Week 4 Assignment

Ben Arancibia

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KJ 8.1

Recreate the simulated data from Exercise 7.2:

```
library(mlbench)
set.seed(200)
simulated <- mlbench.friedman1(200, sd = 1)
simulated <- cbind(simulated$x, simulated$y)
simulated <- as.data.frame(simulated)
colnames(simulated)[ncol(simulated)] <- "y"
```

a) Fit a random forest model to all of the predictors, then estimate the variable importance scores:

```
library(randomForest)
```

```
## randomForest 4.6-10
## Type rfNews() to see new features/changes/bug fixes.
```

```
library(caret)
```

```
## Warning: package 'caret' was built under R version 3.1.3
```

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

```
## Warning: package 'lattice' was built under R version 3.1.3
```

```
## Loading required package: ggplot2
```

```
## Warning: package 'ggplot2' was built under R version 3.1.3
```

```
model1 <- randomForest(y ~ ., data = simulated, importance = TRUE, ntree = 1000)
rfImp1 <- varImp(model1, scale = FALSE)
```

Did the random forest model significantly use the uninformative predic- tors (V6 – V10)?

```
knitr::kable((round(rfImp1,2)))
```

	Overall
V1	8.91
V2	6.50

	Overall
V3	0.79
V4	7.94
V5	2.12
V6	0.18
V7	0.05
V8	-0.12
V9	-0.09
V10	-0.08

The model appears to place most importance on variables 1, 2, 4, and 5, and very little importance on 3 and 6 through 10.

b) Now add an additional predictor that is highly correlated with one of the informative predictors. For example:

```
simulated$duplicate1 <- simulated$V1 + rnorm(200) * .1
cor(simulated$duplicate1, simulated$V1)
```

```
## [1] 0.9304634
```

Fit another random forest model to these data. Did the importance score for V1 change? What happens when you add another predictor that is also highly correlated with V1?

```
model2 <- randomForest(y ~ ., data = simulated, importance = TRUE, ntree = 1000)
rfImp2 <- varImp(model2, scale = FALSE)

vnames <- c('V1', 'V2', 'V3', 'V4', 'V5', 'V6', 'V7', 'V8', 'V9', 'V10', 'duplicate1')

names(rfImp1) <- "Original"
rfImp1$Variable <- factor(rownames(rfImp1), levels = vnames)

names(rfImp2) <- "Extra"
rfImp2$Variable <- factor(rownames(rfImp2), levels = vnames)

rfImps <- merge(rfImp1, rfImp2, all = TRUE)
rownames(rfImps) <- rfImps$Variable
rfImps$Variable <- NULL

knitr::kable((round(rfImps,2)))
```

	Original	Extra
V1	8.91	6.18
V2	6.50	5.89
V3	0.79	0.60

	Original	Extra
V4	7.94	7.15
V5	2.12	2.06
V6	0.18	0.15
V7	0.05	-0.02
V8	-0.12	-0.04
V9	-0.09	-0.12
V10	-0.08	0.06
duplicate1	NA	3.70

When you add another highly correlated predictor the importance score for V1 drops.

c) Use the cforest function in the party package to fit a random forest model using conditional inference trees. The party package function varimp can calculate predictor importance. The conditional argument of that func- tion toggles between the traditional importance measure and the modified version described in Strobl et al. (2007). Do these importances show the same pattern as the traditional random forest model?

```
library(party)
```

```
## Warning: package 'party' was built under R version 3.1.3

## Loading required package: grid
## Loading required package: mvtnorm
## Loading required package: modeltools
## Loading required package: stats4
## Loading required package: strucchange

## Warning: package 'strucchange' was built under R version 3.1.3

## Loading required package: zoo

## Warning: package 'zoo' was built under R version 3.1.3

##
## Attaching package: 'zoo'
##
## The following objects are masked from 'package:base':
##
##     as.Date, as.Date.numeric
##
## Loading required package: sandwich

## Warning: package 'sandwich' was built under R version 3.1.3
```

```
set.seed(147)
cforest1 <- cforest(y ~ ., data = simulated[, 1:11], controls = cforest_control(ntree = 1000))
set.seed(147)
cforest2 <- cforest(y ~ ., data = simulated, controls = cforest_control(ntree = 1000))

cfImps1 <- varimp(cforest1)
cfImps2 <- varimp(cforest2)
cfImps3 <- varimp(cforest1, conditional = TRUE)
cfImps4 <- varimp(cforest2, conditional = TRUE)

cfImps1 <- data.frame(Original = cfImps1, Variable = factor(names(cfImps1), levels = vnames))

cfImps2 <- data.frame(Extra = cfImps2, Variable = factor(names(cfImps2), levels = vnames))

cfImps3 <- data.frame(CondInf = cfImps3, Variable = factor(names(cfImps3), levels = vnames))

cfImps4 <- data.frame("CondInf Extra" = cfImps4, Variable = factor(names(cfImps4), levels = vnames))

cfImps <- merge(cfImps1, cfImps2, all = TRUE)
cfImps <- merge(cfImps, cfImps3, all = TRUE)
cfImps <- merge(cfImps, cfImps4, all = TRUE)
rownames(cfImps) <- cfImps$Variable
cfImps$Variable <- factor(cfImps$Variable, levels = vnames)
cfImps <- cfImps[order(cfImps$Variable),]
cfImps$Variable <- NULL

knitr::kable((round(cfImps,2)))
```

	Original	Extra	CondInf	CondInf.Extra
V1	9.06	5.93	3.04	1.15
V2	6.85	6.25	4.01	3.55
V3	0.05	0.06	0.03	0.02
V4	8.70	8.59	4.87	4.81
V5	2.21	2.07	0.73	0.69
V6	0.02	-0.03	0.01	0.01
V7	0.10	0.05	0.03	0.01
V8	-0.06	-0.03	-0.01	-0.01
V9	-0.06	-0.07	-0.01	0.00
V10	-0.01	0.01	0.00	0.00
duplicate1	NA	3.70	NA	0.49

The conditional inference model has a similar pattern of importance as the random forest model from Part (a), placing most importance on predictors 1, 2, 4, and 5 and very little importance on 3, 6 through 10. Adding a highly correlated predictor has a detrimenal effect on the importance for $V1$.

d) Repeat this process with different tree models, such as boosted trees and Cubist. Does the same pattern occur?

Boosted Trees

```
library(ipred)
set.seed(147)
bagFit1 <- bagging(y ~ ., data = simulated[, 1:11], nbag = 50)

set.seed(147)
bagFit2 <- bagging(y ~ ., data = simulated, nbag = 50)
bagImp1 <- varImp(bagFit1)
```

```
## Loading required package: plyr
```

```
## Warning: package 'plyr' was built under R version 3.1.3
```

```
##
## Attaching package: 'plyr'
##
## The following object is masked from 'package:modeltools':
##
##     empty
##
## Loading required package: rpart
```

```
names(bagImp1) <- "Original"
bagImp1$Variable <- factor(rownames(bagImp1), levels = vnames)

bagImp2 <- varImp(bagFit2)
names(bagImp2) <- "Extra"
bagImp2$Variable <- factor(rownames(bagImp2), levels = vnames)

bagImps <- merge(bagImp1, bagImp2, all = TRUE)
rownames(bagImps) <- bagImps$Variable
bagImps$Variable <- NULL

knitr::kable((round(bagImps,2)))
```

	Original	Extra
V1	1.92	1.83
V2	2.30	2.21
V3	1.37	1.16
V4	2.77	2.72
V5	2.43	2.24
V6	1.00	0.87
V7	0.94	0.92
V8	0.58	0.49
V9	0.68	0.60
V10	0.86	0.74
duplicate1	NA	1.83

Cubist Trees

```
library(Cubist)
set.seed(147)
cbFit1 <- cubist(x = simulated[, 1:10], y = simulated$y, committees = 100)

cbImp1 <- varImp(cbFit1)
names(cbImp1) <- "Original"
cbImp1$Variable <- factor(rownames(cbImp1), levels = vnames)

set.seed(147)
cbFit2 <- cubist(x = simulated[, names(simulated) != "y"], y = simulated$y, committees = 100)

cbImp2 <- varImp(cbFit2)
names(cbImp2) <- "Extra"
cbImp2$Variable <- factor(rownames(cbImp2), levels = vnames)

cbImp <- merge(cbImp1, cbImp2, all = TRUE)
rownames(cbImp) <- cbImp$Variable
cbImp$Variable <- NULL

knitr::kable((round(cbImp,2)))
```

	Original	Extra
V1	71.5	47.5
V2	58.5	57.5
V3	47.0	49.0
V4	48.0	42.5
V5	33.0	27.0
V6	13.0	11.5
V7	0.0	0.5
V8	0.0	3.5
V9	0.0	0.0
V10	0.0	0.0
duplicate1	NA	37.5

KJ 8.6 Return to the permeability problem described in Exercises 6.2 and 7.4. Train several tree-based models and evaluate the resampling and test set performance:

First recreate 6.2 and 7.4.

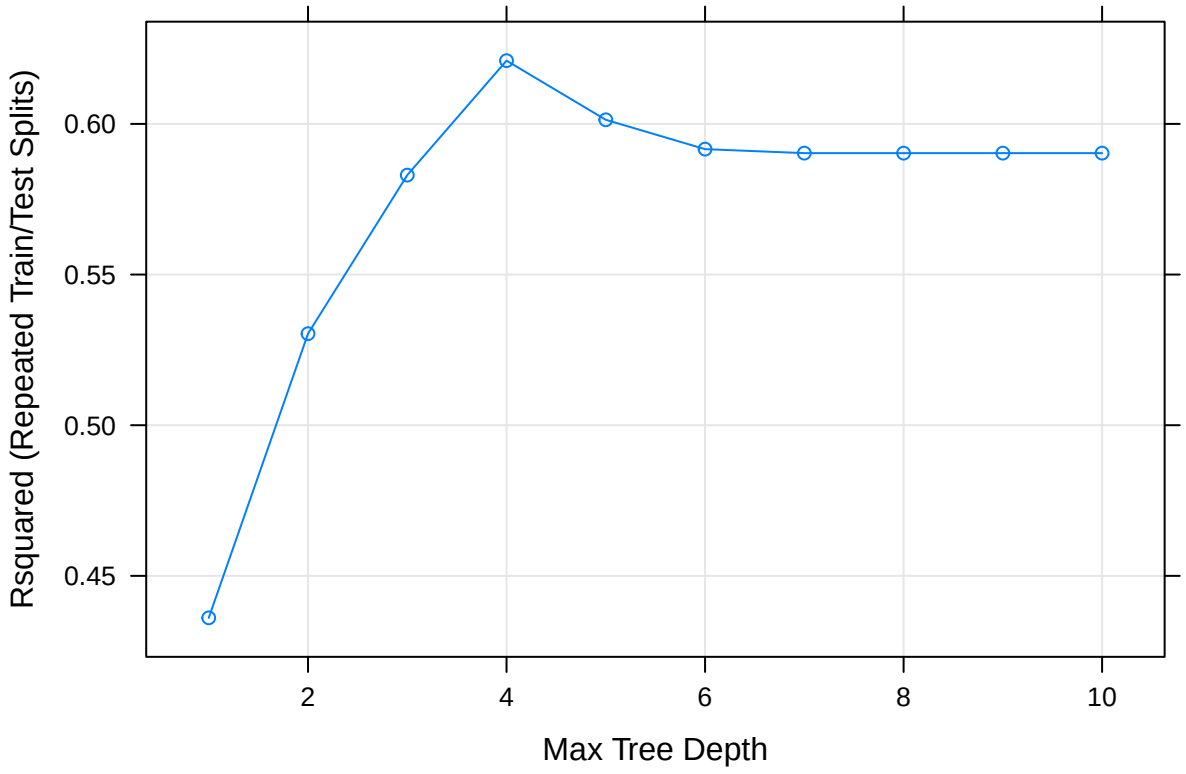
```
library(AppliedPredictiveModeling)
data(permeability)

#Identify and remove NZV predictors
nzvFingerprints <- nearZeroVar(fingerprints)
noNzvFingerprints <- fingerprints[,-nzvFingerprints]
```

```r
#Split data into training and test sets
set.seed(614)
trainingRows <- createDataPartition(permeability, p = 0.75, list = FALSE)

trainFingerprints <- noNzvFingerprints[trainingRows,]
trainPermeability <- permeability[trainingRows,]

testFingerprints <- noNzvFingerprints[-trainingRows,]
testPermeability <- permeability[-trainingRows,]

set.seed(614)
ctrl <- trainControl(method = "LGOCV")
```

(a) Which tree-based model gives the optimal resampling and test set performance?

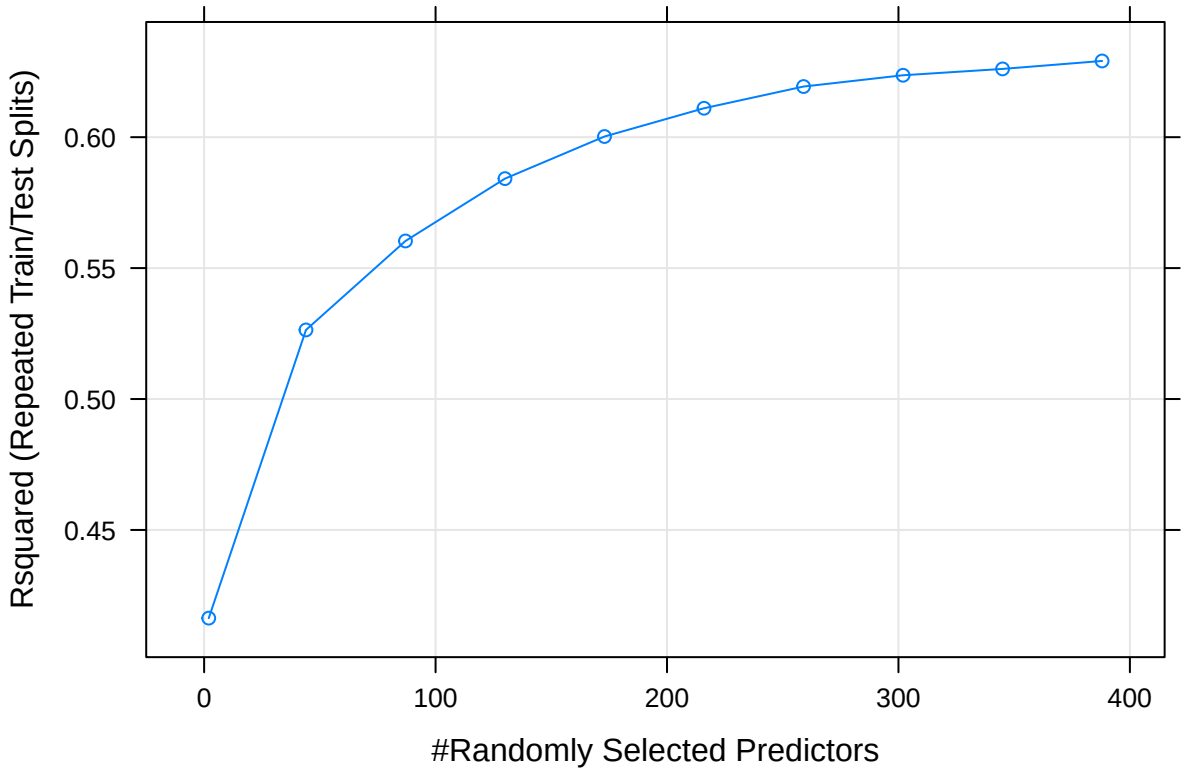
CART

```r
set.seed(614)
rpartGrid <- expand.grid(maxdepth= seq(1,10,by=1))
rpartPermTune <- train(x = trainFingerprints, y = log10(trainPermeability), method = "rpart2", tuneGrid

plot(rpartPermTune,metric="Rsquared")
```



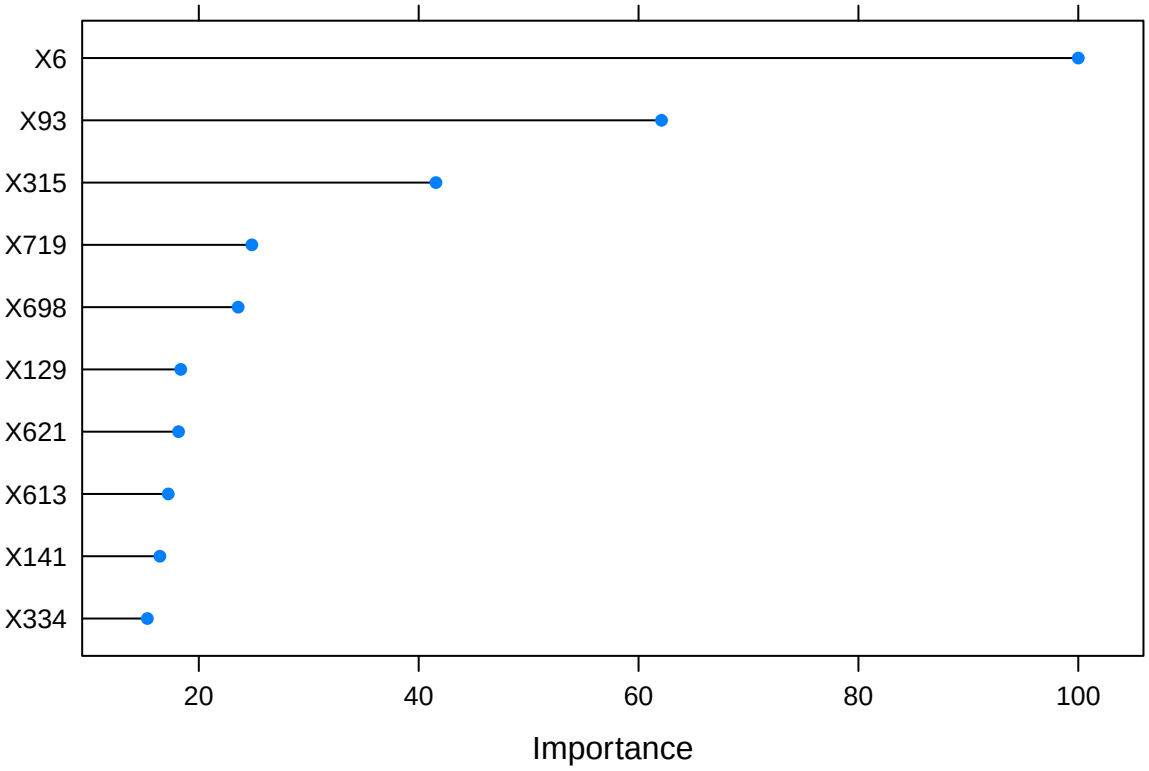
The above plot shows that the tree depth that maximizes R^2 is 4, with an R^2 of 0.62. This is slightly better than what we found with either the selected linear or non-linear based methods. **RF**

```
set.seed(614)
rpartGrid <- expand.grid(maxdepth= seq(1,10,by=1))
rfPermTune <- train(x = trainFingerprints, y = log10(trainPermeability), method = "rf", tuneLength = 10

plot(rfPermTune,metric="Rsquared")
```



The above plot shows that mtry value that maximizes R^2 is 388, with an R^2 of 0.63. It seems the tuning parameter profile has results to the performance results. The modeling process does not seem to benefit from the reduction in variance induced by random forests.

```
rfPermVarImp = varImp(rfPermTune)
plot(rfPermVarImp, top=10, scales = list(y = list(cex = .85)))
```



The above plot shows the variable importance of the top 10 predictors for the random forest model. Clearly a handful of predictors are identified as most important by random forests

GBM

```
######ISSUES WITH THIS NOT WORKING
####Error in train.default(x = trainFingerprints, y = log10(trainPermeability),  :
####The tuning parameter grid should have columns
####n.trees, interaction.depth, shrinkage, n.minobsinnode

set.seed(614)
gbmGrid <- expand.grid(interaction.depth=seq(1,6,by=1),
                       n.trees=c(25,50,100,200),
                       shrinkage=c(0.01,0.05,0.1))
gbmPermTune <- train(x = trainFingerprints, y = log10(trainPermeability), method = "gbm",
                     verbose = FALSE, tuneGrid = gbmGrid, trControl = ctrl)

plot(gbmPermTune,metric="Rsquared")
```

(b) Do any of these models outperform the covariance or non-covariance based regression models you have previously developed for these data? What criteria did you use to compare models' performance?

A siimplr model like a linear-based technique or a single CART tree provides near optimal results while at the same time easier to understand when compared to the best random forest model. The criteria used is the R^2 values and consistency of the importance of variables.

(c) Of all the models you have developed thus far, which, if any, would you recommend to replace the permeability laboratory experiment?

Of all the models so far, the rpart model above with an R^2 value of 0.62 performs just as well as other complex models. I would recommend rpart model as a quick and easy to understand replacement for the permeability laboratory experiment.