

Wine Classification

Final Project

M5364–Data Mining Fall 2016 Tarleton State Univ Dr. Scott Cook Assigned 2016-11-02 Due 2016-12-09

1 Summary of Data and Models

The Wine Quality Data set is a set of data that contains observations of wines. This data comes from the UCI Machine Learning Repository. The data is divided into two sets. The first data set contains 4898 observations of white wines. The second data set has 1599 different red wines. The data contains 12 attributes. The data has 11 numeric attributes. The numeric attributes are fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. The twelfth attribute is quality. This part of the data is usually what is trying to be calculated with a regression problem, or it is also determined via classification techniques. I was not sure how this attribute could be treated. I initially thought about treating it just as a normal numeric value. However, I wanted to see how to treat it as a factor.

I decided to tackle this set of data by combining the red and white rows of data. The combined red and white data had 6,497 different types of wines from Portugal. I wanted to classify the wines between red and white. For this project, I applied classification techniques that we have covered in class throughout the semester to determine the type of wine. The table below describes the techniques applied and the values of accuracy for the respective models. All original models were run with a simple 70-30 split and then cross-validation was applied to the models to determine the mean accuracy for each technique.

Table 1: Accuracy of Models Using Cross-Validation

Model	Accuracy
R Part Decision Trees	0.9804547
C Tree Decision Trees	0.9761422
K Nearest Neighbors	0.9938433
Weighted K nearest Neighbors	0.9943058
Naive Bayes	0.9752199
Support Vector Machines	0.9955366
Artificial Neural Networks	0.9723155

13

14 R Part Decision Trees

When trying to classify the model. I initially ran the decision tree with the `rpart` package. This decision tree started with a depth of 4 and an accuracy of 97.6%. Most of the data in the naive run of the tree was split from the counts of total sulfur dioxides and chlorides. The other factor involved was volatile acidity. Once this model was run, tuning was applied to the complexity parameter, minimum split, and the maximum depth of the trees.

For the complexity parameters, I decided that the best was to test small values from 0.0 to 0.2. After tuning was run, 0.001 was determined to be the most accurate parameter for the model. From our in-class sources, I initially tried to test a minimum split of 5, 10, or 15. However, I was getting the same error rate for all of those values. After looking through the data more, I realized that trying to split with only 5, 10, or 15 observations would be over-fitting the model and not very ideal. I then tried splits of 50, 125 by 5 and I saw that the errors began to change after 50 splits. 50 was determined to be the best minimum split. The maximum depth was decided from values between 1 and 10. The best tree had a depth of 6. Once complexity parameter, minimum split, and maximum depth were set to the optimal parameters, the accuracy of the rerun decision tree was 98%. The best decision tree included fixed acidity in splitting the data into the type of wines, along with the other attributes that were in the naive tree. The optimal decision tree was run using 10 fold cross-validation and the mean of those accuracies was 98%.

28 C Tree Decision Trees

29 In class this semester, our assignments led us to believe that the best decision tree was used with the `rpart` calculations instead
 30 of the `ctree` calculations. I wanted to test the method and determine which method was better for this data. The first attempt
 31 of the model split most frequently with density, alcohol, total sulfur dioxides, sulphates and chlorides. Other attributes used in
 32 the model were pH, residual sugar, volatile acidity, fixed acidity, and chlorides. With these factors, the model had 69 nodes and
 33 the model has a depth of 8. The initial accuracy was 98.1% The model was tuned for the minimum split and the maximum
 34 depth. It was tested for values of minimum split at 50, 100, and 150. The optimal value was 50. At maximum depth, values
 35 between 1 and 10 were tested. The best depth was calculated to be 10. The optimal tree was tested with these values and had
 36 an accuracy of 98.3%. The tree looked similar to the first run of a decision tree. However, the overall depth was increased by
 37 one. Once cross-validation was done with this model, the average accuracy was much lower at 97.6%. I was suprised to see this.
 38 However, I believe that this was done from splits that had more data that was had similar values in certain categories. Overall
 39 after cross-validation of both methods, the `rpart` calculations were proven to be better for this data.

40 K nearest neighbors

41 K nearest neighbors was standardized initially and was calculated with 3 nearest neighbors. This trial resulted in a 99.2%
 42 accuracy. The trial was then tuned with nearest neighbors of 2 through 20. The method was also tuned with three different
 43 types of sampling: cross-validation, fixed sampling, and bootstrapping. The best nearest neighbors for cross-validation was 5.
 44 Fixed sampling had an optimal nearest neighbor count of 11. Bootstrapping was 12. I tested the model with all the values
 45 of k that were determined in the sampling and then cross-validated. Through tuning and cross-validation, the overall average
 46 accuracy was 99.3%

47 Weighted K Nearest Neighbors

48 I wanted to test to see how the kernels of K nearest neighbors affected the values of the model. The first trial was with a
 49 triangular kernel and the accuracy was 99.2%. I tested all eight kernels available. I expected that the optimal kernel would
 50 perform better than my first trial. After testing, the inverted kernel was determined to have minimal errors with 3 nearest
 51 neighbors. The accuracy was run once for a 99.2% accuracy. cross-validation resulted in a mean 99.4% accuracy.

52 Naive Bayes

53 Naive Bayes has the assumption of normality. I had to first test the normality of all attributes of the data. The numerical
 54 values of the data were not normal. At this point I tried to see if I could treat the quality as a factor instead of a numerical
 55 value. All models had obvious curvature in all of the Q-Q Plots. Also, all Shapiro-Wilk tests returned the smallest possible
 56 p-values for a normal distribution. The data had to be cut to assume normality with the `mycut` function that was developed in
 57 this semester. The attributes that needed normalizing were cut into 10 factor levels. Due to time constraints, I was not able to
 58 test multiple cuts. I wish that I had tested multiple cuts to find the best cut for the model. Due to the size of the data, I tried
 59 10 and felt like this was a good estimate. After normalization, the first attempt at the model had a 97.8% accuracy. The model
 60 then underwent 10 fold cross-validation and had a mean accuracy of 97.5%.

61 Support Vector Machines

62 Before we could start Support Vector Machines, I removed the the combined database that was adjusted for normality. Then I
 63 recommitted the combined set of data and ran the support vector machines. The trial support vector machines had an accuracy
 64 of 99.6% percent. The tuning then was tested for gamma and costs parameters. The first time that I tuned the function, the
 65 upper extremities were the best parameters. I then attempted to tune again with the upper extremities as the lower boundaries

of the function. The second attempt at tuning the function resulted in the lower bounds, the original upper extremities, were the optimal gamma and cost. Therefore these values were used and the model after tuning was 99.6%.

Artificial Neural Networks

The neural networks was run using the `nnet` package. The first time it was run with 2 levels and a maximum iteration at 100. The first accuracy was at 99.8% I changed the iterations to 500 and the size of the neural network to 10 hidden layers. During the run of the neural network command. The first iterations stopped at 230 and the accuracy was 99.7%. The network was tuned with sizes of hidden layers between 1 and 15. Also the tuning function was applied with controls of 5 repeats, cross validation sampling, and 10 crosses. The tuning function ran cross validation and resulted in 97.2% accuracy. I was shocked at this low value considering the first values that i got that were extremely high. I think that my first guess of 10 layers was the best for the model and the sum from all other sizes of hidden layers caused the value to overall be lower.

Conclusion

Overall, Support Vector Machines were the optimal model for this data. Neural Networks and the C Tree Decision Trees were the overall worst models for the data. As I was working with the data, I really did not consider the chemical make up of a red wine and the chemical makeup of a white wine. I just wanted to run the data to see how it behaved on it's own. After looking more into the data, there are certain key attributes that really determine the model. Alcohol, density, total sulfur dioxides, free sulfur dioxides, chlorides, and pH were the best attributes that could determine the type of wine. Models where these were these were used instead of the whole data could probably perform at similar accuracies to the models run with all attributes.

Code Appendix

```

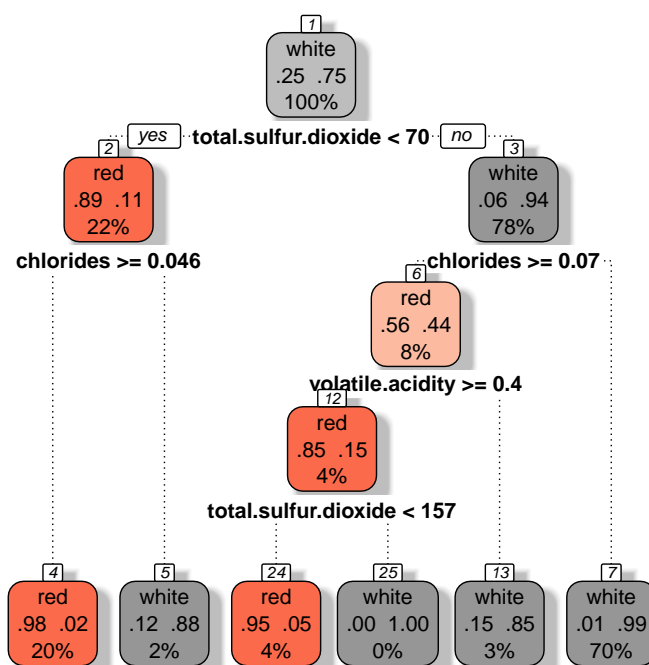
84 set.seed(1506)
85 # Importing Data Sets
86 Red_Wine <- read.csv("~/Downloads/winequality-red.csv", sep = ";")
87 White_Wine <- read.csv("~/Downloads/winequality-white.csv", sep = ";")
88
89 # Adding the Type of Wine to the data set.
90 Red <- c(rep("red", nrow(Red_Wine)))
91 White <- c(rep("white", nrow(White_Wine)))
92 Red_Wine <- cbind(Red_Wine, Red)
93 White_Wine <- cbind(White_Wine, White)
94
95 # Changing the type of wine columns
96 colnames(Red_Wine)[13] <- "wine.type"
97 colnames(White_Wine)[13] <- "wine.type"
98
99 # Combining Both Red and White Wines into one data set
100 Total_Wine <- rbind(Red_Wine, White_Wine)
101 Total_Wine$quality <- as.factor(Total_Wine$quality)
102
103 # Item that will be predicted with the classification.
104 Wine.Type <- Total_Wine$wine.type
105
106 # Splitting Data for testing purposes
107 Wine.Split <- splitdata(Total_Wine, 0.7)
108 Wine.train <- Wine.Split$traindata
109 Wine.test <- Wine.Split$testdata
110

```

```

111 # Decision Trees to determine the type of wine, red or white.
112 wine.tree <- rpart(wine.type ~ ., data = Wine.train)
113 plot.wine.tree <- fancyRpartPlot(wine.tree, palettes = c("Reds", "Greys"))

```



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```

114
115 pred.tree <- predict(wine.tree, newdata = Wine.test, type = "class")
116
117 # Analysis of the decision tree
118 tree.conf <- confusion(Wine.test$wine.type, pred.tree, costs = NULL)
119 tree.conf

```

```

120
121 $counts
122      pred
123 true    red white
124   red   442   36
125   white  10 1461
126
127 $acc
128 [1] 0.9763982
129
130 $rates
131      pred
132 true      red      white
133   red  0.924686192 0.075313808
134   white 0.006798097 0.993201903
135
136 $sensitivities
137      red      white
138 0.9246862 0.9932019
139
140 $precisions
141      red      white
142 0.9778761 0.9759519
143
144 $F1s

```

```

145      red      white
146 0.9505376 0.9845013
147
148 $cost
149 [1] 46
150

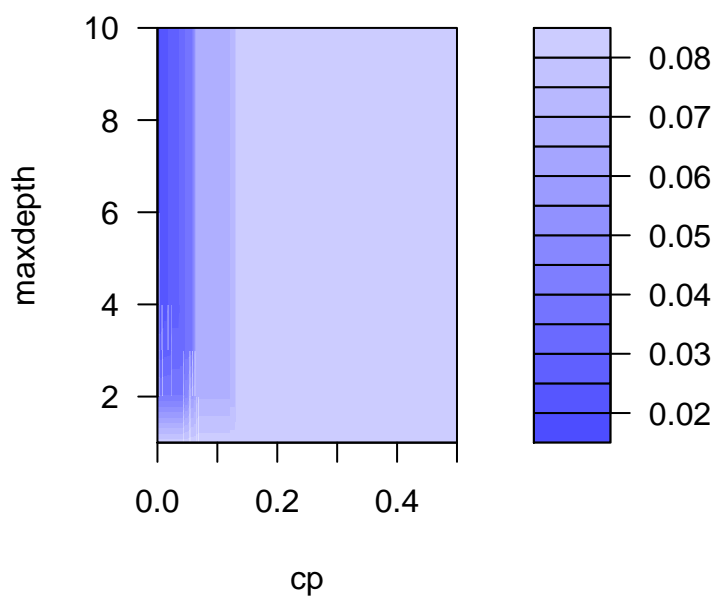
```

```

151 # Tuning decision tree
152 tree.tune <- tune.rpart(wine.type ~ ., data = Total_Wine, cp = seq(0, 0.5, 0.001),
153   maxdepth = 1:10)
154 tree.tune.2 <- tune.rpart(wine.type ~ ., data = Total_Wine, minsplit = seq(50,
155   125, 5))
156 plot(tree.tune)

```

Performance of 'rpart.wrap

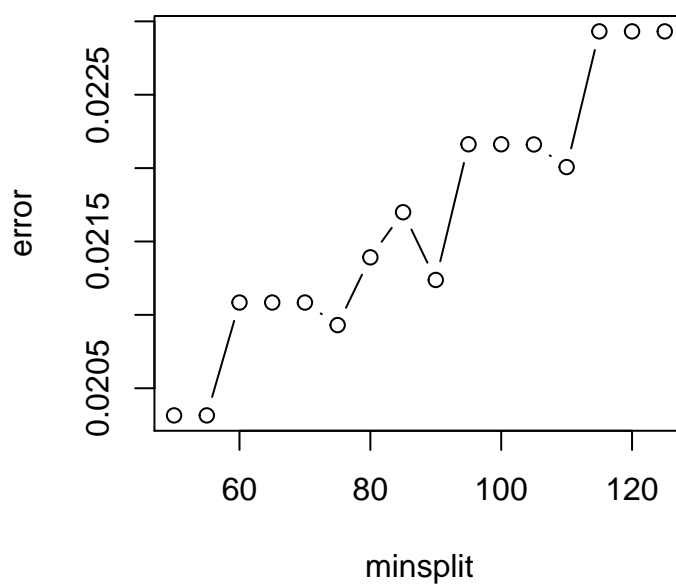


```

157
158 plot(tree.tune.2)

```

Performance of 'rpart.wrapper'



159

```
160 # The best parameters for the rpart decision tree
```

```
161 tree.tune$best.parameters
```

162

```
163      cp maxdepth
```

```
164 2507 0.001      6
```

165

```
166 tree.tune.2$best.parameters
```

167

```
168      minsplit
```

```
169 1          50
```

170

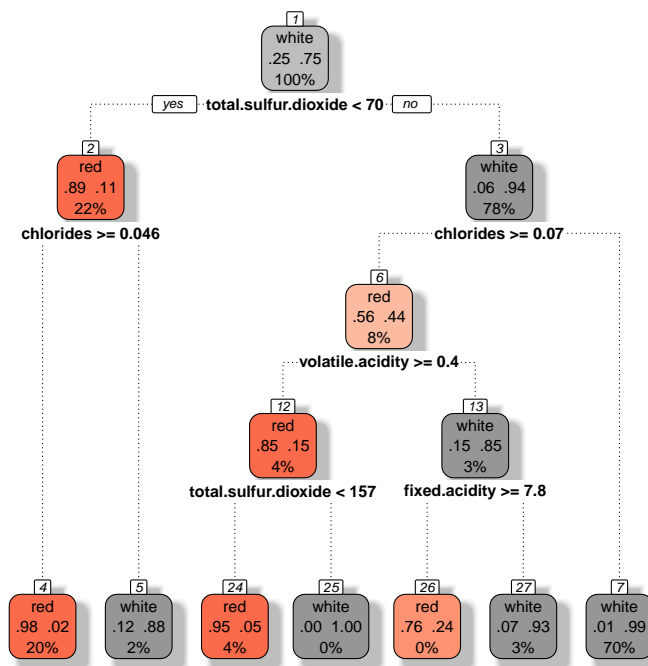
```
171 # Optimal rpart tree
```

```
172 tree.2 <- rpart(wine.type ~ ., data = Wine.train, control = rpart.control(minsplit =
```

```
173   tree.tune.2$best.parameters$minsplit,
```

```
174   cp = tree.tune$best.parameters$cp, maxdepth = tree.tune$best.parameters$maxdepth))
```

```
175 fancyRpartPlot(tree.2, palettes = c("Reds", "Greys"))
```



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```

177 pred.tree.2 <- predict(tree.2, newdata = Wine.test, type = "class")
178
179 # Analysis of optimal decision tree with cross validation
180 tree.conf.2 <- confusion(Wine.test$wine.type, pred.tree.2, costs = NULL)
181 tree.conf.2

```

```

182 $counts
183      pred
184 true    red white
185 red     452   26
186 white   12 1459
187
188 $acc
189 [1] 0.9805028
190
191 $rates
192      pred
193 true    red    white
194 red     0.945606695 0.054393305
195 white  0.008157716 0.991842284
196
197 $sensitivities
198      red    white
199 0.9456067 0.9918423
200
201 $precisions
202      red    white
203 0.9741379 0.9824916
204
205 $F1s
206      red    white
207 0.9596603 0.9871448
208
209 $cost
210 [1] 38

```

212

```

213 kflval <- function(k, data) {
214   folds = createfolds(nrow(data), k)
215   accvector = 1:k
216   for (k in 1:k) {
217     temptrain = data[folds != k, ]
218     temptest = data[folds == k, ]
219     temptree = rpart(wine.type ~ ., data = temptrain, control = rpart.control(minsplit =
220       tree.tune.2$best.parameters$minsplit,
221       cp = tree.tune$best.parameters$cp, maxdepth = tree.tune$best.parameters$maxdepth))
222     temppred = predict(temptree, newdata = temptest, type = "class")
223     analysis = confusion(temptest$wine.type, temppred)
224     accvector[k] = analysis$acc
225   }
226   return(mean(accvector))
227 }
228
229 kflval(10, Total_Wine)

```

230
231
232

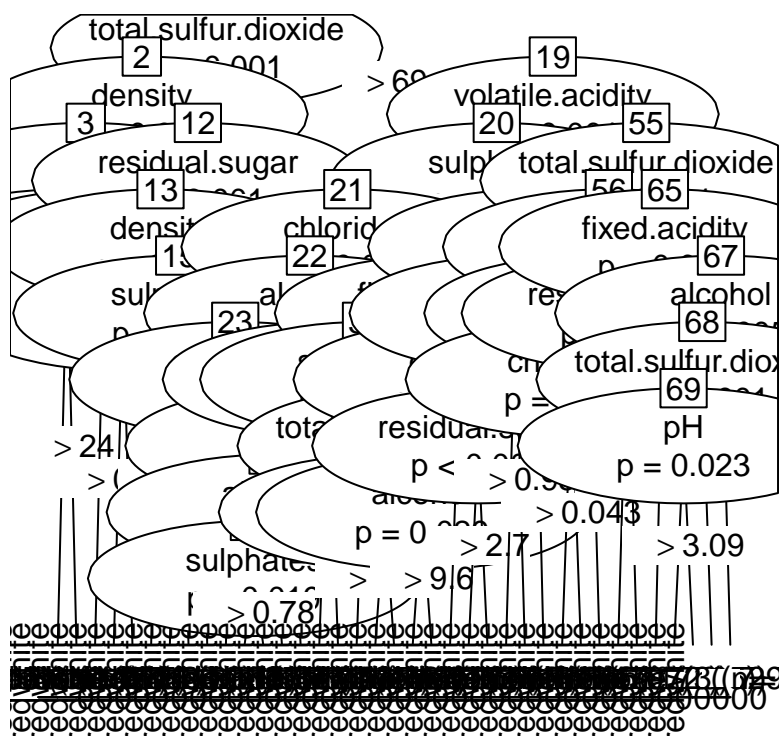
```
[1] 0.9789119
```

233
234
235

```

233 # Ctree
234 wine.ctree <- ctree(wine.type ~ ., data = Wine.train)
235 plot(wine.ctree)

```



236

```

237 # Prediction and confusion of ctree decision tree
238 pred.tree.3 <- predict(wine.ctree, newdata = Wine.test)
239 wine.ctree.conf <- confusion(Wine.test$wine.type, pred.tree.3, costs = NULL)
240 wine.ctree.conf

```

241
242
243
244

```

$counts
      pred
true  red white

```



```

245     red      458      20
246     white    17    1454
247
248 $acc
249 [1] 0.9810159
250
251 $rates
252       pred
253 true      red      white
254   red    0.95815900 0.04184100
255   white 0.01155676 0.98844324
256
257 $sensitivities
258       red      white
259 0.9581590 0.9884432
260
261 $precisions
262       red      white
263 0.9642105 0.9864315
264
265 $F1s
266       red      white
267 0.9611752 0.9874363
268
269 $cost
270 [1] 37

```

```

272 # Testing minsplit and maxdepth of ctree
273 maxdepth <- 1:10
274 # 50 minsplit
275 accvec <- NULL
276 for (i in 1:length(maxdepth)) {
277   temp.tree <- ctree(wine.type ~ ., data = Wine.train, controls = ctree_control(minsplit = 50,
278     maxdepth = maxdepth[i]))
279   temp.pred <- predict(temp.tree, newdata = Wine.test)
280   temp.conf <- confusion(Wine.test$wine.type, temp.pred, costs = NULL)
281   accvec[i] <- temp.conf$acc
282 }
283
284 # 100 misplit
285 accvec.2 <- NULL
286 for (i in 1:length(maxdepth)) {
287   temp.tree <- ctree(wine.type ~ ., data = Wine.train, controls = ctree_control(minsplit = 100,
288     maxdepth = maxdepth[i]))
289   temp.pred <- predict(temp.tree, newdata = Wine.test)
290   temp.conf <- confusion(Wine.test$wine.type, temp.pred, costs = NULL)
291   accvec.2[i] <- temp.conf$acc
292 }
293
294 # 150 minsplit
295 accvec.3 <- NULL
296 for (i in 1:length(maxdepth)) {
297   temp.tree <- ctree(wine.type ~ ., data = Wine.train, controls = ctree_control(minsplit = 150,
298     maxdepth = maxdepth[i]))
299   temp.pred <- predict(temp.tree, newdata = Wine.test)
300   temp.conf <- confusion(Wine.test$wine.type, temp.pred, costs = NULL)
301   accvec.3[i] <- temp.conf$acc
302 }
303

```

```

304 # Creating information matrix
305 max.depth <- as.vector(c(rep(list(1, 2, 3, 4, 5, 6, 7, 8, 9, 10), 3)))
306 min.split <- as.vector(c(rep(list(50, 100, 150), 10)))
307 accuracy <- as.vector(rbind(accvec, accvec.2, accvec.3))
308 acc.matrix <- cbind(max.depth, min.split, accuracy)
309 colnames(acc.matrix)[1] <- "maxdepth"
310 colnames(acc.matrix)[2] <- "misplit"
311 colnames(acc.matrix)[3] <- "accuracy"
312 which.max(accuracy)

```

```

313 [1] 19
314

```

```

316 acc.matrix[which.max(accuracy), ]

```

```

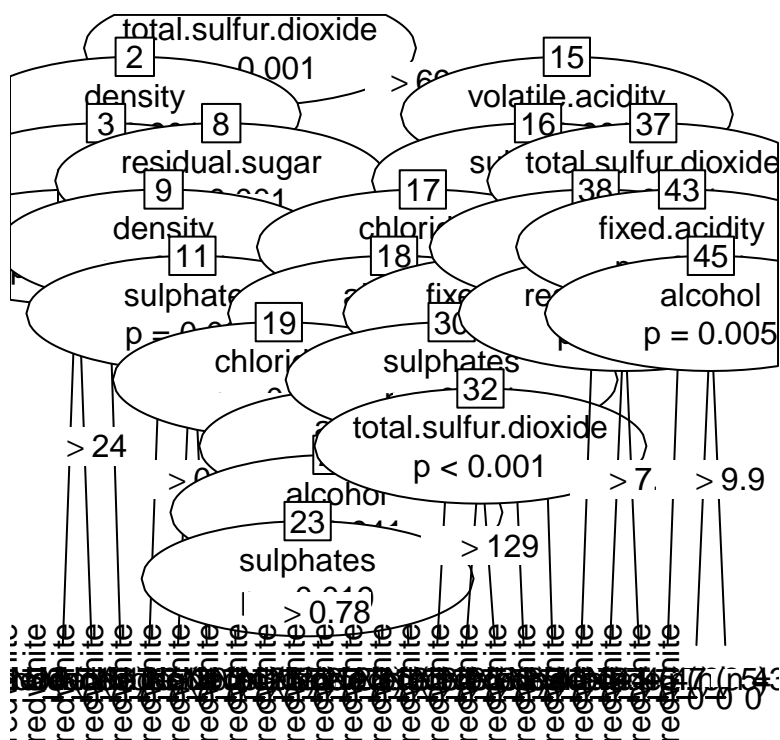
317 $maxdepth
318 [1] 9
319
320 $misplit
321 [1] 50
322
323 $accuracy
324 [1] 0.9712673
325

```

```

327 # Testing Optimal Ctree
328 opt.ctree <- ctree(wine.type ~ ., data = Wine.train, controls = ctree_control(minsplit = 50,
329   maxdepth = 10))
330 plot(opt.ctree)

```



```

331
332 opt.pred <- predict(opt.ctree, newdata = Wine.test)
333 opt.conf <- confusion(Wine.test$wine.type, opt.pred, costs = NULL)
334 opt.conf

```

```

335 $counts
336
337      pred

```

```

338 true      red white
339      red    451    27
340      white   29   1442
341
342 $acc
343 [1] 0.9712673
344
345 $rates
346      pred
347 true      red      white
348      red    0.94351464 0.05648536
349      white 0.01971448 0.98028552
350
351 $sensitivities
352      red      white
353 0.9435146 0.9802855
354
355 $precisions
356      red      white
357 0.9395833 0.9816201
358
359 $F1s
360      red      white
361 0.9415449 0.9809524
362
363 $cost
364 [1] 56
365

```

```

366 # Cross Validation with C Tree
367 ctree.kflval <- function(k, data) {
368   folds = createfolds(nrow(data), k)
369   accvector = 1:k
370   for (k in 1:k) {
371     temptrain = data[folds != k, ]
372     temptest = data[folds == k, ]
373     temptree = ctree(wine.type ~ ., data = temptrain, controls = ctree_control(minsplit = 50,
374       maxdepth = 10))
375     temppred = predict(temptree, newdata = temptest)
376     analysis = confusion(temptest$wine.type, temppred)
377     accvector[k] = analysis$acc
378   }
379   return(mean(accvector))
380 }
381
382 ctree.kflval(10, Total_Wine)
383
384 [1] 0.9738326
385

```

```

386 # K nearest neighbors standardize the data
387 x = Total_Wine[, 1:11]
388 xbar = apply(x, 2, mean)
389 xbarMat = cbind(rep(1, nrow(Total_Wine))) %*% xbar
390 s = apply(x, 2, sd)
391 sMat = cbind(rep(1, nrow(Total_Wine))) %*% s
392 z = (x - xbarMat)/sMat
393
394 # K nearest neighbors sampling the data
395 z.split <- sample(nrow(z), round(nrow(z) * 0.7, 0))
396 z.train <- z[z.split, ]

```

```

397 z.test <- z[-z.split, ]
398
399 # K nearest neighbors Test
400 wine.knn <- knn(train = z.train, test = z.test, k = 3, cl = Wine.Type[z.split])
401 confusion(Wine.Type[-z.split], wine.knn, costs = NULL)

```

```

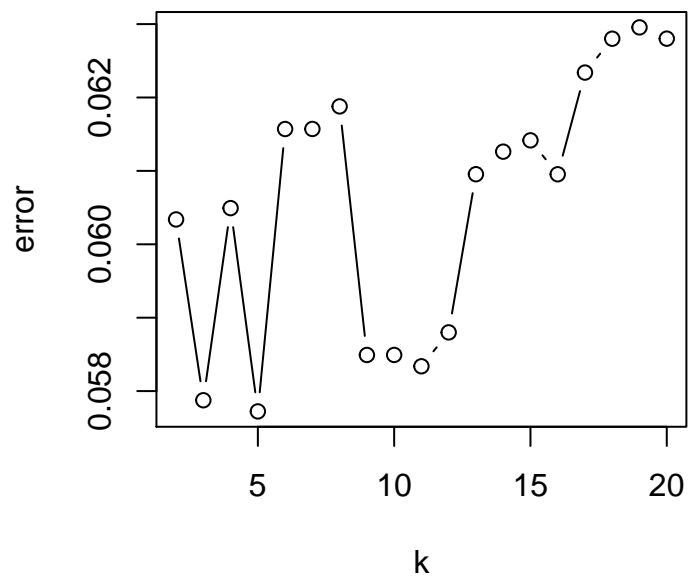
402
403 $counts
404      pred
405 true    red white
406   red   478    7
407   white    6 1458
408
409 $acc
410 [1] 0.9933299
411
412 $rates
413      pred
414 true      red      white
415   red  0.985567010 0.014432990
416   white 0.004098361 0.995901639
417
418 $sensitivities
419      red      white
420 0.9855670 0.9959016
421
422 $precisions
423      red      white
424 0.9876033 0.9952218
425
426 $Fis
427      red      white
428 0.9865841 0.9955616
429
430 $cost
431 [1] 13
432

```

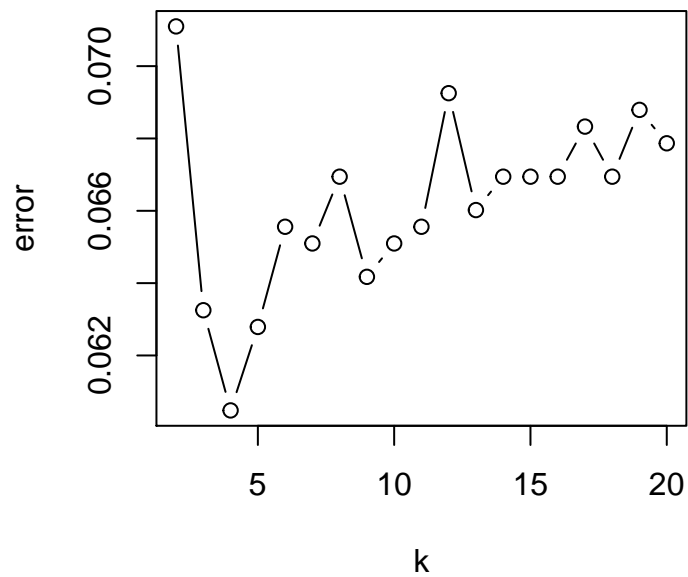
```

433 # Finding the optimal k for K nearest neighbors
434 x <- Total_Wine[, -13]
435 y <- Total_Wine[, 13]
436 knn.tune <- tune.knn(x, y, k = seq(2, 20, 1), tunecontrol = tune.control(sampling = "cross"))
437 knn.tune.2 <- tune.knn(x, y, k = seq(2, 20, 1), tunecontrol = tune.control(sampling = "fix"))
438 knn.tune.3 <- tune.knn(x, y, k = seq(2, 20, 1), tunecontrol = tune.control(sampling = "boot"))
439 plot(knn.tune)

```

Performance of 'knn.wrapper'

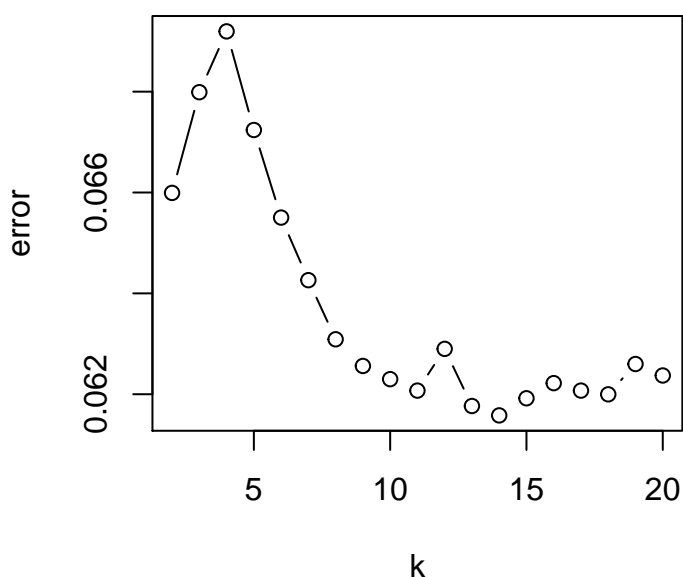
440

441 `plot(knn.tune.2)`**Performance of 'knn.wrapper'**

442

443 `plot(knn.tune.3)`

Performance of 'knn.wrapper'



```
knn.tune$best.parameters$k
```

```
[1] 5
```

```
knn.tune.2$best.parameters$k
```

```
[1] 4
```

```
knn.tune.3$best.parameters$k
```

```
[1] 14
```

```
wine.knn.2 <- knn(train = z.train, test = z.test, k = knn.tune$best.parameters$k,
  cl = Wine.Type[z.split])
wine.knn.3 <- knn(train = z.train, test = z.test, k = knn.tune.2$best.parameters$k,
  cl = Wine.Type[z.split])
wine.knn.4 <- knn(train = z.train, test = z.test, k = knn.tune.3$best.parameters$k,
  cl = Wine.Type[z.split])
wine.knn.2.conf <- confusion(Wine.Type[-z.split], wine.knn.2, costs = NULL)
wine.knn.3.conf <- confusion(Wine.Type[-z.split], wine.knn.3, costs = NULL)
wine.knn.4.conf <- confusion(Wine.Type[-z.split], wine.knn.4, costs = NULL)

# Cross Validation for K nearest neighbors
cross.knn <- knn.cv(train = z, cl = y, k = knn.tune$best.parameters$k)
cross.knn.conf <- confusion(Wine.Type, cross.knn)

# Weighted K nearest neighbors
z <- cbind(z, Wine.Type)
z.train <- z[z.split, ]
z.test <- z[-z.split, ]
weight.knn.wine <- kknn(Wine.Type ~ ., train = z.train, test = z.test, k = knn.tune$best.parameters$k,
  kernel = "triangular")
pred.weight <- predict(weight.knn.wine, newdata = z.test)
confusion(z.test$Wine.Type, pred.weight)
```

479
480
481
482
483
484
485
486
487
488
489
490
491
492
493
494
495
496
497
498
499
500
501
502
503
504
505
506
507
508
509

```
$counts
      pred
true    red white
red     479    6
white    4  1460

$acc
[1] 0.9948692

$rates
      pred
true    red    white
red   0.98762887 0.01237113
white 0.00273224 0.99726776

$sensitivities
      red    white
0.9876289 0.9972678

$precisions
      red    white
0.9917184 0.9959072

$F1s
      red    white
0.9896694 0.9965870

$cost
[1] 10
```

510
511
512
513
514
515
516
517
518
519
520
521
522
523
524
525
526
527
528
529
530
531
532
533
534
535
536
537

```
# Finding the best kernels
tune.kknn <- function(K, kernels) {
  acc <- NULL
  for (i in 1:length(K)) {
    temp.model <- kknn(Wine.Type ~ ., train = z.train, test = z.test, k = i,
      kernel = kernels, distance = 2)
    pred.temp <- predict(temp.model, newdata = z.test)
    temp.conf <- confusion(z.test$Wine.Type, pred.temp)
    acc[i] <- temp.conf$acc
  }
  opt.k <- which.max(acc)
  opt.acc <- acc[opt.k]
  return(list(k = opt.k, accuracy = opt.acc))
}
K <- 2:30
rect <- tune.kknn(K, "rectangular")
triangle <- tune.kknn(K, "triangular")
ep <- tune.kknn(K, "epanechnikov")
biw <- tune.kknn(K, "biweight")
triw <- tune.kknn(K, "triweight")
cosine <- tune.kknn(K, "cos")
invert <- tune.kknn(K, "inv")
gauss <- tune.kknn(K, "gaussian")
rank.weight <- tune.kknn(K, "rank")
optimal <- tune.kknn(K, "optimal")
weighted.accuracy <- list(rect$accuracy, triangle$accuracy, ep$accuracy, biw$accuracy,
  triw$accuracy, cosine$accuracy, invert$accuracy, gauss$accuracy, rank.weight$accuracy,
  optimal$accuracy)
```

```

538 weighted.k ← list(rect$k, triangle$k, ep$k, biw$k, triw$k, cosine$k, invert$k,
539   gauss$k, rank.weight$k, optimal$k)
540
541 opt.weights ← cbind(weighted.k, weighted.accuracy)
542 opt.kknn ← kknn(Wine.Type ~ ., train = z.train, test = z.test, k = 3, kernel = "inv")
543 pred.kknn ← predict(opt.kknn, newdata = z.test)
544 confusion(z.test$Wine.Type, pred.kknn)

```

```

545
546 $counts
547      pred
548 true      red white
549   red      479    6
550   white     5 1459
551
552 $acc
553 [1] 0.9943561
554
555 $rates
556      pred
557 true      red      white
558   red  0.987628866 0.012371134
559   white 0.003415301 0.996584699
560
561 $sensitivities
562      red      white
563 0.9876289 0.9965847
564
565 $precisions
566      red      white
567 0.9896694 0.9959044
568
569 $F1s
570      red      white
571 0.9886481 0.9962445
572
573 $cost
574 [1] 11
575

```

```

576 # Cross Validation fro Weighted K nearest neighbors
577 kknn.kflval ← function(k, data) {
578   folds = createfolds(nrow(data), k)
579   accvector = 1:k
580   for (k in 1:k) {
581     temptrain = data[folds != k, ]
582     temptest = data[folds == k, ]
583     tempmodel = kknn(Wine.Type ~ ., train = temptrain, test = temptest,
584       k = 3, kernel = "inv")
585     temppred = predict(tempmodel, newdata = temptest, type = "raw")
586     analysis = confusion(temptest$Wine.Type, temppred)
587     accvector[k] = analysis$acc
588   }
589   return(mean(accvector))
590 }
591
592 kknn.kflval(10, z)

```

```

593 [1] 0.9941515
594

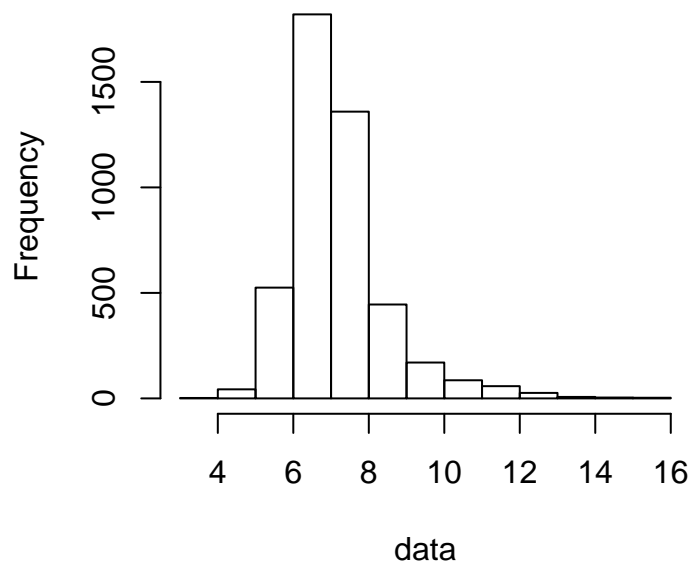
```

```

596 # Investigating qualities of data Naive Bayes
597 normality(Wine.train$fixed.acidity)

```


Histogram of data

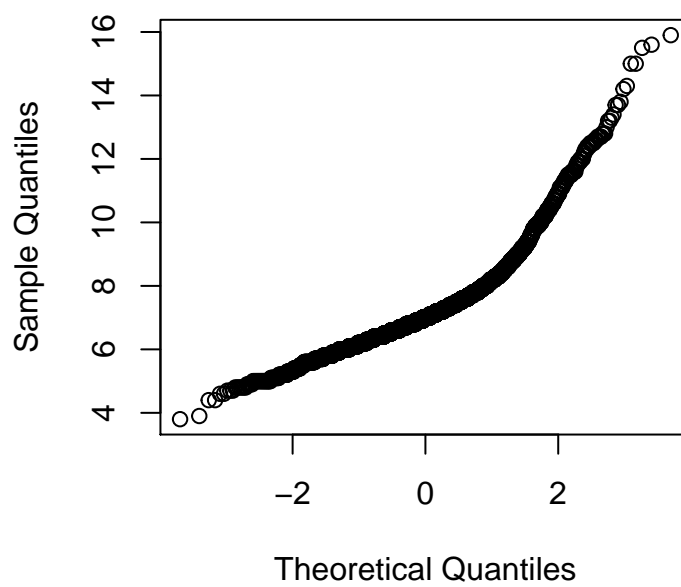


```

598
599
600
601     Shapiro-Wilk normality test
602
603 data:  data
604 W = 0.88403, p-value < 2.2e-16
605

```

Normal Q-Q Plot

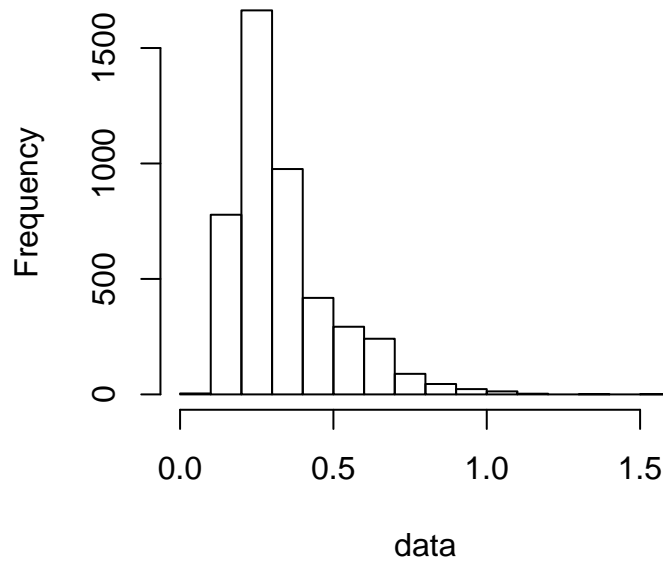


```

606
607 normality(Wine.train$volatile.acidity)

```

Histogram of data

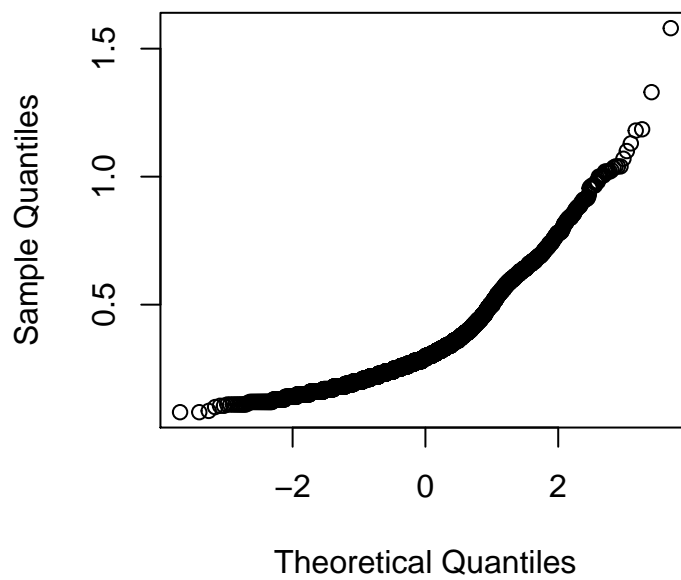


```

608
609
610
611     Shapiro-Wilk normality test
612
613 data:  data
614 W = 0.87268, p-value < 2.2e-16
615

```

Normal Q-Q Plot

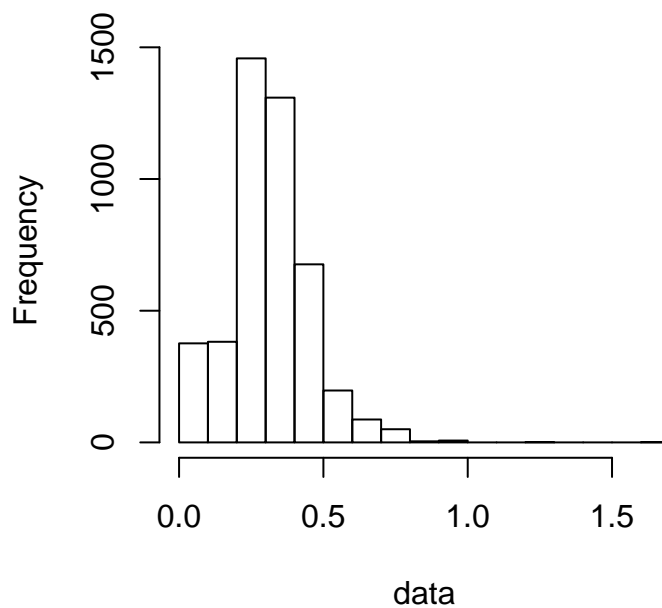


```

616
617 normality(Wine.train$citric.acid)

```

Histogram of data

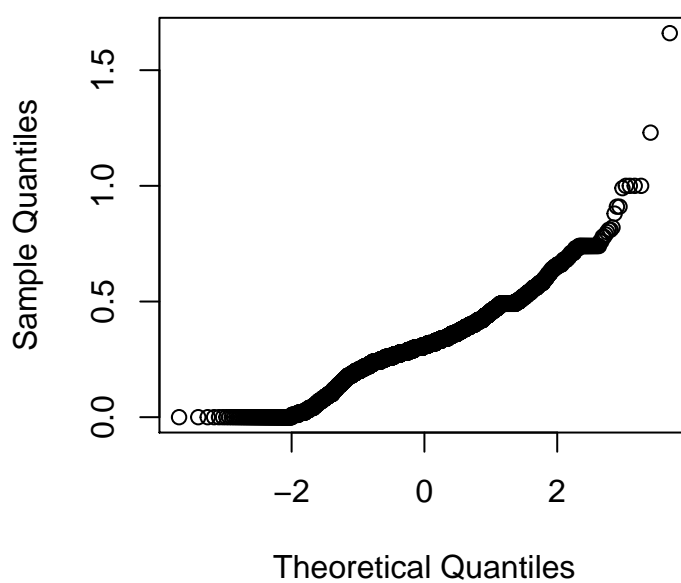


```

618
619
620
621     Shapiro-Wilk normality test
622
623 data:  data
624 W = 0.96462, p-value < 2.2e-16
625

```

Normal Q-Q Plot

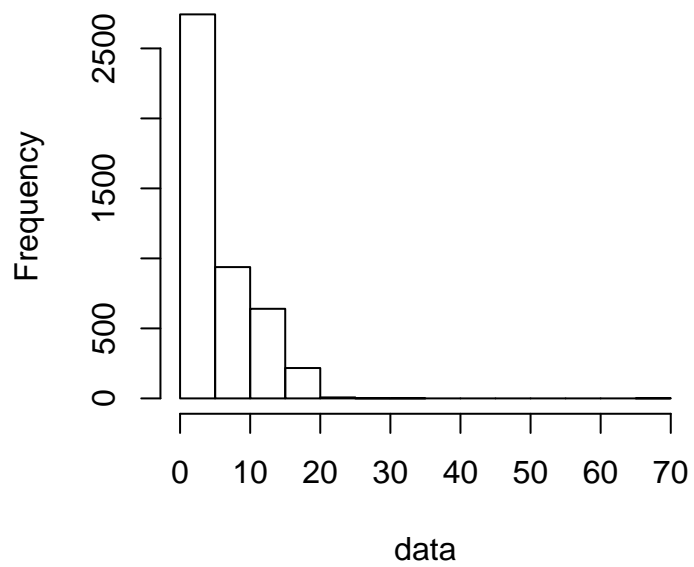


```

626
627 normality(Wine.train$residual.sugar)

```

Histogram of data

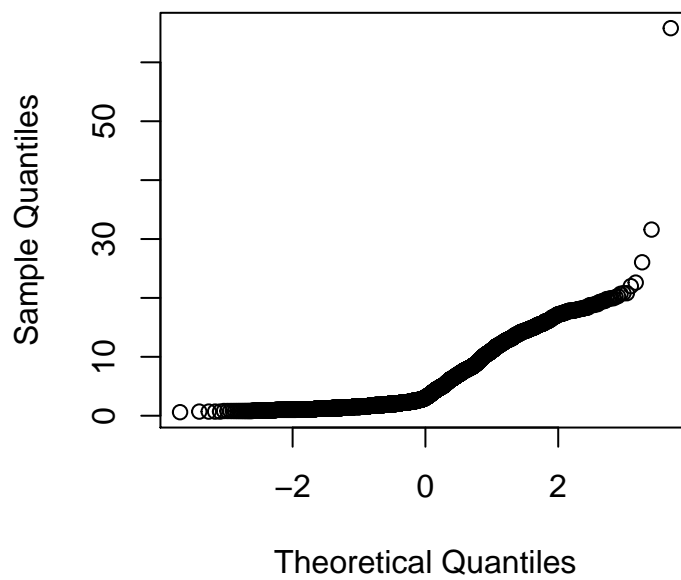


```

628
629
630
631     Shapiro-Wilk normality test
632
633 data:  data
634 W = 0.82197, p-value < 2.2e-16
635

```

Normal Q-Q Plot

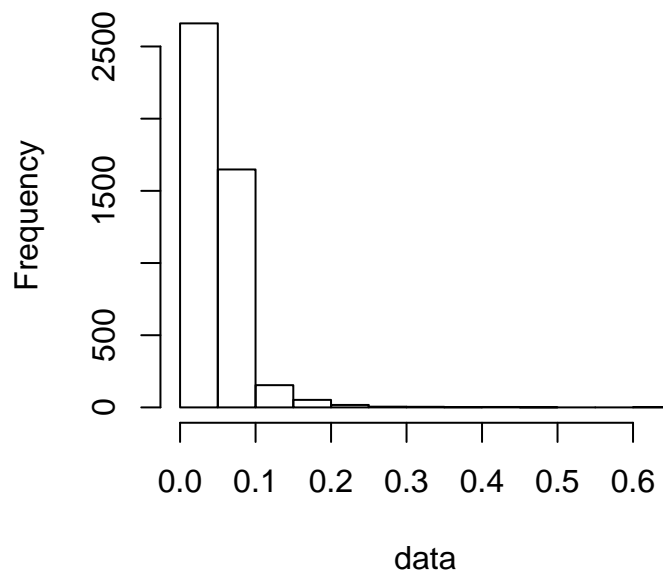


```

636
637 normality(Wine.train$chlorides)

```

Histogram of data

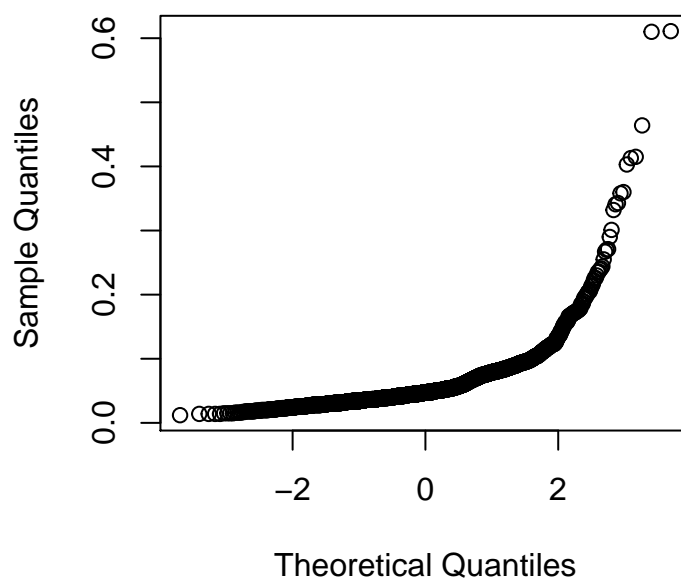


```

638
639
640
641     Shapiro-Wilk normality test
642
643 data:  data
644 W = 0.64501, p-value < 2.2e-16
645

```

Normal Q-Q Plot

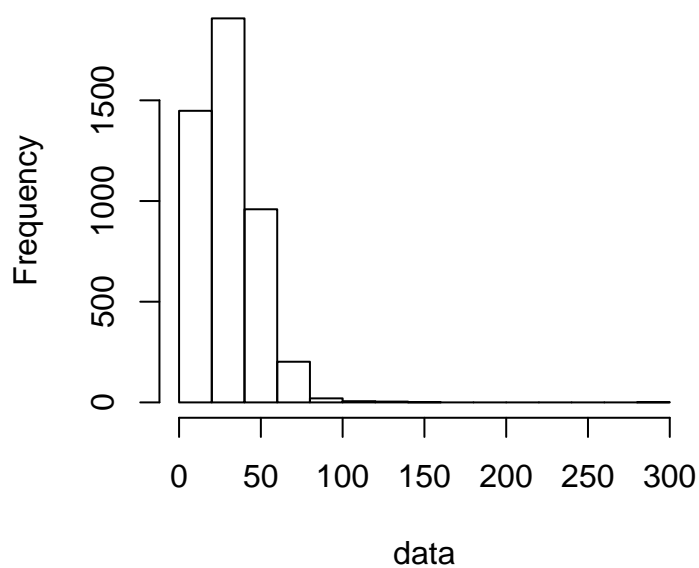


```

646
647 normality(Wine.train$free.sulfur.dioxide)

```

Histogram of data

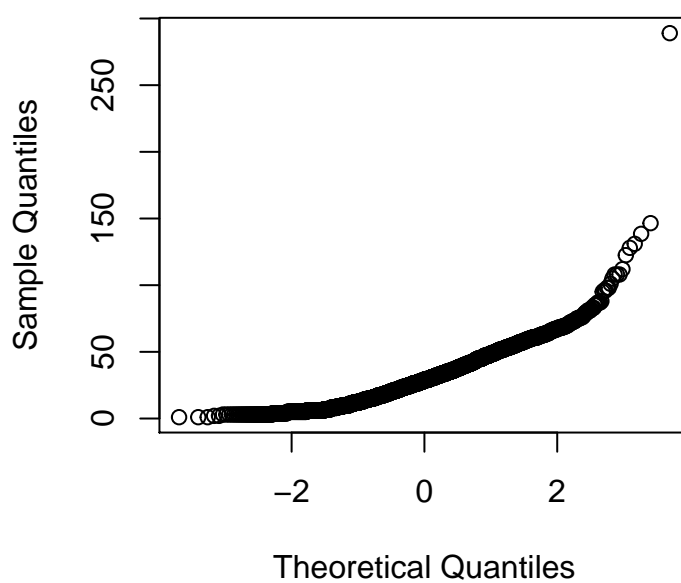


```

648
649
650
651     Shapiro-Wilk normality test
652
653 data:  data
654 W = 0.93333, p-value < 2.2e-16
655

```

Normal Q-Q Plot

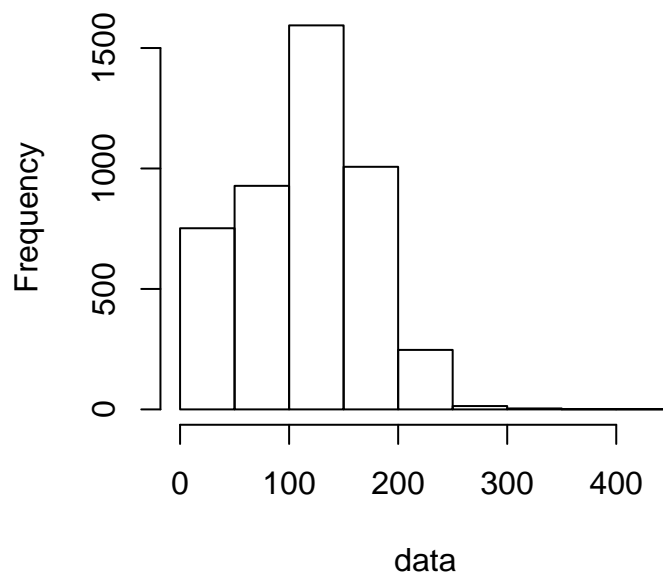


```

656
657 normality(Wine.train$total.sulfur.dioxide)

```

Histogram of data

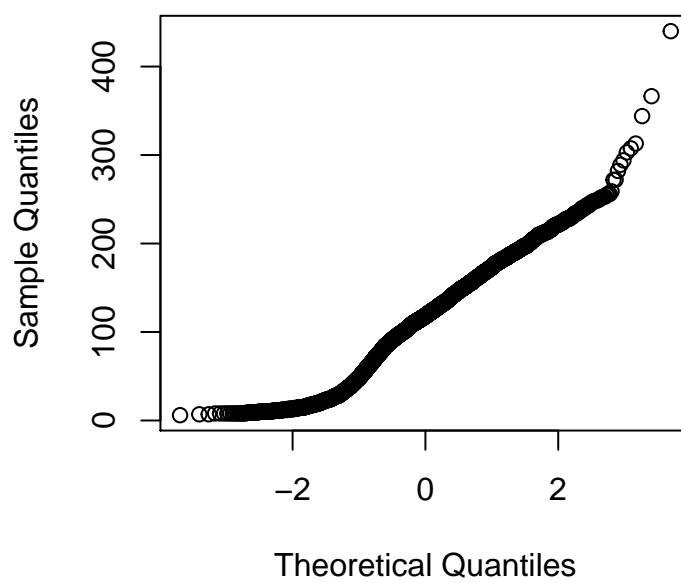


```

658
659
660
661     Shapiro-Wilk normality test
662
663 data:  data
664 W = 0.98268, p-value < 2.2e-16
665

```

Normal Q-Q Plot

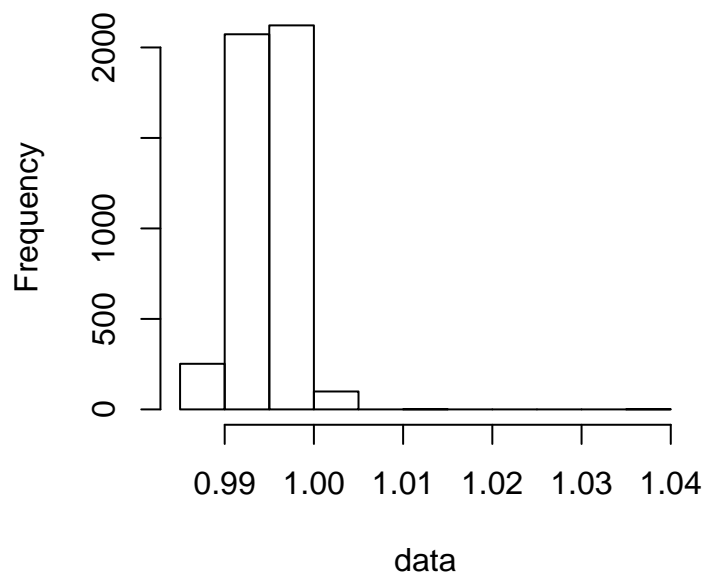


```

666
667 normality(Wine.train$density)

```

Histogram of data

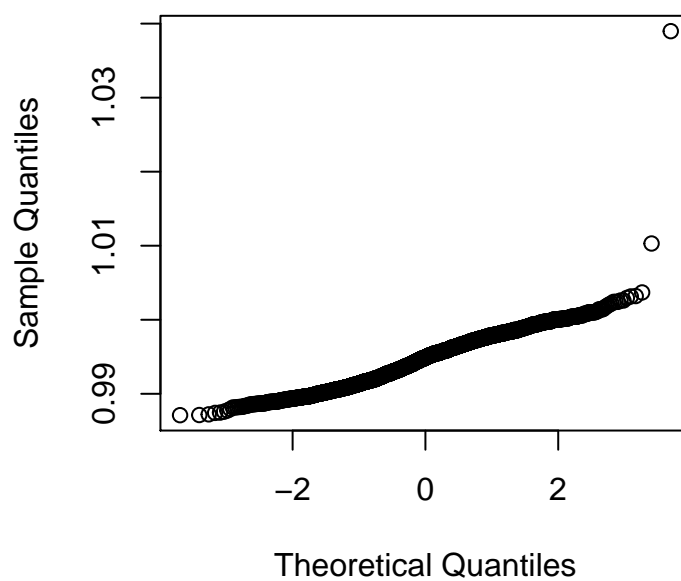


```

668
669
670
671     Shapiro-Wilk normality test
672
673 data:  data
674 W = 0.95975, p-value < 2.2e-16
675

```

Normal Q-Q Plot

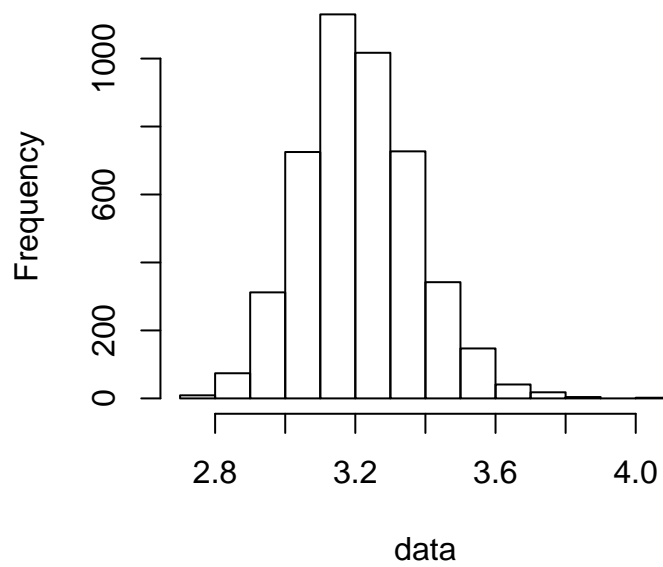


```

676
677 normality(Wine.train$pH)

```


Histogram of data

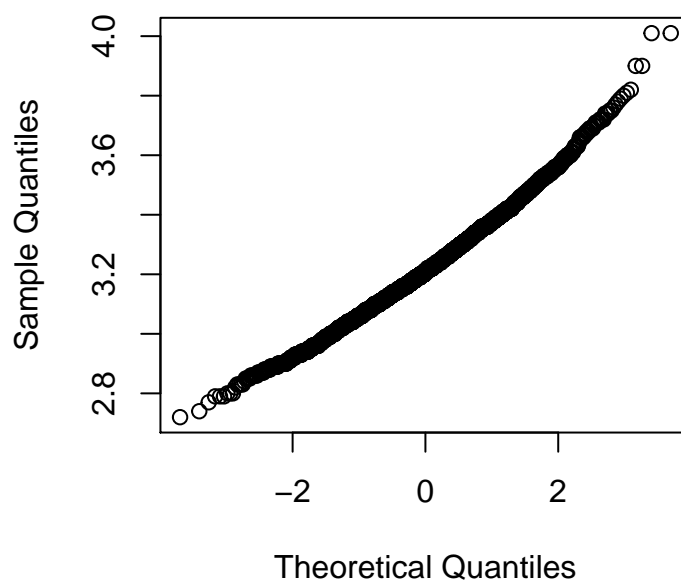


```

678
679
680
681     Shapiro-Wilk normality test
682
683 data:  data
684 W = 0.99181, p-value = 1.555e-15
685

```

Normal Q-Q Plot

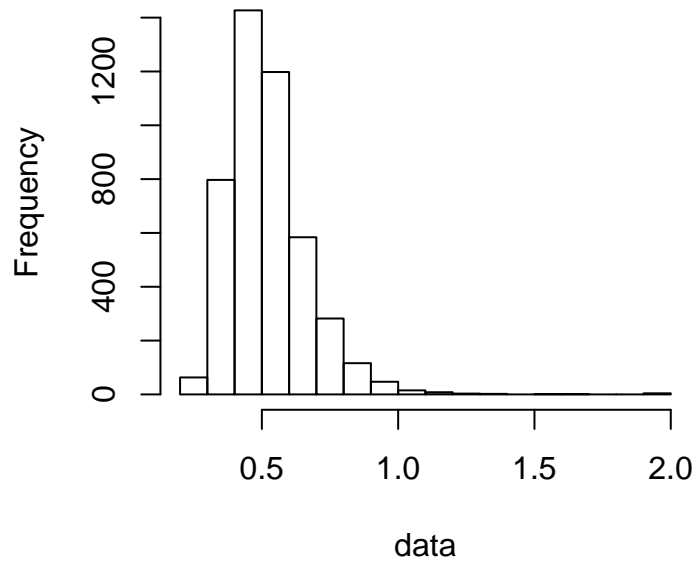


```

686
687 normality(Wine.train$sulphates)

```

Histogram of data

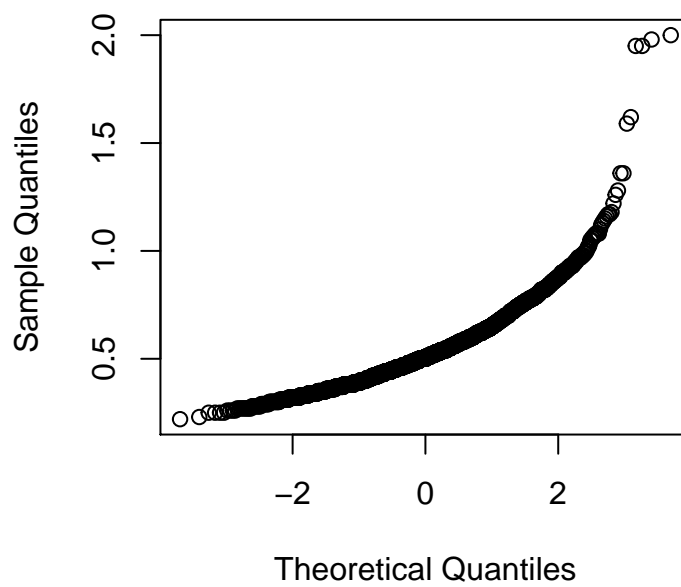


```

688
689
690
691     Shapiro-Wilk normality test
692
693 data:  data
694 W = 0.89657, p-value < 2.2e-16
695

```

Normal Q-Q Plot

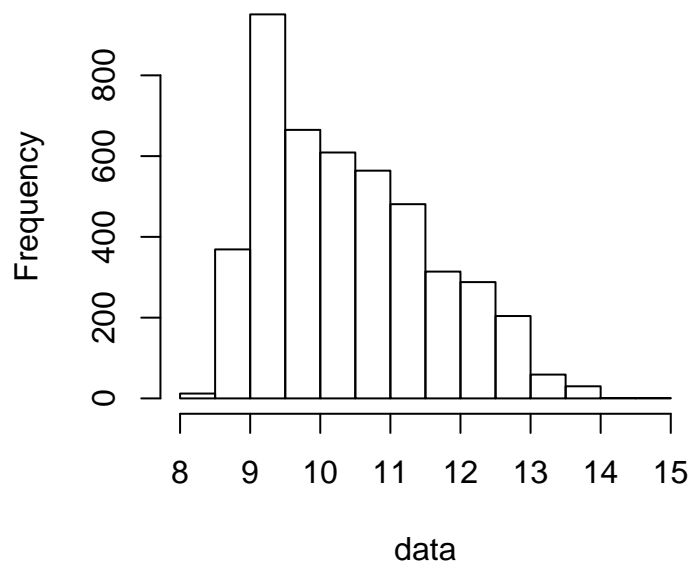


```

696
697 normality(Wine.train$alcohol)

```

Histogram of data

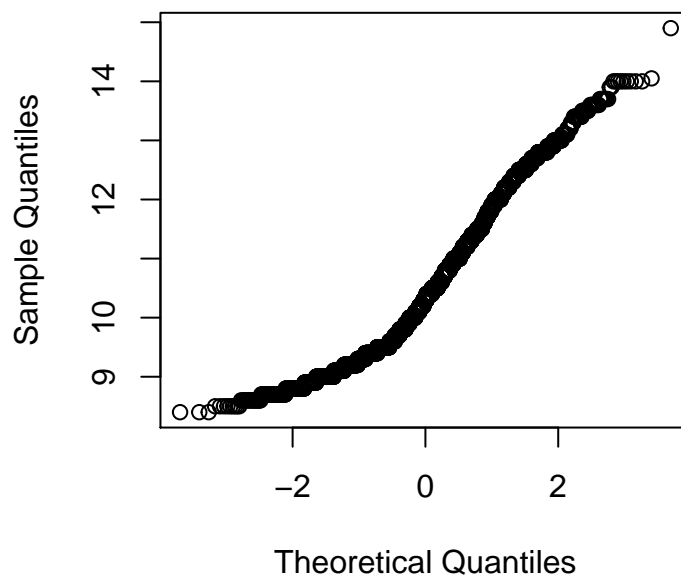


```

698
699
700
701     Shapiro-Wilk normality test
702
703 data:  data
704 W = 0.95221, p-value < 2.2e-16
705

```

Normal Q-Q Plot



```

706
707 # Discretizing data
708 Total_Wine$fixed.acidity <- mycut(Total_Wine$fixed.acidity , 10)
709 Total_Wine$volatile.acidity <- mycut(Total_Wine$volatile.acidity , 10)

```

```

710 Total_Wine$citric.acid <- mycut(Total_Wine$citric.acid , 10)
711 Total_Wine$residual.sugar <- mycut(Total_Wine$residual.sugar , 10)
712 Total_Wine$chlorides <- mycut(Total_Wine$chlorides , 10)
713 Total_Wine$free.sulfur.dioxide <- mycut(Total_Wine$free.sulfur.dioxide , 10)
714 Total_Wine$total.sulfur.dioxide <- mycut(Total_Wine$total.sulfur.dioxide , 10)
715 Total_Wine$density <- mycut(Total_Wine$density , 10)
716 Total_Wine$pH <- mycut(Total_Wine$pH, 10)
717 Total_Wine$sulphates <- mycut(Total_Wine$sulphates , 10)
718 Total_Wine$alcohol <- mycut(Total_Wine$alcohol , 10)
719 Total_Wine$quality <- as.factor(Total_Wine$quality)
720
721 Wine.Split <- splitdata(Total_Wine, 0.7)
722 Wine.train <- Wine.Split$traindata
723 Wine.test <- Wine.Split$testdata
724
725 # Applying Naive Bayes
726 nb.wine <- naiveBayes(wine.type ~ ., data = Wine.train)
727 pred.nb.wine <- predict(nb.wine, newdata = Wine.test, type = "class")
728 nb.conf <- confusion(Wine.test$wine.type, pred.nb.wine)
729
730 # Cross Validation
731 nb.kflval <- function(k, data) {
732   folds = createfolds(nrow(data), k)
733   accvector = 1:k
734   for (k in 1:k) {
735     temptrain = data[folds != k, ]
736     temptest = data[folds == k, ]
737     tempmodel = naiveBayes(wine.type ~ ., data = temptrain)
738     temppred = predict(tempmodel, newdata = temptest, type = "class")
739     analysis = confusion(temptest$wine.type, temppred)
740     accvector[k] = analysis$acc
741   }
742   return(mean(accvector))
743 }
744
745 nb.kflval(10, Total_Wine)

```

```

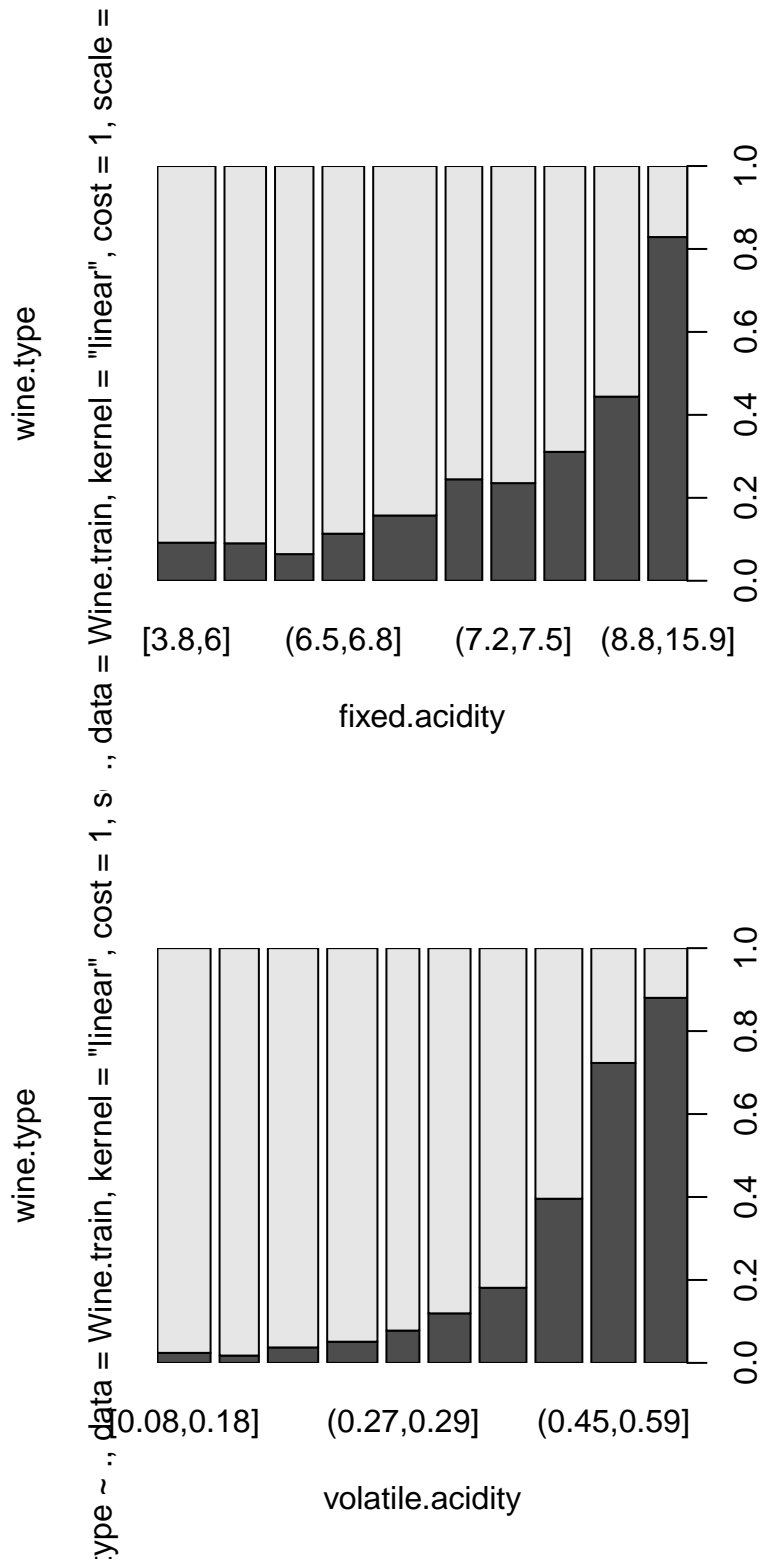
746
747 [1] 0.9898424
748

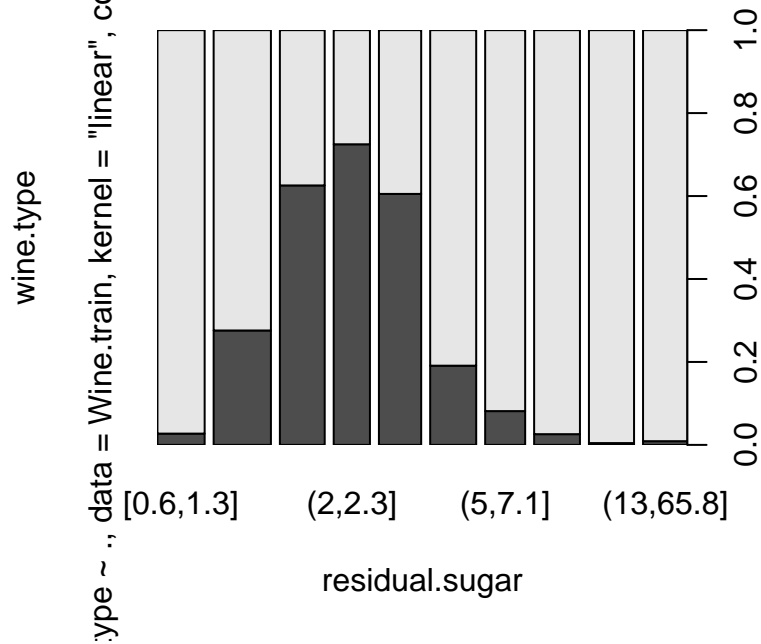
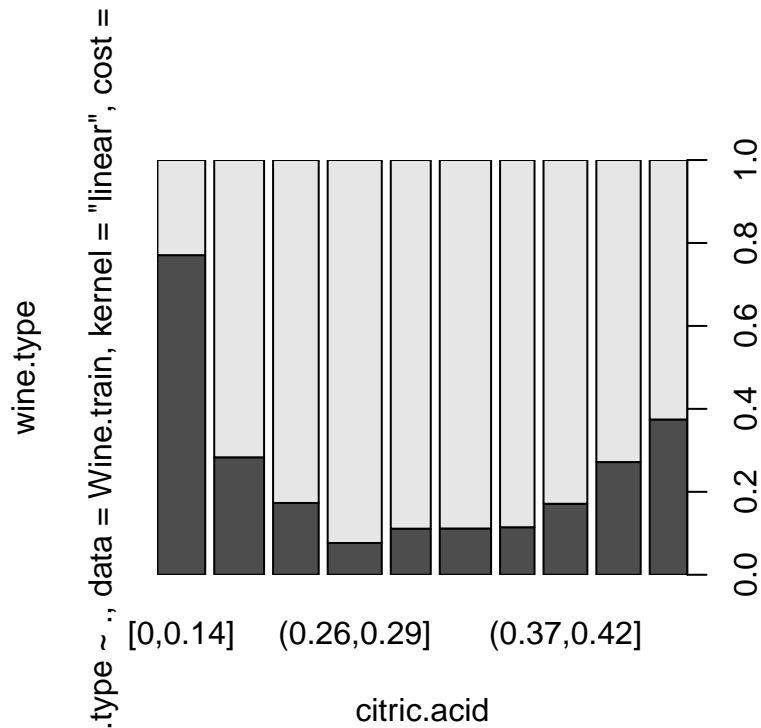
```

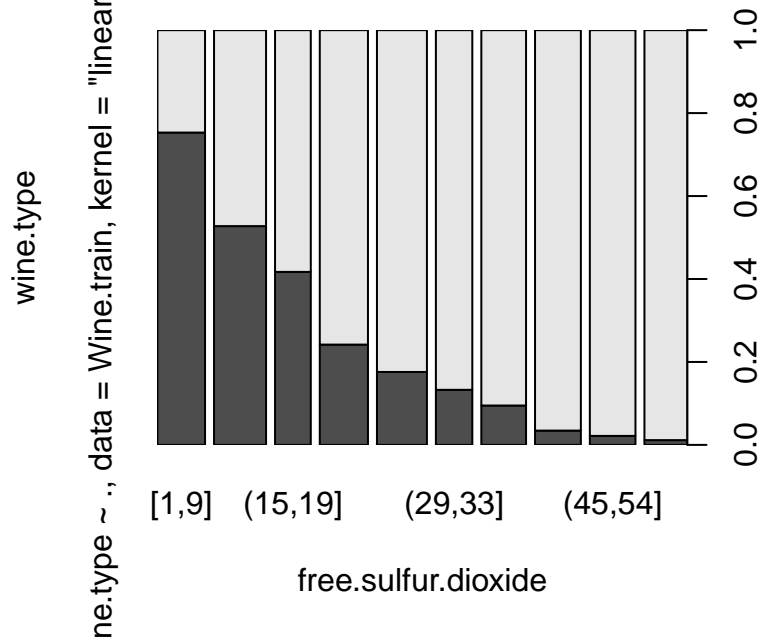
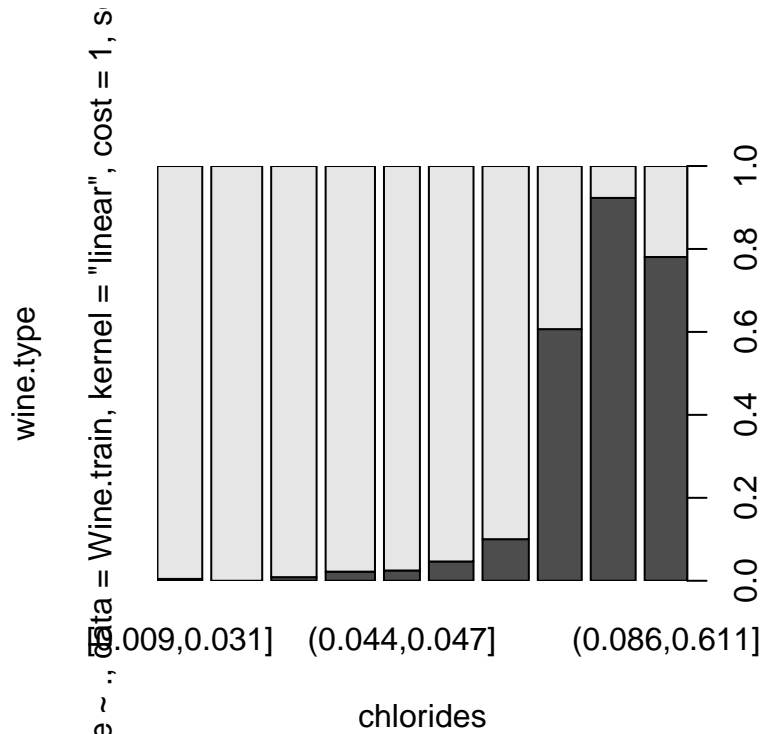
```

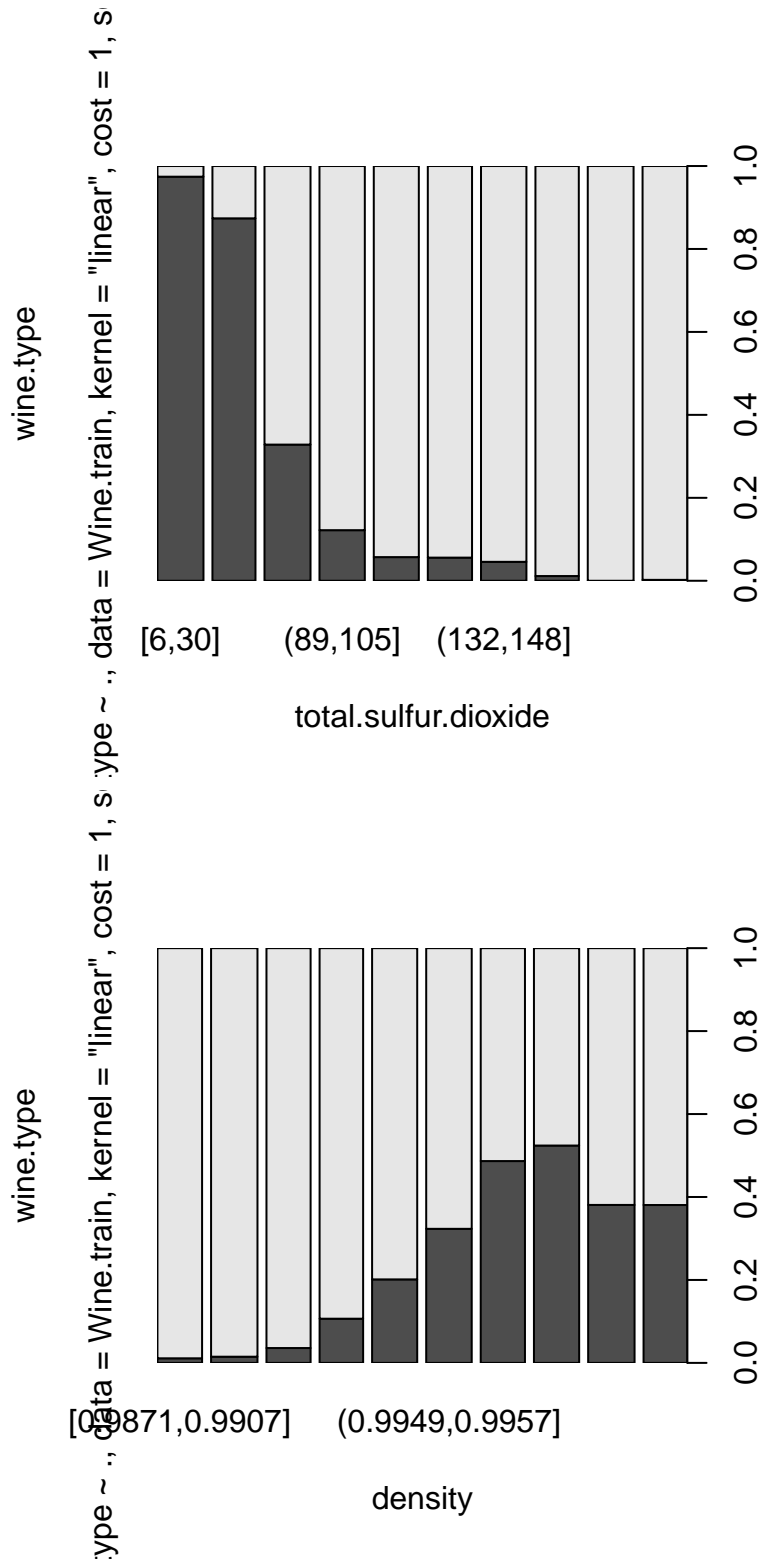
749 # Support Vector Machines
750 rm(Total_Wine)
751 Total_Wine <- rbind(Red_Wine, White_Wine)
752 wine.svm <- svm(wine.type ~ ., data = Wine.train, kernel = "linear", cost = 1,
753   scale = T)
754 pred.svm <- predict(wine.svm, newdata = Wine.test)
755 svm.conf <- confusion(Wine.test$wine.type, pred.svm)
756 plot(wine.type ~ ., wine.svm, data = Wine.train)

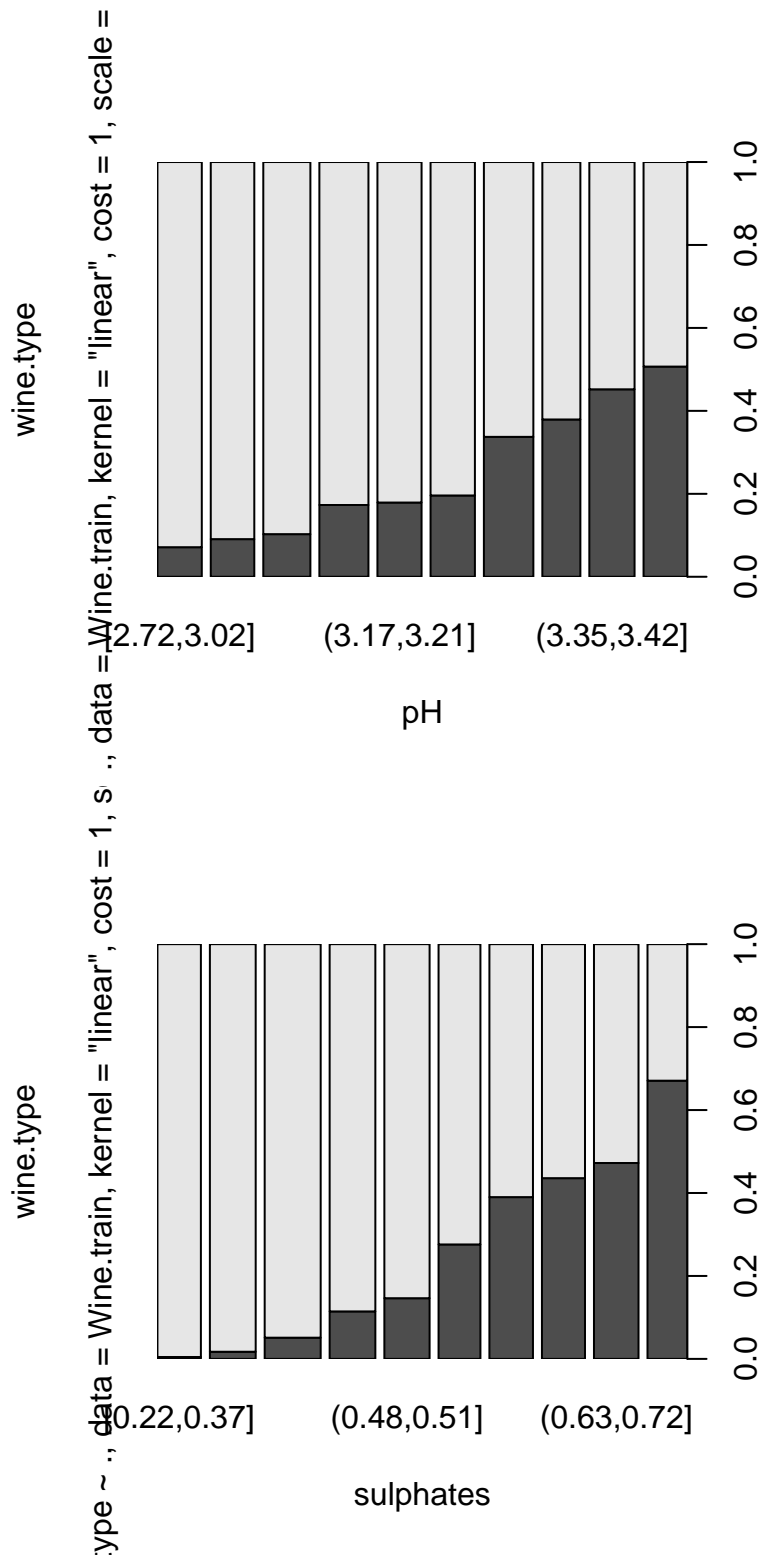
```

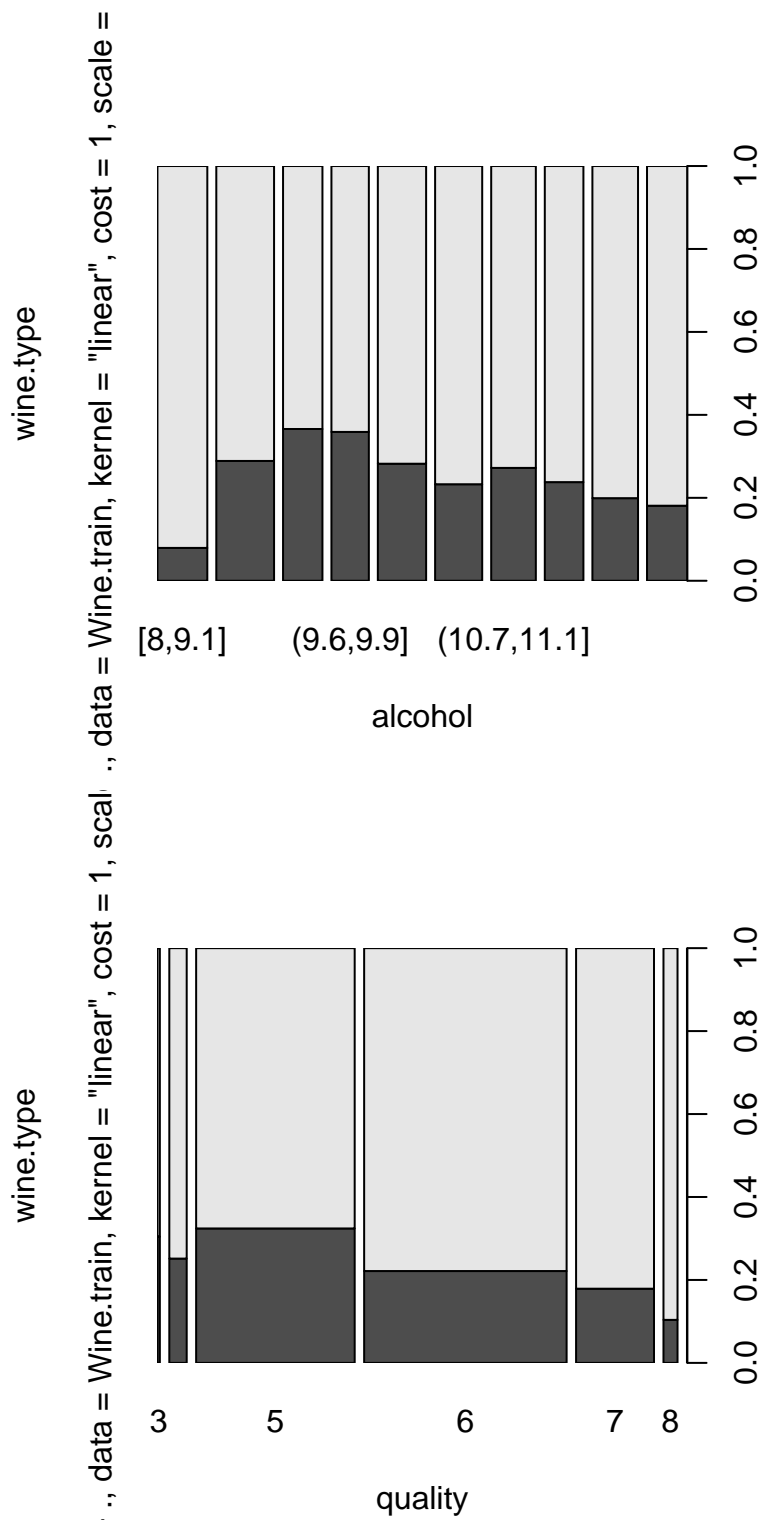












```
# Tuning gamma and cost on SVM
svm.tuning <- tune.svm(wine.type ~ ., data = Total_Wine, gamma = 10^(-6:-3),
  cost = 10^(1:2))
svm.tuning$best.parameters
```

gamma	cost
8	0.001 100

```
svm.tuning.2 <- tune.svm(wine.type ~ ., data = Total_Wine, gamma = 10^(-3:2),
```

```

778     cost = 10^(2:4))
779
780 # Optmal SVM
781 opt.svm <- svm(wine.type ~ ., data = Wine.train, kernel = "linear", gamma =
782     svm.tuning.2$best.parameters$gamma,
783     cost = svm.tuning.2$best.parameters$cost)
784
785 # Cross Validation of SVM
786 svm.kflval <- function(k, data) {
787     folds = createfolds(nrow(data), k)
788     accvector = 1:k
789     for (k in 1:k) {
790         temptrain = data[folds != k, ]
791         temptest = data[folds == k, ]
792         tempmodel = svm(wine.type ~ ., data = Wine.train, kernel = "linear",
793             gamma = svm.tuning.2$best.parameters$gamma, cost = svm.tuning.2$best.parameters$cost)
794         temppred = predict(tempmodel, newdata = temptest)
795         analysis = confusion(temptest$wine.type, temppred)
796         accvector[k] = analysis$acc
797     }
798     return(mean(accvector))
799 }
800
801 svm.kflval(10, Total_Wine)

```

```

802 Error in predict.svm(tempmodel, newdata = temptest): test data does not match model !
803

```

```

805 # Neural Networks
806 wine.nnet <- nnet(wine.type ~ ., data = Wine.test, size = 10, linout = FALSE,
807     maxit = 500)

```

```

808 Error in nnet.default(x, y, w, entropy = TRUE, ...): too many (1071) weights
809

```

```

811 pred.nnet <- predict(wine.nnet, newdata = Wine.test, type = "class")

```

```

812 Error in predict(wine.nnet, newdata = Wine.test, type = "class"): object 'wine.nnet' not found
813

```

```

815 confusion(Wine.test$wine.type, pred.nnet)

```

```

816 Error in table(true, pred): object 'pred.nnet' not found
817

```

```

819 nnet.tuning <- tune.nnet(wine.type ~ ., data = Total_Wine, size = 1:15, trace = FALSE,
820     tunecontrol = tune.control(nrepeat = 5, sampling = "cross", cross = 10,
821     ))
822 1 - mean(nnet.tuning$performances$error)

```

```

823 [1] 0.9754159
824

```

```

826 # Plotting Neaural Networks import the function from Github

```

```

827 library(devtools)

```

```

828 source_url("https://gist.githubusercontent.com/fawda123/7471137/raw/466c1474d0a505ff044412703516c34f1a4684a5/nnet_1")

```

```

829 SHA-1 hash of file is 74c80bd5ddbc17ab3ae5ece9c0ed9be612e87ef
830

```

```

832 plot.nnet(wine.nnet)

```

```

833 Loading required package: scales
834

```

836
837

838 Attaching package: 'scales'
839

840
841

The following object is masked from 'package:kernlab':

842

843 alpha
844

845

846 Error in match(x, table, nomatch = 0L): object 'wine.nnet' not found
847