Statistical Computing with R: Masters in Data Sciences 503 (S25) Third Batch, SMS, TU, 2024

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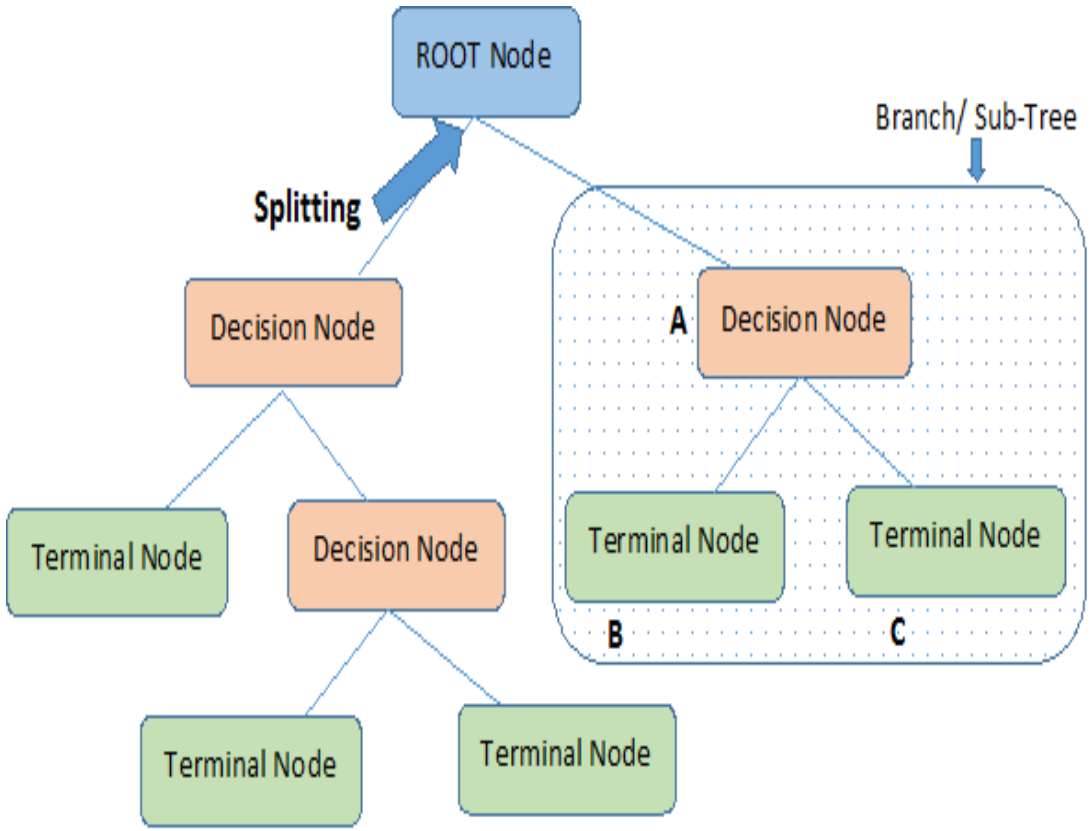
Supervised Learning with classification models

- Decision Tree
  - Model Accuracy
  - Model Prediction
  - Model Validation
- Ensemble learning
  - Bagging
  - Random Forest: Improved Decision Tree Bagging
  - Boosting
  - Random Forest Boosting

Decision Tree: More at ““An Introduction to Statistical Learning with Applications in R” book!

- Decision tree is a type of supervised learning algorithm that can be used in both regression and classification problems.
- It works for both categorical and continuous input and output variables.
- **Today we will focus on the classification tree**

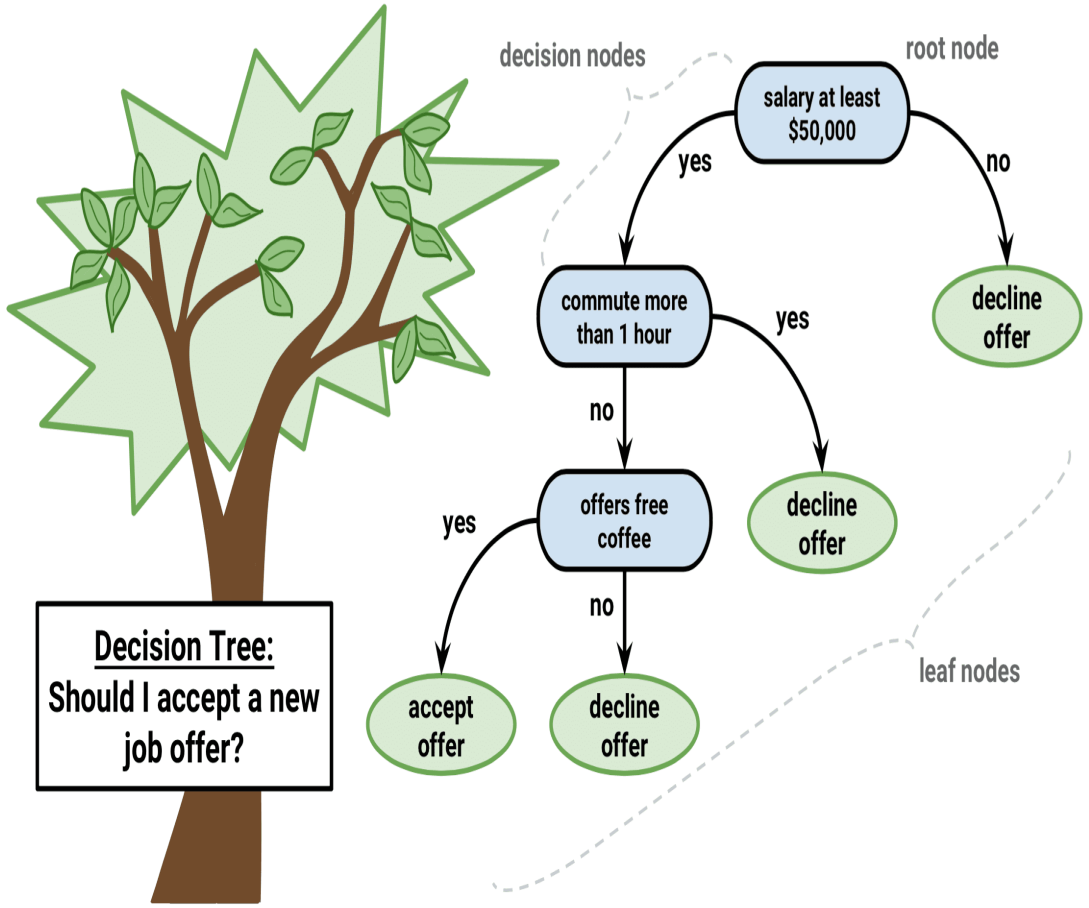


Note:- A is parent node of B and C.

Reference: https://www.datacamp.com/community/tutorials/decision-trees-R

Classification tree:

- Classification Error Rate
- Gini Index
- Cross-Entropy
- **Confusion matrix accuracy and diagnostic measures**



Reference: https://www.datacamp.com/community/tutorials/decision-trees-R

Let’s fit a decision tree classifier in the Cardiotocographic (CTG) data:

#Make sure the data is in the working library of R

- library(readr)
- Cardiotocographic <- read_csv(“Cardiotocographic.csv")

#Save the long name as data

- data <- Cardiotocographic
- str(data)

#The structure correctly shows LB, AC and FM as numerical but incorrectly show NSP as numeric too!

- spec_tbl_df [2,126 x 22] (S3: spec_tbl_df/tbl_df/tbl/data.frame)
- $ LB : num [1:2126] 120 132 133 134 132 134 134 122 122 122 ...
- $ AC : num [1:2126] 0 0.00638 0.00332 0.00256 0.00651 ...
- $ FM : num [1:2126] 0 0 0 0 0 0 0 0 0 0 ...

…

- $ NSP : num [1:2126] 2 1 1 1 1 3 3 3 3 3 ...

Change the NSP as factor variable as this is the dependent variable:

#NSP = Dependent variable (response)

#Three categories of NSP

- NSP = 1 = Normal CTG (No hypoxia or acidosis)
- NSP = 2 = Suspicious CTG (Low probability of hypoxia/acidosis)
- NSP = 3 = Pathological CTG (High probability of hypoxia/acidosis)

#NSP categories were formed using "**Updated 2015 FIGO Intrapartum Fetal Monitoring Guidelines" (figo.org) (Using SisPorto algorithm)**

#Changing NSP as a new factor variable i.e. NSPF

data$NSPF <- factor(data$NSP)

#Checking structure of NSPF

str(data$NSPF)

- Factor w/ 3 levels "1","2","3": 2 1 1 1 1 3 3 3 3 3 ...

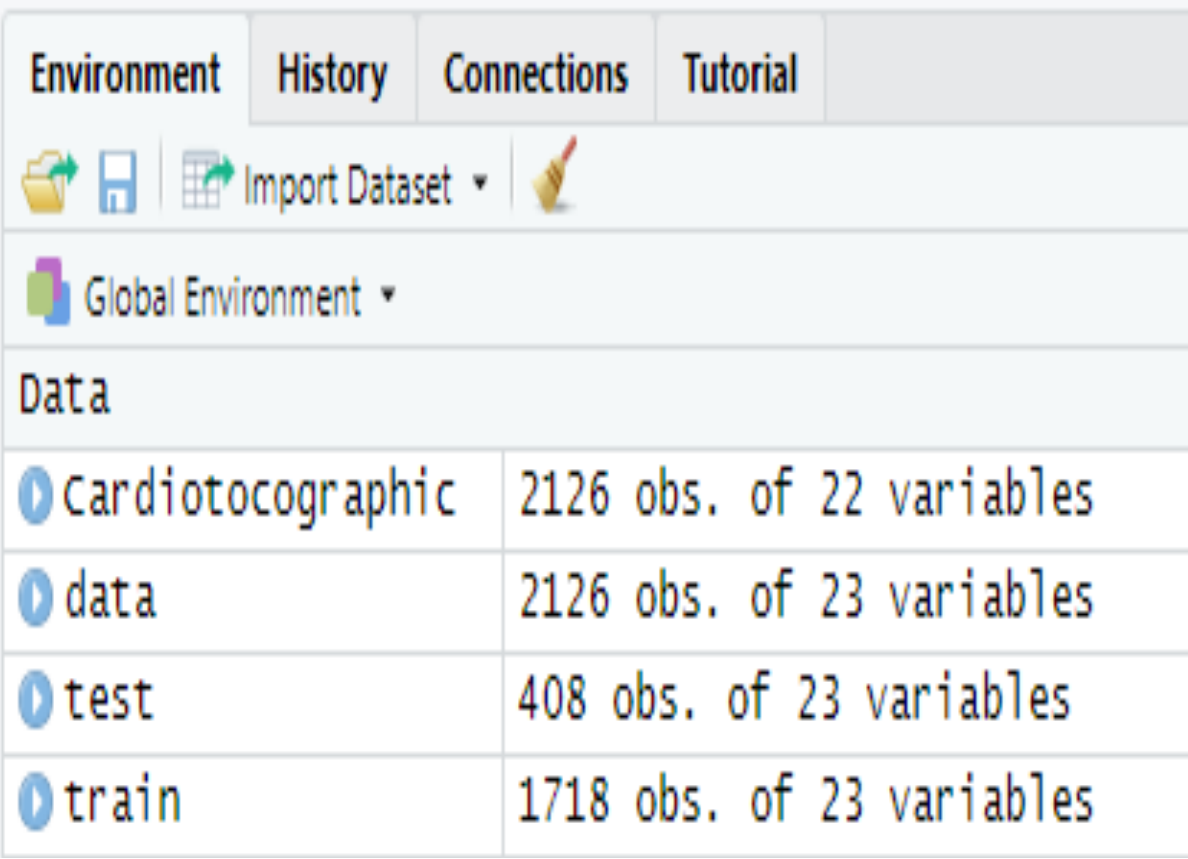
#Key Independent variables (inputs)

- LB = Fetal Hearth Rate
- AC = # of accelerations / minute
- FM = # of fetal movements / minute

Let’s divide the data into train and test sets:

#Data partition

- set.seed(1234)
- ind <- sample(2, nrow(data), replace=T, prob = c(0.8, 0.2))
- train <- data[ind==1,]
- test <- data[ind==2,]



Let’s fit a decision tree classifier in the train data:

#Party package

- install.packages("party")
- library(party)

#Fit the decision tree model with only the first three variable to learn it today

- tree <- ctree(NSPF ~ LB+AC+FM, data=train)

#Check the model

- tree

Conditional inference tree with 10 terminal nodes

- Response: NSPF
- Inputs: LB, AC, FM
- Number of observations: 1718

1) AC <= 0.000834028; criterion = 1, statistic = 263.403

2) LB <= 136; criterion = 1, statistic = 131.511

3) FM <= 0.111898; criterion = 1, statistic = 35.729

Let’s plot the decision tree: plot(tree)

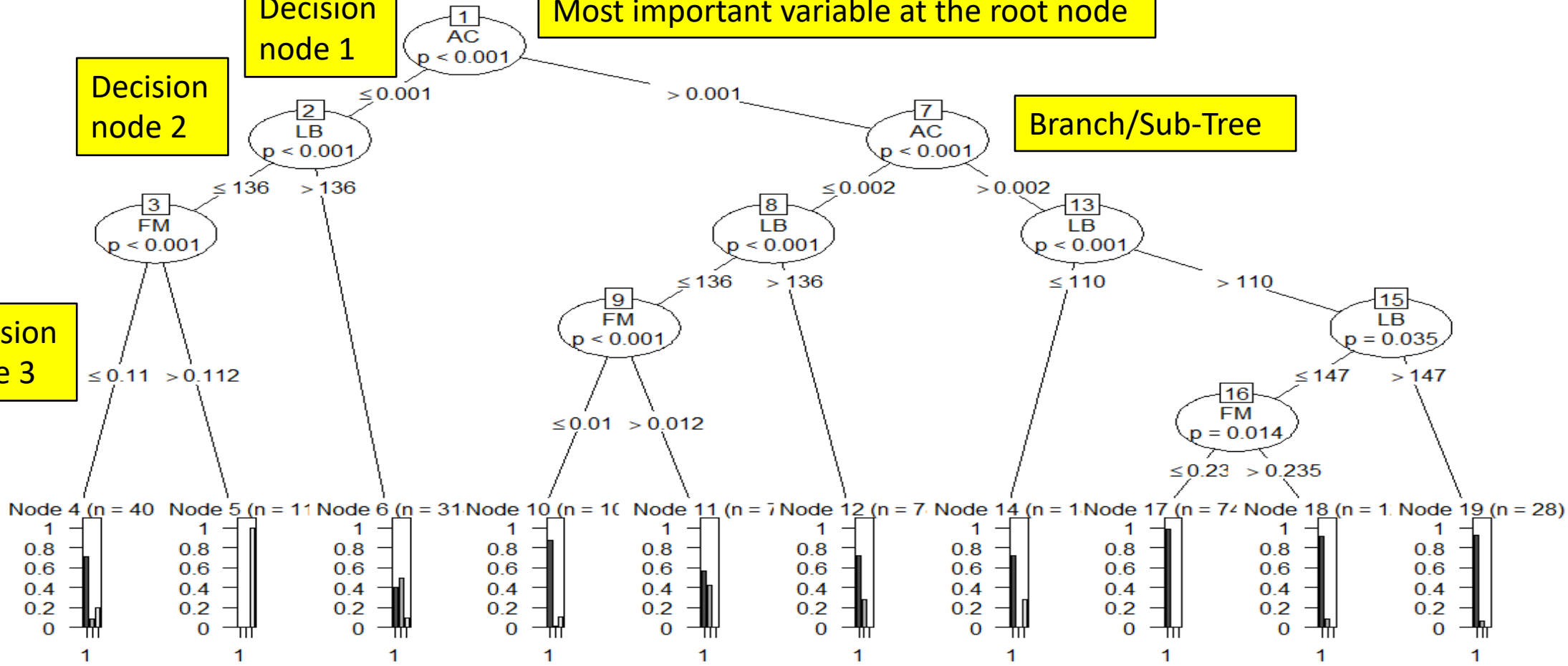
Decision node 1

Most important variable at the root node

Decision node 2

Branch/Sub-Tree

Decision node 3



Terminal node 4: NSP = 1, Terminal node 5: NSP = 3, Terminal node 6: NSP = 2

Terminal node 10, 11, 12, 14, 17, 18, 19: NSP = 1

For predicting 3 variables we have a “tree” with 19 nodes! So, it is a “overfitting”!

#Pruning the tree with 99% confidence interval and split at 500 samples

- tree1 <- ctree(NSPF ~ LB+AC+FM, data=train, controls = ctree_control(mincriterion=0.99, minsplit=500))

- tree1

#Now we have only 9 nodes in the model!

Lets plot it and see how it helps us!

Conditional inference tree with 5 terminal nodes (total 9 nodes)

- Response: NSPF
- Inputs: LB, AC, FM
- Number of observations: 1718

1) AC <= 0.000834028; criterion = 1, statistic = 263.403

2) LB <= 136; criterion = 1, statistic = 131.511

3)* weights = 416

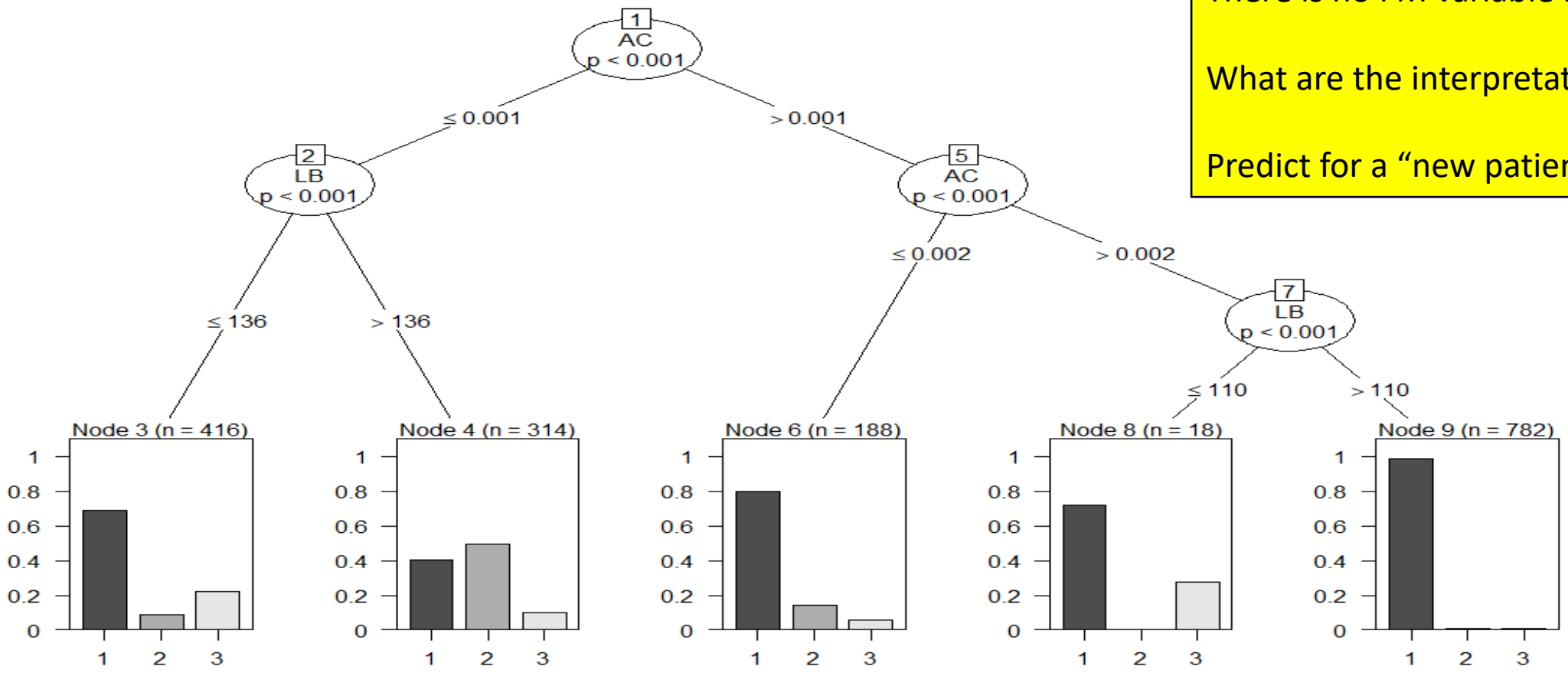
…

7) LB > 110

9)* weights = 782

This is why we need to use ensemble learning i.e. “Random Forest” to avoid overfitting for Decision Tree Model!

Controlled Decision Tree: **plot(tree1)**



There is no FM variable now!

What are the interpretations?

Predict for a “new patient”!

Let’s predict now:

Predict the categorical probabilities for each case in train data

- predict(tree, type="prob")

#Predict the category for each case in test data

- predict(tree, test)

#Predicted probability: case 1

- [[1]]
- 0.71111111 (prob. for NSP=1)
- 0.09135802 (prob. for NSP=2)
- 0.19753086 (prob. for NSP = 3)

#Predicted category for cases:

[1] **1** 1 1 1 1 3 1 1 1 1 1 2 1 1 2 1 1 1 1
1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 1

[40] 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 1 2 2
2 2 2 2 2 1 2 2 2 2 1 1 1 2 2 1 1 2 2 2 1

Let's get the confusion matrix, accuracy and the misclassification error (mce) for "train" data

#Confusion matrix

- (tab <- table(predict(tree), train$NSPF))

#Accuracy

- accuracy <- sum(diag(tab))/sum(tab)

#Misclassification error

- mce <- 1 - accuracy

#Confusion matrix

	1	2	3
1	**1222**	70	101
2	126	**156**	32
3	0	0	**11**

#Accuracy

[1] 0.8084983

#Misclassification error

[1] 0.1915017

NSP classification was done by 3 expert clinicians!

We need to optimize the model so that we can do prediction with confidence with the model rather than clinicians!

Let's get the confusion matrix, accuracy and the misclassification error (mce) for "test" data

#Prediction for test data

pred.test <- predict(tree, newdata=test)

#Confusion matrix

- (tab1 <- table(pred.test, test$NSPF))
- #Accuracy
- accuracy1 <- sum(diag(tab1))/sum(tab1)
- #Misclassification error
- mce1 <- 1 - accuracy1

#Confusion matrix

pred.test	1	2	3
1	**274**	20	27
2	33	**48**	4
3	0	1	**1**

#Accuracy

[1] 0.7916667

(Good, not excellent!)

#Misclassification error

[1] 0.2083333

We must optimize the model so that we can do prediction with confidence with the model rather than clinicians!

Limitations of Decision Tree model:

https://www.datacamp.com/community/tutorials/decision-trees-R

- The decision trees discussed above suffer from *high variance*, meaning if you split the training data into 2 parts at random, and fit a decision tree to both halves, the results that you get could be quite different.
- In contrast, a procedure with *low variance* will yield similar results **if applied repeatedly** to distinct dataset.
- **We must use ensemble learning!**
  - **Bagging, Random Forests and Boosting**

- **Bagging**, or *bootstrap aggregation*, is a technique used to reduce the variance of your predictions by **combining the result of multiple classifiers modeled on different sub-samples** of the same dataset.
- Here is the equation for bagging:

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

Where, we generate B number of bootstrapped (resampled) training datasets and choose one with “vote”.

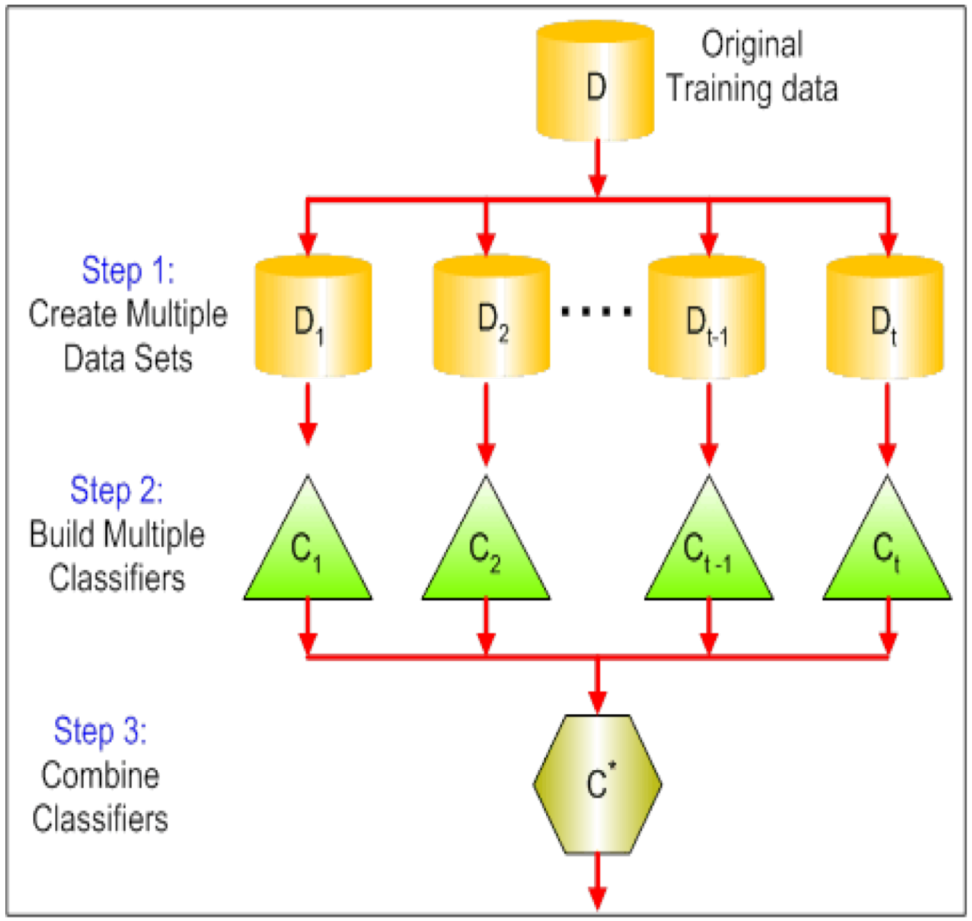
Bagging:

https://www.datacamp.com/community/tutorials/decision-trees-R

- **Step 1**: Here you replace the original data with new data. The new data usually have a fraction of the original data's columns and rows, which then can be used as hyper-parameters in the bagging model.

- **Step 2**: You build classifiers on each dataset. Generally, you can use the same classifier for making models and predictions.

- **Step 3**: Lastly, you use an average value to combine the predictions of all the classifiers, depending on the problem. Generally, these combined values are more robust than a single model.



Bagging in R with “ipred” package for CTG data (NSP = dependent variable):

#Bagging with ipred package

#install.packages(“ipred”) if required

- library(ipred)
- MBTree <- bagging(NSPF~LB+AC+FM, **data = train**, coob=T)
- print(MBTree)

#Prediction

- MBPredict1 <- predict(MBTree, test)
- MBPredict1

#Confusion matrix and accuracy

- confusionMatrix(MBPredict1, test$NSPF)

- Bagging classification trees with 25 bootstrap replications
- Call: bagging.data.frame(formula = NSPF ~ LB + AC + FM, data = train, coob = T)
- Out-of-bag estimate of misclassification error: 0.1717
- **Confusion Matrix and Statistics**

	Reference		
Prediction	1	2	3
1	273	26	17
2	25	37	2
3	9	6	13

Accuracy : 0.7917, 95% CI : (0.749, 0.8301) **(Same!)**

MCE = 1 – 0.7917 = 0.2083 = 20.83%

Random Forest: Improved Bagging model

https://www.datacamp.com/community/tutorials/decision-trees-R

- Random Forest provides an improvement over bagged trees by a small tweak that *decorrelates* the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, a *random sample of **m** predictors (mtry)* is chosen as split candidates from the full set of ***p*** predictors.

- **The split is allowed to use only one of those *m* predictors**

- This is the main difference between random forests and bagging; because as in bagging, the choice of predictor ***m = p i.e. all the predictors are used***.

Random Forest Requisites:

https://www.datacamp.com/community/tutorials/decision-trees-R

- First assume that the number of cases in the training set is K.
- Then, take a random sample of these K cases, and then use this sample as the training set for growing the tree.
- If there are ***p*** Input variables, specify a number ***m < p*** such that at each node, we can select ***m*** random variables out of the ***p***.
- The best split (votes) on these ***m*** is used to split the node.
- Each tree is subsequently grown to the **largest extent** possible and **no pruning** is needed.
- Finally, aggregate the predictions of the target trees to predict new data.
- **Random Forest package in R used 500 trees as "default"!**

Advantages of Random Forests model:

https://www.datacamp.com/community/tutorials/decision-trees-R

- Random Forests is very effective at estimating missing data and maintaining accuracy when a large proportions of the data is missing.
- It can also balance errors in datasets where the **classes are imbalanced**.
- **Most importantly, it can handle massive datasets with large dimensionality.**
- However, one disadvantage of using Random Forests is that you might easily "overfit" noisy datasets, **especially in the case of doing regression**.

Let’s fit the Random Forest model now:

#Random Forests package

#install.packages("randomForest")

- library(randomForest)

#Setting seed for replication

set.seed(222)

#Fitting random forest model

- rfm <- randomForest(NSPF~ LB+AC+FM, data=train)

#Printing random forest model

- print(rfm)

Type of random forest: classification

Number of trees: 500

No. of variables tried at each split: 1

OOB estimate of error rate: 17.35%

Confusion matrix:

	1	2	3	class.error
1	**1295**	52	1	0.03931751
2	119	**104**	3	0.53982301
3.	92	31	**21**	0.85416667

Accuracy = (1295+104+21)/(1718)= 82.83% (Good!)

MCE = 1 – 0.8283 = 0.1717 = 17.17%

Prediction using “caret” package:

#Let us use caret to predict

- library(caret)
- p1 <- predict(rfm, train)
- head(p1)

#Let us see the original values

head(train$NSPF)

> head(p1)

Cases: 1 2 3 4 5 6

Prediction: 1 1 1 1 1 1

- NSP Levels: 1 2 3

>head(train$NSPF)

- Cases: 1 2 3 4 5 6
- [1] 2 1 1 1 1 3
- NSP Levels: 1 2 3

For the first six cases, prediction using train data is “not perfect”!

Let's check the accuracy and misclassification error with Confusion Matrix for "train" data:

- #Confusion matrix
- confusionMatrix(p1, train$NSPF)

Confusion Matrix and Statistics

	Reference		
Prediction	1	2	3
1	1304	82	79
2	44	144	25
3	0	0	40

- Accuracy : **0.8661**

  95% CI : (0.8491, 0.8819)

	Class: 1	Class: 2	Class: 3
Sensitivity	**0.9674**	0.63717	0.27778
Specificity	0.5649	**0.95375**	**1.00000**

- MCE = **1 – 0.8661 = 0.1339**
- Fitted model in the train data is nearly 87% correct!
- **Accuracy of fitted model in the test data = ??% correct??**

Let's check the accuracy and misclassification error with Confusion Matrix for "test" data:

#Prediction for test data

- p2 <- predict(rfm, test)

#Confusion matrix

- confusionMatrix(p2, test$NSP)

Confusion Matrix and Statistics

	Reference		
Prediction	1	2	3
1	293	31	27
2	14	38	2
3	0	0	3

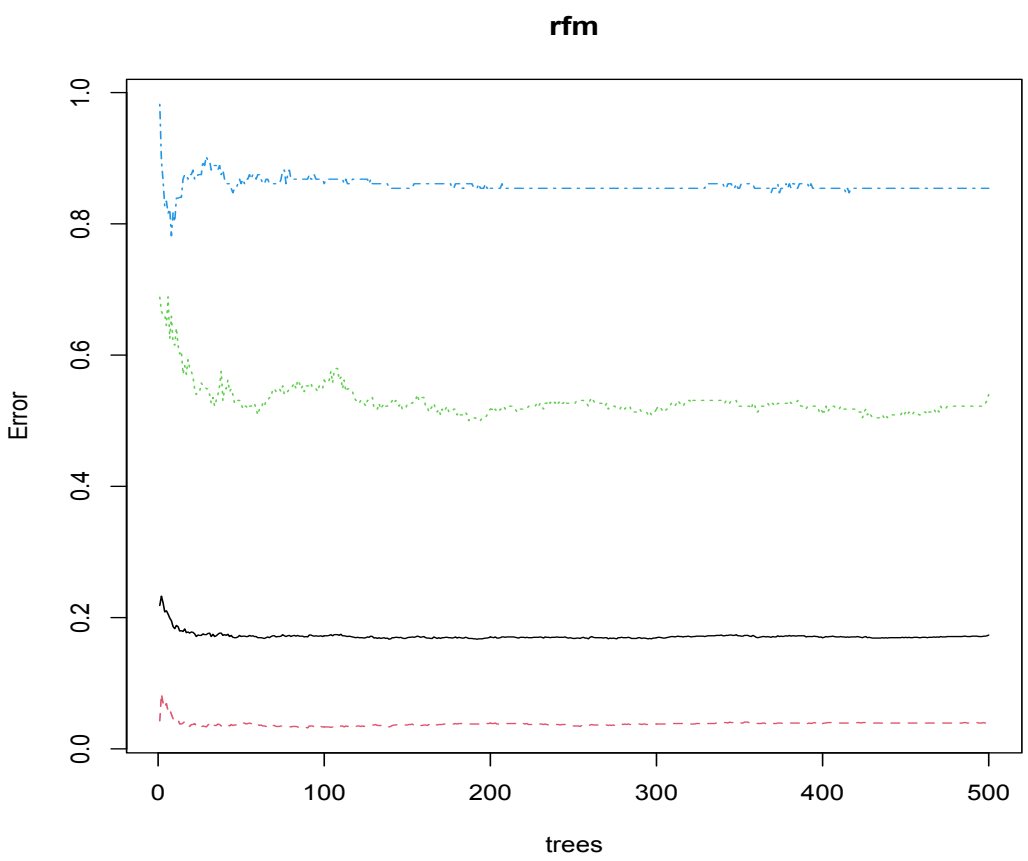
- Accuracy : **0.8186 (Better!)**
- 95% CI : (0.7777, 0.8548)

	Class: 1	Class: 2	Class: 3
Sensitivity	0.9544	0.55072	0.09375
Specificity	0.4257	0.95280	1.00000

- **MCE = 1 – 0.8186 = 0.1814 = 18.14% OOB error?**

Let us evaluate the error and see if we can improve the model with it: **plot(rfm)**

- Here error reduced substantially till 200 trees
- Error did not change between 200-300 trees
- This means the default 500 trees are not required to get the lowest error



Let us use the original data for the subsequent steps:

- NSP as factor instead of creating new variable NSPF
- The divide this data into two partitions with 80% and 20% data
- train = 80% random data
- test = 20% random data

Can we improve the random forest model?

Yes. We can tune the random forest model!

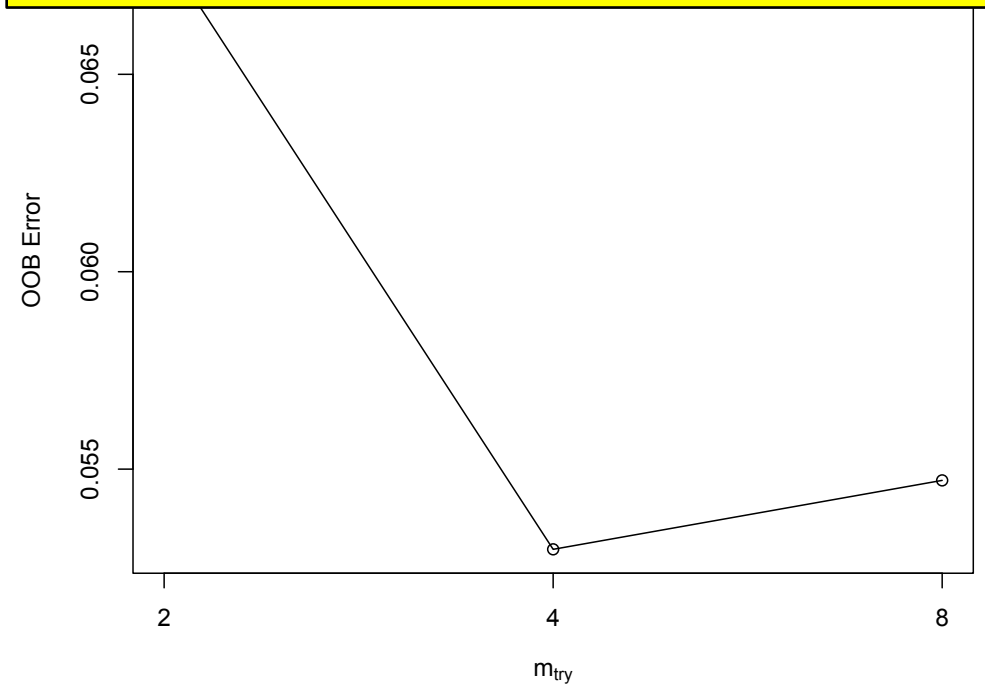
 # We can use "tuneRF" function of the randomForest package but we need to define train as data frame

- train <- as.data.frame(train)

 # We can use the "tuneRF" now

- t <- tuneRF(train[,-22], train[,22],
- stepFactor = 0.5,
- plot = TRUE,
- ntreeTry = 300,
- trace = TRUE,
- improve = 0.05)

Here mtry split parameter i.e. number of variables used in each split have lowest OOB error at 4, with 300 trees instead of default 500 trees!



Lets fit the improved (fineTuned) random forest model and check the OOB error:

 # Improved "rfm" model:

- rfm1 <- randomForest(NSP~ LB+AC+FM, data=train,
- ntree = 300,
- mtry = 4,
- importance = TRUE,
- proximity = TRUE)
- print(rfm1)

Call:

randomForest(formula = NSP ~ LB + AC + FM, data = train, ntree = 300, mtry = 4, importance = TRUE, proximity = TRUE)

Type of random forest: classification

Number of trees: 300

No. of variables tried at each split: 3

OOB estimate of error rate: **16.3%**

(improved a bit but not by much!)

- **Accuracy=?? MSE = ???**
- **(Better than RandomForest or Not?)**

Boosting: Better than Random Forest?

https://www.datacamp.com/community/tutorials/decision-trees-R

- **Boosting** is another approach to improve the predictions resulting from a decision tree.

- Like bagging and random forests, it is a general approach that can be applied to many statistical learning methods for regression or classification.

- Recall that bagging involves creating multiple copies of the original training dataset using the bootstrap, fitting a separate decision tree to each copy, and then combining all of the trees in order to create a single predictive model.

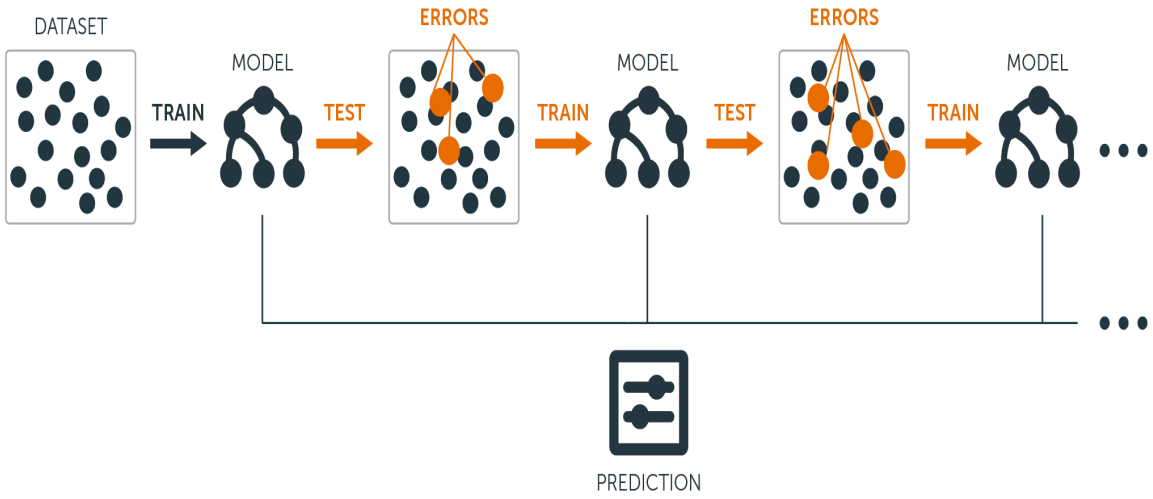
- Notably, each tree is built on a bootstrapped dataset, independent of the other trees.

How Boosting works?

https://www.datacamp.com/community/tutorials/decision-trees-R

- Boosting works in a similar way, except that the trees are grown *sequentially*: each tree is grown using information from previously grown trees.

- Boosting **does not involve bootstrap sampling**; instead, each tree is fitted on a modified version of the original dataset.



Boosting with Generalized Boosting Regression Model (GBM): https://rpubs.com/drwatkins/286356

#Generalized Boosting Regression Model

```
library(caret)
mod.gbm <-
train(NSP~.,data=train,method="gbm",verbose=
F)
print(mod.gbm)
```

#Prediction and confusion matrix

```
pred.mod.gbm <-
predict(mod.gbm,test,data=test)
confusionMatrix(pred.mod.gbm, test$NSP)
```

#Variable importance

```
summary(mod.gbm)
```

Confusion Matrix and Statistics

	Reference		
Prediction	1	2	3
1	288	31	23
2	15	36	2
3	4	2	7

Accuracy : **0.8113 (Lower than Random Forest!)**

95% CI : (0.7699, 0.8481)

Error: 1 – 0.8113 = 0.1887 = **18.87%**

Boosting with GBM did not improve the model!

Because: Our problem is classification not the regression, so this is GIGO!

Boosting of random forest model using “xgboostTree” model with caret package in R: Takes time to fit!

#Boosting with extreme gradient boosting Tree model in caret

```
mod.xgb <-
train(NSP~.,data=train,method="xgb
Tree",verbose=FALSE)
print(mod.xgb)
summary(mod.xgb)
```

#Prediction and confusion matrix

```
pred.mod.xgb <-
predict(mod.xgb,test,data=test)
confusionMatrix(pred.mod.xgb,
test$NSP)
```

Confusion Matrix and Statistics

	Reference		
Prediction	**1**	**2**	**3**
1	**287**	**29**	**23**
2	**14**	**38**	**2**
3	**6**	**2**	**7**

Accuracy : 0.8137

(Lower than Random Forest Model)

OOB Error = 1 – 0.8137 = 0.1853 = **18.53%**

http://www.sthda.com/english/articles/35-statistical-machine-learning-essentials/139-gradient-boosting-essentials-in-r-using-xgboost/

The “best” model?

- Improved random forest model?
- Why?
- What is the lesson learnt?

Self-Learning

- **Try to fit the decision tree, improved decision tree, random forest and boosting models for the same data using all the variables in the model**
- Which model gives the best result?
- Why?

Question/queries?

- Next class

- Unsupervised learning
  - Dimensionality Reduction

- Factor analysis
  - Principal Component Analysis
  - Principal Axis Factoring
  - Confirmative Factor Analysis

Thank you!

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