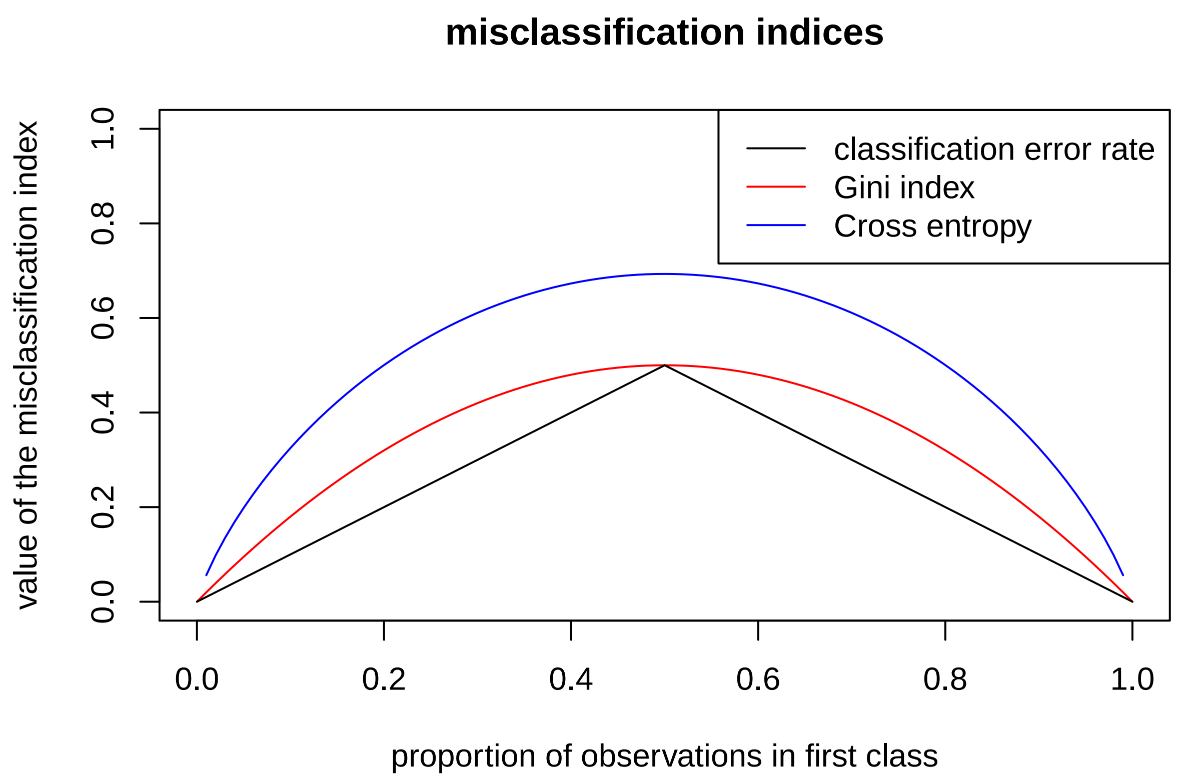
Exercises IOPS course SLP: Trees and ensembles

Exercise 1: Comparing misclassification indices



The plot above, show the values of the different misclassification indices, given the proportion of class-1 observations in a node, on the x-axis.

a) Based on the plot, do you expect each of the criteria to favor the same, or different potential splits?

b) Say, we have a mothernode with .7999 in class 1 (and .2111 in class 0). A given split would result in

- .565 going left, of which a proportion of 1.00 are class 1 observations
- .435 going right, of which a proportion of .54 are class 1 observations

Calculate the (average of the) classification error, Gini index and cross-entropy in the mothernode, and in the two daughternodes. Would the split improve purity according to the classification error, Gini index and cross-entropy?

Classification error in the mothernode is

```
1 - .7999
```

```
## [1] 0.2001
```

Classification in the daughter nodes will be

```
.565 * (1 - 1.0) + .435 * (1 - .54)
```

```
## [1] 0.2001
```

Gini index in the mothernode is

```
.7999 * .2001 + .2001 * .7999
```

```
## [1] 0.32012
```

Gini index in the daughternodes will be

```
.565 * (1.0 * 0.0 + 0.0 * 1.0) + .435 * (.54 * .46 + .46 * .54)
```

```
## [1] 0.216108
```

Cross-entropy in the mothernode is

```
- (.7999 * log(.7999) + .2001 * log(.20011))
```

```
## [1] 0.500531
```

Cross-entropy in the daughternodes will be (have to pick a very small value instead of zero, otherwise log is not defined)

```
- (.565 * (1.00 * log(1.00) + 0.00 * log(1e-50)) +
.435 * (.54 * log(.54) + .46 * log(.46)))
```

```
## [1] 0.3001255
```

Conclusion: According to the classification error rate, purity would not improve and no split would be made. According to the Gini index and cross-entropy, purity would improve and a split would be made.

Exercise 2: Variable selection bias

a) Set the random seed and generate 200 observations from independent variables x1, x2 and e (you are free to choose the shape and parameters of the distribution yourself). Create two datasets consisting of x1, x2 and y: one where $y = e$ (the 'independent' dataset), and one where $y = x2 + e$ (the 'dependent' dataset).

```
set.seed(42)
x1 <- rnorm(200)
x2 <- round(x1)
e <- rnorm(200)
indep.data <- data.frame(x1, x2, y = e)
dep.data <- data.frame(x1, x2, y = x2 + e)
cor(indep.data)
```

```
##              x1          x2           y
## x1  1.00000000  0.95421214 -0.08036539
## x2  0.95421214  1.00000000 -0.08438802
## y  -0.08036539 -0.08438802  1.00000000
```

```
cor(dep.data)
```

```
##           x1        x2         y
## x1 1.0000000 0.9542121 0.6653023
## x2 0.9542121 1.0000000 0.6971071
## y  0.6653023 0.6971071 1.0000000
```

b) Fit a regression tree using x1 and x2 to predict y, using each dataset. Which variable is most often selected for splitting? Is that what you would expect?

```
library(tree)
indep.tree <- tree(y ~ ., data = indep.data)
indep.tree
```

```
## node), split, n, deviance, yval
##       * denotes terminal node
##
##   1) root 200 178.5000  0.01128
##     2) x1 < 0.908147 167 127.8000  0.07600
##       4) x1 < 0.702793 159 123.4000  0.04904
##         8) x1 < 0.642954 152 116.5000  0.08731
##          16) x1 < 0.529576 141 110.0000  0.05215
##            32) x1 < 0.443734 135 105.4000  0.08183
##              64) x1 < -0.611299 50  32.0400  0.24060
##               128) x1 < -1.06408 29  16.2900 -0.05572 *
##               129) x1 > -1.06408 21   9.6790  0.64990 *
##              65) x1 > -0.611299 85  71.3600 -0.01157
##               130) x1 < -0.432308 15   6.5260 -0.43390 *
##               131) x1 > -0.432308 70  61.5900  0.07892 *
##            33) x1 > 0.443734 6   1.7880 -0.61570 *
##          17) x1 > 0.529576 11   4.1010  0.53800 *
##         9) x1 > 0.642954 7   1.8410 -0.78210 *
##       5) x1 > 0.702793 8   2.0080  0.61190 *
##     3) x1 > 0.908147 33  46.4400 -0.31620
##       6) x1 < 1.83186 28  38.2500 -0.46980
##        12) x1 < 1.06526 5   7.8830 -1.08900 *
##        13) x1 > 1.06526 23  28.0300 -0.33510
##          26) x1 < 1.20123 5   0.8233  0.45050 *
##          27) x1 > 1.20123 18  23.2600 -0.55340
##            54) x1 < 1.38103 7   5.7970 -1.05300 *
##            55) x1 > 1.38103 11  14.6100 -0.23540 *
##       7) x1 > 1.83186 5   3.8390  0.54360 *
```

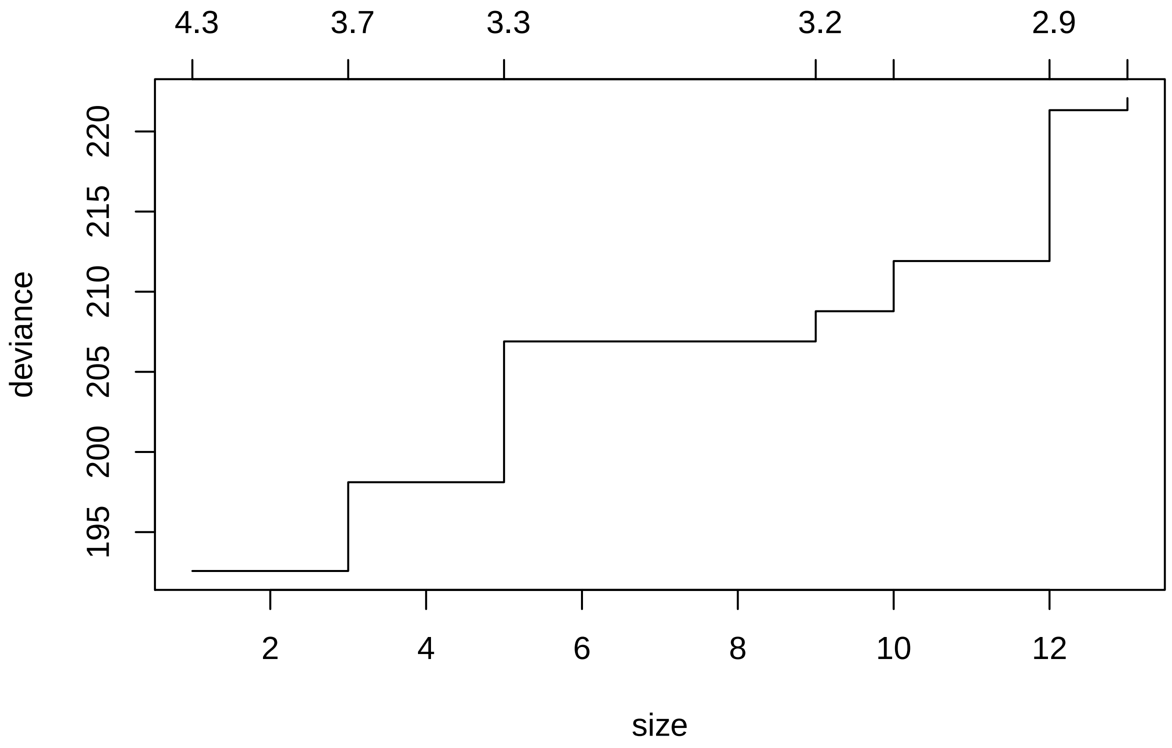
```
dep.tree <- tree(y ~ ., data = dep.data)
dep.tree
```

```
## node), split, n, deviance, yval
##       * denotes terminal node
##
##  1) root 200 344.800  0.011280
##    2) x1 < 0.494074 140 163.800 -0.452700
##      4) x1 < -1.06408 29  22.610 -1.538000
##        8) x1 < -1.52258 12   7.732 -2.065000 *
##        9) x1 > -1.52258 17   9.208 -1.167000 *
##      5) x1 > -1.06408 111  98.070 -0.169000
##       10) x1 < -0.483214 30  17.680 -0.637500
##         20) x1 < -0.611299 21   9.679 -0.350100 *
##         21) x1 > -0.611299 9   2.221 -1.308000 *
##       11) x1 > -0.483214 81  71.360  0.004492 *
##    3) x1 > 0.494074 60  80.500  1.094000
##      6) x1 < 1.83186 55  61.780  0.943900
##       12) x1 < 0.634407 10   4.381  1.542000 *
##       13) x1 > 0.634407 45  53.020  0.811000 *
##      7) x1 > 1.83186 5   3.879  2.744000 *
```

Both the independence and dependence tree use only x1 for splitting. Taking into account the population and sample correlations between x1, x2 and y, one would expect that x2 would be selected at least as often as x1 for splitting.

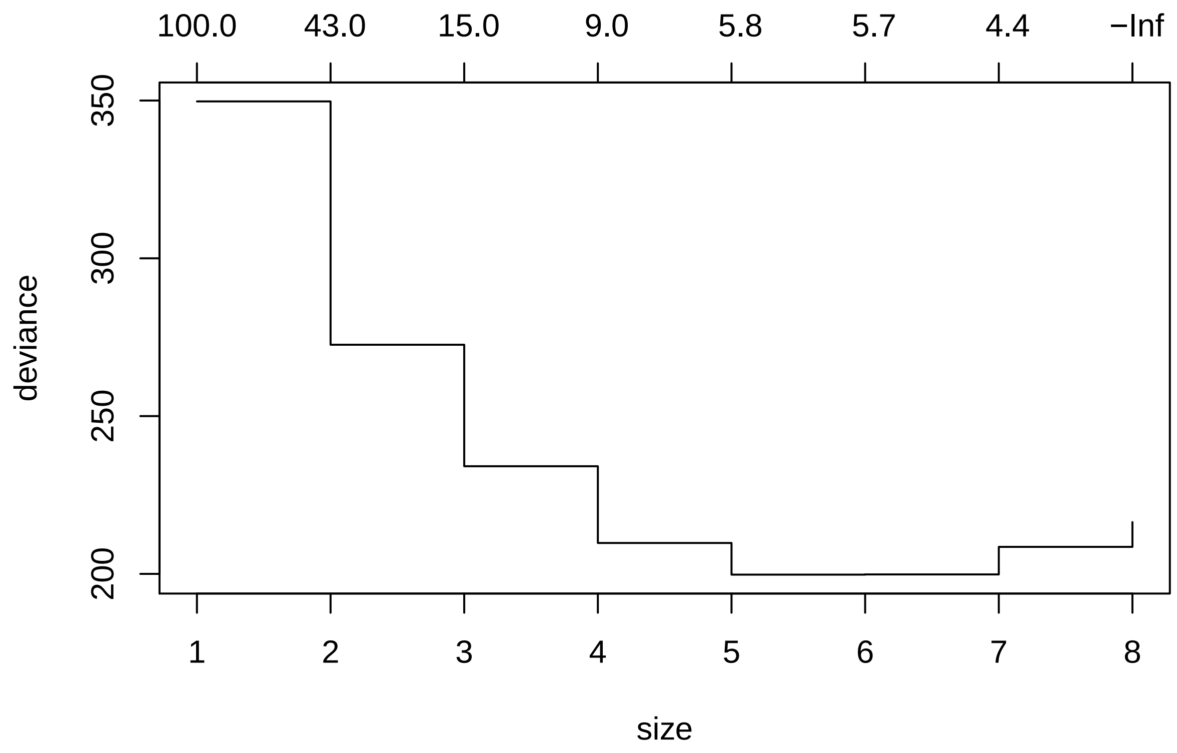
c) Prune the trees. Are there any splits left?

```r
set.seed(4287243)
cv.indeptree <- cv.tree(indep.tree)
plot(cv.indeptree)
```



The independence tree should be pruned to a size-1 tree, so there are no splits left.

```r
set.seed(4287243)
cv.deptree <- cv.tree(dep.tree)
plot(cv.deptree)
```



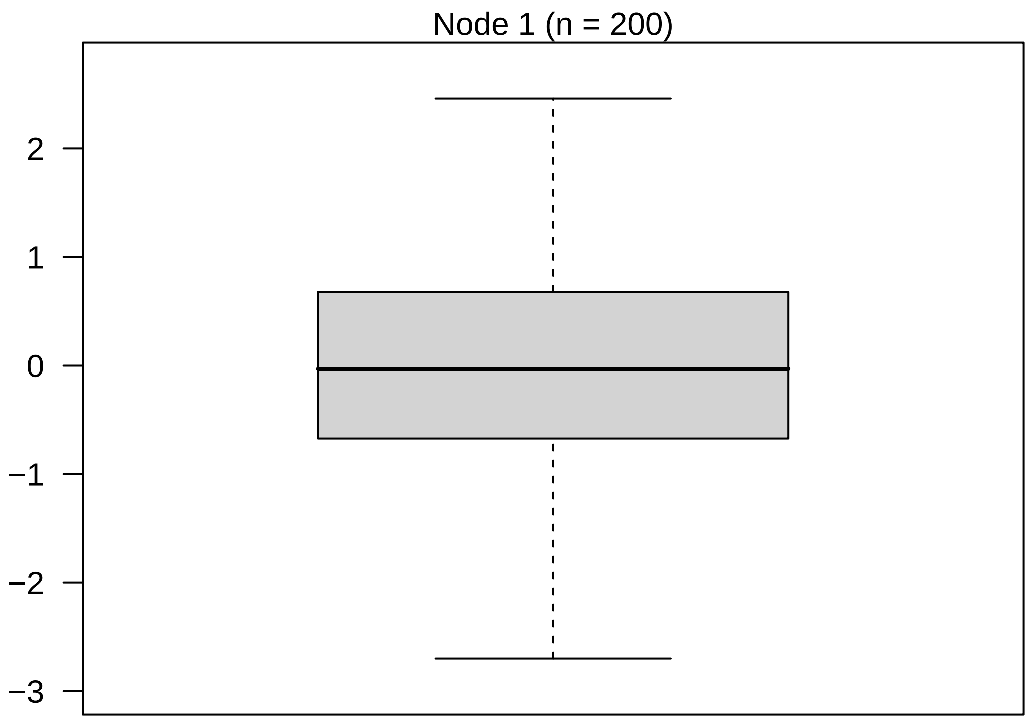
The dependence tree should be pruned to 5 terminal nodes.

c) Use the `ctree()` function from the `partykit` package to fit a conditional inference tree to the independent and dependent data. Also plot the resulting conditional inference tree.

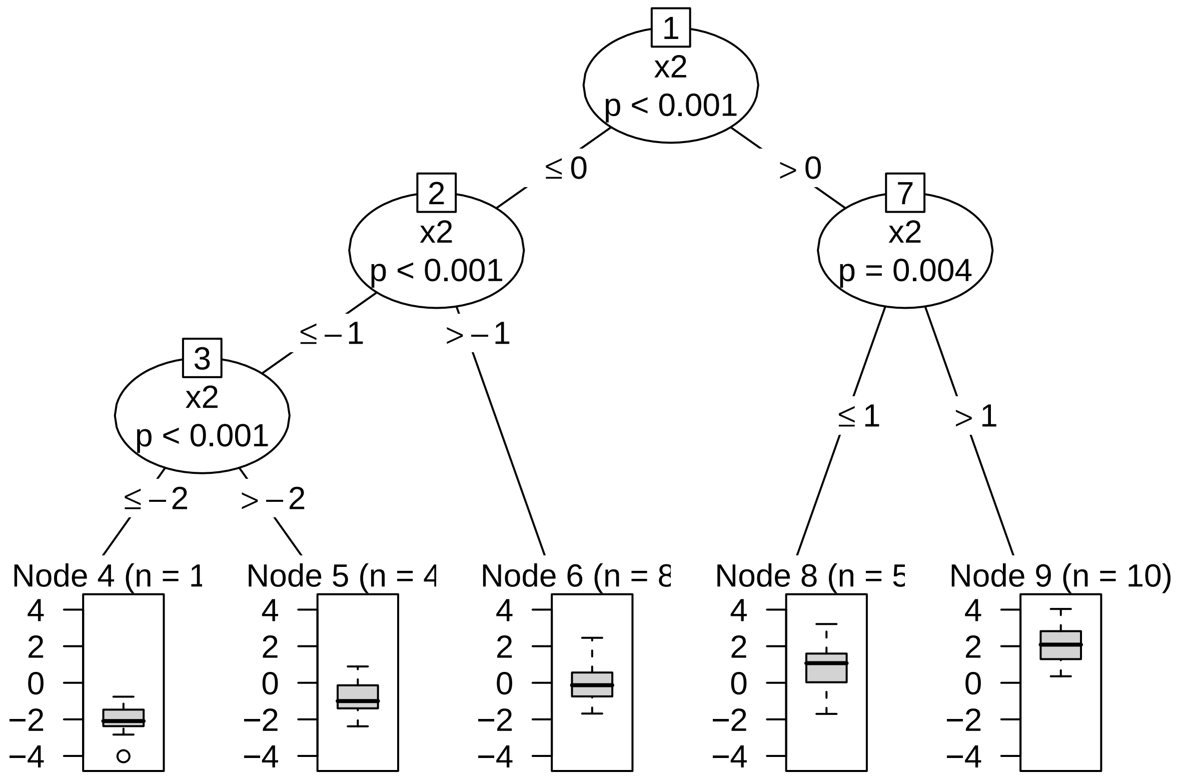
```r
library(partykit)
```

```
## Loading required package: grid

## Loading required package: libcoin

## Loading required package: mvtnorm

## Loading required package: rpart
```

```r
indep.ctree <- ctree(y ~ ., data = indep.data)
plot(indep.ctree)
```



```
dep.ctree <- ctree(y ~ ., data = dep.data)
plot(dep.ctree)
```



d) Compare the results you obtained in part a, b and c.

The conditional inference tree has a preference for x2, as it is slightly higher correlated with y. The CART tree has a preference for x1, as it has more potential splitting values than x2. The conditional inference tree does not need to be pruned, as it quits splitting when there is no significant association between the predictor and outcome variables anymore.

Exercise 3: Fitting trees and ensembles to the Carseats data

(Adaptation of exercise 8.8 ISLR)

In the lab session of chapter 8 (ISLR), a classification tree was applied to the Carseats data set after converting Sales into a qualitative response variable. Now we will seek to predict Sales using regression trees and related approaches, treating the response as a quantitative variable.

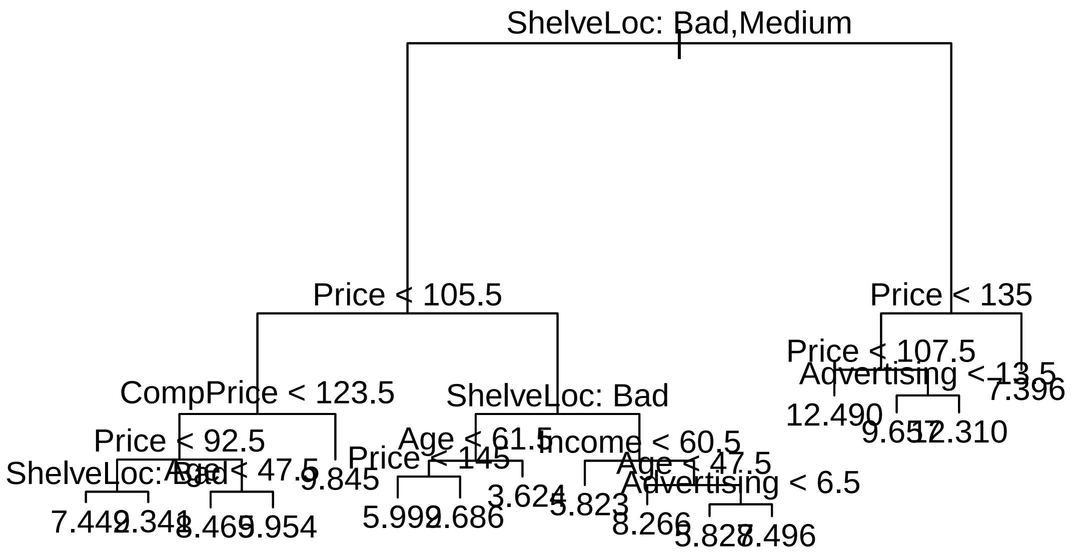
a) Split the data set into a training set and a test set.

```r
library(ISLR)
data(Carseats)
set.seed(42)
train <- sample(nrow(Carseats), 300)
```

b) Fit a regression tree to the training set. Plot the tree, and interpret the results. What test MSE do you obtain?

```r
library(tree)
tree.carseats <- tree(Sales ~ . , data = Carseats[train,])
```

```
plot(tree.carseats)
text(tree.carseats, pretty = 0)
```



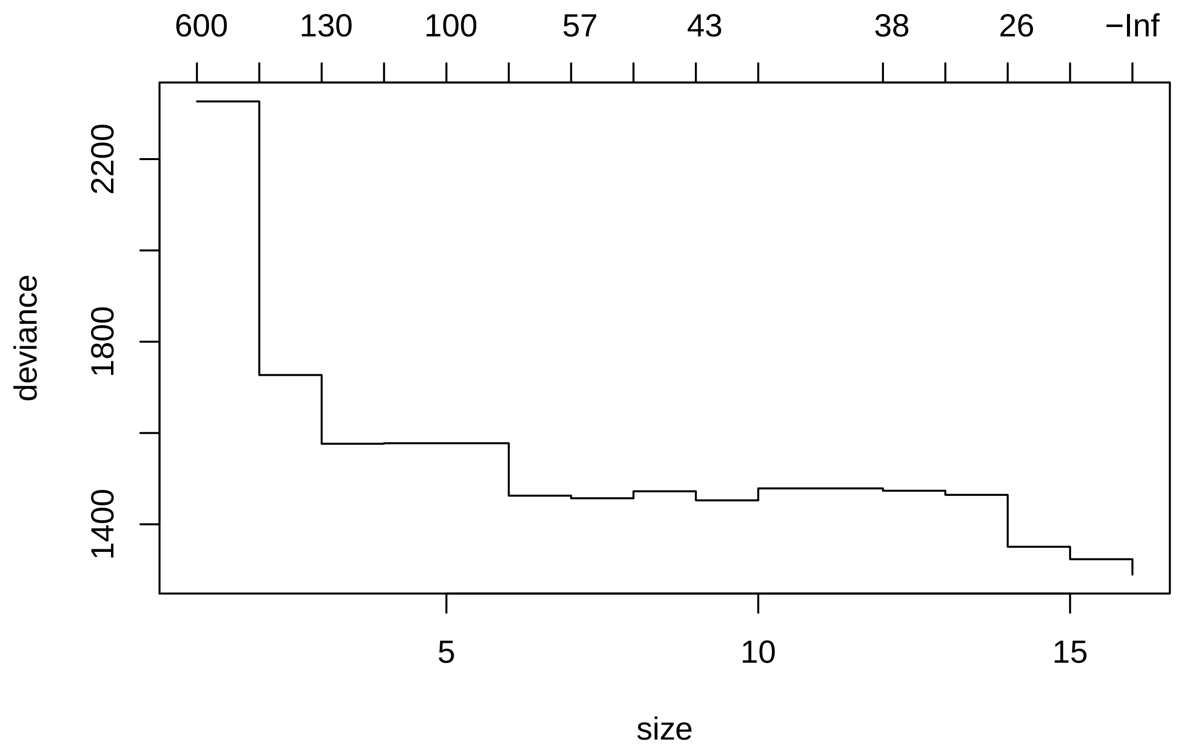
```
tree.pred <- predict(tree.carseats, newdata = Carseats[-train,])
mean((tree.pred - Carseats$Sales[-train])^2)
```

```
## [1] 4.287795
```

Carseats sales go up when shelve location is good and prices are lower. Test MSE is 4.29.

c) Use cross-validation in order to determine the optimal level of tree complexity. Does pruning the tree improve the test MSE?

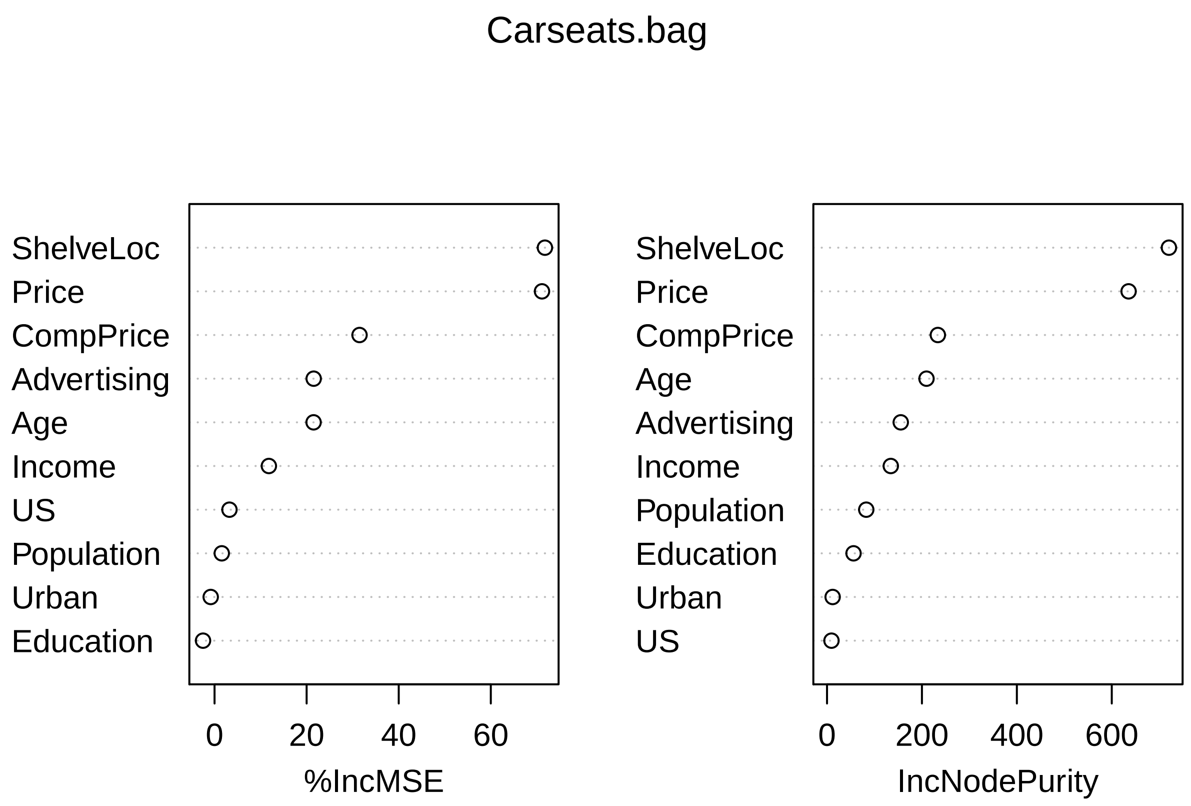
```
set.seed(3)
cv.carseats <- cv.tree(tree.carseats)
plot(cv.carseats)
```



Cross validation suggests that pruning will not improve the prediction error.

d) Use the bagging approach in order to analyze this data. What test MSE do you obtain? Use the importance() function to determine which variables are most important.

```
library(randomForest)
set.seed(432)
Carseats.bag <- randomForest(Sales ~ ., data = Carseats[train,],
                             mtry = ncol(Carseats) - 1, ntree = 500,
                             importance = TRUE)
par(mfrow = c(1,2))
varImpPlot(Carseats.bag)
```



Price, ShelveLocation and Competitor Price are most important in predicting car seat sales.

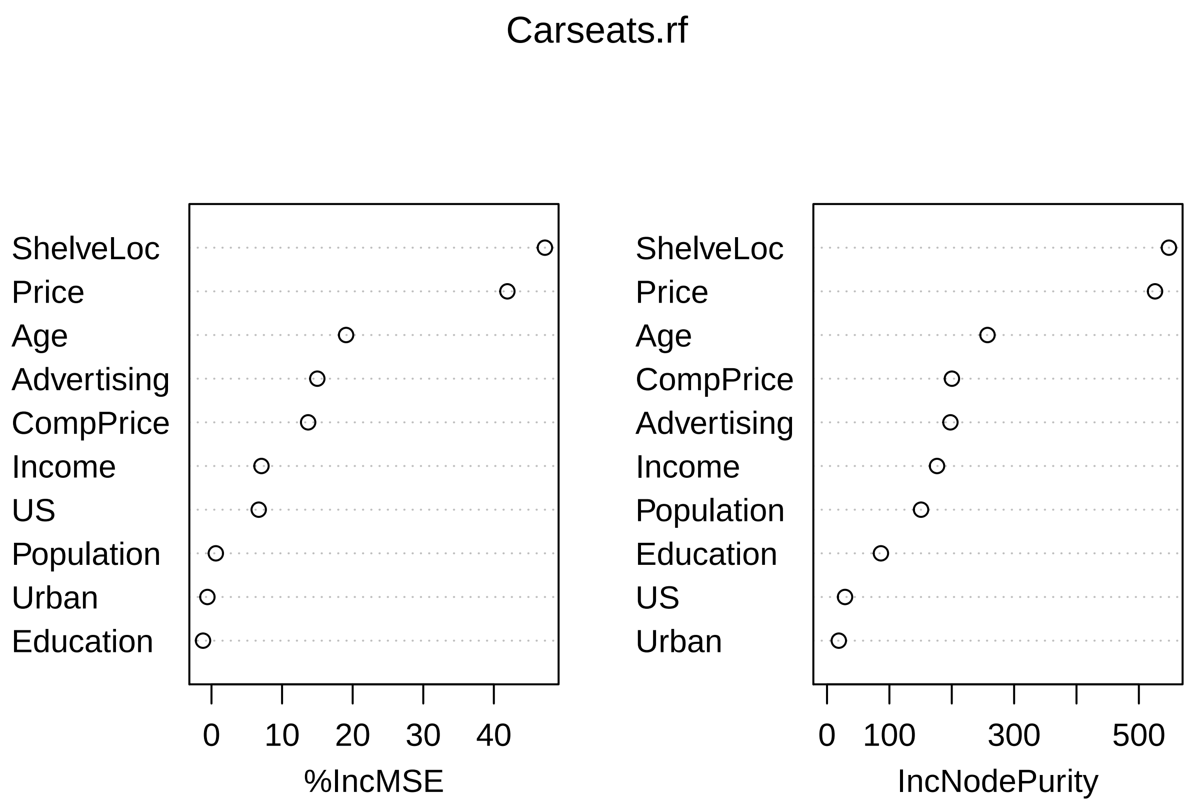
```
pred.bag <- predict(Carseats.bag, newdata = Carseats[-train,])
mean((pred.bag - Carseats[-train,]$Sales)^2)
```

```
## [1] 2.423866
```

The test MSE for the bagged ensemble is 2.41, lower than the tree.

e) Use random forests to analyze this data. What test MSE do you obtain? Use the importance() function to determine which variables are most important. Describe the effect of mtry, the number of variables considered at each split, on the error rate obtained.

```
set.seed(526)
Carseats.rf <- randomForest(Sales ~ ., data =  Carseats[train,],
                            mtry = round(sqrt(ncol(Carseats)-1)),
                            ntree = 500, importance = TRUE)
varImpPlot(Carseats.rf)
```



We see that Price, ShelveLocation and Age are most important in predicting carseat sales, according to the random forest.

```
pred.rf <- predict(Carseats.rf, newdata = Carseats[-train,])
mean((pred.rf - Carseats[-train,]$Sales)^2)
```

```
## [1] 2.98506
```

The test MSE for the random forest is 2.99, which is higher than that of the bagged ensemble. In this case, a lower value of mtry did not improve predictive accuracy on test data.

f) Create a boosted ensemble to predict Sales. Compare the boosted ensemble with the bagged and random forest ensemble in terms of test MSE and (the effect of) important predictor variables. (Additional: Before creating the ensemble, use cross validation to determine the optimal parameter settings.)

```
library(caret)
set.seed(49493)
tunegrid <- expand.grid(n.trees = c(500, 750, 1000),
                        shrinkage = c(.001, .01, .1),
                        interaction.depth = 3:4,
                        n.minobsinnode = 10)
Sales_ind <- which(names(Carseats) == "Sales")
garbage <- capture.output(
cvpars <- train(x = Carseats[train, -Sales_ind], y = Carseats[train, Sales_ind],
                method = 'gbm', distribution = "gaussian", tuneGrid = tunegrid)
)
```

```
cvpars
```

```
## Stochastic Gradient Boosting
##
## 300 samples
##  10 predictor
##
## No pre-processing
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 300, 300, 300, 300, 300, 300, ...
## Resampling results across tuning parameters:
##
##   shrinkage  interaction.depth  n.trees  RMSE      Rsquared   MAE
##   0.001      3                   500     2.401686  0.5157323  1.942670
##   0.001      3                   750     2.269564  0.5507395  1.839020
##   0.001      3                  1000     2.160417  0.5812896  1.750004
##   0.001      4                   500     2.364035  0.5488383  1.910048
##   0.001      4                   750     2.220636  0.5822615  1.797525
##   0.001      4                  1000     2.103397  0.6102495  1.701777
##   0.010      3                   500     1.471345  0.7539361  1.181249
##   0.010      3                   750     1.373137  0.7716804  1.099205
##   0.010      3                  1000     1.345161  0.7758402  1.074105
##   0.010      4                   500     1.434176  0.7590768  1.146882
##   0.010      4                   750     1.363103  0.7719211  1.085770
##   0.010      4                  1000     1.349937  0.7728073  1.074335
##   0.100      3                   500     1.431881  0.7433187  1.138449
##   0.100      3                   750     1.450029  0.7373050  1.154715
##   0.100      3                  1000     1.459616  0.7341140  1.164318
##   0.100      4                   500     1.436147  0.7404844  1.142538
##   0.100      4                   750     1.447009  0.7366812  1.153192
##   0.100      4                  1000     1.452943  0.7346340  1.158843
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were n.trees = 1000,
##  interaction.depth = 3, shrinkage = 0.01 and n.minobsinnode = 10.
```

```r
library(gbm)
```

```
## Loading required package: survival
```

```
##
## Attaching package: 'survival'
```

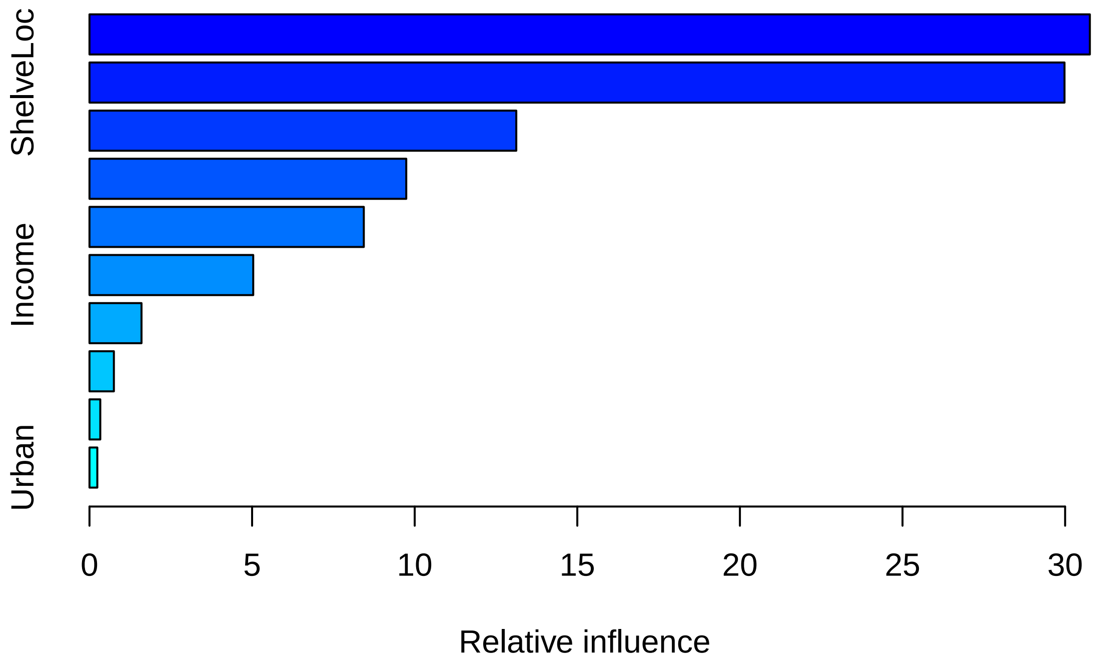
```
## The following object is masked from 'package:caret':
##
##     cluster
```

```
## Loading required package: splines
```

```
## Loading required package: parallel
```

```
## Loaded gbm 2.1.3
```

```r
set.seed(47895321)
boost.ens <- gbm(Sales ~ ., data =  Carseats[train,],
                 distribution = "gaussian",
                 n.trees = 1000, shrinkage = .01, interaction.depth = 3)
summary(boost.ens)
```



```
##                     var    rel.inf
## Price             Price 30.7601045
## ShelveLoc     ShelveLoc 29.9803757
## CompPrice     CompPrice 13.1235582
## Age                 Age  9.7407170
## Advertising Advertising  8.4358885
## Income           Income  5.0353704
## Population   Population  1.5993559
## Education     Education  0.7509441
## US                   US  0.3326009
## Urban             Urban  0.2410849
```

```
yhat.boost <- predict(boost.ens, newdata = Carseats[-train,], n.trees = 1000)
mean((yhat.boost - Carseats$Sales[-train])^2)
```

```
## [1] 1.428045
```

Price, ShelveLocation, Competitor Price and Age were also important in the bagged and random forest ensemble. Test MSE is lowest for the boosted ensemble.

Exercise 4: Boston housing and OOB error estimates

(Adaptation of exercise 8.7 ISLR).

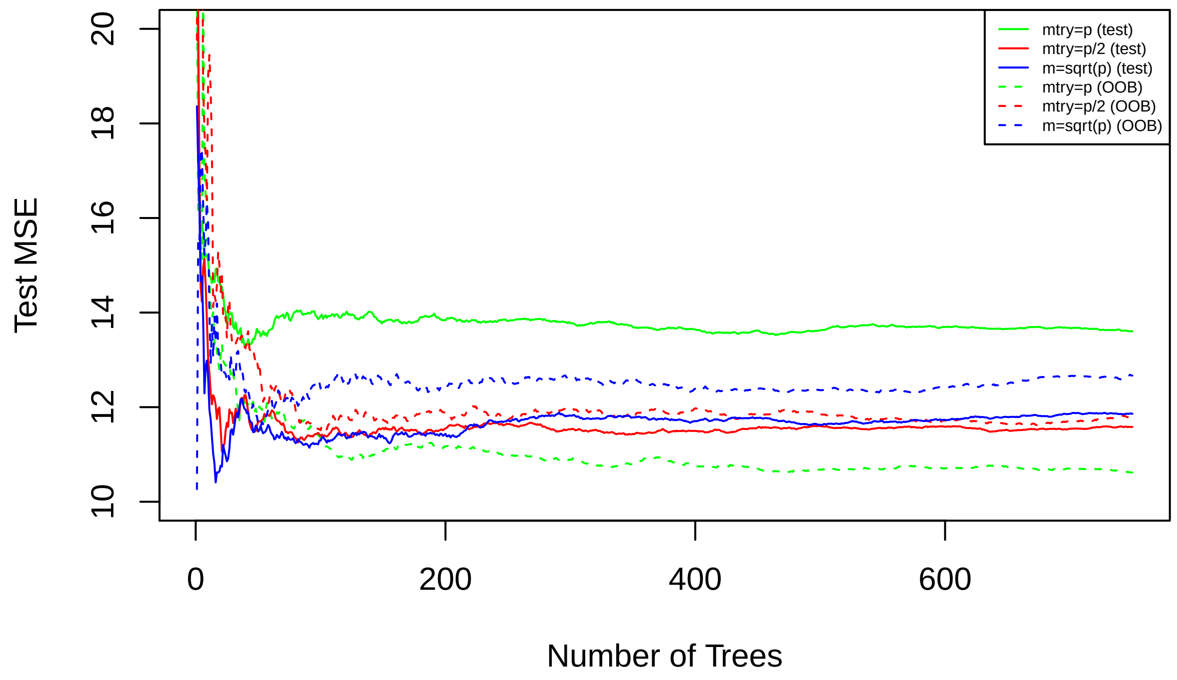
In the lab, a random forest was created for the Boston data using mtry=6 and using ntree=25 and ntree=500. For mtry values of p, $p/2$, and $\sqrt{p}$. Use ntree values of 1:750. Create a plot with the number of trees on the x-axis and the error rate on the y-axis. Plot both the OOB and test error.

Hints: Note that you only need to fit 3 ensembles, one for each value of mtry, because the fitted randomForest object contains a slot $mse, of which the i-th element ($1 \leq i \leq ntree$) is the OOB estimate of the MSE for all trees up to the i-th; and a slot $test$mse, of which the i-th element ($1 \leq i \leq ntree$) is the test MSE for the ensemble of trees up to the i-th.

To obtain both OOB and test eror, first separate the data in a test and training set and supply these to the `X.train`, `Y.train`, `xtest` and `ytest` arguments of the `randomForest()` function:

```
library(MASS)
set.seed(1)
train <- sample(1:nrow(Boston), nrow(Boston)/2)
X.train <- Boston[train, -14]
X.test <- Boston[-train, -14]
Y.train <- Boston[train, 14]
Y.test <- Boston[-train, 14]
```

```
set.seed(443329)
rf.boston.p <- randomForest(X.train, Y.train, xtest = X.test, ytest = Y.test,
                            mtry = 13, ntree = 750)
rf.boston.p2 <- randomForest(X.train, Y.train, xtest = X.test, ytest = Y.test,
                             mtry = round(13/2), ntree = 750)
rf.boston.p.sq <- randomForest(X.train, Y.train, xtest = X.test, ytest = Y.test,
                               mtry = round(sqrt(13)), ntree = 750)
par(mfrow = c(1,1))
# Plot lines for mtry = p:
plot(1:750, rf.boston.p$test$mse, col = "green", type = "l", xlab = "Number of Trees",
     ylab = "Test MSE", ylim = c(10, 20))
lines(1:750, rf.boston.p$mse, col = "green", type = "l", lty = 2)
# Plot lines for mtry = p/2:
lines(1:750, rf.boston.p2$test$mse, col = "red", type = "l")
lines(1:750, rf.boston.p2$mse, col = "red", type = "l", lty = 2)
# Plot lines for mtry = sqrt(p)
lines(1:750, rf.boston.p.sq$test$mse, col = "blue", type = "l")
lines(1:750, rf.boston.p.sq$mse, col = "blue", type = "l", lty = 2)
# Add legend:
legend("topright", paste(rep(c("mtry=p", "mtry=p/2", "m=sqrt(p)"), times=2),
                         rep(c("(test)", "(OOB)"), each = 3)),
       col = rep(c("green", "red", "blue"), times = 2), cex = .5, lty = rep(1:2,each = 3))
```



a) Based on the plot, does the default setting of ntree=500 seem reasonable to you?

Yes, all error rates stabilize after about 200 trees.

b) Based on the plot, would you prefer a random forest over a bagged ensemble?

I would prefer the random forest (mtry $< p$) over the bagged ensemble (mtry $= p$), as it yields lower test error.

c) Does the OOB error give a more realistic estimate of test error for bagged ensembles or for random forests? Can you explain this?

The OOB error is closer to the test error, so seems more realistic, for the random forests. Random sampling of predictor variables in the random forest drives down the performance of individual trees, yielding a higher error estimate for the OOB observations in the random forest, compared to the bagged ensemble. OOB error estimates may therefore be more realistic for random forests than for bagged ensembles.