8 PQHS 471 Notes Week 8

8.1 Week 8 Day 1

8.1.1 Random Forests

Random forests are a model averaging technique using trees as base models. Bagging is a special case of random forests.

1. Specify B, the number of bootstrap samples, and $m \leq p$, the number of features to consider at each split.
2. For $b = 1, \ldots, B$, create a bootstrap sample of the training data, build a maximal-depth tree $\hat{r}_b$ *without pruning*. For every split during tree building, only m randomly selected features are considered.
3. The final RF model is $\hat{r}_{\text{rf}} = \frac{1}{B}\hat{r}_b$ for continuous outcome, or majority vote over $\hat{r}_b$ for categorical outcomes.

When $m = p$ for every split, the method is called **bagging**. In R `randomForest` package, by default, m (`mtry`) is $m = \sqrt{p}$ for classification trees and $m = p/3$ for regression trees, B (`ntree`) is 500. The measure of impurity is MSE for regression trees and Gini index for classification trees.

Notes:

- m is a hyperparameter. Once m is specified, RF is an automatic procedure and no tuning is needed. The choice of m determines the complexity of the final model.
- B is not a tuning parameter because a large value of B will not lead to overfitting.
- The random forest algorithm is non-deterministic.
- Majority vote is a type of average.
- Maximal-depth severely overfits as an individual tree. But this reduces correlation from one tree to another. The randomization due to using a subset of features leads to a higher variance, but a lot less correlation.
- Maximal-depth can be slow for very large n. In `randomForest()`, one can set `nodesize=` (minimum size of terminal nodes; default 1 for classification and 5 for regression) and `maxnodes=` (maximum number of terminal nodes).
- RFs are **adaptive nearest-neighbor estimators** with neighborhood-defining features selected adaptively. The value m implicitly determines the definition of neighborhood; the smaller m the larger neighborhood.
- Model averaging can be used with any base models besides trees.

Justification for model averaging: Let $\hat{a}_1, \ldots, \hat{a}_B$ be estimates of μ that have the same mean μ and variance σ^2. If their pairwise correlation is $cor(\hat{a}_i, \hat{a}_j) = \rho$ for any $i \neq j$, then their average $\frac{1}{B}\sum \hat{a}_i$ has mean μ and variance

$$\frac{\sigma^2}{B^2}[B + B(B-1)\rho] = \sigma^2[\rho + \frac{1}{B}(1-\rho)].$$

We can pick a large B to make $\frac{1}{B}\sigma^2(1-\rho)$ very small. If ρ is very small and σ^2 is not too high, then $\sigma^2\rho$ can be small. Thus, we seek to define a base model (or classifier) that (1) is unbiased, (2) is fast to build (so that B can be large), (3) has very small correlation from one to another and a variance not too large.

```r
library(randomForest)

Heart = read.csv("Heart.csv", row.names=1)  ## first column is row name, not a variable
names(Heart); dim(Heart)  ## 303, 14
Heart$Thal = factor(Heart$Thal, c('normal', 'reversable', 'fixed'), ordered=T)
Heart$ChestPain = factor(Heart$ChestPain, levels(Heart$ChestPain), ordered=T)

rf = randomForest(AHD ~ ., data=Heart)  ## error due to missing data

apply(is.na(Heart), 2, sum)  ## check which variable has missing data
apply(is.na(Heart), 1, sum)  ## check which observation has missing data

Heart2 = na.omit(Heart); dim(Heart2)  ## 297, 14
set.seed(899); rf1 = randomForest(AHD ~ ., data=Heart2)
set.seed(899); rf2 = randomForest(AHD ~ ., data=Heart, na.action=na.omit)
```

```r
all.equal(rf1$predicted, rf2$predicted, check.attributes=F)  ## True
table(Heart2$AHD)
```

Here I prefer creating a new data frame than using `na.action=na.omit`. Now we create training and test sets, and then fit a RF model:

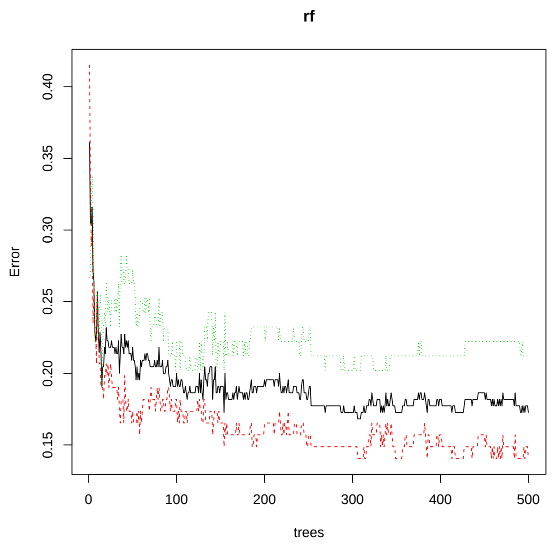
```r
set.seed(2018)
trainidx = sample(1:nrow(Heart2), 220)
Heart2.train = Heart2[trainidx, ] ## training set
Heart2.test = Heart2[-trainidx, ] ## test set

## Fit the RF model
rf = randomForest(AHD ~ ., data = Heart2.train)
rf ## print general results
names(rf) ## all details are here
rf$mtry; rf$ntree  ## check what default values were used
```

Out-of-bag (OOB) error estimation: RF allows CV-like error estimation without CV. For every tree, those in the bootstrap sample are training data and those left out are test data. Let w_{bi} be the number of copies of observation i is in bootstrap sample b. Let $B_i = \#\{b : w_{bi} = 0\}$ be the number of bootstrap samples not containing observation i. (Note that $E(B_i) = e^{-1}B \approx 0.37B$.) For observation i, let $\hat{r}_{\text{rf}}^{(i)}(x_i) = \frac{1}{B_i}\sum_{b:w_{bi}=0} \hat{r}_b(x_i)$, or majority vote. Then $\text{OOB}_i = L(y_i, \hat{r}_{\text{rf}}^{(i)}(x_i))$, and $\text{OOB} = \frac{1}{n}\sum_i \text{OOB}_i$. When B is sufficiently large, the OOB error estimate is equivalent to leave-one-out cross-validation error.

```r
mean(rf$oob.times/rf$ntree); exp(-1)  ## they are close
```

For a model fitted with `randomForest()`, its component `err.rate` contains the overall OOB error and the OOB errors stratified by the outcome categories as the number of trees increases. The function `plot.randomForest()` displays these errors in a plot (black is the overall OOB error).

```r
plot(rf)  ## same as matplot(rf$err.rate, type='l', xlab='trees', ylab='Error')
matplot(rf$err.rate[,'OOB'], type='l', xlab='trees', ylab='Error')  ## overall OOB error only
```



All measures of model performance are based on the OOB samples: `votes` contains the distribution of OOB predictions, `predicted` is the result of majority vote, `confusion` is the corresponding confusion matrix.

```r
table(rf$predicted, rf$votes[,2] > 0.5)  ## "predicted" is based on "votes"
rf$confusion  ## same as table(Heart2.train$AHD, rf$predicted)
rf$err.rate[rf$ntree, ]  ## the FPR and FNR can also be obtained here
```

We can make predictions on new data using `predict()`. But we should NOT re-predict the training set because it would give near perfect accuracy. This is called the **apparent error rate** and is known for being wildly optimistic.

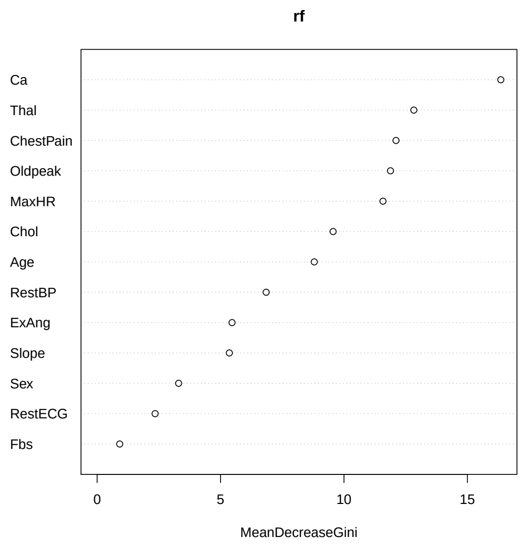
```
## Out-of-bag prediction
rfyhat = predict(rf)  ## without newdata, this returns rf$predicted
all.equal(rfyhat, rf$predicted)  ## True
table(Heart2.train$AHD, predict(rf))  ## OOB confusion matrix

table(Heart2.train$AHD, predict(rf, Heart2.train))  ## This is wrong!
rfyhat.test = predict(rf, Heart2.test)  ## This is correct.
table(Heart2.test$AHD, rfyhat.test)  ## test set confusion matrix
```

In `predict(rf, Heart2.train)`, the whole RF model is used to make prediction on every observation in `Heart2.train`. Since the individual trees severely overfit data and every observation is in 63% of the bootstrap samples, 63% of the individual trees probably "predict" the observation correctly. As a result, the final majority vote from all trees will give the "correct" prediction.

Variable importance: To measure the importance of a variable, we record the reduction of impurity (MSE, Gini, etc.) whenever the variable is used to split a node, compute the total reduction for every tree, and then average over all trees.

For a classification model fitted with `randomForest()`, its component `importance` contains `MeanDecreaseGini`. The function `importance()` and `varImpPlot()` display the importance values.

```
importance(rf)  ## show rf$importance
varImpPlot(rf)  ## same as dotchart(rf$importance[, 'MeanDecreaseGini']) except order
```



The results can vary quite a bit between runs because of the randomness introduced during model fitting: (1) bootstrap sampling, and (2) a random subset of features are considered at each split.

```
varImpPlot(randomForest(AHD ~ ., data=Heart2.train))  ## repeat a few times
```

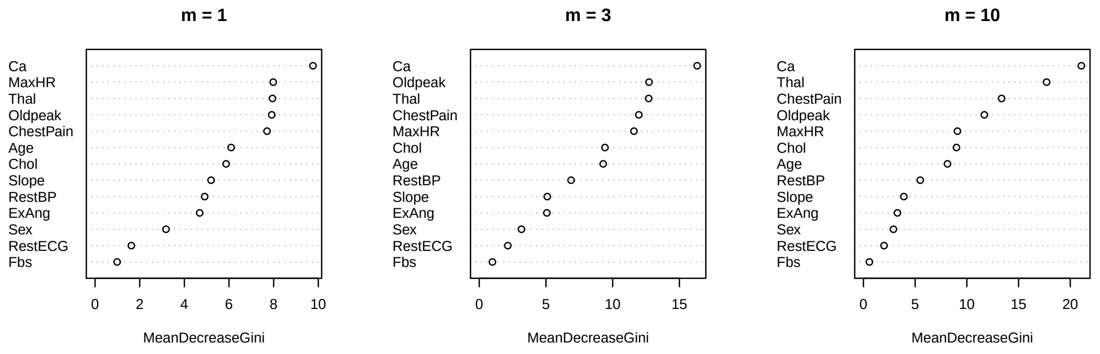
Below we evaluate the variation of results across runs.

```
importance.multirun = matrix(,20,13)
for(i in 1:20)
  importance.multirun[i,] = randomForest(AHD ~ ., data=Heart2.train, ntree=500)$importance
colnames(importance.multirun) = rownames(rf$importance)
idx = order(apply(importance.multirun, 2, median))

par(mar=c(4,6,1,1))
```

```r
boxplot(importance.multirun[, idx], horizontal=T, las=1, ylim=c(0,20))
#dotchart(importance.multirun[, idx], las=1, ylim=c(0,20))
```

The smaller m the more spread-out of importance over the variables. A small m has some similarity to ridge regression, which tends to share the coefficients evenly among correlated variables.

```r
set.seed(2018)
varImpPlot(randomForest(AHD ~ ., data=Heart2.train, mtry=1))
varImpPlot(randomForest(AHD ~ ., data=Heart2.train, mtry=3))
varImpPlot(randomForest(AHD ~ ., data=Heart2.train, mtry=10))
```



Another measure of **variable importance** is the *mean decrease in accuracy*, which is calculated by `randomForest()` when `importance=T` is specified.

```r
rf = randomForest(AHD ~ ., data=Heart2.train, importance=T)
rf$importance
importance(rf)  ## different from rf$importance except the last column
varImpPlot(rf)
```

The help page for `importance()` explains what the measure is: For each tree b, the prediction error e_b on the OOB portion of the data is recorded (error rate for classification, MSE for regression). Then for each predictor j, permute it in the OOB portion, calculate the prediction error again as e_{bj}, and $d_{bj} = e_{bj} - e_b$, which is the amount of additional error caused by permuting predictor j (effectively making it noninformative). The mean of d_{bj} over all trees is stored in the component `importance` while the standard deviation is stored in `importanceSD`. The coefficient of variation (i.e., mean/SD) is reported when `importance()` is called.

```r
all.equal(importance(rf)[,'MeanDecreaseAccuracy'],
  rf$importance[,'MeanDecreaseAccuracy']/rf$importanceSD[,'MeanDecreaseAccuracy'])  ## True
```

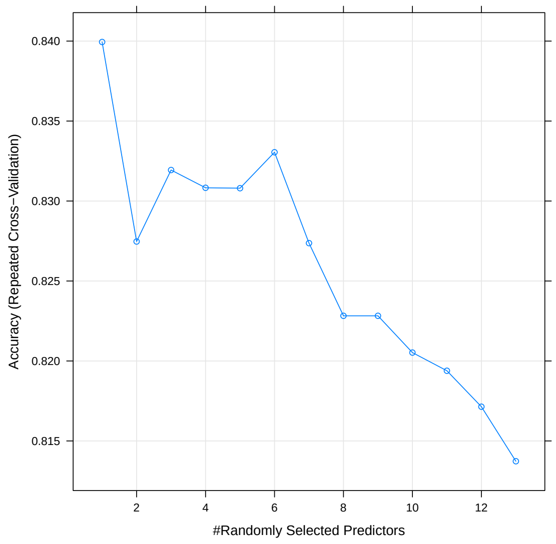
One can also get **local variable importance**, which is the mean decrease of accuracy of the predictors for each observation when it is OOB. To do this, set `localImp=T`. The results are stored in the component `localImportance`.

```r
rf = randomForest(AHD ~ ., data=Heart2.train, localImp=T)
dim(rf$localImportance)  ## 13 x 220
matplot(rf$localImportance[,1:5], type='l')  ## first 5 observations
#rf$localImportance %*% rf$oob.times
```

Cross-validation to select m: The R `caret` package can do cross-validation to select the hyperparameter m. By default, a grid over the hyperparameter is selected by the `train()` function. To change that, use either `tuneLength=` to specify the number of values in a grid or `tuneGrid=` to specify the values in a data frame. Note that by default, `summaryFunction=defaultSummary` and `metric=Accuracy`; when `summaryFunction` is set to be `twoClassSummary`, `metric` can only be `ROC`.

```r
library(caret)
cvCtrl = trainControl(method="repeatedcv", number=5, repeats=4,  ## 5-fold CV repeated 4 times
                      #summaryFunction=twoClassSummary,
                      classProbs=TRUE)
```

```
set.seed(2018)
fitRFcaret = train(x=Heart2.train[,1:13], y=Heart2.train$AHD, trControl=cvCtrl,
                   tuneGrid=data.frame(mtry=1:13),
                   #tuneLength=4,
                   #metric="ROC",  ## when summaryFunction=twoClassSummary
                   method="rf", ntree=500)  ## takes 24 sec on my laptop
fitRFcaret
plot(fitRFcaret)
```



`fitRFcaret` contains other results. It also contains the final model using the ‘optimal’ hyperparameter selected from `train()`.

```
names(fitRFcaret)
fitRFcaret$results
fitRFcaret$bestTune$mtry

fitRFcaret$finalModel
fitRFcaret$finalModel$confusion  ## OOB confusion matrix
```

The following gives test set confusion matrix.

```
table(Heart2.test$AHD, predict(fitRFcaret$finalModel, Heart2.test))
```

Again, the following generate “apparent error rates” that are too good.

```
table(Heart2.train$AHD, predict(fitRFcaret))
table(Heart2.train$AHD, predict(fitRFcaret, Heart2.train))
table(Heart2.train$AHD, predict(fitRFcaret$finalModel, Heart2.train))
```

`train()` can be called in two ways. `train(x,y)` is recommended because it handles categorical predictors nicely. If you use `train(formula, data)`, dummy variables are created for categorical predictors with more than two categories, which can cause problems when using functions such as `predict()`.

```
fitRFcaret2 = train(AHD ~ ., data=Heart2.train, trControl=cvCtrl,
                    method="rf", ntree=200)
predict(fitRFcaret2$finalModel, Heart2.test)  ## Error, due to reason below
fitRFcaret2$finalModel$importance  ## notice the variable names
fitRFcaret$finalModel$importance
```

`caret` also has a function `tuneRF()`, which is not as useful as the `train()` approach above.

```r
tuneRF(x=Heart2.train[,1:13], y=Heart2.train$AHD, stepFactor=1.5, improve=0.01, ntreeTry=50)
```

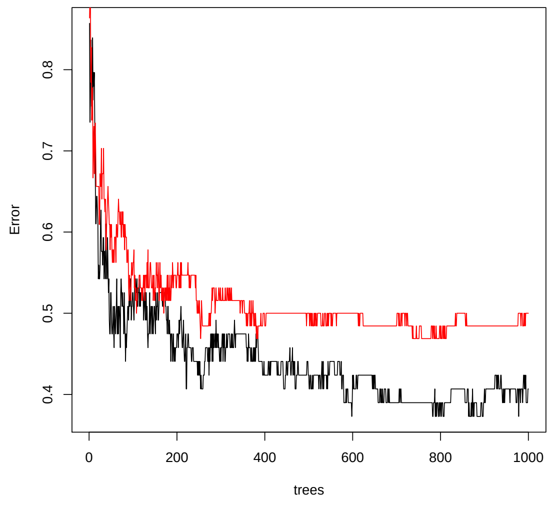
Other evaluations using caret: We can try several models under different settings, put them together into a list, and evaluate them using `resamples()`. As an example, I fit 4 RF models with different ntree values and compare them.

```r
modellist = list()
for (ntree in c(200, 400, 600, 800))
    modellist[[toString(ntree)]] = train(x=Heart2.train[,1:13], y=Heart2.train$AHD,
                                         method="rf", trControl=cvCtrl, ntree=ntree)

results = resamples(modellist)
names(results)
results$timings
summary(results)
dotplot(results)
```

`caret` allows users to define a new method for `train()`. An example is in https://machinelearningmastery.com/tune-machine-learning-algorithms-in-r/, under "Extend Caret" in Section 3, where the author defines a new RF method so that the grid search can be done over a grid of combinations of mtry and ntree.

Example: Classification RF on the `NCI60` dataset, which contains gene expression of 6830 genes for 64 tumor samples. The tumors are classified into 14 types.

```r
library(ISLR)
str(NCI60)
table(NCI60$labs)
dd = data.frame(NCI60$data)
dd$labs = as.factor(NCI60$labs)  ## randomForest() requires categorical outcome to be a factor

set.seed(2018)
rf = randomForest(labs ~ ., data=dd, ntree=1000)
plot(rf$err.rate[,1], type='l', xlab='trees', ylab='Error')

## Remove those rare/unknown tumor types (those with only one obs)
idx = dd$labs %in% names(table(NCI60$labs))[table(NCI60$labs) > 1]
dd2 = dd[idx,]
dd2$labs = as.factor(as.character(dd2$labs))  ## redefine the factor levels
rf2 = randomForest(labs ~ ., data=dd2, ntree=1000)

plot(rf2$err.rate[,1], type='l', xlab='trees', ylab='Error')
points(rf$err.rate[,1], type='l', col=2)
```



Example: Regression RF on the `Wage` dataset:

```
library(ISLR)
str(Wage)
levels(Wage$education)
Wage$education = factor(Wage$education, levels(Wage$education), ordered=T)

rf = randomForest(wage ~ .-logwage, data=Wage)  ## all predictors except `logwage`
rf
names(rf)
rf$mtry; rf$ntree
```

The counterpart of `err.rate` is `mse`.

```
plot(rf)  ## same as plot(rf$mse, type='l', xlab='trees', ylab='Error')
plot(Wage$wage, rf$predicted)
cor(Wage$wage, rf$predicted, method='spearman')

## Again, below is wrong.
plot(Wage$wage, predict(rf, Wage))
cor(Wage$wage, predict(rf, Wage), method='spearman')
```

For a regression model fitted with `randomForest()`, its component `importance` contains `IncNodePurity`. When `importance=T` is used, `%IncMSE` is the counterpart of `MeanDecreaseAccuracy` in classification RF.

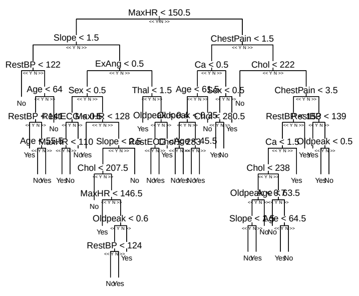
```
rf = randomForest(wage ~ .-logwage, data=Wage, importance=T)
importance(rf)
varImpPlot(rf)
```

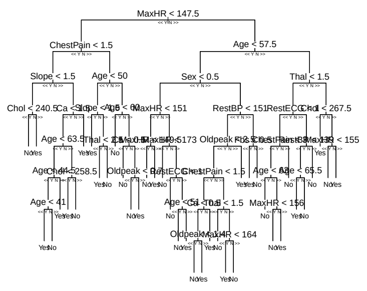
The smaller m the more spread-out of importance over the variables.

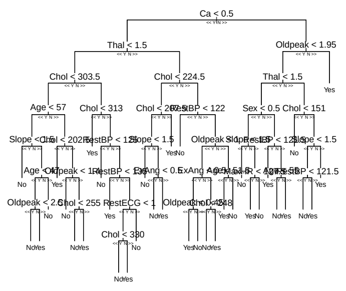
```
varImpPlot(randomForest(wage ~ .-logwage, data=Wage, mtry=1))
varImpPlot(randomForest(wage ~ .-logwage, data=Wage, mtry=3))
varImpPlot(randomForest(wage ~ .-logwage, data=Wage, mtry=5))
```

Individuals trees can be obtained with `getTree()`. For example, to get the 100th tree from the object `rf`, use `getTree(rf, 100)`. Unfortunately, the result of `getTree()` is in a format different from the frame format used by the `rpart` and `tree` packages, we cannot use the graphics functions from those packages. An R package `reprtree` posted on the GitHub can plot the individual trees. The plots are often not useful because the indivial trees often have a high depth. To install the `reprtree` package, use `devtools::install_github('araastat/reprtree')`.

```r
set.seed(2018)
rf = randomForest(AHD ~ ., data=Heart2.train)
reprtree:::plot.getTree(rf, k=20)
reprtree:::plot.getTree(rf, k=30)
reprtree:::plot.getTree(rf, k=50)
```







To redraw a tree without text

```r
library(rpart)
tr100 = reprtree:::as.tree(getTree(rf, k=20, labelVar=T), rf)
plot(tr100, type='uniform')
#text(tr100, split=T, cex=.8)  ## adding text may make the plot look too crowded
```

The `reprtree` package also implements a method to generate "representative trees" for random forests (Banerjee, Ding, Noone (2012). Identifying representative trees from ensembles. *Statistics in Medicine*).

```r
rep = reprtree::ReprTree(rf, Heart2.train)  ## representative tree
reprtree:::plot.reprtree(rep)
```

Notes on other R packages for bagging and random forests:

- caret (document) provides a unified interface (and a wrapper) for using `randomForest` and many other R packages. For example, it offers bagging of base models of type: lda, pls, nb (naive Bayes), ctree, svm, nnet. `names(getModelInfo())` provides a list of all trainable model types.
- party privides functions to build "conditional inference trees" (ctree) and to fit random forest models with conditional inference trees as base models.

8.1.2 Assignment

1. Reading for next lecture: ISLR 8.2, HOML 7.
2. ISLR Chapter 8 R Labs

8.2 Week 8 Day 2 (off for midterm)