Module 8: Solutions to Recommended Exercises

TMA4268 Statistical Learning V2021

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Problem 1 – Theoretical

a)

- 1. Recursive binary splitting: We find the best single partitioning of the data such that the reduction of RSS is the greatest. This process is applied sequencially to each of the split parts until a predefined minimum number of leave observation is reached.
- 2. Cost complexity pruning of the large tree from previous step, in order to obtain a sequence of best trees as a function of a parameter α . Each value of α corresponds to a subtree that minimize the following equation (several α s for the same tree):

$$\sum_{m=1}^{|T|} \sum_{i:x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|,$$

where |T| is the numb er of terminal nodes.

- 3. K-fold cross-validation to choose α . For each fold:
- Repeat Steps 1 and 2 on all but the kth folds of the training data.
- Evaluate the mean squared prediction on the data in the left-out kth fold, as a function of α .
- Average the results for each value of α and choose α to minimize the average error.
- 4. Return the subtree from Step 2 that corresponds to the chosen value of α .

For a classification tree we replace RSS with Gini index or entropy.

b)

Advantages

- Very easy to explain
- Can be displayed graphically
- Can handle both quantitative and qualitative predictors without the need to create dummy variables

Disadvantages

- The predictive accuracy is usualy not very high
- They are non-robust. That is a small change in the data can cause a large change in the estimated tree

c)

Decision trees suffer from high variance. Recall that if we have B i.i.d observations of a random variable X with the same mean and variance σ^2 . We calculate the mean $\bar{X} = \frac{1}{B} \sum_{b=1}^{B} X_b$, and the variance of the mean is $\text{Var}(\bar{X}) = \frac{\sigma^2}{B}$. That is by averaging we get reduced variance.

For decision trees, if we have B training sets, we could estimate $\hat{f}_1(\boldsymbol{x}), \hat{f}_2(\boldsymbol{x}), \dots, \hat{f}_B(\boldsymbol{x})$ and average them as

$$\hat{f}_{avg}(\boldsymbol{x}) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b(\boldsymbol{x}) .$$

However we do not have many data independent data sets, and we bootstraping to create B datasets. These datasets are however not completely independent and the reduction in variance is therefore not as large as for independent training sets.

To make the different trees that are built from each bootstrapped dataset more different, random forests use a random subset of the predictors to split the tree into new branches at each step. This decorrelates the different trees that are built from the B bootstrapped datasets, and consequently reduces variance.

d) An OOB is the set of observations that were not chosen to be in a specific bootstrap sample. From RecEx5-Problem 4c we have that on average 1 - 0.632 = 0.368 are included in the OOB sample.

e)

Variable importance based on node impurity

Regression Trees: The total amount that the RSS is decreased due to splits of each predictor, averaged over the B trees.

Classification Trees: The importance is the mean decrease (over all B trees) in the Gini index by splits of a predictor.

Variable importance based on randomization

This measure is based on how much the predictive accuracy (MSE or gini indiex) is decreased when the variable is replaced by a permuted version of it. You find a drawing here.

Problem 2 – Regression (Book Ex. 8)

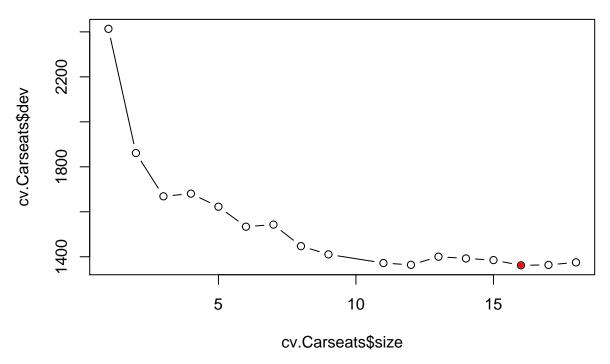
```
a)
library(ISLR)
data("Carseats")
set.seed(4268)
n = nrow(Carseats)
train = sample(1:n, 0.7 * nrow(Carseats), replace = F)
test = (1:n)[-train]
Carseats.train = Carseats[train, ]
Carseats.test = Carseats[-train, ]
  b)
library(tree)
tree.mod = tree(Sales ~ ., Carseats, subset = train)
summary(tree.mod)
##
## Regression tree:
## tree(formula = Sales ~ ., data = Carseats, subset = train)
## Variables actually used in tree construction:
## [1] "ShelveLoc"
                     "Price"
                                    "Age"
                                                  "Income"
                                                                 "CompPrice"
```

```
## [6] "Population" "Advertising" "Education"
## Number of terminal nodes: 18
## Residual mean deviance: 2.609 = 683.6 / 262
## Distribution of residuals:
        Min. 1st Qu. Median
                                        Mean 3rd Qu.
                                                              Max.
## -3.74000 -1.12400 -0.06522 0.00000 1.06800 4.47200
plot(tree.mod)
text(tree.mod, pretty = 0)
                                     ShelveLoc: Bad,Medium
                     Price < 105.5
                                                               Advertising < 13.5
                                                          13.280 Income < 49
                                                               7.658 9.762
        ShelveLoc: Bad
Income < 58.5 Price k 80.5 Shelvelloc: Bad CompPride < 171.5
8.149 10.040
8.26410.760<sup>10.040</sup>
                              Age < 60
                 5.717 7.913 3.033 5.898 3.422
                                       Price < 137 8.755 6.973 5.812 3.740
yhat = predict(tree.mod, newdata = Carseats.test)
mse = mean((yhat - Carseats.test$Sales)^2)
mse
## [1] 4.585249
  c)
set.seed(4268)
cv.Carseats = cv.tree(tree.mod)
tree.min = which.min(cv.Carseats$dev)
```

points(cv.Carseats\$size[tree.min], cv.Carseats\$dev[tree.min], col = "red", pch = 20)

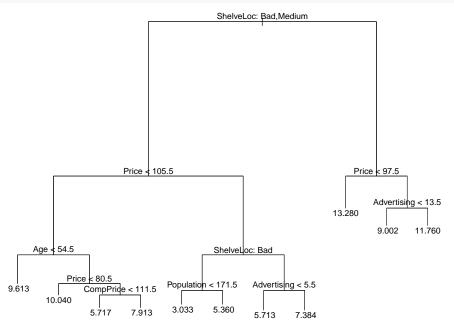
best = cv.Carseats\$size[tree.min]

plot(cv.Carseats\$size, cv.Carseats\$dev, type = "b")



We see that trees with sizes 11, 12, 16 and 17 have similar deviance values. We should ideally choose the tree of size 11 as it gives the simpler tree.

```
pr.tree = prune.tree(tree.mod, best = 11)
plot(pr.tree)
text(pr.tree, pretty = 0)
```



```
yhat = predict(pr.tree, newdata = Carseats.test)
mse = mean((yhat - Carseats.test$Sales)^2)
mse
```

[1] 4.378499

There is a slight reduction in MSE for the pruned tree with 11 leaves.

d)

```
library(randomForest)
dim(Carseats)

## [1] 400 11

bag.Carseats = randomForest(Sales ~ ., Carseats.train, mtry = ncol(Carseats) - 1,
    ntree = 500, importance = TRUE)
yhat.bag = predict(bag.Carseats, newdata = Carseats.test)
mse.bag = mean((yhat.bag - Carseats.test$Sales)^2)
mse.bag
```

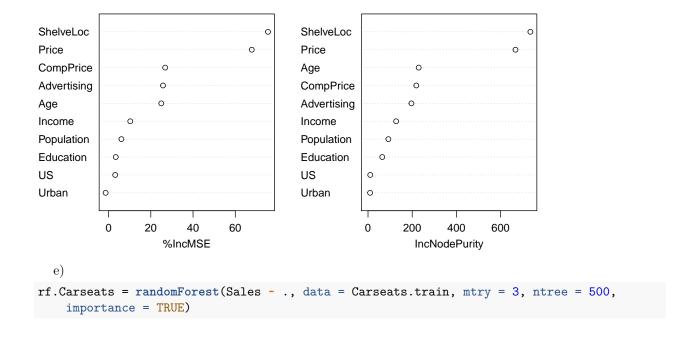
[1] 2.122958

Bagging decreases the test MSE significantly to 2.12. From the importance plots we might conclude that Priceand ShelveLoc are the most important Variables.

importance(bag.Carseats)

```
##
                 %IncMSE IncNodePurity
## CompPrice
               26.803869
                             218.740455
               10.284817
                             127.447480
## Income
## Advertising 25.795425
                             196.438893
## Population
                6.084270
                              92.149065
## Price
               67.791459
                             667.696518
## ShelveLoc
               75.485534
                             734.902022
               24.961130
                             229.491494
## Age
## Education
                3.423565
                              64.510742
## Urban
                               9.423406
               -1.373635
## US
                3.141449
                              10.105870
varImpPlot(bag.Carseats)
```

bag.Carseats



```
yhat.rf = predict(rf.Carseats, newdata = Carseats.test)
mse_forest <- mean((yhat.rf - Carseats.test$Sales)^2)
mse_forest</pre>
```

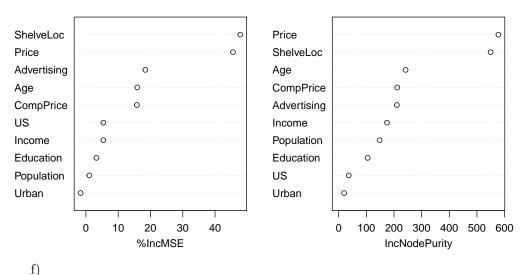
[1] 2.25397

We use $p/3 = 10/3 \approx 3$ trees, and we obtain an MSE of 2.25 which is slightly larger than Bagging MSE. The two most important Variables are again Priceand ShelveLoc.

importance(rf.Carseats)

```
##
                 %IncMSE IncNodePurity
## CompPrice
               15.789484
                              211.79213
## Income
                5.415374
                              174.79625
                             210.47149
## Advertising 18.402600
## Population
                1.076874
                             148.09993
## Price
               45.548596
                             577.68865
## ShelveLoc
               47.810006
                             549.62278
## Age
               15.936114
                             241.99130
## Education
                3.275725
                             104.89503
## Urban
               -1.646580
                               19.63668
## US
                5.427599
                               36.45647
varImpPlot(rf.Carseats)
```

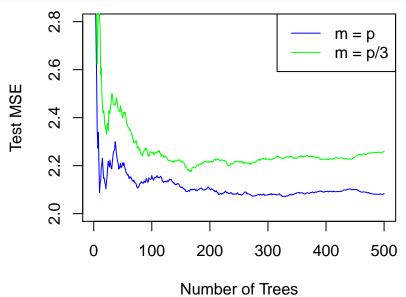
rf.Carseats



```
library(gbm)
r.boost = gbm(Sales ~ ., Carseats.train, distribution = "gaussian", n.trees = 500,
    interaction.depth = 4, shrinkage = 0.1)
yhat.boost = predict(r.boost, newdata = Carseats.test, n.trees = 500)
mse_boost <- mean((yhat.boost - Carseats.test$Sales)^2)
mse_boost</pre>
```

[1] 2.151292

We see a further decrease in MSE by boosing our trees.



Problem 3 – Classification

```
library(kernlab)
data(spam)
```

a)

Do this in R and read the Description.

b)

```
library(ISLR)
set.seed(4268)
n = nrow(spam)
train = sample(1:n, 0.7 * n, replace = F)
test = (1:n)[-train]
spam.train = spam[train, ]
spam.test = spam[-train, ]
```

```
c)
spam.tree = tree(type ~ ., spam, subset = train)
plot(spam.tree)
text(spam.tree, pretty = 1)
                                     charExclamation < 0.0795
                          remove < 0.045
                                                     charDollar < 0.0065
                 charDollar < 0.0575
                                    spam
                                                remove < 0.065
                                                             spam nonspam
 hp < capitalLqng < 9.5
                   nonspam spam nonspam
                                           capitalAve < 2.7545
our < 1.105 nonspam
                                     charExclamation < 0.838
                                       nonspam spam
summary(spam.tree)
##
## Classification tree:
## tree(formula = type ~ ., data = spam, subset = train)
## Variables actually used in tree construction:
## [1] "charExclamation" "remove"
                                                "charDollar"
                                                                    "george"
## [5] "hp"
                           "capitalLong"
                                                "our"
                                                                    "capitalAve"
## [9] "hpl"
## Number of terminal nodes: 14
## Residual mean deviance: 0.4801 = 1539 / 3206
## Misclassification error rate: 0.08975 = 289 / 3220
  d)
yhat = predict(spam.tree, spam[test, ], type = "class")
response.test = spam$type[test]
misclass = table(yhat, response.test)
misclass
##
             response.test
## yhat
             nonspam spam
     nonspam
                  781
                         67
##
     spam
                    67 466
1 - sum(diag(misclass))/sum(misclass)
## [1] 0.09703114
```

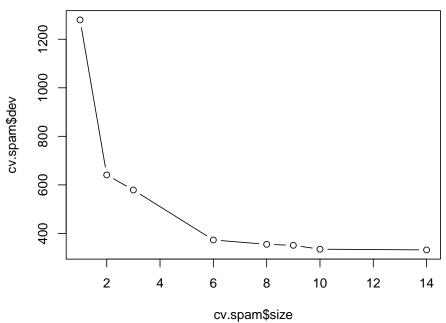
8

e)

```
set.seed(4268)

cv.spam = cv.tree(spam.tree, FUN = prune.misclass)

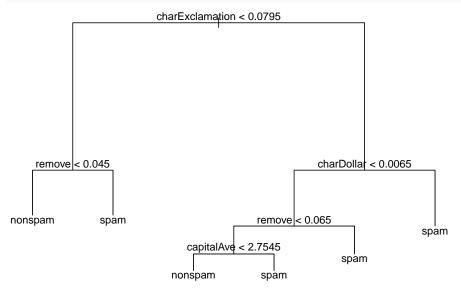
plot(cv.spam$size, cv.spam$dev, type = "b")
```



According to the plot the optimal number of terminal nodes is 6 (or larger). We choose 6 as this gives the simplest tree, and prune the tree according to this value.

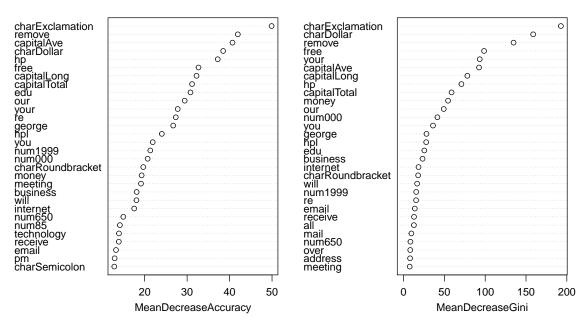
```
prune.spam = prune.misclass(spam.tree, best = 6)

plot(prune.spam)
text(prune.spam, pretty = 1)
```



We predict the response for the test data:

```
yhat.prune = predict(prune.spam, spam[test, ], type = "class")
misclass.prune = table(yhat.prune, response.test)
misclass.prune
             response.test
## yhat.prune nonspam spam
##
      nonspam
                   796 104
##
      spam
                    52 429
The misclassification rate is
1 - sum(diag(misclass.prune))/sum(misclass.prune)
## [1] 0.1129616
  f)
library(randomForest)
bag.spam = randomForest(type ~ ., data = spam, subset = train, mtry = ncol(spam) -
    1, ntree = 500, importance = TRUE)
We predict the response for the test data as before:
yhat.bag = predict(bag.spam, newdata = spam[test, ])
misclass.bag = table(yhat.bag, response.test)
misclass.bag
##
            response.test
## yhat.bag nonspam spam
     nonspam
                 810
                   38 490
##
     spam
The misclassification rate is
1 - sum(diag(misclass.bag))/sum(misclass.bag)
## [1] 0.05865315
We now use the random forest-algorithm and consider only \sqrt{57} \approx 8 of the predictors at each split. This is
specified in mtry.
set.seed(4268)
rf.spam = randomForest(type ~ ., data = spam, subset = train, mtry = round(sqrt(ncol(spam) -
    1)), ntree = 500, importance = TRUE)
We study the importance of each variable
importance(rf.spam)
If MeanDecreaseAccuracy and MeanDecreaseGini are large, the corresponding covariate is important.
varImpPlot(rf.spam)
```



In this plot we see that charExclamation is the most important covariate, followed by remove and charDollar. This is as expected as these variables are used in the top splits in the classification trees we have seen so far.

We now predict the response for the test data.

```
yhat.rf = predict(rf.spam, newdata = spam[test, ])
misclass.rf = table(yhat.rf, response.test)
1 - sum(diag(misclass.rf))/sum(misclass.rf)
```

[1] 0.044895

The misclassification rate is given by

misclass.rf

```
## response.test
## yhat.rf nonspam spam
## nonspam 824 38
## spam 24 495
```

The gbm() function does not allow factors, so we have to use '1' and '0' instead of spam and nonspam

We predict the response for the test data

```
yhat.boost = predict(boost.spam, newdata = spamboost[-train, ], n.trees = 5000, distribution = "bernoul"
    type = "response")
yhat.boost = ifelse(yhat.boost > 0.5, 1, 0) #Transform to 0 and 1 (nonspam and spam).
misclass.boost = table(yhat.boost, spamboost$type[test])
misclass.boost
##
## yhat.boost
                0
            0 812 52
##
            1 36 481
##
and the misclassification rate is
1 - sum(diag(misclass.boost))/sum(misclass.boost)
## [1] 0.06372194
  i)
```

We get lower missclassification rates for bagging, random forest and boosting than for a simple tree, which is expected.