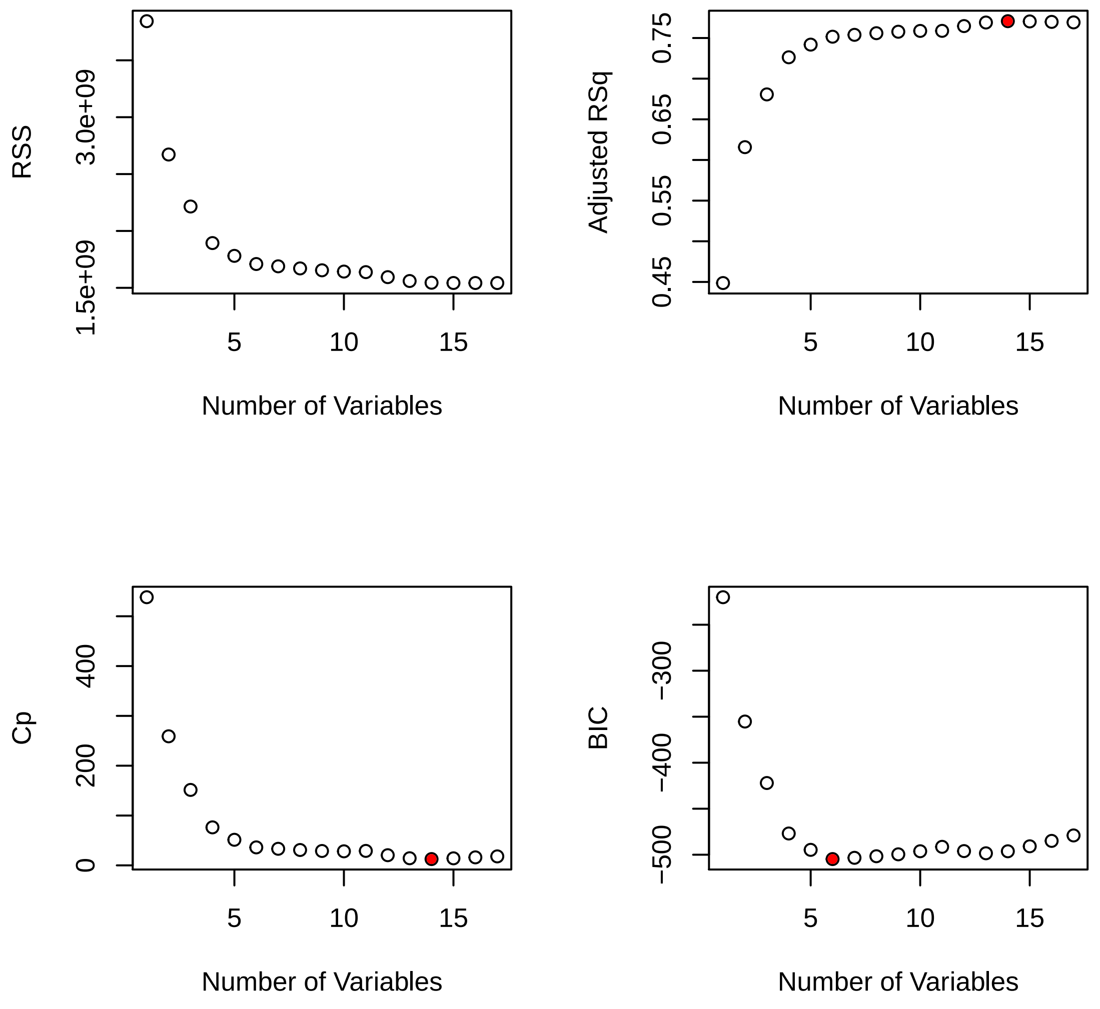
c)

(i) True
(ii) False
(iii) False
(iv) True

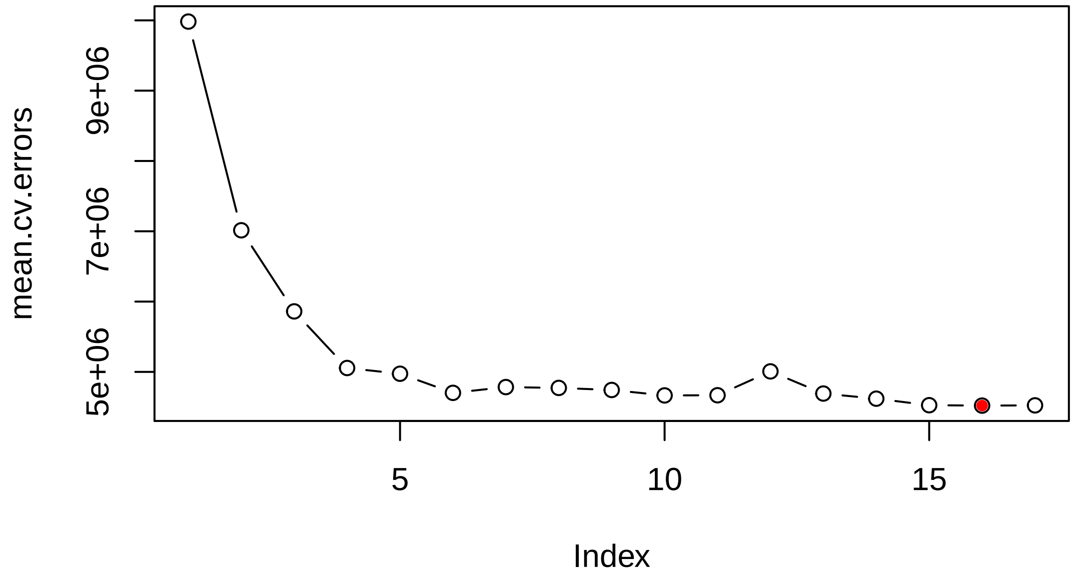
d)

Forward selection will be performed with `Outstate` as response using the `regsubsets` function.

```r
set.seed(1)
train.ind = sample(1:nrow(College), 0.5 * nrow(College))
college.train = College[train.ind, ]
college.test = College[-train.ind, ]
n_predictors = dim(College)[2] - 1
fwd.fit = regsubsets(Outstate ~ ., college.train, nvmax = n_predictors, method = "forward")
fwd.fit.summary = summary(fwd.fit)
par(mfrow = c(2, 2))
plot(fwd.fit.summary$rss, xlab = "Number of Variables", ylab = "RSS", type = )
plot(fwd.fit.summary$adjr2, xlab = "Number of Variables", ylab = "Adjusted RSq")
fwd_best_adjr2 = which.max(fwd.fit.summary$adjr2)
points(fwd_best_adjr2, fwd.fit.summary$adjr2[fwd_best_adjr2], col = "red", cex = 1,
    pch = 20)
plot(fwd.fit.summary$cp, xlab = "Number of Variables", ylab = "Cp")
fwd_best_cp = which.min(fwd.fit.summary$cp)
points(fwd_best_cp, fwd.fit.summary$cp[fwd_best_cp], col = "r ed", cex = 1, pch = 20)
fwd_best_bic = which.min(fwd.fit.summary$bic)
plot(fwd.fit.summary$bic, xlab = "Number of Variables", ylab = "BIC")
points(fwd_best_bic, fwd.fit.summary$bic[fwd_best_bic], col = "red", cex = 1, pch = 20)
```



```
predict.regsubsets = function(object, newdata, id, ...) {
    form = as.formula(object$call[[2]])
    mat = model.matrix(form, newdata)
    coefi = coef(object, id = id)
    xvars = names(coefi)
    mat[, xvars] %*% coefi
}
k = 10
set.seed(1)
folds = sample(1:k, nrow(college.train), replace = TRUE)
cv.errors = matrix(NA, k, n_predictors, dimnames = list(NULL, paste(1:n_predictors)))
# Perform CV
for (j in 1:k) {
    best_subset_method = regsubsets(Outstate ~ ., data = college.train[folds != j,
        ], nvmax = n_predictors, method = "forward")
    for (i in 1:n_predictors) {
        pred = predict(best_subset_method, college.train[folds == j, ], id = i)
        cv.errors[j, i] = mean((college.train$Outstate[folds == j] - pred)^2)
    }
}
# Compute mean cv errors for each model size
mean.cv.errors = apply(cv.errors, 2, mean)
# mean.cv.errors Plot the mean cv errors
par(mfrow = c(1, 1))
plot(mean.cv.errors, type = "b")
min_cverror = which.min(mean.cv.errors)
points(min_cverror, mean.cv.errors[min_cverror], col = "red", cex = 1, pch = 20)
```



```
# Calculating the MSE for model with 6 predictors
x.test = model.matrix(Outstate ~ ., data = college.test)
coef6 = coef(fwd.fit, id = 6)
co.names = names(coef6)[-1]
co.names[1] = "Private"
```

```r
pred = x.test[, names(coef6)] %*% coef6
MSE.forward = mean((college.test$Outstate - pred)^2)
```

The obvious choice might be the model with 14 predictors, as this had both the highest adjusted R^2 and the smallest C_p. However, since the improvement is very small for the larger models it may be unnecesary to have such a large model. See that the model with 6 predictors has the smallest BIC. BIC is defined in a way that normally favors a smaller model. Cross validation also shows that 6 would be a good choice. It is not the one with the lowest mean error, but it is quite good compared to the rest and better than both 5 and 7. The model with 6 predictors has a MSE of 3.8448572×10^6. The 6 predictors are Private, Room.Board, Terminal, perc.alumni, Expend, Grad.Rate.

e)

Model selection using the Lasso method. Since the package `glmnet` does not use the model formula language we need to set up `x` and `y`.

```r
x.train = model.matrix(Outstate ~ ., data = college.train)[, -1]  # -1 is to remove intercept
y.train = college.train$Outstate
x.test = model.matrix(Outstate ~ ., data = college.test)[, -1]
y.test = college.test$Outstate
lasso.fit = glmnet(x.train, y.train, alpha = 1)  # alpha = 1 gives the Lasso method
set.seed(1)
lasso.fit.cv = cv.glmnet(x.train, y.train, alpha = 1)
lasso.lambda = lasso.fit.cv$lambda.1se
lasso.pred = predict(lasso.fit, s = lasso.lambda, newx = x.test)
MSE.lasso = mean(as.numeric((lasso.pred - y.test)^2))
lasso.coeffs = coef(lasso.fit, s = lasso.lambda)
nonzero.names = rownames(lasso.coeffs)[lasso.coeffs[, 1] != 0]
nonzero.names[2] = "Private"
```

Used the function `cv.glmnet` to perform 10 fold cross validation and choose a value for λ. Instead of choosing the model with the lowest MSE in the cross validation, which used all the predictors, we chose the value `lamdba.1se` which is the largest value of λ which gives an error within 1 standard error of the minimum. The value was $\lambda = 367.77$. The reason for this is that it is a much smaller model, which only uses 8 predictors. The predictors were Private, Top10perc, Room.Board, Personal, Terminal, S.F.Ratio, perc.alumni, Expend, Grad.Rate. The MSE on the test set was 3.9033653×10^6.

Problem 2

a)

(i) False
(ii) False
(iii) True
(iv) True (fra video om smoothing splines)

b)

The basis functions are

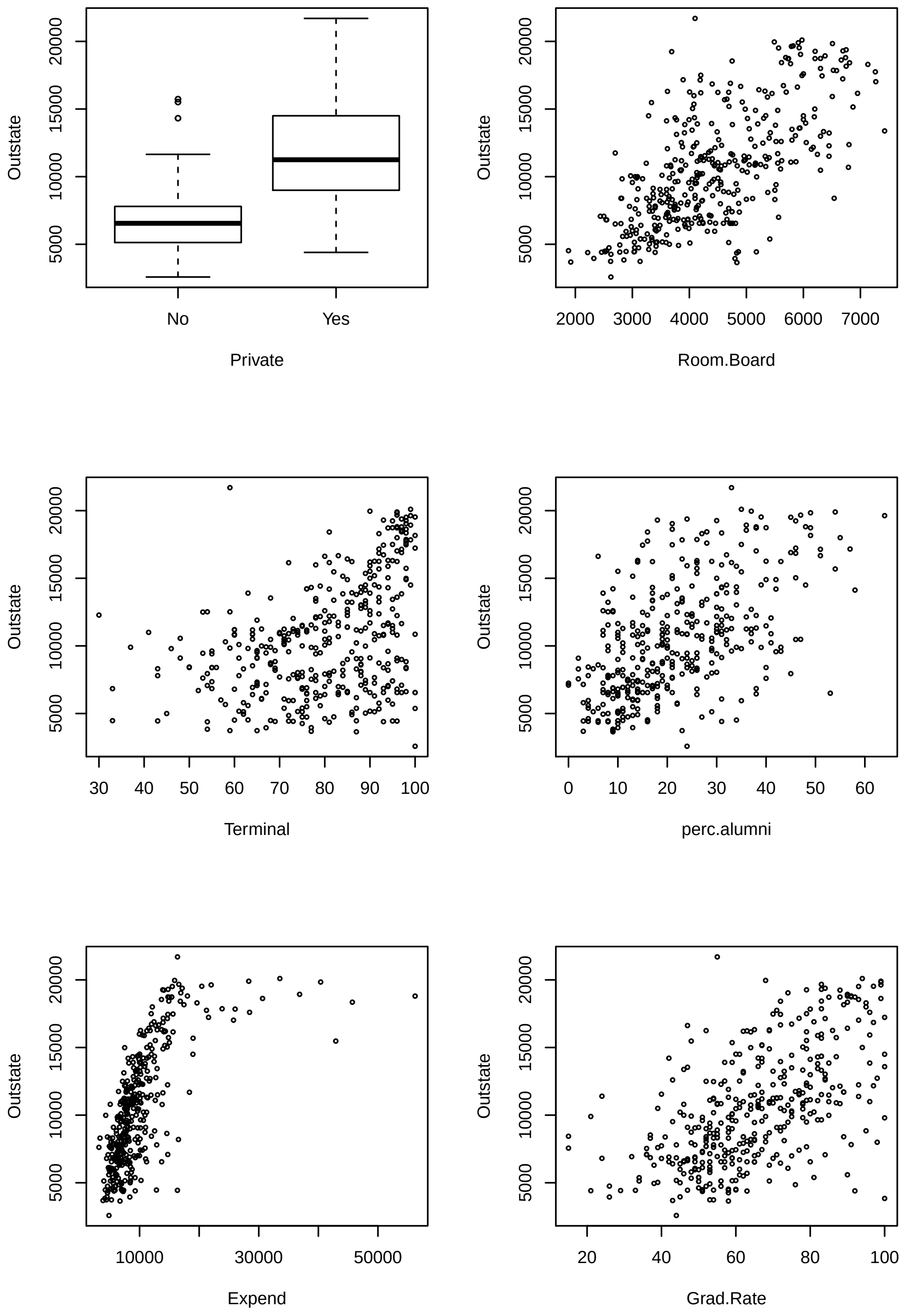
$$
\begin{aligned}
b_1(x) &= x^1 && \text{(7a)}\\
b_2(x) &= x^2 && \text{(7b)}\\
b_3(x) &= x^3 && \text{(7c)}\\
b_4(x) &= (x-q_1)_+^3 && \text{(7d)}\\
b_5(x) &= (x-q_2)_+^3 && \text{(7e)}\\
b_6(x) &= (x-q_3)_+^3 && \text{(7f)}
\end{aligned}
$$

c)

```r
for.reg = regsubsets(Outstate ~ ., data = college.train, method = "forward")
coef.for = coef(for.reg, id = 6)
co.names = names(coef.for)[-1]
co.names[1] = "Private"
```

Will investigate the relationship between `Outstate` and the following 6 predictors: Private, Room.Board, Terminal, perc.alumni, Expend, Grad.Rate.

```r
par(mfrow = c(3, 2))
plot(Outstate ~ Private, data = college.train)
plot(Outstate ~ Room.Board, data = college.train, cex = 0.5)
plot(Outstate ~ Terminal, data = college.train, cex = 0.5)
plot(Outstate ~ perc.alumni, data = college.train, cex = 0.5)
plot(Outstate ~ Expend, data = college.train, cex = 0.5)
plot(Outstate ~ Grad.Rate, data = college.train, cex = 0.5)
```

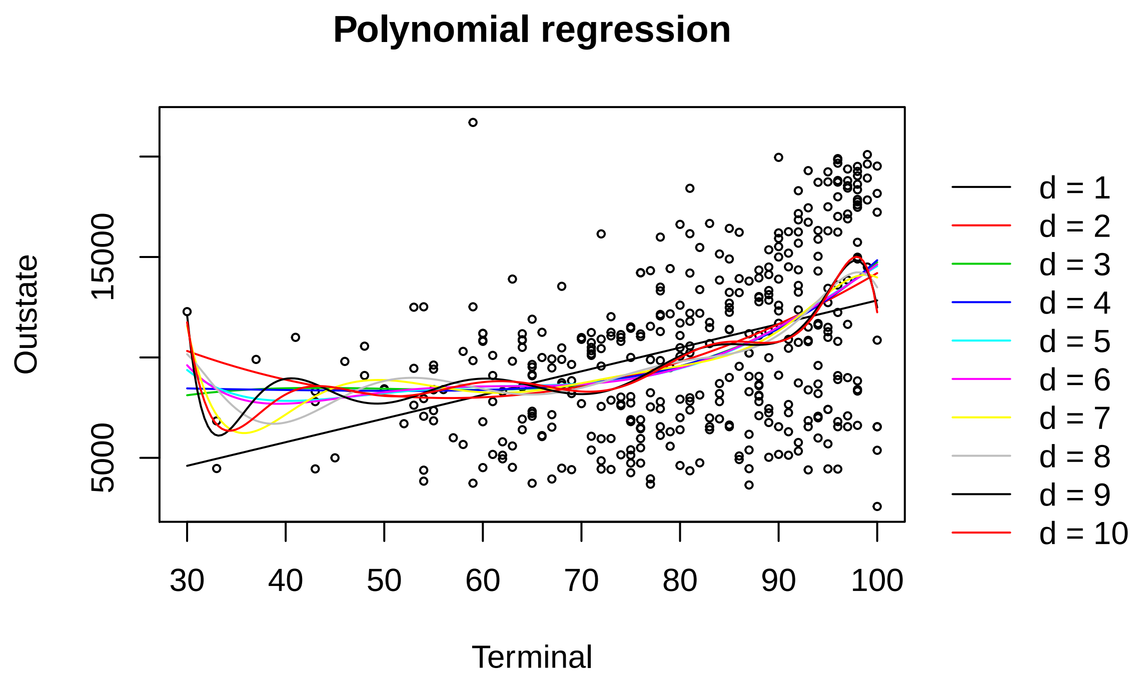

Outstate
5000
10000
15000
20000
No
Yes
Private
Room.Board
2000
3000
4000
5000
6000
7000
Terminal
30
40
50
60
70
80
90
100
perc.alumni
0
10
20
30
40
50
60
Expend
10000
30000
50000
Grad.Rate
20
40
60
80
100

The relationship between `Outstate` and `Room.Board` seems to be approximately linear, same for `perc.alumni`. For `Terminal` on the other hand the slope seems to increase with increasing value for `Terminal`, it could maybe benefit from a non-linear transformation. The relation between `Outstate` and `Expend` does not seem linear, however the relation between `Outstate` and `Grad.Rate` does.

d)

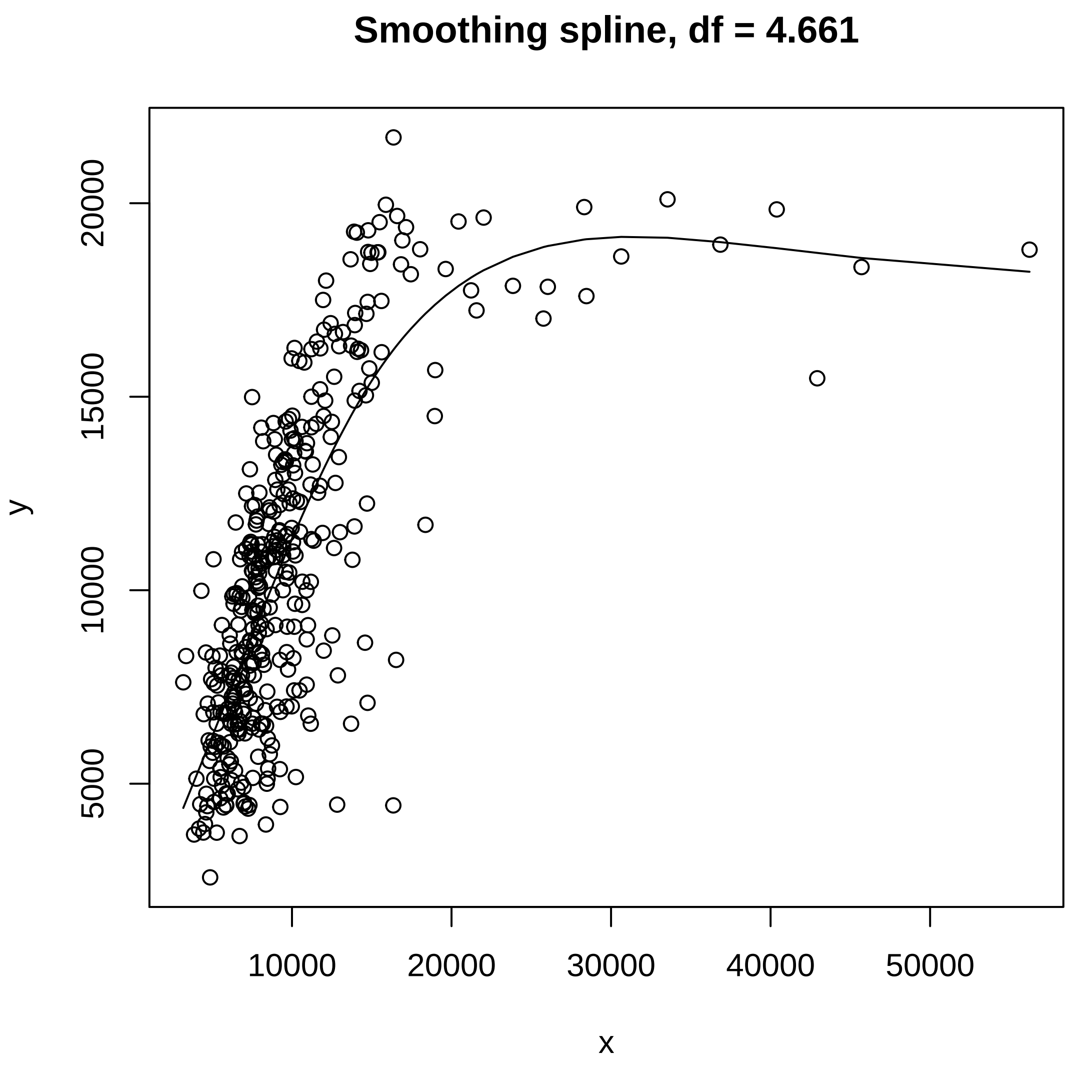
(i) Fit polynomial regression models for `Outstate` as a function of `Terminal` with polynomial degrees $d = 1, \ldots, 10$.

```r
par(mar = c(5.1, 4.1, 4.1, 6.5), xpd = TRUE)
degs = 10
MSE.poly.train = rep(NA, degs)
MSE.poly.test = rep(NA, degs)
plot(Outstate ~ Terminal, data = college.train, main = "Polynomial regression", cex = 0.5)
d <- seq(min(college.train$Terminal), max(college.train$Terminal), length.out = 200)
for (degree in 1:degs) {
    fm <- lm(Outstate ~ poly(Terminal, degree), data = college.train)
    assign(paste("college.train", degree, sep = "."), fm)
    lines(d, predict(fm, data.frame(Terminal = d)), col = degree)
    # Calculate training MSE
    MSE.poly.train[degree] = mean((predict(fm, college.train) - college.train$Outstate)^2)
    MSE.poly.test[degree] = mean((predict(fm, college.test) - college.test$Outstate)^2)
}
legend("topright", inset = c(-0.32, 0.1), legend = paste("d =", 1:degs), col = c(1:degs),
    lty = 1, bty = "n")
```



(ii) Choose a suitable smoothing spline model to predict `Outstate` as a function of `Expend`.

```r
x = college.train$Expend
y = college.train$Outstate
smthspl.fit = smooth.spline(x, y, cv = T)
plot(y ~ x, main = paste("Smoothing spline, df =", round(smthspl.fit$df, 3)))
lines(smthspl.fit)
```



```r
# points(college.test$Expend, college.test$Outstate, pch=2, col=2)
MSE.smthspl.train = mean((predict(smthspl.fit, x)$y - y)^2)
MSE.smthspl.test = mean((predict(smthspl.fit, college.test$Expend)$y - college.test$Outstate)^2)
MSE.smthspl.train
```

```
## [1] 6871281
```

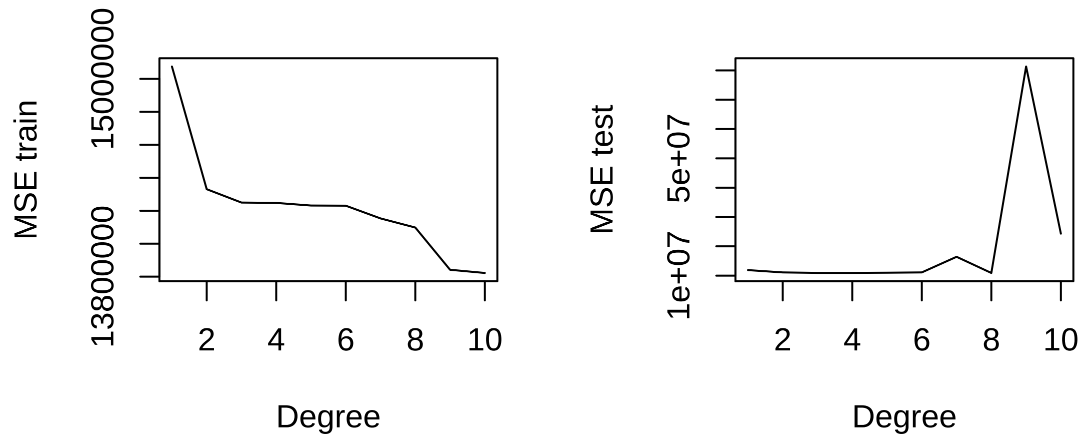
```
MSE.smthspl.test
```

```
## [1] 5943680
```

By putting `cv=T` cross validation is used to determine the degrees of freedom. They are determined to be 4.660711, higher values of `df` gives a more overfitted line.

(iii) Training MSE

```
par(mfrow = c(1, 2))
plot(1:degs, MSE.poly.train, type = "l", xlab = "Degree", ylab = "MSE train")
plot(1:degs, MSE.poly.test, type = "l", xlab = "Degree", ylab = "MSE test")
```



The training MSE for the smoothing spline is 6.8712814×10^6.

Problem 3

a)

(i) False
(ii) True
(iii) True
(iv) False

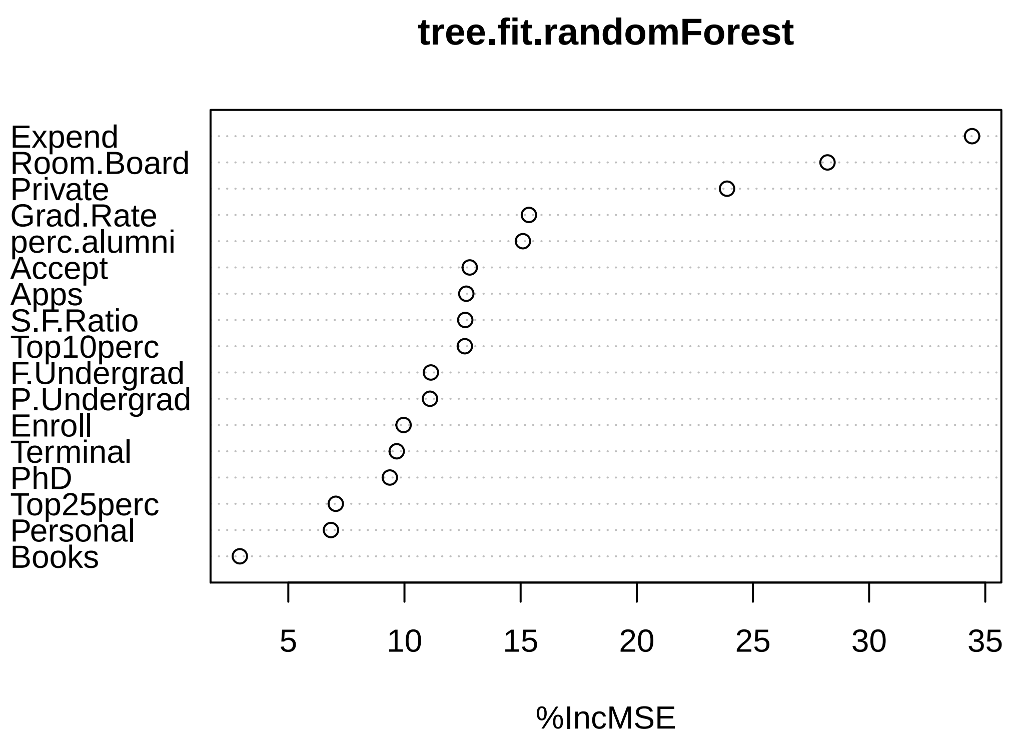
b)

Will use random forest as there are a few strong predictors which makes the trees correlated. A random forest can help decrease the variance by decorrelating the trees. This this is a regression tree $m = p/3$ will be used. A disadvantage of using a random forest is that t does not give one tree, which makes it difficult to visualize.

```r
set.seed(1)
tree.fit.randomForest = randomForest(Outstate ~ ., data = college.train, mtry = ncol(college.train)/3,
    ntree = 500, importance = TRUE)
yhat.randomForest = predict(tree.fit.randomForest, newdata = college.test)
MSE.randomForest = mean((yhat.randomForest - college.test$Outstate)^2)
importance(tree.fit.randomForest)
```

```
##               %IncMSE IncNodePurity
## Private     23.884645     572396197
## Apps        12.660213     119525827
## Accept      12.809286     113271754
## Enroll       9.960338     105290813
## Top10perc   12.597062     367734616
## Top25perc    7.042636     161501521
## F.Undergrad 11.136443     122819717
## P.Undergrad 11.097160     164097235
## Room.Board  28.209705    1012135468
## Books        2.912269      71226082
## Personal     6.834351     119306116
## PhD          9.369483     225362542
## Terminal     9.665515     196862503
## S.F.Ratio   12.615659     390623584
## perc.alumni 15.097476     337449297
## Expend      34.432054    2218648378
## Grad.Rate   15.356554     545391655
```

```r
varImpPlot(tree.fit.randomForest, type = 1)
```



c)

Compare MSEs of the different methods.

```
MSE.forward
```

```
## [1] 3844857
```

```
MSE.lasso
```

```
## [1] 3903365
```

```
MSE.poly.test
```

```
##  [1] 11892400 11103379 10937428 10936549 11005681 11105882 16429293 10914136
##  [9] 81326931 24310822
```

```
MSE.smthspl.test
```

```
## [1] 5943680
```

```
MSE.randomForest
```

```
## [1] 2566908
```

Problem 4

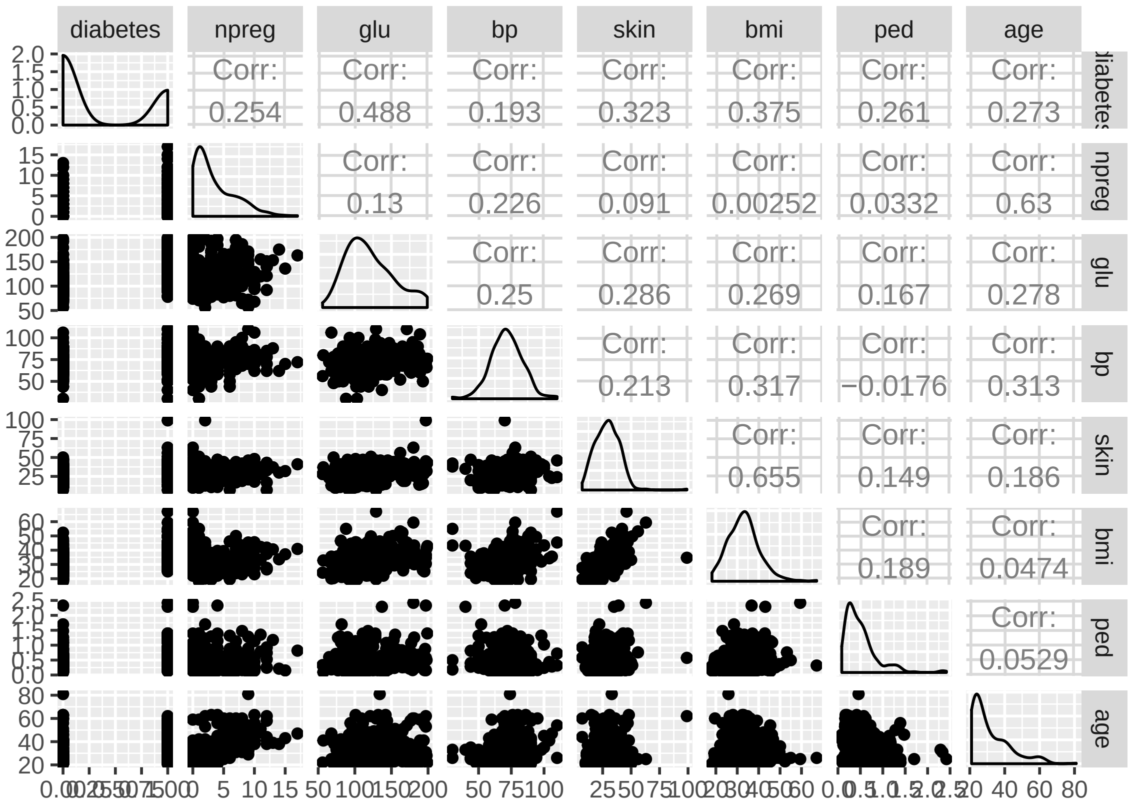
```r
id <- "1Fv6xwKLSZHldRAC1MrcK2mzdOYnbgv0E"  # google file ID
d.diabetes <- dget(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
d.train = d.diabetes$ctrain
d.test = d.diabetes$ctest
```

a)

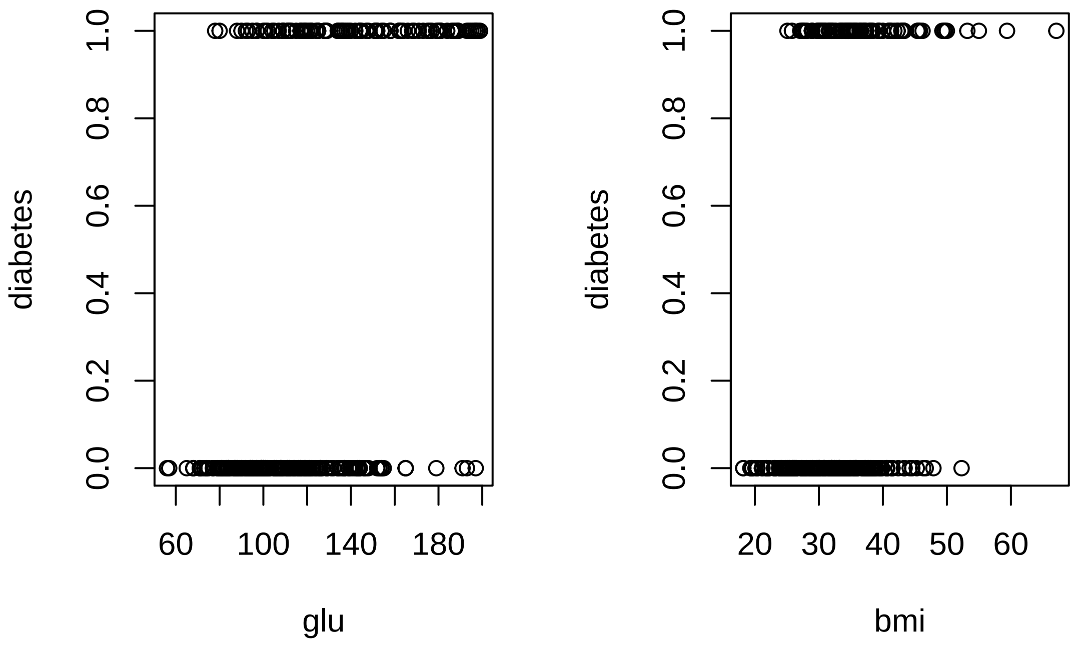
```r
summary(d.train)
```

```
##     diabetes          npreg             glu               bp        
##  Min.   :0.0000   Min.   : 0.000   Min.   : 56.00   Min.   : 30.00  
##  1st Qu.:0.0000   1st Qu.: 1.000   1st Qu.: 96.75   1st Qu.: 64.00  
##  Median :0.0000   Median : 2.000   Median :114.00   Median : 71.00  
##  Mean   :0.3333   Mean   : 3.467   Mean   :120.13   Mean   : 71.56  
##  3rd Qu.:1.0000   3rd Qu.: 5.250   3rd Qu.:140.25   3rd Qu.: 80.00  
##  Max.   :1.0000   Max.   :17.000   Max.   :199.00   Max.   :110.00  
##       skin            bmi             ped              age       
##  Min.   : 7.00   Min.   :18.20   Min.   :0.0850   Min.   :21.00  
##  1st Qu.:22.00   1st Qu.:27.98   1st Qu.:0.2567   1st Qu.:23.00  
##  Median :29.00   Median :32.80   Median :0.4150   Median :27.00  
##  Mean   :29.14   Mean   :33.03   Mean   :0.5004   Mean   :31.55  
##  3rd Qu.:36.00   3rd Qu.:37.12   3rd Qu.:0.6210   3rd Qu.:37.25  
##  Max.   :99.00   Max.   :67.10   Max.   :2.4200   Max.   :81.00
```

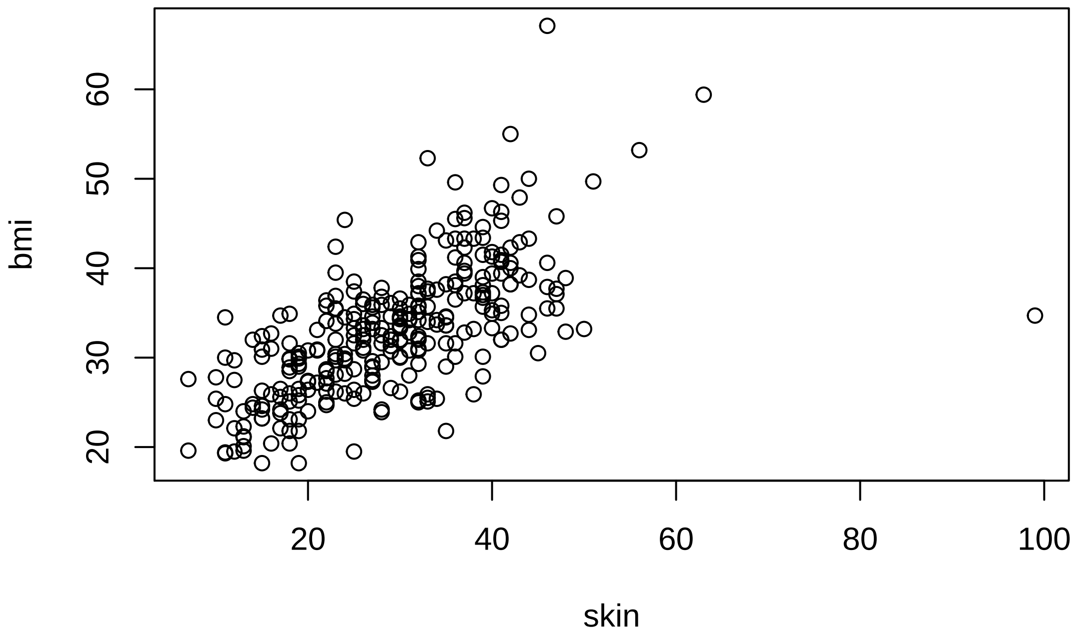
```r
ggpairs(d.train)
```



```r
par(mfrow = c(1, 2))
plot(diabetes ~ glu, data = d.train)
plot(diabetes ~ bmi, data = d.train)
```



```r
par(mfrow = c(1, 1))
plot(bmi ~ skin, data = d.train)
```



(i) True
(ii) True
(iii) True
(iv) True? Ser på ggpairs plotet at sannsynlighetsfordeligen er forskjøvet mot 0

b)

```
d.train$diabetes <- as.factor(d.train$diabetes)
d.test$diabetes <- as.factor(d.test$diabetes)
svmfit_linear = svm(diabetes ~ ., data = d.train, kernel = "linear", cost = 1, scale = FALSE)
dim(d.train)
```

```
## [1] 300   8
```

```
summary(d.train)
```

```
##  diabetes     npreg             glu               bp              skin
##  0:200    Min.   : 0.000   Min.   : 56.00   Min.   : 30.00   Min.   : 7.00
##  1:100    1st Qu.: 1.000   1st Qu.: 96.75   1st Qu.: 64.00   1st Qu.:22.00
##           Median : 2.000   Median :114.00   Median : 71.00   Median :29.00
##           Mean   : 3.467   Mean   :120.13   Mean   : 71.56   Mean   :29.14
##           3rd Qu.: 5.250   3rd Qu.:140.25   3rd Qu.: 80.00   3rd Qu.:36.00
##           Max.   :17.000   Max.   :199.00   Max.   :110.00   Max.   :99.00
##       bmi              ped               age
##  Min.   :18.20   Min.   :0.0850   Min.   :21.00
##  1st Qu.:27.98   1st Qu.:0.2567   1st Qu.:23.00
##  Median :32.80   Median :0.4150   Median :27.00
##  Mean   :33.03   Mean   :0.5004   Mean   :31.55
##  3rd Qu.:37.12   3rd Qu.:0.6210   3rd Qu.:37.25
##  Max.   :67.10   Max.   :2.4200   Max.   :81.00
```

```
summary(svmfit_linear)
```

```
##
## Call:
## svm(formula = diabetes ~ ., data = d.train, kernel = "linear", cost = 1,
##     scale = FALSE)
##
##
## Parameters:
##    SVM-Type:  C-classification
##  SVM-Kernel:  linear
##        cost:  1
##
## Number of Support Vectors:  140
##
##  ( 70 70 )
##
##
## Number of Classes:  2
##
## Levels:
##  0 1
```

To run cross-validation over a grid of two tuning parameters, you can use the `tune()` function where `ranges` defines the grid points as follows:

```
CV_linear = tune(svm, diabetes ~ ., data = d.train, kernel = "linear", ranges = list(cost = c(0.001,
    0.01, 0.1, 1, 5, 10, 50)))
summary(CV_linear)
best_model = CV_linear$best.model
summary(best_model)
# best_model = svm(diabetes~., data = d.train, kernel = 'linear', cost = 0.1,
# scale=FALSE)
y_pred = predict(best_model, d.test)
table(predict = y_pred, truth = d.test[, 1])
```