1. Analysis of the ALL data set.

(a) Define an indicator variable IsB such that IsB=TRUE for B-cell patients and IsB=FALSE for T-cell patients.

(b) Use two genes "39317_at" and "38018_g_at" to fit a classification tree for IsB. Print out the confusion matrix. Plot ROC curve for the tree.

(c) Find its empirical misclassification rate (mcr), false negative rate (fnr) and specificity. Find the area under curve (AUC) for the ROC curve.

(d) Use 10-fold cross-validation to estimate its real false negative rate (fnr). What is your estimated fnr?

(e) Do a logistic regression, using genes "39317_at" and "38018_g_at" to predict IsB. Find an 80% confidence interval for the coefficient of gene "39317_at".

(f) Use n-fold cross-validation to estimate misclassification rate (mcr) of the logistic regression classifier. What is your estimated mcr?

(g) Conduct a PCA on the scaled variables of the whole ALL data set (NOT just the two genes used above). We do this to reduce the dimension in term of genes (so this PCA should be done on the transpose of the matrix of expression values). To simply our future analysis, we use only the first K principal components (PC) to represent the data. How many PCs should be used? Explain how you arrived at your conclusion. Provide graphs or other R outputs to support your choice.

(h) Do a SVM classifier of IsB using only the first five PCs. (The number K=5 is fixed so that we all use the same classifier. You do not need to choose this number in the previous part (g).) What is the sensitivity of this

(i) Use leave-one-out cross-validation to estimate misclassification rate (mcr) of the SVM classifier. Report your estimate.

(j) If you had to choose between classifiers in part (e) and in part (h), which one would you choose? Why?

You should put answers to the questions in the PDF file. That means, for (a), provide the R command; for (b), provide the printout and the plot; for (c) provide the numerical answers; et al. Remember to answer each question directly. The grader should not have to pick out the numerical answers from the R outputs.

The R commands that you used to get those printout/plots et al. should be submitted in the separate R script file.

A)

Rscript:

```
library(ALL);data(ALL)
```

```
IsB <- factor(ALL$BT %in% c("B","B1","B2","B3","B4"))
IsB
```

Answer:

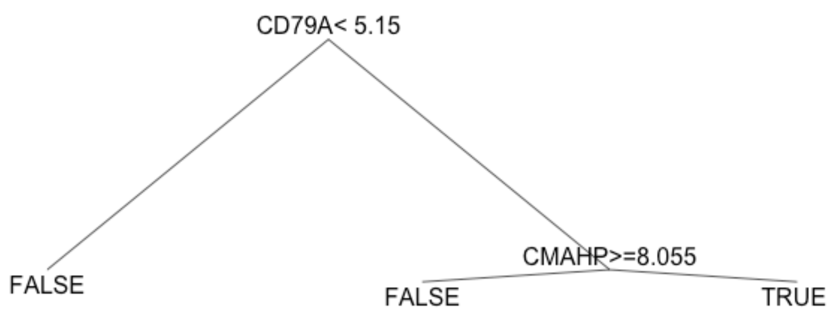
```
[1] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE
 [14] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [27] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [40] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [53] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [66] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [79] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
TRUE  TRUE
 [92] TRUE  TRUE  TRUE  TRUE  FALSE FALSE FALSE FALSE FALSE FALSE FALSE
FALSE FALSE
[105] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
FALSE FALSE
[118] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
Levels: FALSE TRUE
```

B)
Rscript:

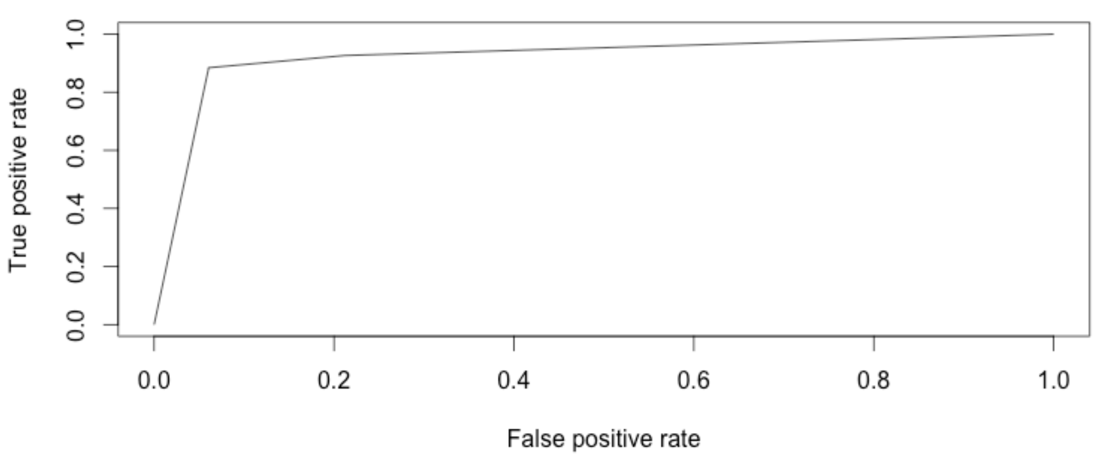
```
install.packages('rpart')
library("hgu95av2.db")
library(ALL);data(ALL)

names <- c("39317_at", "38018_g_at")
expr.data <- exprs(ALL)[names,]
symb <- mget(names, env = hgu95av2SYMBOL)
ALLBTnames <- ALL[names, ]
probedat <- as.matrix(exprs(ALLBTnames))
row.names(probedat) <- unlist(symb)

require(rpart)
B.stage <- factor(IsB)
c.tr <- rpart(B.stage~., data = data.frame(t(probedat)))
plot(c.tr, branch=0,margin=0.1)
text(c.tr, digits=3,)
rpartpred <- predict(c.tr, type="class")
table(rpartpred, B.stage)
```

```
install.packages('ROCR')
library("ROCR")
pred.prob <- predict(c.tr, type="prob")[,2]
pred <- prediction(pred.prob, IsB=="TRUE")
perf <- performance(pred,"tpr","fpr")
plot(perf)
```

Answer:




```
  B.stage
rpartpred FALSE TRUE
   FALSE    31   11
   TRUE      2   84
```



C)
Rscript:

```
mcr<-(11+2)/(31+11+2+84)
mcr
fnr<-11/(11+84)
fnr
spe<-31/(2+31)
spe
performance(pred,"auc")
```

Answer:
empirical misclassification rate (mcr) = 0.1015625
false negative rate (fnr) = 0.1157895
specificity = 0.9393939
area under curve (AUC) for the ROC curve = 0.922807
Slot "y.values":
[[1]]
[1] 0.922807

D)
Rscript:

```
require(caret)
n <- length(rpartpred)
index <- 1:n
K <- 10
folds <- createFolds(index, k=K)
fnr.cv.raw <- rep(NA, K)
for (i in 1:K) {
  testID <- folds[[i]]
  c.tr <- rpart(IsB[-testID]~., data=data.frame(t(expr.data)[-testID,]))
  tr.pred <- predict(c.tr, newdata=data.frame(t(expr.data)[-testID,]), type="class")
  fnr.cv.raw[i] <- mean(tr.pred[testID] == 'FALSE' & IsB[testID] ==
'TRUE')/mean(IsB[testID] == 'TRUE')
}
fnr.cv <- mean(fnr.cv.raw)
fnr.cv
```

Answer:
estimated fnr: 0.1630556

E)
Rscript:

```
prob.name <- c("39317_at", "38018_g_at")
expr.data <- exprs(ALL)[prob.name,]
data.lgr <- data.frame(IsB, t(expr.data))
fit.lgr <- glm(IsB~., family=binomial(link='logit'), data=data.lgr)
```

```
pred.prob <- predict(fit.lgr, data=data.lgr$expr.data, type="response")
pred.B1 <- factor(pred.prob> 0.5, levels=c(TRUE,FALSE), labels=c("Bcell","not
Bcell"))
IsBcell <- factor(IsB, levels=c(TRUE,FALSE), labels=c("Bcell","not Bcell"))
table(pred.B1, IsBcell)


y <- as.numeric(IsB==TRUE)
data.CI <- exprs(ALL)["39317_at", ]
data <- glm(data.frame(y, data.CI))
confint(data, level=0.8)
```

Answer:
Logistic regression:

```
       IsBcell
pred.B1     Bcell not Bcell
  Bcell       90        6
  not Bcell    5       27
```

80% confidence interval for “39317_at”

```
               10 %       90 %
(Intercept)  1.7157421  2.1038847
data.CI     -0.2039277 -0.1469204
```

80% CI for B_0 = (1.72,2.01)
80% CI for B_1 = (-0.2, -0.15)

F)
Rscript:

```
install.packages('caret');
require(caret);
data.lgr <- data.frame(IsB,t(expr.data))
n <- dim(data.lgr)[1]
index <- 1:n
K <- 10
flds <- createFolds(index, k=K)
mcr.cv.raw <- rep(NA, K)
for (i in 1:K) {
  testID <- flds[[i]]
  data.tr <- data.lgr[-testID,]
  data.test <- data.lgr[testID,]
  fit.lgr <- glm(IsB~., family=binomial(link='logit'), data=data.tr)
  pred.prob <- predict(fit.lgr, newdata=data.test, type="response")
  pred <- (pred.prob> 0.5)
```

```
  mcr.cv.raw[i] <- sum(pred!=data.test$IsB)/length(pred)
}
mcr.cv <- mean(mcr.cv.raw)
mcr.cv
```

Answer:
estimated mcr = .09386447 = 9.4%

G)
Rscript:

```
pca.all <- prcomp(t(exprs(ALL)), scale=TRUE)
summary(pca.all)
PropVar <- summary(pca.all)$importance[2,]
plot(1:length(PropVar), PropVar, xlab='number of principal components',
ylab='proportion of variance explained',cex=0.3)
```

Answer:

```
Importance of components:
                        PC1     PC2      PC3     PC4      PC5      PC6      PC7
Standard deviation     47.8103 36.9157 27.73208 24.0204 21.29449 19.64675
18.00937
Proportion of Variance  0.1811  0.1079  0.06092  0.0457  0.03592  0.03057  0.02569
Cumulative Proportion   0.1811  0.2890  0.34991  0.3956  0.43153  0.46211
0.48780
                         PC8      PC9     PC10     PC11     PC12     PC13    PC14
Standard deviation     16.52815 16.08110 15.68492 14.73970 13.49120 13.46128
13.1528
Proportion of Variance  0.02164  0.02048  0.01949  0.01721  0.01442  0.01435
0.0137
Cumulative Proportion   0.50943  0.52992  0.54940  0.56661  0.58103  0.59538
0.6091
                        PC15     PC16     PC17     PC18     PC19     PC20    PC21
Standard deviation     12.50326 11.62651 11.33948 10.95969 10.56977 10.27269
9.98280
Proportion of Variance  0.01238  0.01071  0.01018  0.00951  0.00885  0.00836
0.00789
Cumulative Proportion   0.62147  0.63217  0.64236  0.65187  0.66072  0.66908
0.67698
                       PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29
Standard deviation     9.76071 9.69351 9.35307 9.07879 8.97473 8.85997 8.72421
8.59119
Proportion of Variance 0.00755 0.00744 0.00693 0.00653 0.00638 0.00622 0.00603
0.00585
Cumulative Proportion  0.68452 0.69196 0.69889 0.70542 0.71180 0.71802
0.72405 0.72989
                       PC30    PC31    PC32    PC33    PC34    PC35    PC36   PC37
```

Standard deviation 8.53111 8.27069 8.23309 8.08897 8.07028 7.83775 7.80235 7.7043
Proportion of Variance 0.00576 0.00542 0.00537 0.00518 0.00516 0.00487 0.00482 0.0047
Cumulative Proportion 0.73566 0.74108 0.74645 0.75163 0.75679 0.76165 0.76648 0.7712

PC38 PC39 PC40 PC41 PC42 PC43 PC44 PC45
Standard deviation 7.56167 7.54920 7.47852 7.40003 7.33338 7.21207 7.18165 7.07957
Proportion of Variance 0.00453 0.00451 0.00443 0.00434 0.00426 0.00412 0.00409 0.00397
Cumulative Proportion 0.77571 0.78022 0.78465 0.78899 0.79325 0.79737 0.80145 0.80542

PC46 PC47 PC48 PC49 PC50 PC51 PC52 PC53
Standard deviation 7.00761 6.88692 6.86142 6.81489 6.79102 6.70541 6.68737 6.61719
Proportion of Variance 0.00389 0.00376 0.00373 0.00368 0.00365 0.00356 0.00354 0.00347
Cumulative Proportion 0.80931 0.81307 0.81680 0.82048 0.82413 0.82769 0.83123 0.83470

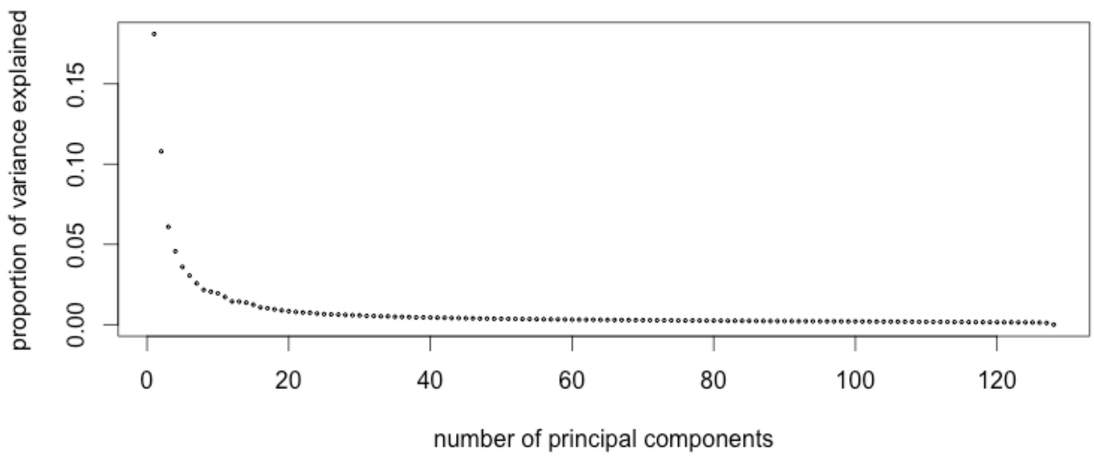
PC54 PC55 PC56 PC57 PC58 PC59 PC60 PC61
Standard deviation 6.58283 6.51855 6.4543 6.42488 6.40876 6.33493 6.2549 6.22671
Proportion of Variance 0.00343 0.00337 0.0033 0.00327 0.00325 0.00318 0.0031 0.00307
Cumulative Proportion 0.83813 0.84150 0.8448 0.84807 0.85132 0.85450 0.8576 0.86067

PC62 PC63 PC64 PC65 PC66 PC67 PC68 PC69
Standard deviation 6.19791 6.17728 6.13009 6.07863 6.0457 6.00987 5.98143 5.95744
Proportion of Variance 0.00304 0.00302 0.00298 0.00293 0.0029 0.00286 0.00283 0.00281
Cumulative Proportion 0.86371 0.86674 0.86971 0.87264 0.8755 0.87839 0.88123 0.88404

PC70 PC71 PC72 PC73 PC74 PC75 PC76 PC77
Standard deviation 5.87113 5.84515 5.82817 5.76546 5.74950 5.69443 5.67019 5.66516
Proportion of Variance 0.00273 0.00271 0.00269 0.00263 0.00262 0.00257 0.00255 0.00254
Cumulative Proportion 0.88677 0.88948 0.89217 0.89480 0.89742 0.89999 0.90253 0.90508

PC78 PC79 PC80 PC81 PC82 PC83 PC84 PC85
Standard deviation 5.64871 5.60202 5.56279 5.53503 5.5092 5.48405 5.44800 5.42787
Proportion of Variance 0.00253 0.00249 0.00245 0.00243 0.0024 0.00238 0.00235 0.00233

Cumulative Proportion 0.90760 0.91009 0.91254 0.91497 0.9174 0.91975 0.92210 0.92444
PC86 PC87 PC88 PC89 PC90 PC91 PC92 PC93
Standard deviation 5.36975 5.33498 5.29293 5.28715 5.25939 5.22066 5.18953 5.17319
Proportion of Variance 0.00228 0.00225 0.00222 0.00221 0.00219 0.00216 0.00213 0.00212
Cumulative Proportion 0.92672 0.92898 0.93119 0.93341 0.93560 0.93776 0.93989 0.94201
PC94 PC95 PC96 PC97 PC98 PC99 PC100 PC101
Standard deviation 5.1529 5.10942 5.09202 5.07675 5.03399 5.0260 4.99505 4.96053
Proportion of Variance 0.0021 0.00207 0.00205 0.00204 0.00201 0.0020 0.00198 0.00195
Cumulative Proportion 0.9441 0.94618 0.94824 0.95028 0.95228 0.9543 0.95626 0.95821
PC102 PC103 PC104 PC105 PC106 PC107 PC108 PC109
Standard deviation 4.92004 4.8988 4.86395 4.85237 4.81879 4.80002 4.72967 4.69107
Proportion of Variance 0.00192 0.0019 0.00187 0.00186 0.00184 0.00182 0.00177 0.00174
Cumulative Proportion 0.96013 0.9620 0.96390 0.96577 0.96761 0.96943 0.97120 0.97295
PC110 PC111 PC112 PC113 PC114 PC115 PC116 PC117
Standard deviation 4.68160 4.64703 4.61168 4.59981 4.56873 4.54519 4.45476 4.42230
Proportion of Variance 0.00174 0.00171 0.00168 0.00168 0.00165 0.00164 0.00157 0.00155
Cumulative Proportion 0.97468 0.97639 0.97808 0.97975 0.98141 0.98304 0.98462 0.98616
PC118 PC119 PC120 PC121 PC122 PC123 PC124 PC125
Standard deviation 4.38206 4.36821 4.30457 4.27980 4.25439 4.18120 4.16837 4.14619
Proportion of Variance 0.00152 0.00151 0.00147 0.00145 0.00143 0.00138 0.00138 0.00136
Cumulative Proportion 0.98769 0.98920 0.99066 0.99212 0.99355 0.99493 0.99631 0.99767
PC126 PC127 PC128
Standard deviation 4.00554 3.65401 1.028e-13
Proportion of Variance 0.00127 0.00106 0.000e+00
Cumulative Proportion 0.99894 1.00000 1.000e+00



I think 1 to 11 PCs should be used because there is a rapid drop of proportion of variance till PC11.

H)

Rscript:

```
install.packages('e1071');
library(e1071)
data.pca <- pca.all$x[,1:5]
svmest <- svm(IsB~data.pca,type="C-classification",kernel="linear")
svmpred <- predict(svmest,data.pca)
table(svmpred,IsB)
tpr.svm <- mean(svmpred==IsB &
IsB==TRUE)/(mean(svmpred==IsB&IsB==TRUE)+mean(svmpred!=IsB&IsB==TRU
E))
tpr.svm
```

Answer:

```
     IsB
svmpred FALSE TRUE
  FALSE    30    1
  TRUE      3   94
```

Sensitivity = 0.9894737

I)

Rscript:

```
n <- length(IsB)
mcr.cv.raw <-rep (NA,n)
```

```
for (i in 1:n) {
  svmest <- svm(data.pca[-i,],IsB[-i],type="C-classification",kernel="linear")
  svmpred <- predict(svmest,t(data.pca[i,]))
  mcr.cv.raw[i] <-mean(svmpred!=IsB[i])
}
mcr.cv <- mean(mcr.cv.raw)
mcr.cv
```

Answer:
estimate misclassification rate = 0.0390625 = 3.9%

J)
Answer:
MCR in E part is 11/128 = .0859 = 8.6%
MCR in H part is 4/128 = 0.0312= 3.12%
As MCR for SVM method is less than logistic regression so I will choose SVM method i.e. h part.

2**. Choosing Classifiers and Number of Principal Components for PCA reduced iris data set.**

In the last example of this module, we compared three classifiers on the iris data by working on the first three principal components. We choose the best classifiers based on cross-validated misclassification rate. We can also choose the number of principal components to use by cross-validation, instead of fixing it at K=3.

Use the leave-one-out cross-validation to choose the number of principal components together with the classifier. Please report the empirical misclassification rates (on whole data set) and the leave-one-out cross-validation misclassification rates for each value of K=1, 2, 3, 4 principal components and for each of the three classifiers: logistic regression, support vector machine and classification tree. Based on those rates, what is your choice?

Note: when you fit the logistic regression with K=1 principal component, then the PC1 becomes a vector instead of a matrix. You will need to modify the code for logistic regression for K=1 differently from the other values of K=2, 3, 4.

2)

Rscript:

```
# Answer 2
install.packages("VGAM")
library("VGAM")
pca.iris <- prcomp(iris[,1:4], scale=TRUE)
Species <- iris$Species
data.pca <- pca.iris$x[,1]

n <- length(Species)
iris2 <- data.frame(Species, data.pca)
iris2.lgr <- vglm(Species~., family=multinomial, data=iris2)
pred.prob <- predict(iris2.lgr, iris2[,2,drop=F], type="response")
pred.lgr <- apply(pred.prob, 1, which.max)
pred.lgr <- factor(pred.lgr, levels=c("1","2","3"), labels=levels(iris2$Species))
mcr.lgr <- mean(pred.lgr!=iris2$Species)
### leave-one-out cross validation
mcr.cv.raw<-rep(NA, n)
for (i in 1:n) {
  fit.lgr <- vglm(Species~., family=multinomial, data=iris2[-i,])
  pred.prob <- predict(fit.lgr, iris2[i,-1, drop=F], type="response")
  pred <- apply(pred.prob, 1, which.max)
  pred <- factor(pred, levels=c("1","2","3"), labels=levels(iris2$Species))
```

```
  mcr.cv.raw[i] <- mean(pred!=Species[i])
}
mcr.cv <- mean(mcr.cv.raw)
c(mcr.lgr, mcr.cv)
# SVM mcr
svmest <- svm(data.pca, Species, type = "C-classification", kernel = "linear") #train
SVM
svmpred <- predict(svmest , data.pca)
mcr.svm<- mean(svmpred!=Species)
mcr.svm
mat<-data.frame(data.pca)
### leave-one-out cross validation
mcr.cv.raw<-rep(NA, n)
for (i in 1:n) {
  svmest <- svm(mat[-i,], Species[-i], type = "C-classification", kernel ="linear")
  svmpred <- predict(svmest, t(mat[i,]))
  mcr.cv.raw[i]<- mean(svmpred!=Species[i])
}
mcr.cv<-mean(mcr.cv.raw)
c(mcr.svm, mcr.cv)

#Classification tree
fit <- rpart(Species ~ ., data = iris2, method = "class")
pred.tr<-predict(fit, iris2, type = "class")
mcr.tr <- mean(pred.tr!=Species)
### leave-one-out cross validation
mcr.cv.raw <- rep(NA, n) #A vector to save mcr validation
for (i in 1:n) {
  fit.tr <- rpart(Species ~ ., data = iris2[-i,], method = "class") #train the tree without
i-th observation
  pred <- predict(fit.tr, iris2[i,], type = "class")#use tree to predict i-th observation
class
  mcr.cv.raw[i] <- mean(pred!=Species[i]) #check misclassifion
}
mcr.cv<-mean(mcr.cv.raw) #average the mcr over all n rounds.
c(mcr.tr, mcr.cv)


get_mcr_values <- function(k){
  data.pca <- pca.iris$x[,1:k]
  n <- length(Species)
  iris2 <- data.frame(Species, data.pca)
  iris2.lgr <- vglm(Species~., family=multinomial, data=iris2)
  pred.prob <- predict(iris2.lgr, iris2[,-1,drop=F], type="response")
  pred.lgr <- apply(pred.prob, 1, which.max)
  pred.lgr <- factor(pred.lgr, levels=c("1","2","3"), labels=levels(iris2$Species))
```

```
  mcr.lgr <- mean(pred.lgr!=iris2$Species)
  ### leave-one-out cross validation
  mcr.cv.raw<-rep(NA, n)
  for (i in 1:n) {
    fit.lgr <- vglm(Species~., family=multinomial, data=iris2[-i,])
    pred.prob <- predict(fit.lgr, iris2[i,-1, drop=F], type="response")
    pred <- apply(pred.prob, 1, which.max)
    pred <- factor(pred, levels=c("1","2","3"), labels=levels(iris2$Species))
    mcr.cv.raw[i] <- mean(pred!=Species[i])
  }
  mcr.cv <- mean(mcr.cv.raw)
  print(c("Logistic regression",mcr.lgr, mcr.cv))

  # SVM mcr
  svmest <- svm(data.pca, Species, type = "C-classification", kernel = "linear") #train
SVM
  svmpred <- predict(svmest , data.pca)
  mcr.svm<- mean(svmpred!=Species)
  ### leave-one-out cross validation
  mcr.cv.raw<-rep(NA, n)
  for (i in 1:n) {
    svmest <- svm(data.pca[-i,], Species[-i], type = "C-classification", kernel ="linear")
    svmpred <- predict(svmest, t(data.pca[i,]))
    mcr.cv.raw[i]<- mean(svmpred!=Species[i])
  }
  mcr.cv<-mean(mcr.cv.raw)
  print(c("SVM",mcr.svm, mcr.cv))

  #Classification tree
  fit <- rpart(Species ~ ., data = iris2, method = "class")
  pred.tr<-predict(fit, iris2, type = "class")
  mcr.tr <- mean(pred.tr!=Species)
  ### leave-one-out cross validation
  mcr.cv.raw <- rep(NA, n) #A vector to save mcr validation
  for (i in 1:n) {
    fit.tr <- rpart(Species ~ ., data = iris2[-i,], method = "class") #train the tree without
i-th observation
    pred <- predict(fit.tr, iris2[i,], type = "class")#use tree to predict i-th observation
class
    mcr.cv.raw[i] <- mean(pred!=Species[i]) #check misclassifion
  }
  mcr.cv<-mean(mcr.cv.raw) #average the mcr over all n rounds.
  print(c("Classification tree",mcr.tr, mcr.cv))

}
get_mcr_values(2)
```

get_mcr_values(3)
get_mcr_values(4)

Answer:

	Empirical	Leave one out
K=1		
Logistic Regression =	0.07333333	0.07333333
SVM =	0.07333333	0.08000000
Classification tree =	0.06666667	0.10666667
K=2		
Logistic Regression =	0.08	0.08
SVM =	0.08667	0.08667
Classification tree =	0.0667	0.10667
K=3		
Logistic Regression =	0.0133	0.02667
SVM =	0.02667	0.04667
Classification tree =	0.0667	0.14
K=4		
Logistic Regression =	0.0133	0.02
SVM =	0.02	0.02667
Classification tree =	0.0667	0.14

Based on the above rates I would choose K=4 as the values for empirical and leave one out is really close for K=4.
I would also consider SVM as the best classifier method as both the values are really close