STA 235H - Prediction: Bagging, Random Forests, and Boosting

Fall 2022

McCombs School of Business, UT Austin

Announcements

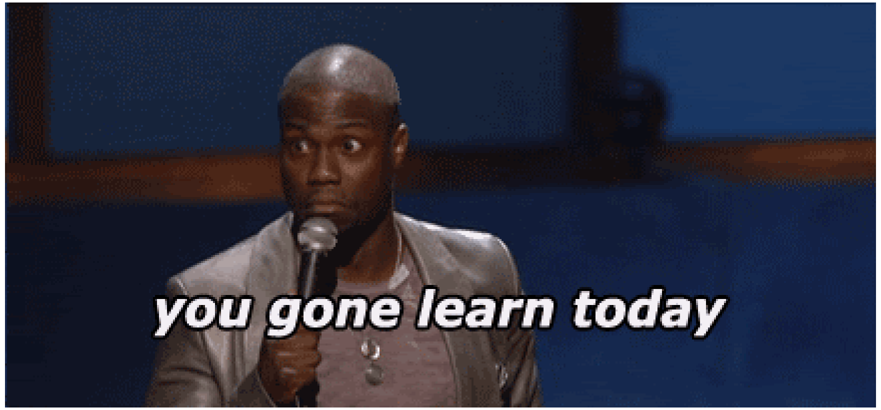
- Homework 6 is due this Friday
- Homework 7 will be posted this Friday as well (shorter homework)
  - Remember that it is due Thursday Dec. 1st and you cannot submit late.
- Next class: No new content, only a review! (Final TRIVIA)
- One final JITT: No content, but you will need to make sure Proctorio works.
  - No video recording, no websites blocked.
  - You will need to show an ID before starting. Only one device and one screen.

What we have seen...

- Decision trees:
  - Classification and Regression Trees
  - When to split? Complexity parameter
  - Advantages and disadvantages.

What we'll cover today

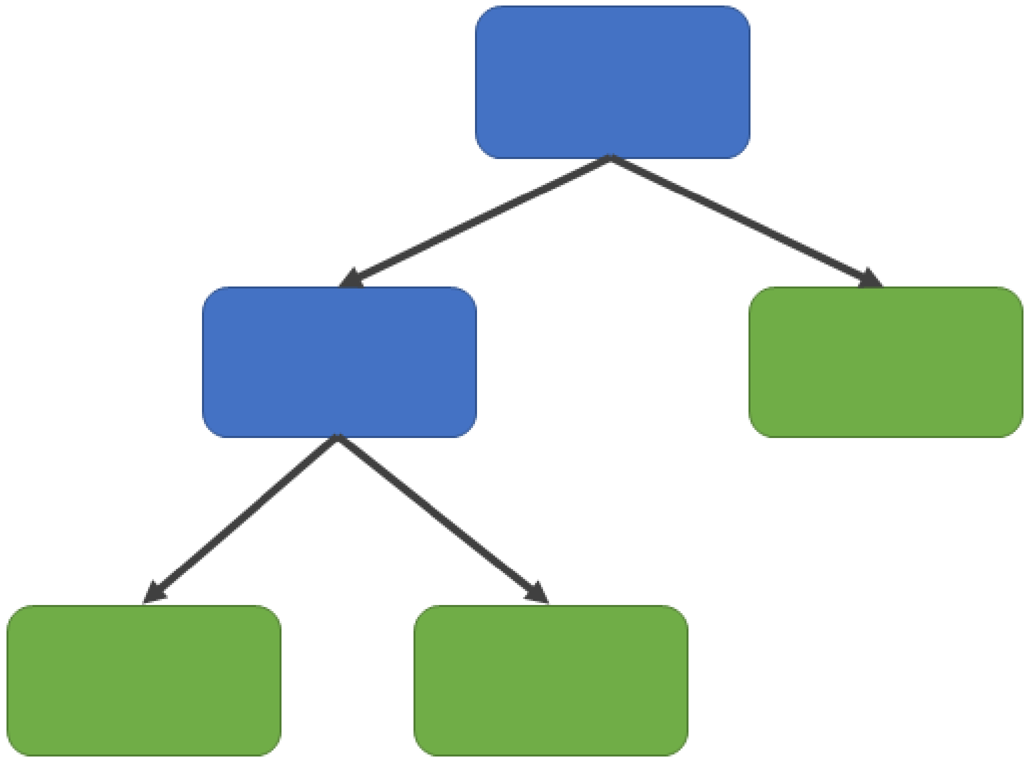
- Ensemble methods:
  - Bagging (e.g. tree bagging)
  - Random Forests
  - Boosting



Quick recap on trees

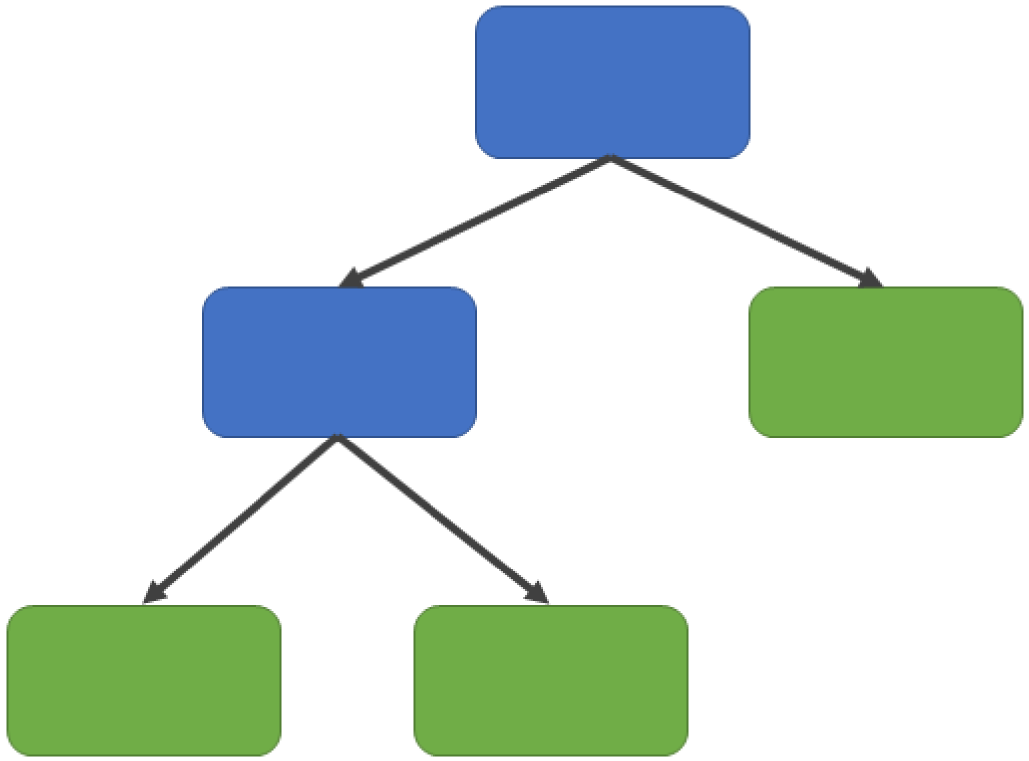
Quick refresher on decision trees

- A decision tree is a structure that works like a flowchart
- You start at the root node, make your way down the branches through the (internal) nodes, and get to the leaves (terminal nodes).
    - At the leaves is where prediction happens!



To split or not to split

- In general, we will only increase the size of our tree (additional split) if we gain some additional information for prediction
- How do we measure that information gain?
    - Classification: Impurity measure (like Gini Index).
    - Regression: Decrease in RMSE.



Q1) In term of bias, which one is better: A deep tree or a shallow tree?

Let's look at an example: Car seat prices

```r
library(ISLR)
data(Carseats)

head(Carseats)
```

```
##   Sales CompPrice Income Advertising Population Price ShelveLoc Age Education
## 1  9.50       138     73          11        276   120       Bad  42        17
## 2 11.22       111     48          16        260    83      Good  65        10
## 3 10.06       113     35          10        269    80    Medium  59        12
## 4  7.40       117    100           4        466    97    Medium  55        14
## 5  4.15       141     64           3        340   128       Bad  38        13
## 6 10.81       124    113          13        501    72       Bad  78        16
##   Urban  US
## 1   Yes Yes
## 2   Yes Yes
## 3   Yes Yes
## 4   Yes Yes
## 5   Yes  No
## 6    No Yes
```

Do you wanna build a... tree?

```r
library(caret)
library(rpart)
library(rattle)
library(rsample)
library(modelr)

set.seed(100)

split <- initial_split(Carseats, prop = 0.7, strata = "Sales")

carseats.train  <- training(split)
carseats.test   <- testing(split)

tuneGrid <- expand.grid(cp = seq(0, 0.015, length = 100))

mcv <- train(Sales ~., data = carseats.train, method = "rpart",
  trControl = trainControl("cv", number = 10), tuneGrid = tuneGrid)
```

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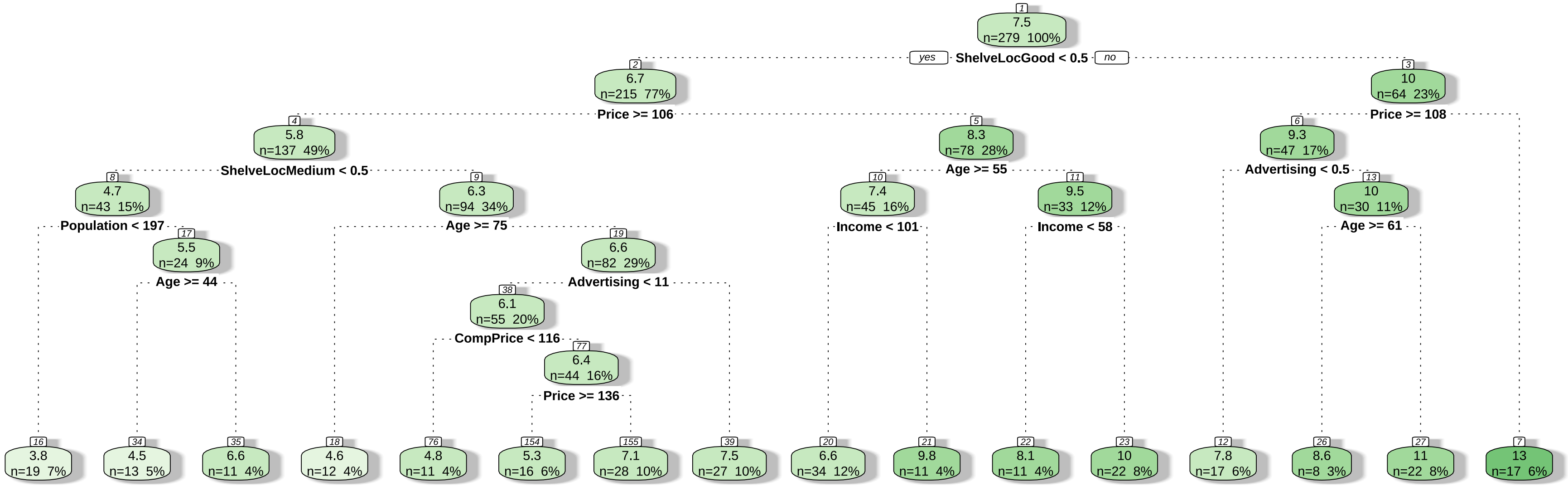
```

Do you wanna build a... tree?

```
fancyRpartPlot(mcv$finalModel, caption="Decision Tree for Car Seats Sales")
```



Decision Tree for Car Seats Sales

Q2) We are trying to predict Sales. How many different prediction values for sales will I have, at most, considering the previous decision tree?

Seems a pretty complex tree… can we improve it?

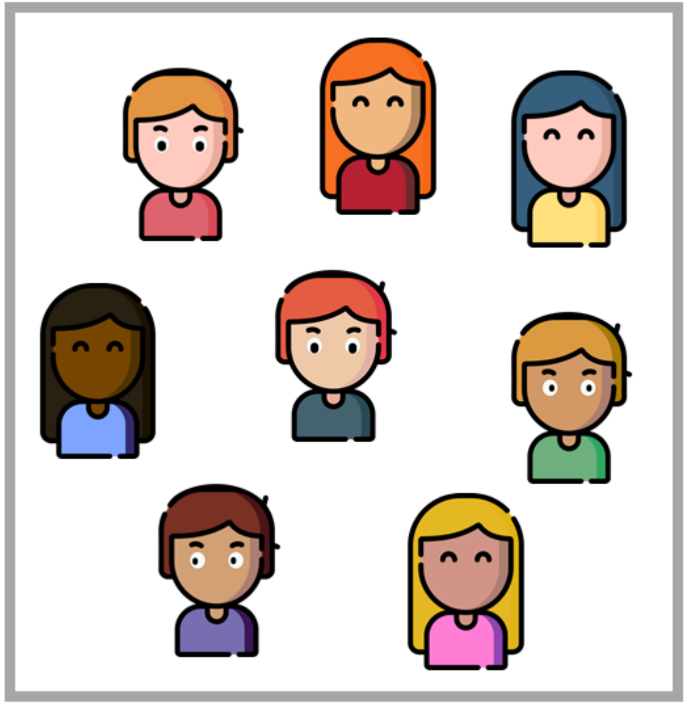
Bagging

Q3) What is the main objective of bagging?

Introduction to Bagging

- Bagging (Bootstrap Aggregation): Meant to reduce variance.
- Remember bootstrap sampling?

Sample



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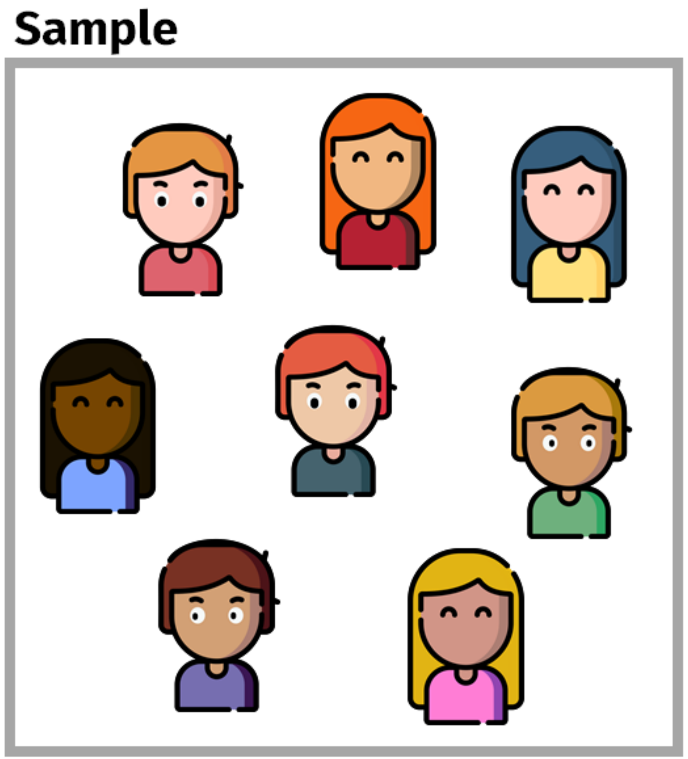

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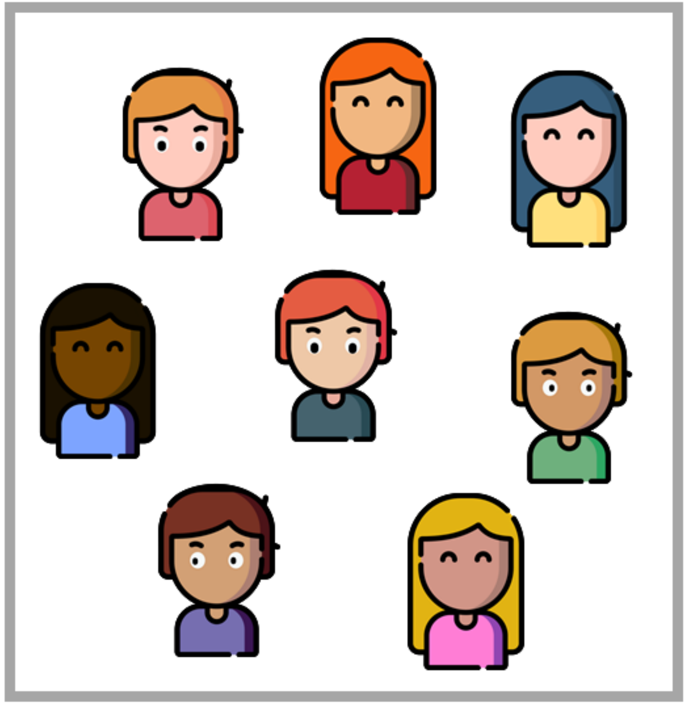

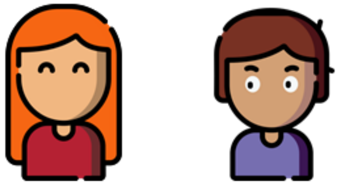

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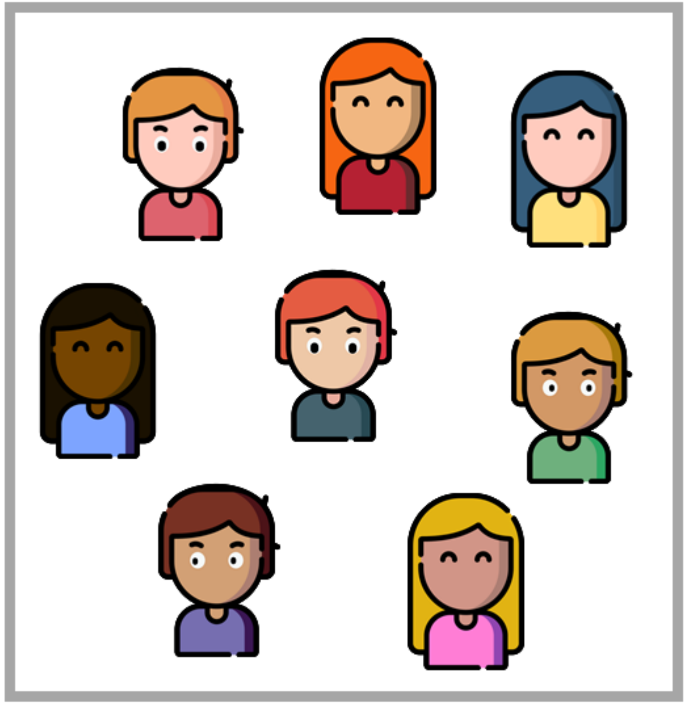

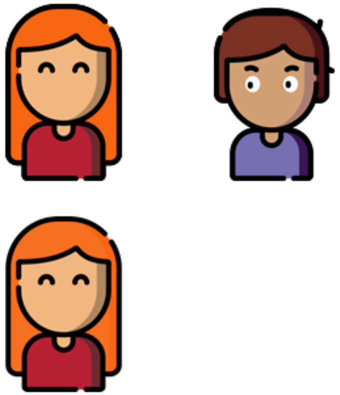

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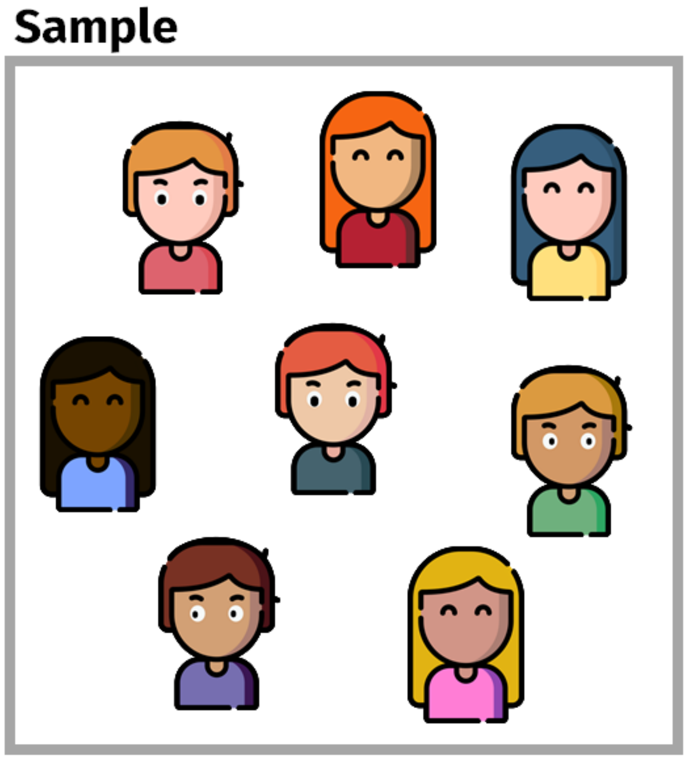
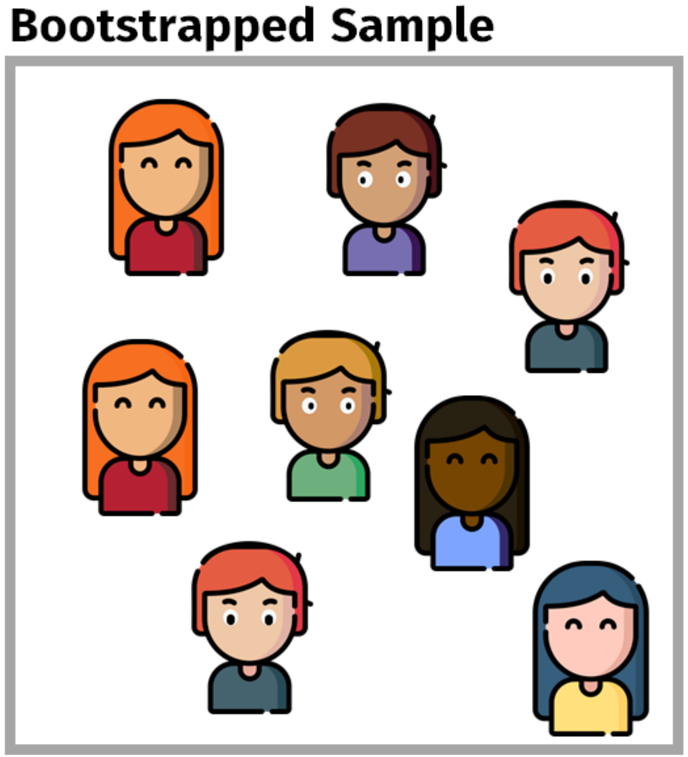




Bagging and Decision Trees

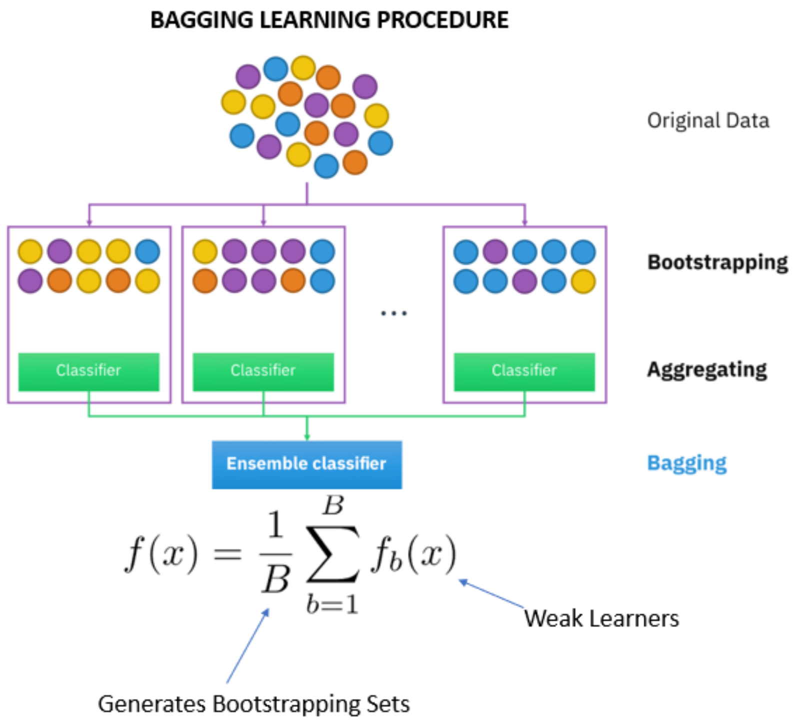
1. Bootstrap your training sample B times

2. For each sample b, build a full-grown tree (no pruning).

3. Predict your outcomes!

   a) Regression: Average the outcomes

   b) Classification: Majority vote



Source: Singhal (2020)

But... how does this reduce variance?

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

- If $Var(\hat{f}^{b}(x)) = \sigma^2 \ \ \forall\, b$, then:

$$Var(\hat{f}_{bag}(x)) = Var(\frac{1}{B}\sum_{b=1}^{B}\hat{f}^{b}(x)) = \frac{B}{B^2}\sigma^2 = \frac{\sigma^2}{B}$$

How do we do this in R?

```
set.seed(100)

bt <- train(Sales ~ ., data = carseats.train,
            method = "treebag",
            trControl = trainControl("cv", number = 10),
            nbagg = 100,
            control = rpart.control(cp = 0))
```

How do we do this in R?

```r
set.seed(100)

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            nbagg = 100,
            control = rpart.control(cp = 0))
```

How does it compare to the best single decision tree?

Let's see!

Best DT vs Bagging

- RMSE for single decision tree:

```
rmse(mcv, carseats.test)
```

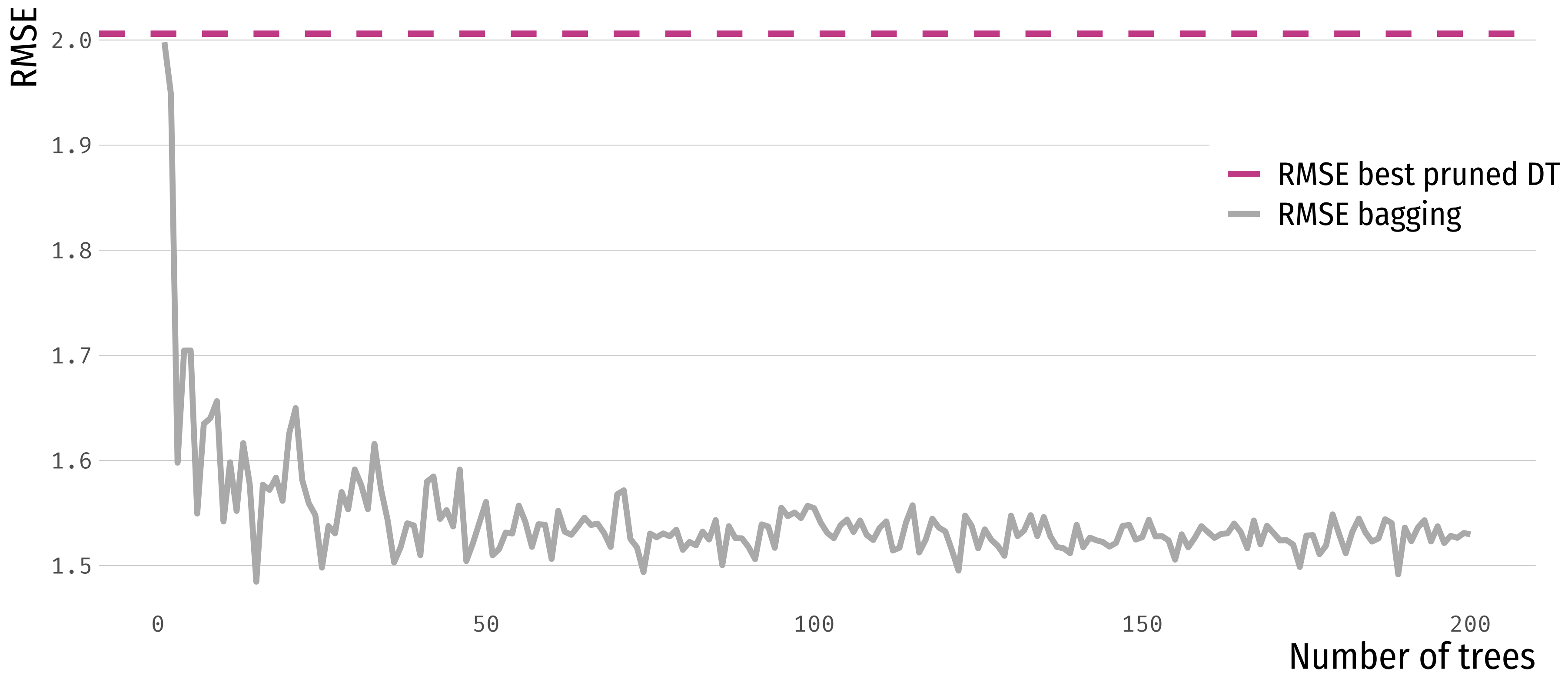
```
## [1] 2.025994
```

- RMSE for bagged trees (100):

```
rmse(bt, carseats.test)
```

```
## [1] 1.523912
```

Best DT vs Bagging



Interpretability?

```r
set.seed(100)

bt <- train(Sales ~ ., data = carseats.train, method = "treebag",
            trControl = trainControl("cv", number = 10),
            nbagg = 100, control = rpart.control(cp = 0))

plot(varImp(bt, scale = TRUE))
```

We can do better...

Random forests

Bringing trees together

- Random Forests uses both the concepts of decision trees and bagging, but also de-correlates the trees.

Bootstrap: Vary n dimension (rows/obs)

De-correlation: Vary p dimension (number of predictors)

- For each bagged tree, choose m out of p regressors.

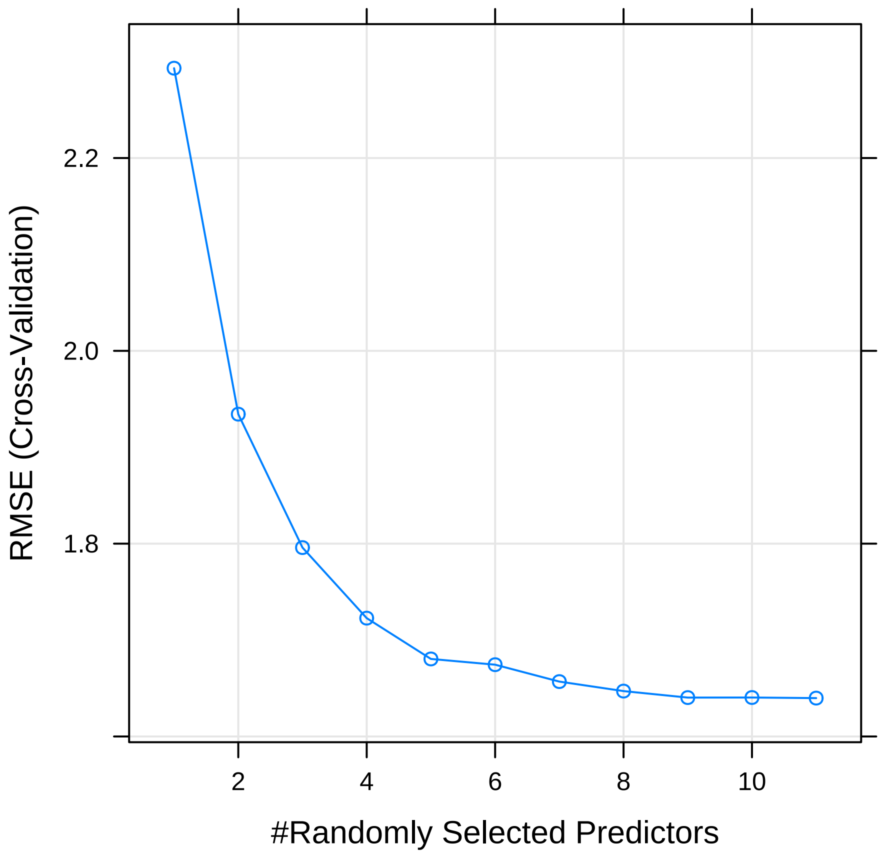
Basic algorithm

```
1.  Given a training data set
2.  Select number of trees to build (n_trees)
3.  for i = 1 to n_trees do
4.  |  Generate a bootstrap sample of the original data
5.  |  Grow a regression/classification tree to the bootstrapped data
6.  |  for each split do
7.  |  | Select m_try variables at random from all p variables
8.  |  | Pick the best variable/split-point among the m_try
9.  |  | Split the node into two child nodes
10. |  end
11. | Use typical tree model stopping criteria to determine when a
    | tree is complete (but do not prune)
12. end
13. Output ensemble of trees
```

Source: Boehmke & Greenwell (2020)

Back to our example!

```
set.seed(100)

tuneGrid <- expand.grid(
  mtry = seq(1:11),
  splitrule = "variance",
  min.node.size = 5
)

rfcv <- train(Sales ~ ., data = carseats.train
             method = "ranger",
             trControl = trainControl("cv", nu
             importance = "permutation",
             tuneGrid = tuneGrid)

plot(rfcv)
```

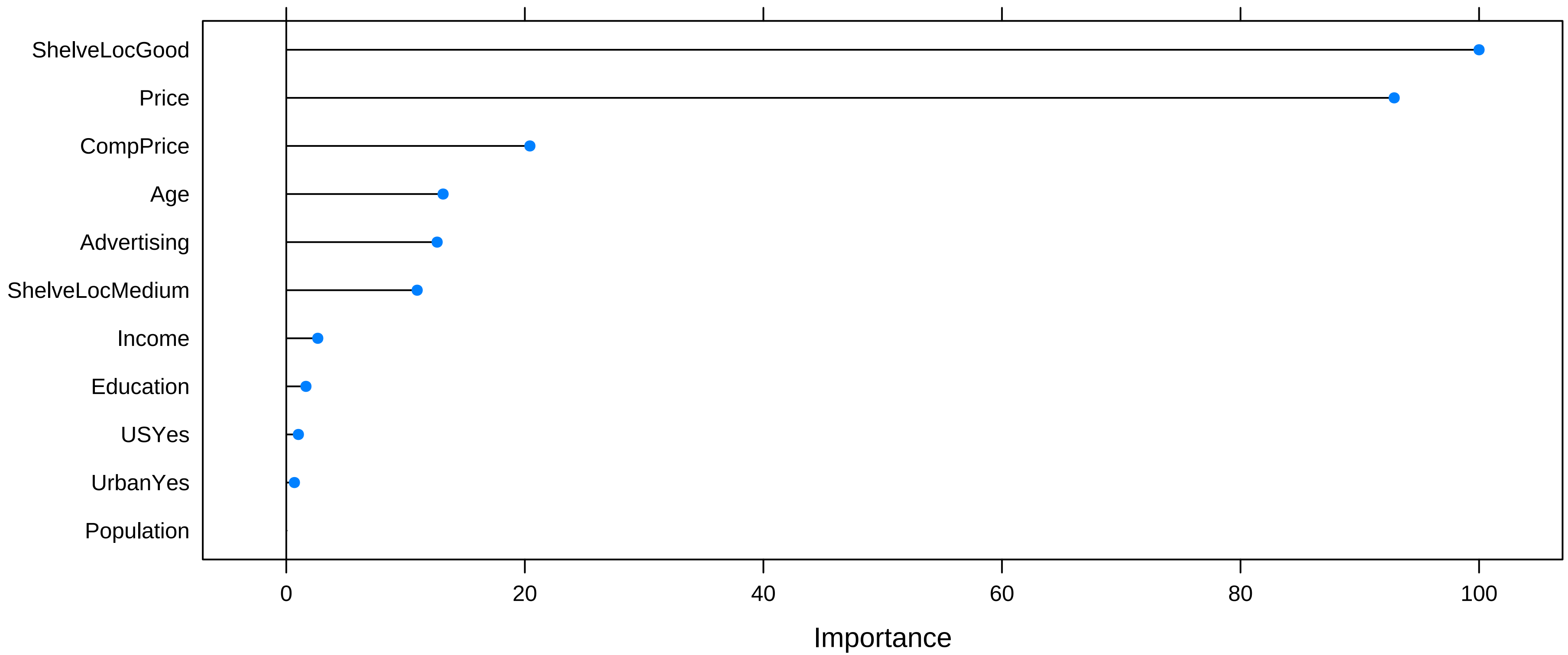


Back to our example! (Runs faster: 30s vs 11s)

```
library(doParallel)
cl <- makePSOCKcluster(7)
registerDoParallel(cl)

set.seed(100)

rfcv_fast <- train(Sales ~ ., data = carseats.train,
                   method = "ranger",
                   trControl = trainControl("cv", number = 10,
                                            allowParallel = TRUE),
                   tuneGrid = tuneGrid)

stopCluster(cl)
registerDoSEQ()
```

Covariance importance?

```
plot(varImp(rfcv, scale = TRUE))
```



Q4) In a Random Forest, a higher number of trees will yield an... underfitted model? overfitted model? doesn't affect?

Let's compare our models:

```r
# Pruned tree
rmse(mcv, carseats.test)
```

```
## [1] 2.025994
```

```r
# Bagged trees
rmse(bt, carseats.test)
```

```
## [1] 1.523912
```

```r
# Random Forest
rmse(rfcv, carseats.test)
```

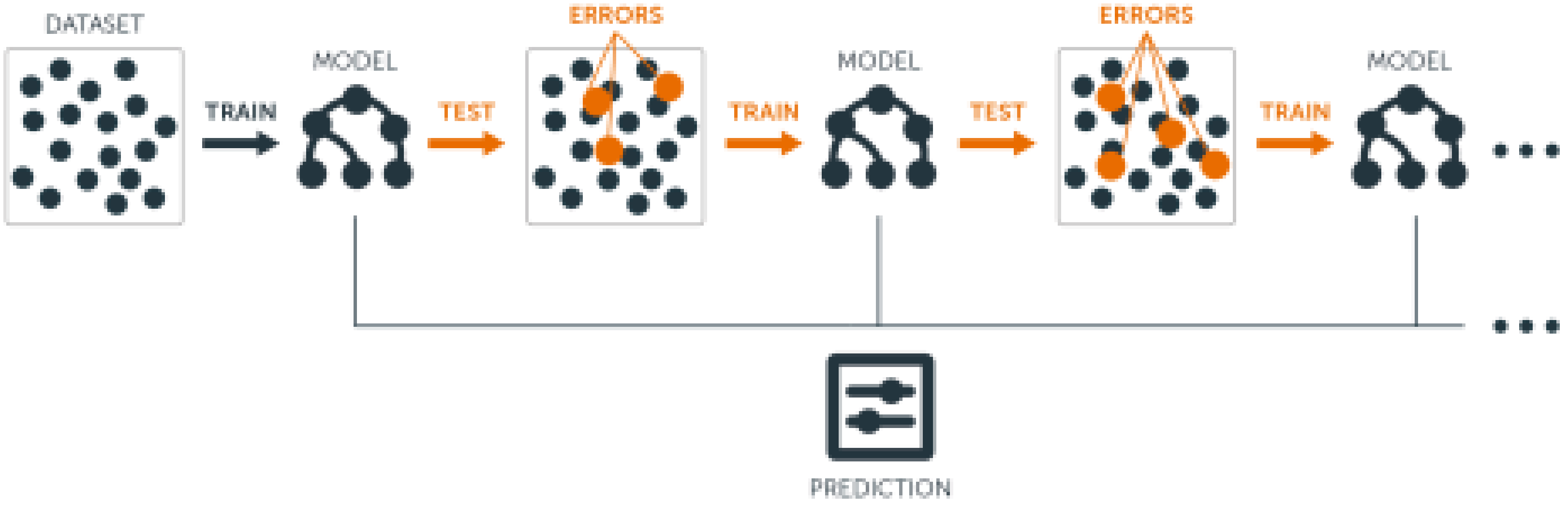
```
## [1] 1.476309
```

Can we do better than this?

Boosting!

What is boosting?

- Similar to bagging, but now trees grow sequentially.
- Slowly learning!
- More effective on models with high bias and low variance



Tuning parameters for boosting

- Number of trees: We need to select the B number of trees we will fit. We can get this through cross-validation.
- Shrinkage parameter: λ determines how fast the boosting will learn. Typical numbers range are 0.001 to 0.01. If your algorithm is learning too slow (low λ), you're going to need a lot of trees!
- Number of splits: Number of splits d controls the complexity of your trees. We usually work with low-complexity trees (d=1)

Q5) A tree with just a root and two leaves is called a stomp. Are these high or low-bias trees?

Boosting in R

- We have seen **gradient boosting** so far.
- There are other types of boosting, like **adaptive boosting** (you saw it in the video!)
  - For classification problems

```
modelLookup("ada")
```

```
##   model parameter          label forReg forClass probModel
## 1   ada      iter         #Trees  FALSE     TRUE      TRUE
## 2   ada  maxdepth Max Tree Depth  FALSE     TRUE      TRUE
## 3   ada        nu  Learning Rate  FALSE     TRUE      TRUE
```

```
modelLookup("gbm")
```

```
##   model         parameter                   label forReg forClass probModel
## 1   gbm           n.trees   # Boosting Iterations   TRUE     TRUE      TRUE
## 2   gbm interaction.depth          Max Tree Depth   TRUE     TRUE      TRUE
## 3   gbm         shrinkage               Shrinkage   TRUE     TRUE      TRUE
## 4   gbm    n.minobsinnode Min. Terminal Node Size   TRUE     TRUE      TRUE
```

Gradient Boosting in R

```r
set.seed(100)

gbm <- train(Sales ~ ., data = carseats.train,
             method = "gbm",
             trControl = trainControl("cv", number = 10),
             tuneLength = 20)
```

Gradient Boosting in R

```r
# Final Model information
gbm$finalModel
```

```
## A gradient boosted model with gaussian loss function.
## 400 iterations were performed.
## There were 11 predictors of which 11 had non-zero influence.
```

```r
# Best Tuning parameters?
gbm$bestTune
```

```
##   n.trees interaction.depth shrinkage n.minobsinnode
## 8     400                 1       0.1             10
```

Let's do a comparison!

```r
# Pruned tree
rmse(mcv, carseats.test)
```

```
## [1] 2.025994
```

```r
# Bagged trees
rmse(bt, carseats.test)
```

```
## [1] 1.523912
```

```r
# Random Forest
rmse(rfcv, carseats.test)
```

```
## [1] 1.476309
```

```r
# Gradient Boosting
rmse(gbm, carseats.test)
```

```
## [1] 1.212779
```


COMEDY

Q6) What is the main objective of boosting?

Main takeaway points

- There's a lot we can do to **improve our prediction models!**
- Decision trees by itself are not great…
  - … but they are awesome for building other stuff like **random forests**.
- **Bagging** and **boosting** can be used with other learners, not only DT!

There are a lot of other methods out there and ways to combine them! (e.g. stacking)

References

- Boehmke, B. & B. Greenwell. (2020). "Hands-on Machine Learning with R"
- James, G. et al. (2021). "Introduction to Statistical Learning with Applications in R". *Springer. Chapter 8.*
- Singhal, G. (2020). "Ensemble methods in Machine Learning: Bagging vs. Boosting"