DS 8002 Machine Learning Project 2 – Unsupervised and Supervised Learning (December 2016)

Najlis, Bernardo J. (Student Number: 500744793)

Abstract—**In this project, you will apply several algorithms to two data sets. Please answer each question in the order they appear. Do not skip to later steps to answer earlier questions that ask you to predict outcomes based on your analysis of the data and understanding of the algorithms.**
Submit your report in D2L by midnight on the due date.

I. Introduction

In this project we perform analysis on two the same data sets (iris and contact lens) as in the previous project using five different types of machine learning algorithms and techniques:

- Clustering – Simple K-means
- PCA – Principal Component Analysis
- SVM – Support Vector Machines
- Random Forest
- AdaBoost

The analysis was done using R and libraries for each type of algorithm used.

This report is accompanied by an R markup document with all the code and its output to support all answers and reasoning presented here.

II. SVM

Which kernel works better? Why?

With **Iris**, using tune() to select the best cost for each of the four kernels evaluated (linear, polynomial, radial and sigmoid). As the accuracy varies depending on the test set, through several runs the best kernel is **Polynomial.** Here is one of the sample runs:

SVM Kernel	Best Cost	Accuracy
Linear	100	0.9623
Polynomial	10	1
Radial	1	0.98
Sigmoid	1	0.931

With **Contact Lenses** I also used tune() to select the best cost for each of the four kernels evaluated (linear, polynomial, radial and sigmoid), and the best kernel through multiple runs is also **Polynomial.**

SVM Kernel	Best Cost	Accuracy
Linear	1	0.6364
Polynomial	10	0.9091
Radial	10	0.7273
Sigmoid	10	0.6364

Polynomial is the best probably because it can provide a model to separate classes with higher complexity than linear, radial and sigmoid.

How did the SVM compare to the classifiers from Project 1 in terms of training time and performance?

The table below summarizes my conclusions when comparing SVM with the classifiers from project 1 (KNN, Decision Trees and Multilayer Perceptron). I also added the "Knowledge Extraction" as another variable to consider (if required by the use case). Overall, SVM provides higher performance than KNN and Decision trees but at a higher cost, still providing some degree of knowledge that can be extracted. For classifiers, SVM is probably the mid-range best option if the training time can be afforded (i.e. batch training use case): provides high performance at a reasonable increase in training time.

	Training Time	Performance	Knowledge Extraction
SVM	**MED**	**HIGH**	**MED**
KNN	**LOW**	**LOW**	**MED**
Decision Trees	**LOW**	**LOW**	**HIGH**
Perceptron	**HIGH**	**HIGH**	**LOW**

III. PCA – SVM

Run PCA and then run SVM on the reduced data.

With both data sets we first apply log() transformation on the data, and we center and scale when doing PCA analysis.

How many principal components did you pick? Why?

On Iris, I picked the first two components, which account for 96% of the total variance.

On Contact lenses, I picked three components as they all have the same variance, leading to 75% percent of total variance. Accuracy will suffer by losing 25% of the total variance, but it is worth trying to see by how much.

How did the SVM perform on the reduced data compared to the original data?

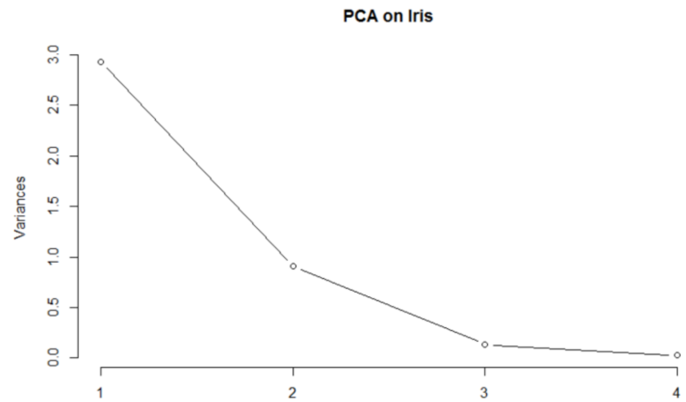
On Iris, as the best kernel is Polynomial, the comparison analysis is based just on that kernel. **The accuracy is about 10% lower than when using all original features.** This is expected as we are only using a subset of the features, but still a good tradeoff ratio: reducing 50 percent of features (which means we also reduced training time by half) we only lost 10 percent of accuracy.

On contact lenses, the best we can get by is trying with three principal components and 75% total variance. **The accuracy went down to 0.4545 (about half of using four components).** This indicates that for this data set (also considering its size) it is not worth using PCA to do dimensionality reduction. Also, any variance in accuracy are more related to the training/test data sets used than to the specific alternatives and tweaks done to the models.

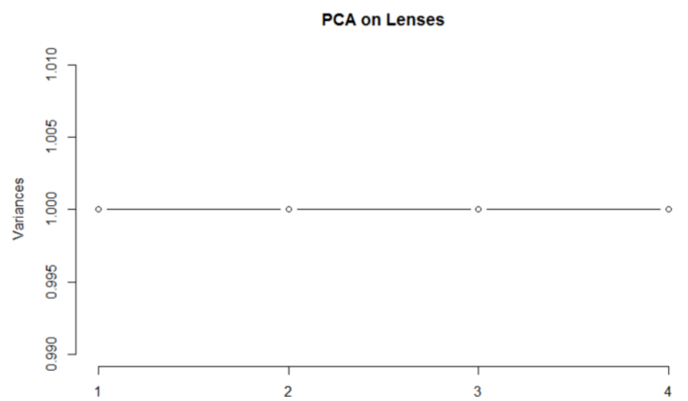
How much of the variance in the data is described by the first two or three principal components? Show visually.

In iris, after normalization and centering, the first two components describe 96% of the variance, and the first three describe 99.3% of the variance.

In Contact Lens, the variance is equal among all variables, the first two describe 50% and the first three describe 75% of the total variance.



	PC1	PC2	PC3	PC4
Cumulative Proportion	**0.7331**	**0.9599**	**0.99314**	**1.0000**



	PC1	PC2	PC3	PC4
Cumulative Proportion	**0.25**	**0.50**	**0.75**	**1.00**

IV. AdaBoost – Random Forest

How did the boosting or bagging compare to the J48 results from Project 1?

On **Iris**, J48 in Project 1 had 0.8936 accuracy, and using Random Forest I obtained 0.9362 accuracy. **Performance is better using Random Forest**.

On **lenses**, as the data set is too small, I used 3-fold cross validation to evaluate performance on J48. **Surprisingly accuracy went down to 0.6667 with Random Forest vs. 0.8333 using J48.**

V. Clustering (K-Means) / Decision Tree / SVM

Run clustering (k-means) and then apply decision tree and SVM on clustered data.

Compare the performance with the previous results.

With Iris, adding a cluster feature to the data set before running SVM varies the accuracy by a very small factor (reducing from 1 to 0.9821). In other cases, it may increase the performance as well. Results are very tight to draw a definitive conclusion. One important detail that can be noted is that **when adding the cluster feature** based on the columns suggested by NbClust() (two clusters) **the SVM accuracy is higher than when using 3 centroids**, even though the underlying data is really split into three classes.
Still with Iris, running decision trees with the additional cluster feature doesn't affect the performance as the cluster feature is not used at all in any of the tree stumps.

With lenses, adding a cluster feature reduces accuracy significantly (down to 0.6667 from 0.9091). It is as if adding the additional cluster number feature (being based on two or three centroids) makes it more difficult to run SVM. Also, if running decision trees with the additional cluster feature does not make any difference, as the cluster feature is not used by any of the stumps in the decision tree.

This leads to the conclusion that adding clustering features to the set can or cannot improve accuracy, and it must be determined based on the data set.

DS8002 - Machine Learning Project 2 - Unsupervised and Supervised Learning (December 2016)

Najlis, Bernardo

December 2nd, 2016

This is the R code, illustrations and examples that go together with the report for DS8002 - Project 2.

0 - Data Preparation

Load required libraries, data sets, split train and test sets, label sets, etc.

```
library(ggplot2)
library(e1071)
library(caret)
```

```
## Loading required package: lattice
```

```
library(randomForest)
```

```
## Warning: package 'randomForest' was built under R version 3.3.2
```

```
## randomForest 4.6-12
```

```
## Type rfNews() to see new features/changes/bug fixes.
```

```
##
## Attaching package: 'randomForest'
```

```
## The following object is masked from 'package:ggplot2':
##
##     margin
```

```
library(RWeka)
library(NbClust)
```

```
## Warning: package 'NbClust' was built under R version 3.3.2
```

```
library(rpart)
library(partykit)
```

```
## Loading required package: grid
```

```
data(iris)  #load iris data
nrow(iris)
```

```
## [1] 150
```

```r
head(iris)
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         0.2  setosa
## 5          5.0         3.6          1.4         0.2  setosa
## 6          5.4         3.9          1.7         0.4  setosa
```

```r
iris.data <- iris[, 1:4]  # features
iris.class <- iris[, 5] # labels

ind.iris <- sample(2, nrow(iris), replace=TRUE, prob=c(0.67, 0.33)) # get random indices for training /
iris.training <- iris[ind.iris==1,1:4]                              # get training set
iris.trainingWithLabels <- iris[ind.iris==1,]                       # training set with labels
iris.test <- iris[ind.iris==2,]                                     # get test set
iris.trainLabels <- iris[ind.iris==1, 5]                            # get labels for training
iris.testLabels <- iris[ind.iris==2, 5]                             # get labels for set

lenses <- read.table("lenses.data", # name of file reading, this requires setting the working directory
                     header= FALSE, # header is not included in first line
                     col.names =    # to provide names for columns
                       c("id", "age", "spectacle_prescription", "astigmatic", "tear_production_rate", "c
                     colClasses=    # data types for columns
                       c("NULL",    # as first column is specified as "NULL", read.table will skip this
                         rep("integer", 4), # all other attributes are integer
                          "factor"          # the last column is the class, typified as factor
                         ))
nrow(lenses)
```

```
## [1] 24
```

```r
head(lenses)
```

```
##   age spectacle_prescription astigmatic tear_production_rate class
## 1   1                      1          1                    1     3
## 2   1                      1          1                    2     2
## 3   1                      1          2                    1     3
## 4   1                      1          2                    2     1
## 5   1                      2          1                    1     3
## 6   1                      2          1                    2     2
```

```r
lenses.data <- lenses[, 1:4]
lenses.class <- lenses[, 5]

ind.lenses <- sample(2, nrow(lenses), replace=TRUE, prob=c(0.8, 0.2)) # get random indices for training
lenses.training <- lenses[ind.lenses==1,1:4]                            # get training set
lenses.trainingWithLabels <- lenses[ind.lenses==1,]                     # training set with labels
lenses.test <- lenses[ind.lenses==2,]                                   # get test set
lenses.trainLabels <- lenses[ind.lenses==1, 5]                          # get labels for training
lenses.testLabels <- lenses[ind.lenses==2, 5]                           # get labels for set
```

1 - SVM

Run SVM with different kernels and then compare.

Iris

```r
# First use tune to select best model parameters

iris.svm.linear.tuned <- tune.svm(Species~.,                                # class and features
                                  data=iris.trainingWithLabels,             # data frame
                                  kernel="linear",                          # kernel
                                  cost=c(0.001, 0.01, 0.1, 1, 10, 100)      # parameter values to try mode
                                  )

iris.svm.linear.tuned <- tune.svm(Species~.,                                # class and features
                                  data=iris.trainingWithLabels,                       # data frame
                                  kernel="linear",                          # kernel
                                  cost=c(0.001, 0.01, 0.1, 1, 10, 100)      # parameter values to try mode
                                  )
summary(iris.svm.linear.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  cost
##    10
##
## - best performance: 0.04222222
##
## - Detailed performance results:
##    cost      error dispersion
## 1 1e-03 0.61555556 0.14686481
## 2 1e-02 0.28555556 0.10975093
## 3 1e-01 0.06444444 0.07640769
## 4 1e+00 0.04333333 0.07670334
## 5 1e+01 0.04222222 0.05463434
## 6 1e+02 0.04222222 0.05463434
```

```r
iris.svm.polynomial.tuned <- tune.svm(Species~., data=iris.trainingWithLabels, kernel="polynomial",
                                      degree = c(3, 4, 5),              # degree of polynomial
                                      coef0=c(0.1, 0.5, 1, 2, 3, 4))    # kernel coefficient

summary(iris.svm.polynomial.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
```

```
##
## - best parameters:
##  degree coef0
##       3   0.5
##
## - best performance: 0.04333333
##
## - Detailed performance results:
##    degree coef0      error dispersion
## 1       3   0.1 0.07444444 0.08733990
## 2       4   0.1 0.09555556 0.09416444
## 3       5   0.1 0.12666667 0.08367420
## 4       3   0.5 0.04333333 0.07670334
## 5       4   0.5 0.04333333 0.07670334
## 6       5   0.5 0.05444444 0.07776896
## 7       3   1.0 0.04333333 0.07670334
## 8       4   1.0 0.05444444 0.07776896
## 9       5   1.0 0.05444444 0.07776896
## 10      3   2.0 0.05444444 0.07776896
## 11      4   2.0 0.05444444 0.07776896
## 12      5   2.0 0.05444444 0.07776896
## 13      3   3.0 0.05444444 0.07776896
## 14      4   3.0 0.05444444 0.07776896
## 15      5   3.0 0.05333333 0.07694439
## 16      3   4.0 0.05444444 0.07776896
## 17      4   4.0 0.06555556 0.07706018
## 18      5   4.0 0.07333333 0.08689113
```

```
iris.svm.radial.tuned <- tune.svm(Species~., data=iris.trainingWithLabels, kernel="radial",
                                  gamma = c(0.1, 0.5, 1, 2, 3, 4))          # gamma coefficient
summary(iris.svm.radial.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  gamma
##      3
##
## - best performance: 0.04222222
##
## - Detailed performance results:
##   gamma      error dispersion
## 1   0.1 0.05333333 0.07694439
## 2   0.5 0.04333333 0.07670334
## 3   1.0 0.04333333 0.07670334
## 4   2.0 0.04333333 0.07670334
## 5   3.0 0.04222222 0.07568616
## 6   4.0 0.05333333 0.07694439
```

```r
iris.svm.sigmoid.tuned <- tune.svm(Species~., data=iris.trainingWithLabels, kernel="sigmoid",
                                   gamma = c(0.1, 0.5, 1, 2, 3, 4),          # gamma
                                   coef0=c(0.1, 0.5, 1, 2, 3, 4))            # kernel coefficient
summary(iris.svm.sigmoid.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  gamma coef0
##    0.1   0.1
##
## - best performance: 0.05111111
##
## - Detailed performance results:
##    gamma coef0      error dispersion
## 1    0.1   0.1 0.05111111 0.08577893
## 2    0.5   0.1 0.29777778 0.16603171
## 3    1.0   0.1 0.40666667 0.23136738
## 4    2.0   0.1 0.40111111 0.12983581
## 5    3.0   0.1 0.38666667 0.13102948
## 6    4.0   0.1 0.38888889 0.15449373
## 7    0.1   0.5 0.05333333 0.05636448
## 8    0.5   0.5 0.30666667 0.15583749
## 9    1.0   0.5 0.41222222 0.18632611
## 10   2.0   0.5 0.35777778 0.13984118
## 11   3.0   0.5 0.36777778 0.16105363
## 12   4.0   0.5 0.37777778 0.14487116
## 13   0.1   1.0 0.11555556 0.16247401
## 14   0.5   1.0 0.31444444 0.17870514
## 15   1.0   1.0 0.33444444 0.16088319
## 16   2.0   1.0 0.29333333 0.20529346
## 17   3.0   1.0 0.32555556 0.19647441
## 18   4.0   1.0 0.32555556 0.13878268
## 19   0.1   2.0 0.29333333 0.17948257
## 20   0.5   2.0 0.32333333 0.16156386
## 21   1.0   2.0 0.36555556 0.14791185
## 22   2.0   2.0 0.36555556 0.20009943
## 23   3.0   2.0 0.36444444 0.18934585
## 24   4.0   2.0 0.36333333 0.20102959
## 25   0.1   3.0 0.61000000 0.15726137
## 26   0.5   3.0 0.38888889 0.22246900
## 27   1.0   3.0 0.45333333 0.20772463
## 28   2.0   3.0 0.40555556 0.16457536
## 29   3.0   3.0 0.37555556 0.21505733
## 30   4.0   3.0 0.40444444 0.18711586
## 31   0.1   4.0 0.61000000 0.15726137
## 32   0.5   4.0 0.61000000 0.15726137
## 33   1.0   4.0 0.44777778 0.20448000
## 34   2.0   4.0 0.48111111 0.20641628
## 35   3.0   4.0 0.38555556 0.15538350
```

```
## 36   4.0   4.0 0.41555556 0.22105868
```

```r
# Now use the best model with the best cost as selected by tune()

iris.svm.linear.best <- iris.svm.linear.tuned$best.model
iris.svm.linear.best.pred <- predict(iris.svm.linear.best, iris.test)
confusionMatrix(iris.svm.linear.best.pred, iris.testLabels)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         12         0
##   virginica       0          1        22
##
## Overall Statistics
##
##                Accuracy : 0.9818
##                  95% CI : (0.9028, 0.9995)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.972
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.9231           1.0000
## Specificity                 1.0000            1.0000           0.9697
## Pos Pred Value              1.0000            1.0000           0.9565
## Neg Pred Value              1.0000            0.9767           1.0000
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2182           0.4000
## Detection Prevalence        0.3636            0.2182           0.4182
## Balanced Accuracy           1.0000            0.9615           0.9848
```

```r
iris.svm.polynomial.best <- iris.svm.polynomial.tuned$best.model
iris.svm.polynomial.best.pred <- predict(iris.svm.polynomial.best, iris.test)
confusionMatrix(iris.svm.polynomial.best.pred, iris.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         13         2
##   virginica       0          0        20
##
## Overall Statistics
##
##                Accuracy : 0.9636
```

```
##                  95% CI : (0.8747, 0.9956)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9447
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            1.0000           0.9091
## Specificity                 1.0000            0.9524           1.0000
## Pos Pred Value              1.0000            0.8667           1.0000
## Neg Pred Value              1.0000            1.0000           0.9429
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2364           0.3636
## Detection Prevalence        0.3636            0.2727           0.3636
## Balanced Accuracy           1.0000            0.9762           0.9545
```

```
iris.svm.radial.best <- iris.svm.radial.tuned$best.model
iris.svm.radial.best.pred <- predict(iris.svm.radial.best, iris.test)
confusionMatrix(iris.svm.radial.best.pred, iris.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         19          0         0
##   versicolor      0         12         2
##   virginica       1          1        20
##
## Overall Statistics
##
##                Accuracy : 0.9273
##                  95% CI : (0.8241, 0.9798)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : 2.361e-16
##
##                   Kappa : 0.8888
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 0.9500            0.9231           0.9091
## Specificity                 1.0000            0.9524           0.9394
## Pos Pred Value              1.0000            0.8571           0.9091
## Neg Pred Value              0.9722            0.9756           0.9394
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3455            0.2182           0.3636
## Detection Prevalence        0.3455            0.2545           0.4000
## Balanced Accuracy           0.9750            0.9377           0.9242
```

```r
iris.svm.sigmoid.best <- iris.svm.sigmoid.tuned$best.model
iris.svm.sigmoid.best.pred <- predict(iris.svm.sigmoid.best, iris.test)
confusionMatrix(iris.svm.sigmoid.best.pred, iris.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         13         2
##   virginica       0          0        20
##
## Overall Statistics
##
##                Accuracy : 0.9636
##                  95% CI : (0.8747, 0.9956)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9447
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            1.0000           0.9091
## Specificity                 1.0000            0.9524           1.0000
## Pos Pred Value              1.0000            0.8667           1.0000
## Neg Pred Value              1.0000            1.0000           0.9429
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2364           0.3636
## Detection Prevalence        0.3636            0.2727           0.3636
## Balanced Accuracy           1.0000            0.9762           0.9545
```

Contact Lenses

```r
lenses.svm.linear.tuned <- tune.svm(class~., data=lenses.trainingWithLabels, kernel="linear", cost=c(0.0
summary(lenses.svm.linear.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  cost
##    10
##
## - best performance: 0.2833333
##
## - Detailed performance results:
```

```
##    cost     error dispersion
## 1 1e-03 0.3666667  0.3122993
## 2 1e-02 0.3666667  0.3122993
## 3 1e-01 0.4166667  0.2859897
## 4 1e+00 0.3333333  0.4082483
## 5 1e+01 0.2833333  0.2490724
## 6 1e+02 0.2833333  0.2490724
```

```
lenses.svm.polynomial.tuned <- tune.svm(class~., data=lenses.trainingWithLabels, kernel="polynomial", de
summary(lenses.svm.polynomial.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  degree coef0
##       3   0.5
##
## - best performance: 0.1833333
##
## - Detailed performance results:
##    degree coef0     error dispersion
## 1       3   0.1 0.2833333  0.2490724
## 2       4   0.1 0.3166667  0.2283867
## 3       5   0.1 0.3333333  0.3333333
## 4       3   0.5 0.1833333  0.2415229
## 5       4   0.5 0.2000000  0.2581989
## 6       5   0.5 0.2000000  0.2581989
## 7       3   1.0 0.2333333  0.2509242
## 8       4   1.0 0.1833333  0.2415229
## 9       5   1.0 0.2000000  0.2581989
## 10      3   2.0 0.2333333  0.2509242
## 11      4   2.0 0.2333333  0.2509242
## 12      5   2.0 0.1833333  0.2415229
## 13      3   3.0 0.2333333  0.2509242
## 14      4   3.0 0.2333333  0.2509242
## 15      5   3.0 0.2333333  0.2509242
## 16      3   4.0 0.2333333  0.2509242
## 17      4   4.0 0.2333333  0.2509242
## 18      5   4.0 0.2333333  0.2509242
```

```
lenses.svm.radial.tuned <- tune.svm(class~., data=lenses.trainingWithLabels, kernel="radial", gamma = c
summary(lenses.svm.radial.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  gamma
```

```
##    0.5
##
## - best performance: 0.3333333
##
## - Detailed performance results:
##   gamma     error dispersion
## 1   0.1 0.3833333  0.3147603
## 2   0.5 0.3333333  0.3333333
## 3   1.0 0.3333333  0.3333333
## 4   2.0 0.3333333  0.3333333
## 5   3.0 0.3333333  0.3333333
## 6   4.0 0.3333333  0.3333333
```

```
lenses.svm.sigmoid.tuned <- tune.svm(class~., data=lenses.trainingWithLabels, kernel="sigmoid", gamma =
summary(lenses.svm.sigmoid.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  gamma coef0
##      3     3
##
## - best performance: 0.3333333
##
## - Detailed performance results:
##    gamma coef0     error dispersion
## 1    0.1   0.1 0.4000000  0.3258417
## 2    0.5   0.1 0.4000000  0.3258417
## 3    1.0   0.1 0.4000000  0.3258417
## 4    2.0   0.1 0.4333333  0.3351801
## 5    3.0   0.1 0.4333333  0.3351801
## 6    4.0   0.1 0.4333333  0.3351801
## 7    0.1   0.5 0.3500000  0.2539807
## 8    0.5   0.5 0.3500000  0.3464992
## 9    1.0   0.5 0.4500000  0.2944969
## 10   2.0   0.5 0.4000000  0.3258417
## 11   3.0   0.5 0.4333333  0.3351801
## 12   4.0   0.5 0.4333333  0.3351801
## 13   0.1   1.0 0.3500000  0.2539807
## 14   0.5   1.0 0.4500000  0.2944969
## 15   1.0   1.0 0.4500000  0.2944969
## 16   2.0   1.0 0.4500000  0.2944969
## 17   3.0   1.0 0.4500000  0.2944969
## 18   4.0   1.0 0.4833333  0.2986596
## 19   0.1   2.0 0.3500000  0.2539807
## 20   0.5   2.0 0.3500000  0.2539807
## 21   1.0   2.0 0.5000000  0.2484520
## 22   2.0   2.0 0.3833333  0.3147603
## 23   3.0   2.0 0.4500000  0.2944969
## 24   4.0   2.0 0.4500000  0.2944969
## 25   0.1   3.0 0.3500000  0.2539807
```

```
## 26   0.5   3.0 0.3500000  0.2539807
## 27   1.0   3.0 0.3500000  0.2539807
## 28   2.0   3.0 0.5000000  0.2484520
## 29   3.0   3.0 0.3333333  0.3333333
## 30   4.0   3.0 0.4500000  0.2944969
## 31   0.1   4.0 0.3500000  0.2539807
## 32   0.5   4.0 0.3500000  0.2539807
## 33   1.0   4.0 0.3833333  0.3147603
## 34   2.0   4.0 0.5000000  0.2484520
## 35   3.0   4.0 0.5000000  0.2484520
## 36   4.0   4.0 0.3666667  0.3496029
```

```r
# Now create the best model with the best cost as selected by tune()

lenses.svm.linear.best <- lenses.svm.linear.tuned$best.model
lenses.svm.linear.best.pred <- predict(lenses.svm.linear.best, lenses.test)
confusionMatrix(lenses.svm.linear.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```

```r
lenses.svm.polynomial.best <- lenses.svm.polynomial.tuned$best.model
lenses.svm.polynomial.best.pred <- predict(lenses.svm.polynomial.best, lenses.test)
confusionMatrix(lenses.svm.polynomial.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
```

```
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```

```r
lenses.svm.radial.best <- lenses.svm.radial.tuned$best.model
lenses.svm.radial.best.pred <- predict(lenses.svm.radial.best, lenses.test)
confusionMatrix(lenses.svm.radial.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 0 0 0
##          2 0 0 0
##          3 1 0 1
##
## Overall Statistics
##
##                Accuracy : 0.5
##                  95% CI : (0.0126, 0.9874)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.75
##
##                   Kappa : 0
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
```

```
## Sensitivity               0.0       NA      1.0
## Specificity               1.0        1      0.0
## Pos Pred Value            NaN       NA      0.5
## Neg Pred Value            0.5       NA      NaN
## Prevalence                0.5        0      0.5
## Detection Rate            0.0        0      0.5
## Detection Prevalence      0.0        0      1.0
## Balanced Accuracy         0.5       NA      0.5
```

```
lenses.svm.sigmoid.best <- lenses.svm.sigmoid.tuned$best.model
lenses.svm.sigmoid.best.pred <- predict(lenses.svm.sigmoid.best, lenses.test)
confusionMatrix(lenses.svm.sigmoid.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 0 0 0
##          2 0 0 0
##          3 1 0 1
##
## Overall Statistics
##
##                Accuracy : 0.5
##                  95% CI : (0.0126, 0.9874)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.75
##
##                   Kappa : 0
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               0.0       NA      1.0
## Specificity               1.0        1      0.0
## Pos Pred Value            NaN       NA      0.5
## Neg Pred Value            0.5       NA      NaN
## Prevalence                0.5        0      0.5
## Detection Rate            0.0        0      0.5
## Detection Prevalence      0.0        0      1.0
## Balanced Accuracy         0.5       NA      0.5
```

2 - PCA - SVM

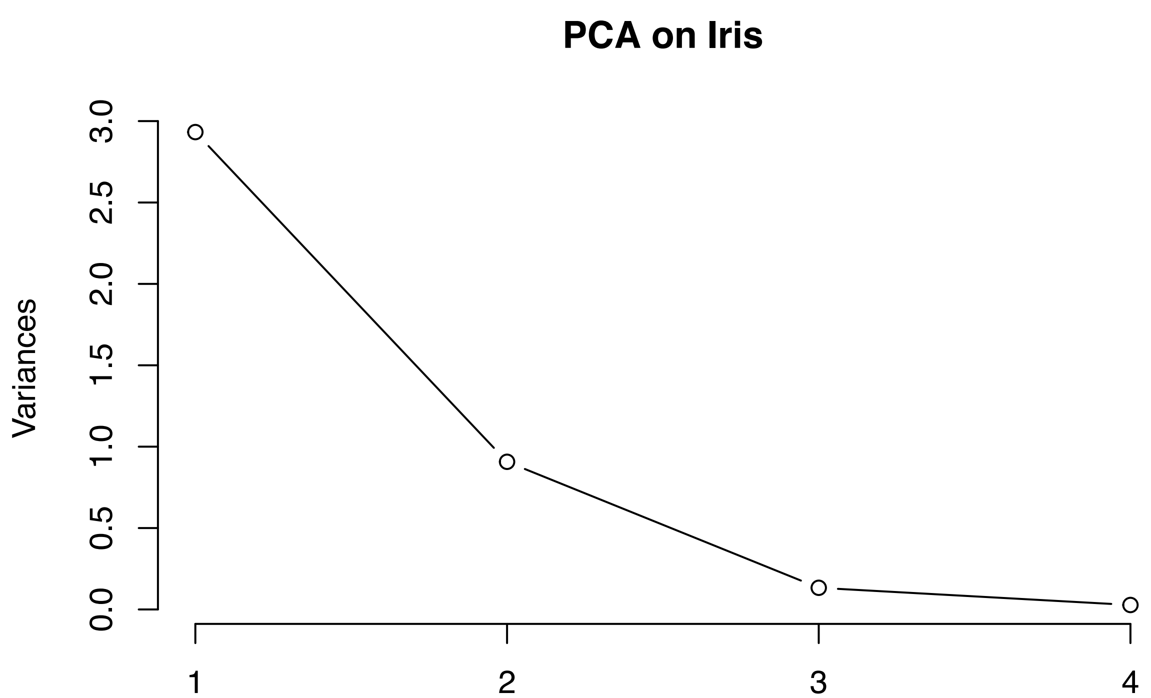
Run PCA and then run SVM on the reduced data.

Iris

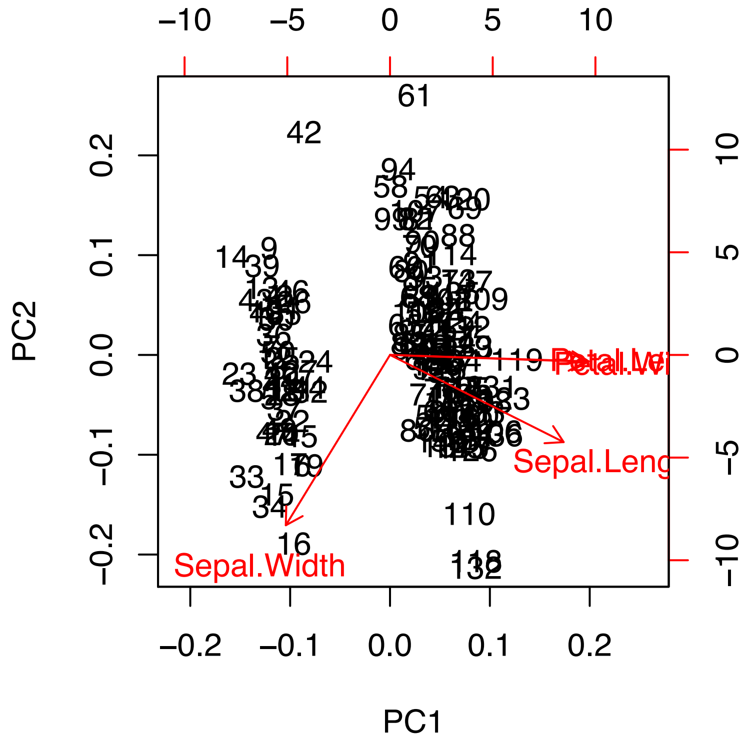
```r
iris.log <- log(iris.data)
iris.pca <- prcomp(iris.log, center=TRUE, scale. = TRUE) # do PCA analysis on iris data
summary(iris.pca)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4
## Standard deviation     1.7125 0.9524 0.36470 0.16568
## Proportion of Variance 0.7331 0.2268 0.03325 0.00686
## Cumulative Proportion  0.7331 0.9599 0.99314 1.00000
```

```r
plot(iris.pca, main="PCA on Iris", type="l")                # plot PCA comparison
```




```r
biplot(iris.pca)
```




```
# SVM on reduced set

iris.training.reduced <- cbind.data.frame(iris.pca$x[ind.iris==1, c(1,2)], Species=iris.trainLabels) #
iris.test.reduced <- cbind.data.frame(iris.pca$x[ind.iris==2, c(1,2)], Species=iris.testLabels)#reduced

iris.svm.polynomial.reduced.tuned <- tune.svm(Species~., data=iris.training.reduced, kernel="polynomial
summary(iris.svm.polynomial.reduced.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  degree coef0
##       4     1
##
## - best performance: 0.1177778
##
## - Detailed performance results:
##    degree coef0     error dispersion
## 1       3   0.1 0.1688889 0.17652335
## 2       4   0.1 0.1800000 0.17745341
## 3       5   0.1 0.1900000 0.16207248
## 4       3   0.5 0.1688889 0.17652335
## 5       4   0.5 0.1588889 0.13709208
```

```
## 6       5   0.5 0.1688889 0.12752794
## 7       3   1.0 0.1477778 0.15135873
## 8       4   1.0 0.1177778 0.13159359
## 9       5   1.0 0.1477778 0.12744724
## 10      3   2.0 0.1777778 0.14083817
## 11      4   2.0 0.1366667 0.08607427
## 12      5   2.0 0.1366667 0.08607427
## 13      3   3.0 0.1677778 0.15021247
## 14      4   3.0 0.1255556 0.08081376
## 15      5   3.0 0.1477778 0.07258692
## 16      3   4.0 0.1577778 0.15115468
## 17      4   4.0 0.1366667 0.08607427
## 18      5   4.0 0.1477778 0.07258692
```

```r
# Now create polynomial SVM with optimal parameters

iris.svm.polynomial.reduced.best <- iris.svm.polynomial.reduced.tuned$best.model
iris.svm.polynomial.reduced.best.pred <- predict(iris.svm.polynomial.reduced.best, iris.test.reduced)

confusionMatrix(iris.svm.polynomial.reduced.best.pred, iris.testLabels)  # Confusion matrix
```

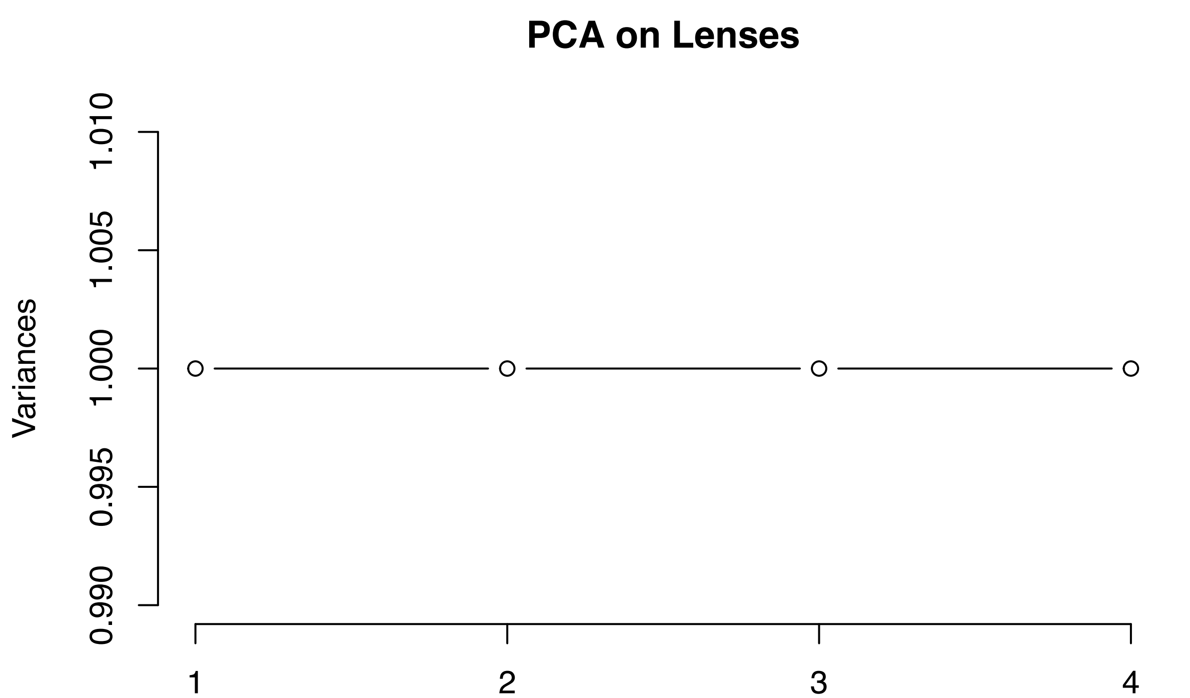
```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         11         4
##   virginica       0          2        18
##
## Overall Statistics
##
##                Accuracy : 0.8909
##                  95% CI : (0.7775, 0.9589)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : 4.653e-14
##
##                   Kappa : 0.8342
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.8462           0.8182
## Specificity                 1.0000            0.9048           0.9394
## Pos Pred Value              1.0000            0.7333           0.9000
## Neg Pred Value              1.0000            0.9500           0.8857
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2000           0.3273
## Detection Prevalence        0.3636            0.2727           0.3636
## Balanced Accuracy           1.0000            0.8755           0.8788
```

Contact Lenses

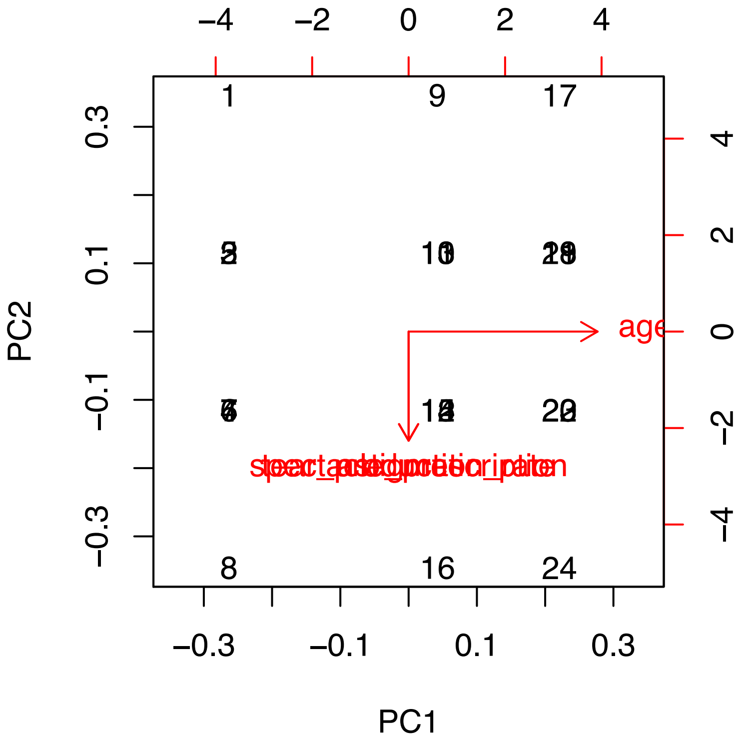
```
lenses.log <- log(lenses.data)
lenses.pca <- prcomp(lenses.log, center=TRUE, scale. = TRUE) # do PCA analysis on iris data
summary(lenses.pca)
```

```
## Importance of components:
##                         PC1  PC2  PC3  PC4
## Standard deviation     1.00 1.00 1.00 1.00
## Proportion of Variance 0.25 0.25 0.25 0.25
## Cumulative Proportion  0.25 0.50 0.75 1.00
```

```
plot(lenses.pca, main="PCA on Lenses", type="l")                # plot PCA comparison
```




```
biplot(lenses.pca)
```




```
lenses.training.reduced <- cbind.data.frame(lenses.pca$x[ind.lenses==1, c(1,2,3)], class=lenses.trainLal
lenses.test.reduced <- cbind.data.frame(lenses.pca$x[ind.lenses==2, c(1,2, 3)], class=lenses.testLabels)

lenses.svm.polynomial.reduced.tuned <- tune.svm(class~., data=lenses.training.reduced, kernel="polynomia
summary(lenses.svm.polynomial.reduced.tuned)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##  degree coef0
##       3   0.1
##
## - best performance: 0.3333333
##
## - Detailed performance results:
##    degree coef0     error dispersion
## 1       3   0.1 0.3333333  0.3767961
## 2       4   0.1 0.3833333  0.3604695
## 3       5   0.1 0.3833333  0.3604695
## 4       3   0.5 0.4333333  0.4097575
## 5       4   0.5 0.4333333  0.4097575
## 6       5   0.5 0.4833333  0.3804643
```

```
## 7       3   1.0 0.4833333  0.3804643
## 8       4   1.0 0.4833333  0.3804643
## 9       5   1.0 0.4833333  0.3804643
## 10      3   2.0 0.4833333  0.3804643
## 11      4   2.0 0.4833333  0.3804643
## 12      5   2.0 0.4833333  0.3804643
## 13      3   3.0 0.4833333  0.3804643
## 14      4   3.0 0.4833333  0.3804643
## 15      5   3.0 0.4833333  0.3804643
## 16      3   4.0 0.4833333  0.3804643
## 17      4   4.0 0.4833333  0.3804643
## 18      5   4.0 0.4833333  0.3804643
```

```r
# Now create polynomial SVM with optimal parameters

lenses.svm.polynomial.reduced.best <- lenses.svm.polynomial.reduced.tuned$best.model
lenses.svm.polynomial.reduced.best.pred <- predict(lenses.svm.polynomial.reduced.best, lenses.test.reduc

confusionMatrix(lenses.svm.polynomial.reduced.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```

3 - Random Forest

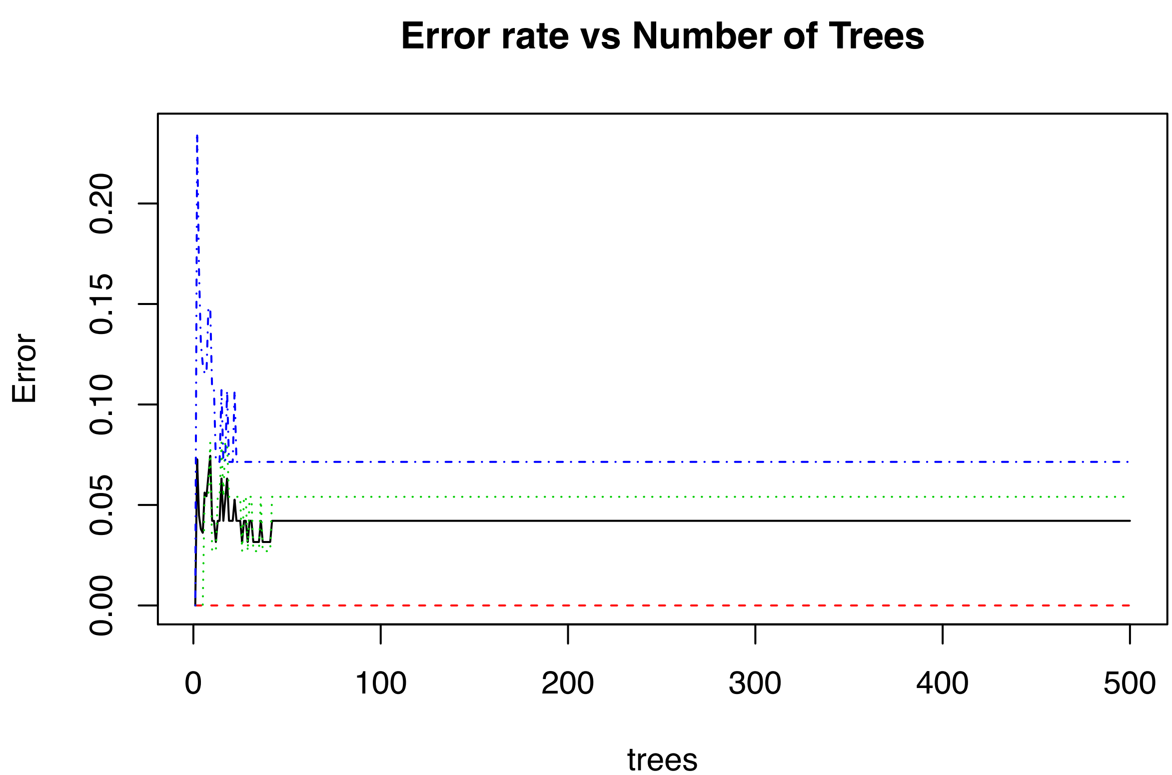
How did the boosting or bagging compare to the J48 results from Project 1?

Iris

```r
set.seed(1234)
iris.rf <- randomForest(Species~., data=iris.trainingWithLabels)
print(iris.rf)
```

```
##
## Call:
##  randomForest(formula = Species ~ ., data = iris.trainingWithLabels)
##                Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 2
##
##         OOB estimate of  error rate: 4.21%
## Confusion matrix:
##            setosa versicolor virginica class.error
## setosa         30          0         0  0.00000000
## versicolor      0         35         2  0.05405405
## virginica       0          2        26  0.07142857
```

```r
plot(iris.rf, main="Error rate vs Number of Trees")
```



```r
which.min(iris.rf$err.rate[,1])     # this returns how mamy trees are needed
```

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

```r
iris.rf.ntree <- randomForest(Species~., data=iris.trainingWithLabels,
                              ntree = which.min(iris.rf$err.rate[,1]) ) # specify the number of trees t

print(iris.rf.ntree)
```

```
##
## Call:
##  randomForest(formula = Species ~ ., data = iris.trainingWithLabels,      ntree = which.min(iris.rf$e
##                Type of random forest: classification
##                      Number of trees: 1
## No. of variables tried at each split: 2
##
##         OOB estimate of  error rate: 8.33%
## Confusion matrix:
##            setosa versicolor virginica class.error
## setosa         11          0         0   0.0000000
## versicolor      0         14         0   0.0000000
## virginica       0          3         8   0.2727273
```

```r
iris.rf.ntree.pred <- predict(iris.rf.ntree, newdata = iris.test)
confusionMatrix(iris.rf.ntree.pred, iris.testLabels)
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         12         2
##   virginica       0          1        20
##
## Overall Statistics
##
##                Accuracy : 0.9455
##                  95% CI : (0.8488, 0.9886)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9167
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            0.9231           0.9091
## Specificity                 1.0000            0.9524           0.9697
## Pos Pred Value              1.0000            0.8571           0.9524
## Neg Pred Value              1.0000            0.9756           0.9412
```

```
## Prevalence                      0.3636            0.2364           0.4000
## Detection Rate                  0.3636            0.2182           0.3636
## Detection Prevalence            0.3636            0.2545           0.3818
## Balanced Accuracy               1.0000            0.9377           0.9394
```

```
# J48 (from Project 1) to compare with Random Forest

weka_j48 <- make_Weka_classifier("weka/classifiers/trees/J48")
# non-prunned version of J48 tree
iris.j48 <- weka_j48(Species~., data=iris.trainingWithLabels, control=Weka_control(U=TRUE))
evaluate_Weka_classifier(iris.j48, newdata = iris.test, class=TRUE)
```

```
##
## === Summary ===
##
## Correctly Classified Instances          51               92.7273 %
## Incorrectly Classified Instances         4                7.2727 %
## Kappa statistic                          0.8893
## Mean absolute error                      0.0521
## Root mean squared error                  0.216
## Relative absolute error                 11.9789 %
## Root relative squared error             46.3404 %
## Total Number of Instances               55
##
## === Detailed Accuracy By Class ===
##
##                  TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
##                  0.950    0.000    1.000      0.950    0.974      0.961    0.975     0.968     setosa
##                  0.923    0.071    0.800      0.923    0.857      0.812    0.926     0.757     versi
##                  0.909    0.030    0.952      0.909    0.930      0.886    0.956     0.921     virgi
## Weighted Avg.    0.927    0.029    0.934      0.927    0.929      0.896    0.956     0.899
##
## === Confusion Matrix ===
##
##   a  b  c   <-- classified as
##  19  1  0 |  a = setosa
##   0 12  1 |  b = versicolor
##   0  2 20 |  c = virginica
```

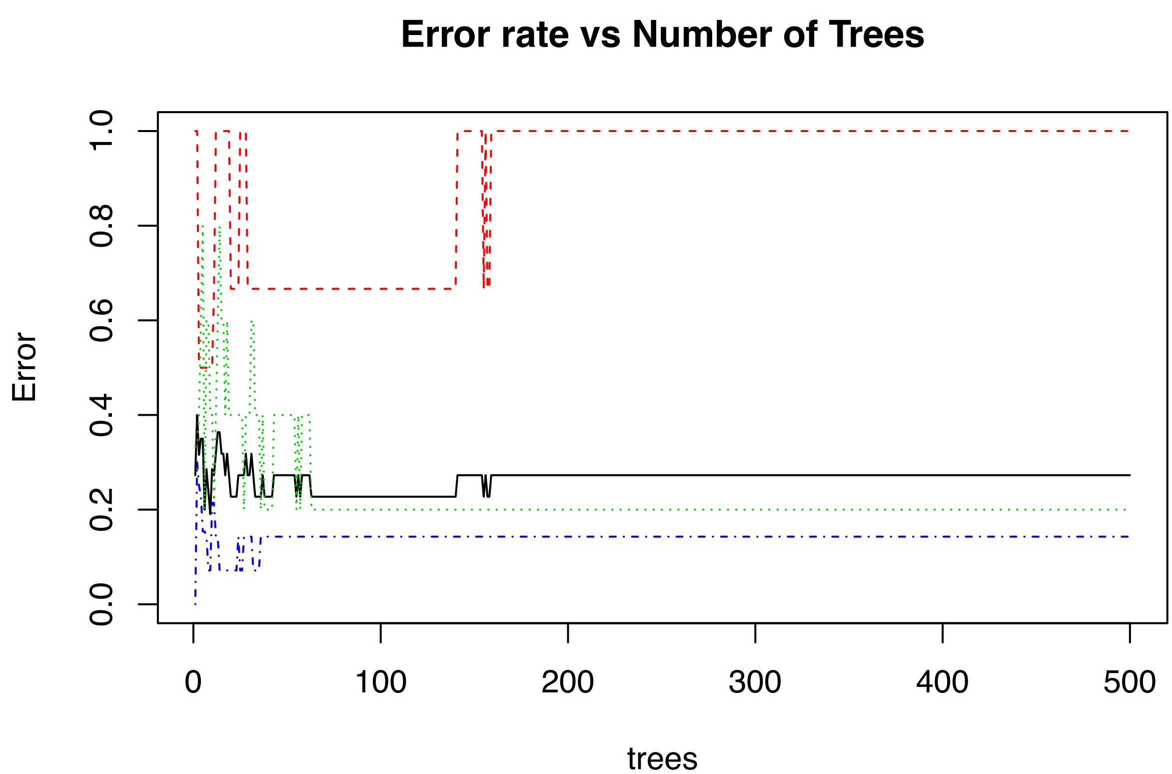
Contact Lenses

```
set.seed(1234)
lenses.rf <- randomForest(class~., data=lenses.trainingWithLabels)
print(lenses.rf)
```

```
##
## Call:
##  randomForest(formula = class ~ ., data = lenses.trainingWithLabels)
##                Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 2
```

```
##
##         OOB estimate of  error rate: 27.27%
## Confusion matrix:
##   1 2  3 class.error
## 1 0 0  3   1.0000000
## 2 0 4  1   0.2000000
## 3 1 1 12   0.1428571
```

```r
plot(lenses.rf, main="Error rate vs Number of Trees")
```




```r
which.min(lenses.rf$err.rate[,1])      # this returns how mamy trees are needed
```

```
## [1] 9
```

```r
lenses.rf.ntree <- randomForest(class~., data=lenses.trainingWithLabels,
                               ntree = which.min(lenses.rf$err.rate[,1]) ) # specify the number of trees

print(lenses.rf.ntree)
```

```
##
## Call:
##  randomForest(formula = class ~ ., data = lenses.trainingWithLabels,      ntree = which.min(lenses.r
##               Type of random forest: classification
##                     Number of trees: 9
```

```
## No. of variables tried at each split: 2
##
##         OOB estimate of  error rate: 33.33%
## Confusion matrix:
##   1 2  3 class.error
## 1 1 0  2   0.6666667
## 2 0 2  3   0.6000000
## 3 1 1 11   0.1538462
```

```r
lenses.rf.ntree.pred <- predict(lenses.rf.ntree, newdata = lenses.test)
confusionMatrix(lenses.rf.ntree.pred, lenses.testLabels)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```

```r
# J48 (from Project 1) to compare with Random Forest

weka_j48 <- make_Weka_classifier("weka/classifiers/trees/J48")
# non-prunned version of J48 tree
lenses.j48 <- weka_j48(class~., data=lenses, control=Weka_control(U=TRUE))
evaluate_Weka_classifier(lenses.j48, numFolds = 3, class=TRUE)
```

```
## === 3 Fold Cross Validation ===
##
## === Summary ===
##
```

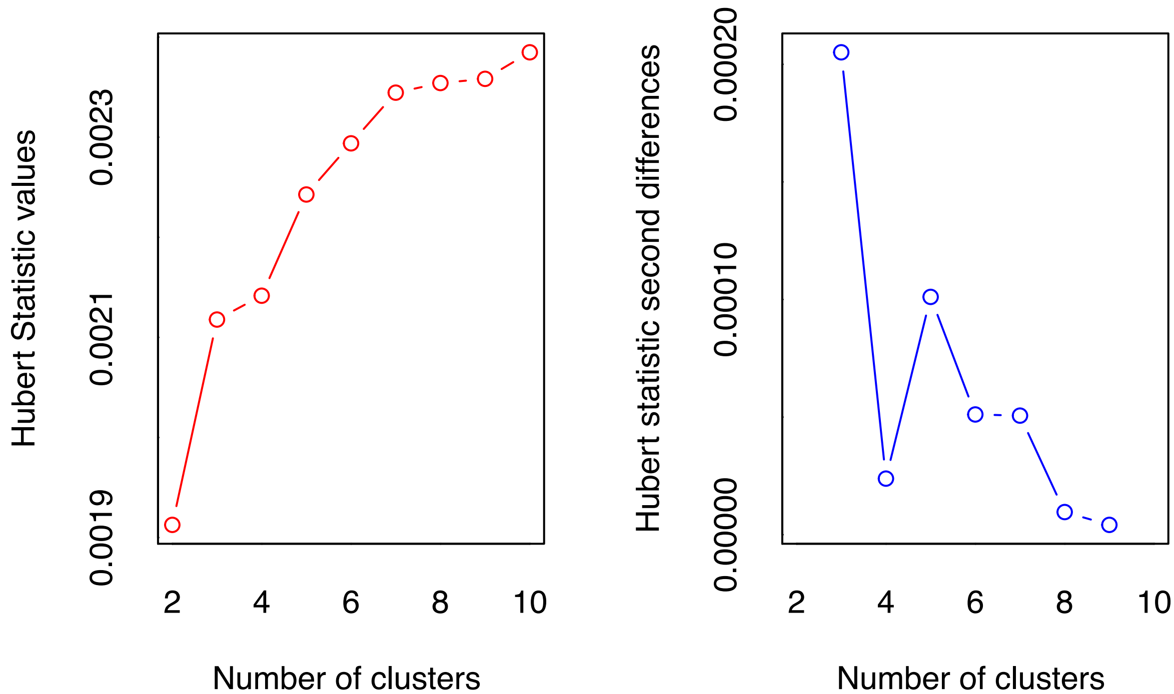
```
## Correctly Classified Instances          20               83.3333 %
## Incorrectly Classified Instances         4               16.6667 %
## Kappa statistic                          0.71
## Mean absolute error                      0.1398
## Root mean squared error                  0.3099
## Relative absolute error                 37.3568 %
## Root relative squared error             72.4701 %
## Total Number of Instances               24
##
## === Detailed Accuracy By Class ===
##
##                  TP Rate  FP Rate  Precision  Recall   F-Measure  MCC      ROC Area  PRC Area  Class
##                  0.750    0.100    0.600      0.750    0.667      0.596    0.819     0.467     1
##                  1.000    0.053    0.833      1.000    0.909      0.889    0.958     0.750     2
##                  0.800    0.111    0.923      0.800    0.857      0.669    0.848     0.881     3
## Weighted Avg.    0.833    0.097    0.851      0.833    0.836      0.703    0.866     0.785
##
## === Confusion Matrix ===
##
##   a  b  c   <-- classified as
##   3  0  1 |  a = 1
##   0  5  0 |  b = 2
##   2  1 12 |  c = 3
```

4 - Clustering (k-means) / Decision Tree / SVM

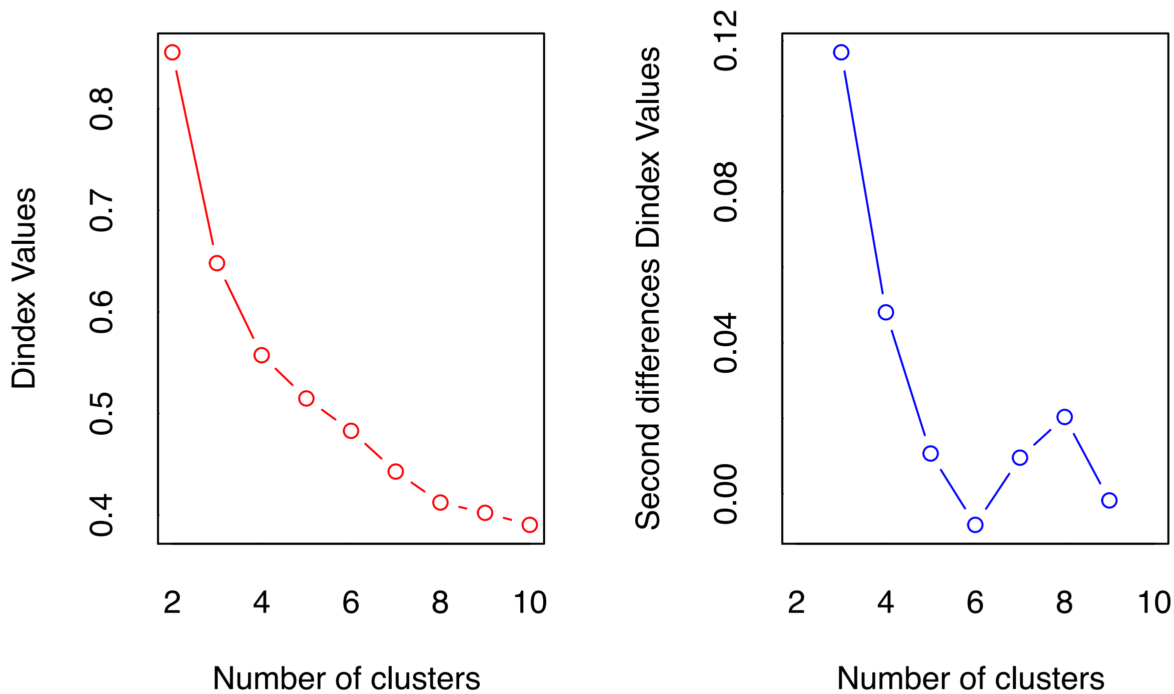
Run clustering (k-means) ant then apply decision tree and SVM on clustered data.

Iris

```r
NbClust(iris.data,          # using the complete set with no labels
        min.nc = 2,         # minimum number of clusters
        max.nc = 10,        # maximum number of clusters
        method = "kmeans")
```




```
## *** : The Hubert index is a graphical method of determining the number of clusters.
##                 In the plot of Hubert index, we seek a significant knee that corresponds to a
##                 significant increase of the value of the measure i.e the significant peak in Hubert
##                 index second differences plot.
##
```

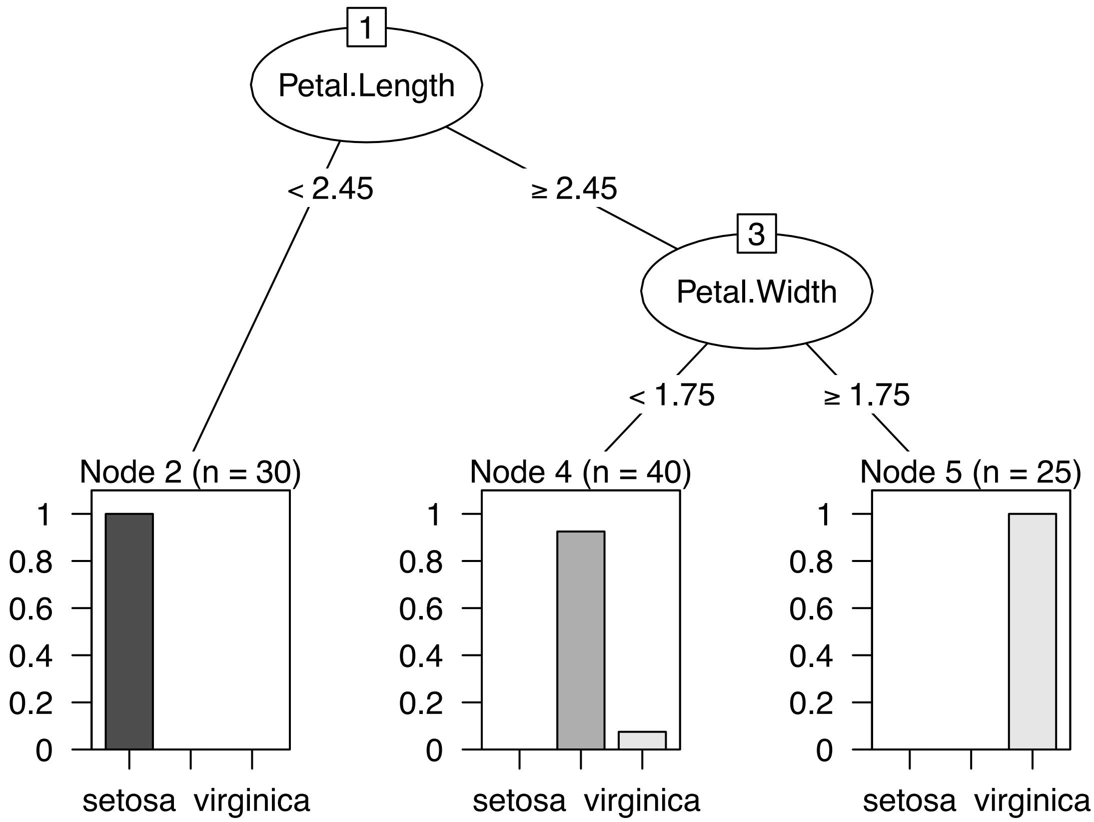



```
## *** : The D index is a graphical method of determining the number of clusters.
##                 In the plot of D index, we seek a significant knee (the significant peak in Dindex
##                 second differences plot) that corresponds to a significant increase of the value of
##                 the measure.
##
## *******************************************************************
## * Among all indices:
## * 10 proposed 2 as the best number of clusters
## * 8 proposed 3 as the best number of clusters
## * 2 proposed 4 as the best number of clusters
## * 1 proposed 5 as the best number of clusters
## * 1 proposed 7 as the best number of clusters
## * 1 proposed 8 as the best number of clusters
## * 1 proposed 10 as the best number of clusters
##
##                    ***** Conclusion *****
##
## * According to the majority rule, the best number of clusters is  2
##
##
## *******************************************************************


## $All.index
##        KL       CH Hartigan     CCC    Scott  Marriot    TrCovW   TraceW
## 2  5.9068 513.9245 137.9491 35.9428 1044.605 467371.6 1045.9696 152.3480
```

```
## 3  3.5663 561.6278  55.5419 37.6701 1246.668 273408.6  248.9814  78.8514
## 4  7.2495 530.7658  21.7032 36.4682 1359.280 229428.4  173.8973  57.2285
## 5  0.4117 459.5058  25.1578 34.3409 1415.662 246163.9  140.6758  49.8223
## 6  0.6156 433.4067  31.8988 33.3747 1502.213 199064.5   87.7420  42.4561
## 7  1.6869 443.3948  22.7349 33.4645 1583.366 157734.8   79.7038  34.7567
## 8  5.3825 440.6205   6.2958 33.2318 1653.207 129330.2   49.7924  29.9889
## 9  1.3278 400.5825   9.3700 31.9307 1683.279 133948.2   38.7655  28.7158
## 10 2.2038 378.0763   7.6187 31.1083 1712.825 135802.5   35.2030  26.9264
##     Friedman    Rubin Cindex     DB Silhouette   Duda Pseudot2   Beale
## 2   732.8086  62.6152 0.2728 0.4744     0.6810 1.9253 -52.8667 -1.1380
## 3   801.6490 120.9780 0.3450 0.7256     0.5528 1.1915  -9.3224 -0.3776
## 4   874.3981 166.6878 0.3211 0.8436     0.4981 0.5112  45.9014  2.2615
## 5   936.2996 191.4664 0.3327 0.9987     0.3728 1.1340  -5.1981 -0.2746
## 6  1033.8843 224.6862 0.3594 1.0923     0.3263 0.8469   5.2430  0.4175
## 7  1173.6099 274.4586 0.3965 1.0070     0.3462 3.9365 -17.9033 -1.5008
## 8  1289.5807 318.0936 0.4007 1.0403     0.3519 0.9269   1.5780  0.1799
## 9  1381.7100 332.1968 0.3919 1.0573     0.3536 0.7926   6.5424  0.6084
## 10 1443.8573 354.2725 0.3831 1.0993     0.3114 1.0204  -0.5210 -0.0452
##    Ratkowsky    Ball Ptbiserial    Frey McClain   Dunn Hubert SDindex
## 2     0.5462 76.1740     0.8345  1.7571  0.2723 0.0765 0.0019  1.2820
## 3     0.4967 26.2838     0.7146  1.5949  0.5255 0.0988 0.0021  1.7259
## 4     0.4413 14.3071     0.6361  6.0985  0.7120 0.1365 0.0021  2.4707
## 5     0.4067  9.9645     0.5521  1.3762  0.9903 0.0624 0.0022  3.1993
## 6     0.3737  7.0760     0.5023 -0.1138  1.2099 0.0739 0.0023  3.3704
## 7     0.3498  4.9652     0.5119  1.1261  1.1407 0.0872 0.0023  3.4409
## 8     0.3302  3.7486     0.4690  1.3658  1.3416 0.0974 0.0024  3.8586
## 9     0.3131  3.1906     0.4567  3.0876  1.4108 0.0974 0.0024  4.4503
## 10    0.2989  2.6926     0.4249  0.6407  1.6368 0.0974 0.0024  4.9241
##    Dindex   SDbw
## 2  0.8556 0.1618
## 3  0.6480 0.2257
## 4  0.5574 0.3186
## 5  0.5148 0.1542
## 6  0.4829 0.1158
## 7  0.4428 0.1341
## 8  0.4123 0.0713
## 9  0.4022 0.0612
## 10 0.3904 0.0311
##
## $All.CriticalValues
##    CritValue_Duda CritValue_PseudoT2 Fvalue_Beale
## 2          0.5633            85.2756       1.0000
## 3          0.5131            55.0440       1.0000
## 4          0.5551            38.4707       0.0640
## 5          0.4590            51.8597       1.0000
## 6          0.4284            38.6922       0.7956
## 7          0.0772           287.0296       1.0000
## 8          0.3773            33.0071       0.9481
## 9          0.4590            29.4657       0.6575
## 10         0.3357            51.4462       1.0000
##
## $Best.nc
##                     KL       CH Hartigan     CCC    Scott  Marriot
## Number_clusters 4.0000   3.0000   3.0000  3.0000   3.0000      3.0
```

```
## Value_Index     7.2495 561.6278  82.4072 37.6701 202.0631 149982.9
##                   TrCovW  TraceW Friedman    Rubin Cindex     DB
## Number_clusters   3.0000  3.0000   7.0000   8.0000 2.0000 2.0000
## Value_Index     796.9882 51.8735 139.7256 -29.5317 0.2728 0.4744
##                 Silhouette   Duda PseudoT2  Beale Ratkowsky    Ball
## Number_clusters      2.000 2.0000   2.0000  2.000    2.0000  3.0000
## Value_Index          0.681 1.9253 -52.8667 -1.138    0.5462 49.8902
##                 PtBiserial   Frey McClain   Dunn Hubert SDindex Dindex
## Number_clusters     2.0000 5.0000  2.0000 4.0000      0   2.000      0
## Value_Index         0.8345 1.3762  0.2723 0.1365      0   1.282      0
##                    SDbw
## Number_clusters 10.0000
## Value_Index      0.0311
##
## $Best.partition
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2
##  [71] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 2 2 2 2 1 2 2 2 2 2 2
## [106] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
## [141] 2 2 2 2 2 2 2 2 2 2
```

```r
## Two centroids

iris.kmeans.2 <- kmeans(iris.data, centers = 2) # two centroids as suggested by NbClust
iris.with.kmeans.2 <- cbind.data.frame(iris, Cluster = iris.kmeans.2$cluster) # add cluster feature
iris.with.kmeans.2.training = iris.with.kmeans.2[ind.iris==1,]
iris.with.kmeans.2.test = iris.with.kmeans.2[ind.iris==2,]

## Decision tree on clustered data
iris.kmeans.2.dtree <- rpart(Species~., data = iris.with.kmeans.2.training)
plot(as.party(iris.kmeans.2.dtree))
```

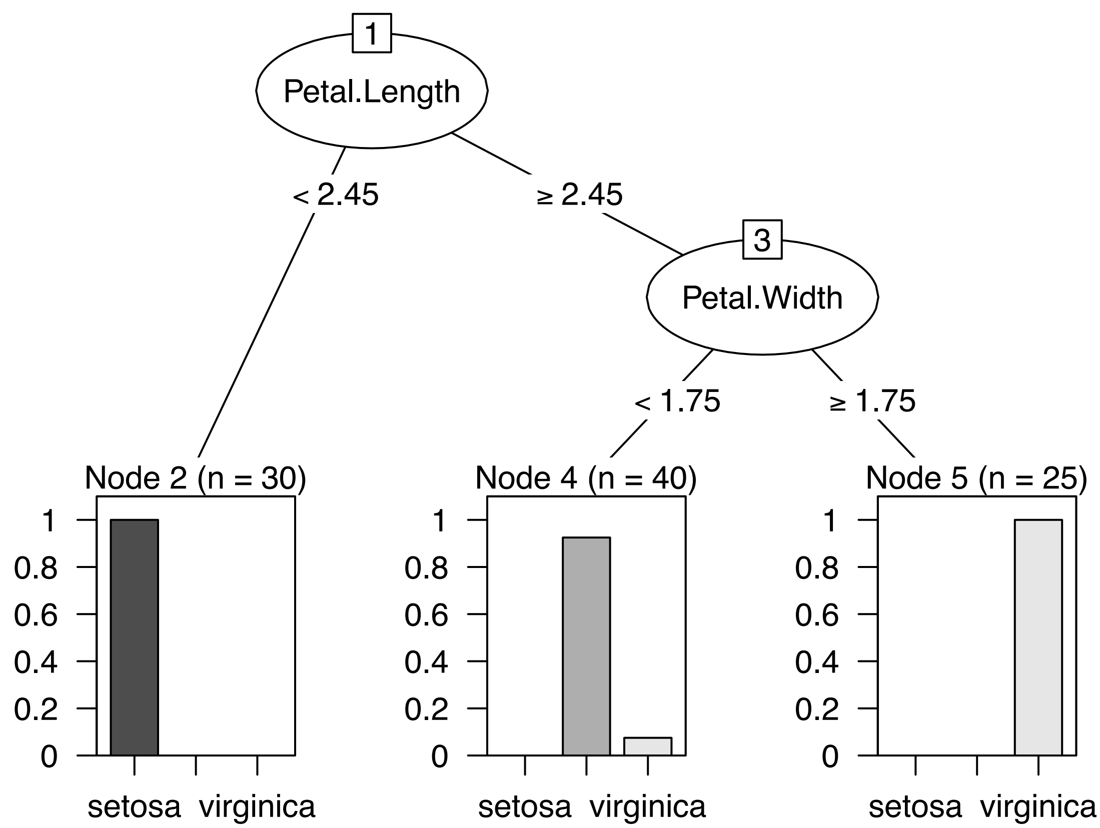



```
## SVM on clustered data

# tune svm once more
iris.kmeans.2.svm.polynomial.tuned <- tune.svm(Species~., data=iris.with.kmeans.2.training, kernel="pol
# select best model
iris.kmeans.2.svm.polynomial.best <- iris.kmeans.2.svm.polynomial.tuned$best.model
iris.kmeans.2.svm.polynomial.best.pred <- predict(iris.kmeans.2.svm.polynomial.best, iris.with.kmeans.2

confusionMatrix(iris.kmeans.2.svm.polynomial.best.pred, iris.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         13         2
##   virginica       0          0        20
##
## Overall Statistics
##
##                Accuracy : 0.9636
##                  95% CI : (0.8747, 0.9956)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9447
```

```
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            1.0000           0.9091
## Specificity                 1.0000            0.9524           1.0000
## Pos Pred Value              1.0000            0.8667           1.0000
## Neg Pred Value              1.0000            1.0000           0.9429
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2364           0.3636
## Detection Prevalence        0.3636            0.2727           0.3636
## Balanced Accuracy           1.0000            0.9762           0.9545
```

```
## Three centroids

iris.kmeans.3 = kmeans(iris.data, centers = 3) # three centroids as data is really 3 classes
iris.with.kmeans.3 <- cbind.data.frame(iris.data, Cluster = iris.kmeans.3$cluster)

iris.with.kmeans.3 <- cbind.data.frame(iris, Cluster = iris.kmeans.3$cluster) # add cluster feature
iris.with.kmeans.3.training = iris.with.kmeans.3[ind.iris==1,]
iris.with.kmeans.3.test = iris.with.kmeans.3[ind.iris==2,]

## Decision tree on clustered data
iris.kmeans.3.dtree <- rpart(Species~., data = iris.with.kmeans.3.training)
plot(as.party(iris.kmeans.3.dtree))
```

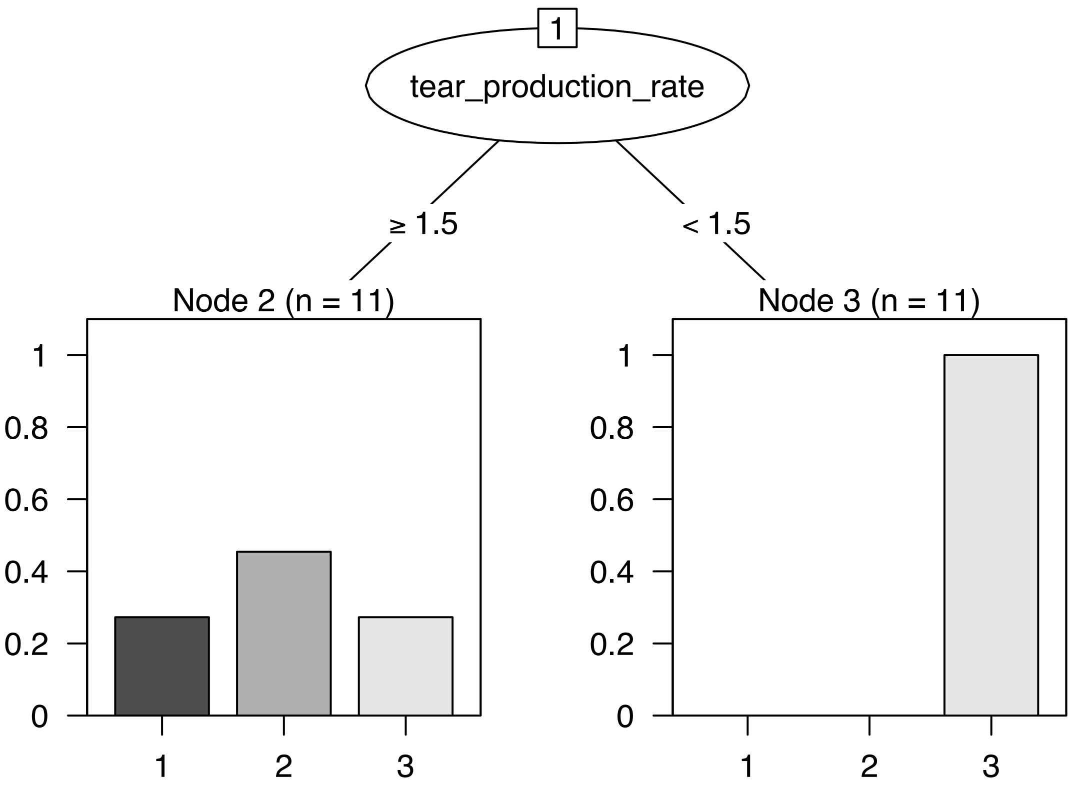


```
## SVM on clustered data

# tune svm once more
iris.kmeans.3.svm.polynomial.tuned <- tune.svm(Species~., data=iris.with.kmeans.3.training, kernel="pol
# select best model
iris.kmeans.3.svm.polynomial.best <- iris.kmeans.3.svm.polynomial.tuned$best.model
iris.kmeans.3.svm.polynomial.best.pred <- predict(iris.kmeans.3.svm.polynomial.best, iris.with.kmeans.3

confusionMatrix(iris.kmeans.3.svm.polynomial.best.pred, iris.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##             Reference
## Prediction   setosa versicolor virginica
##   setosa         20          0         0
##   versicolor      0         13         2
##   virginica       0          0        20
##
## Overall Statistics
##
##                Accuracy : 0.9636
##                  95% CI : (0.8747, 0.9956)
##     No Information Rate : 0.4
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9447
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: setosa Class: versicolor Class: virginica
## Sensitivity                 1.0000            1.0000           0.9091
## Specificity                 1.0000            0.9524           1.0000
## Pos Pred Value              1.0000            0.8667           1.0000
## Neg Pred Value              1.0000            1.0000           0.9429
## Prevalence                  0.3636            0.2364           0.4000
## Detection Rate              0.3636            0.2364           0.3636
## Detection Prevalence        0.3636            0.2727           0.3636
## Balanced Accuracy           1.0000            0.9762           0.9545
```

Contact Lenses

```
## Can't apply NbClust for this dataset, will use 2 and 3 centroids as with iris
## Two centroids
lenses.kmeans.2 <- kmeans(lenses.data, centers = 2)
lenses.with.kmeans.2 <- cbind.data.frame(lenses, cluster=lenses.kmeans.2$cluster)
lenses.with.kmeans.2.training = lenses.with.kmeans.2[ind.lenses==1,]
lenses.with.kmeans.2.test = lenses.with.kmeans.2[ind.lenses==2,]

## Decision tree on clustered data
lenses.kmeans.2.dtree <- rpart(class~., data = lenses.with.kmeans.2.training)
plot(as.party(lenses.kmeans.2.dtree))
```

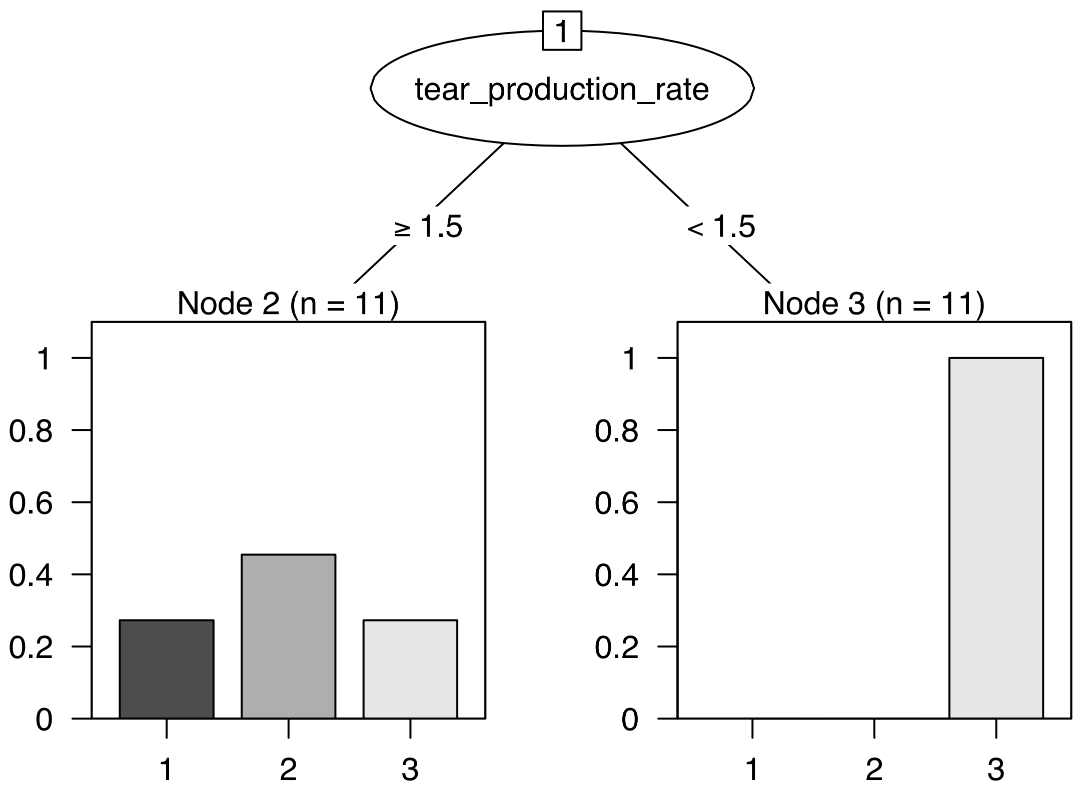



```
## SVM on clustered data

# tune svm once more
lenses.kmeans.2.svm.polynomial.tuned <- tune.svm(class~., data=lenses.with.kmeans.2.training, kernel="p
# select best model
lenses.kmeans.2.svm.polynomial.best <- lenses.kmeans.2.svm.polynomial.tuned$best.model
lenses.kmeans.2.svm.polynomial.best.pred <- predict(lenses.kmeans.2.svm.polynomial.best, lenses.with.km

confusionMatrix(lenses.kmeans.2.svm.polynomial.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
```

```
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```

```
## Three centroids
lenses.kmeans.3 <- kmeans(lenses.data, centers = 3)
lenses.with.kmeans.3 <- cbind.data.frame(lenses, cluster=lenses.kmeans.3$cluster)
lenses.with.kmeans.3.training = lenses.with.kmeans.3[ind.lenses==1,]
lenses.with.kmeans.3.test = lenses.with.kmeans.3[ind.lenses==2,]

## Decision tree on clustered data
lenses.kmeans.3.dtree <- rpart(class~., data = lenses.with.kmeans.3.training)
plot(as.party(lenses.kmeans.3.dtree))
```



```
## SVM on clustered data
# tune svm once more
lenses.kmeans.3.svm.polynomial.tuned <- tune.svm(class~., data=lenses.with.kmeans.3.training, kernel="po
# select best model
lenses.kmeans.3.svm.polynomial.best <- lenses.kmeans.3.svm.polynomial.tuned$best.model
lenses.kmeans.3.svm.polynomial.best.pred <- predict(lenses.kmeans.3.svm.polynomial.best, lenses.with.kme

confusionMatrix(lenses.kmeans.3.svm.polynomial.best.pred, lenses.testLabels)  # Confusion matrix
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction 1 2 3
##          1 1 0 0
##          2 0 0 0
##          3 0 0 1
##
## Overall Statistics
##
##                Accuracy : 1
##                  95% CI : (0.1581, 1)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.25
##
##                   Kappa : 1
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity               1.0       NA      1.0
## Specificity               1.0        1      1.0
## Pos Pred Value            1.0       NA      1.0
## Neg Pred Value            1.0       NA      1.0
## Prevalence                0.5        0      0.5
## Detection Rate            0.5        0      0.5
## Detection Prevalence      0.5        0      0.5
## Balanced Accuracy         1.0       NA      1.0
```