STA 235 - Bagging, Random Forests, and Boosting

Spring 2021

McCombs School of Business, UT Austin

Some reminders

Prediction Project due next Friday

Remember not to leave it for the last minute!

Some reminders (Cont.)

No highlight session this week + OH moved to Wednesday

There is going to be a review session (+ highlight) the week of May 3rd

I'll send out a Doodle to pick the best time

Some reminders (Cont.)

Review of Homework 3 tomorrow at 6.00pm

What we have seen...

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

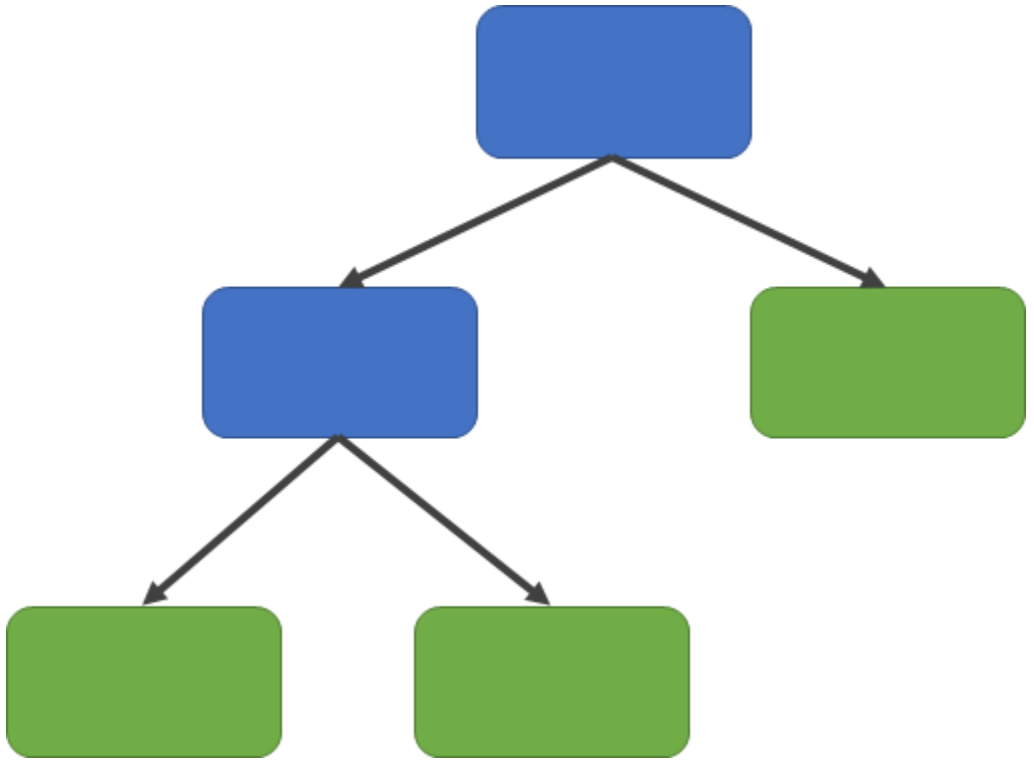
What we'll cover today

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

Quick recap on trees

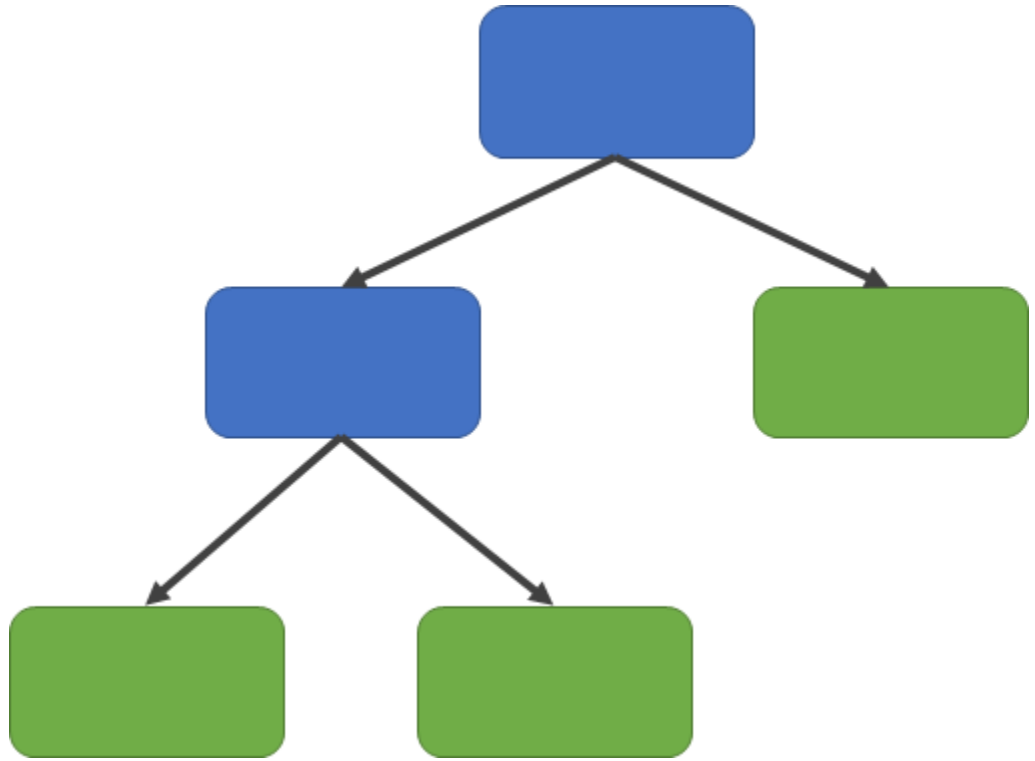
Quick refresher on decision trees

- 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 RSS.



One tree, two ways

- We mentioned in class that there are **two ways to build trees**:
    - **Recursive binary splitting**: Top-down approach, greedy algorithm.
    - **Tree pruning**: Build full-grown tree and prune it.
- The complexity parameter (in R) works in both these settings.

Poll Time!

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

Let's look at an example: Car seat prices

```
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?

```
library(caret)
library(rattle)
library(rsample)

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, 0.01, 0.0001))

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

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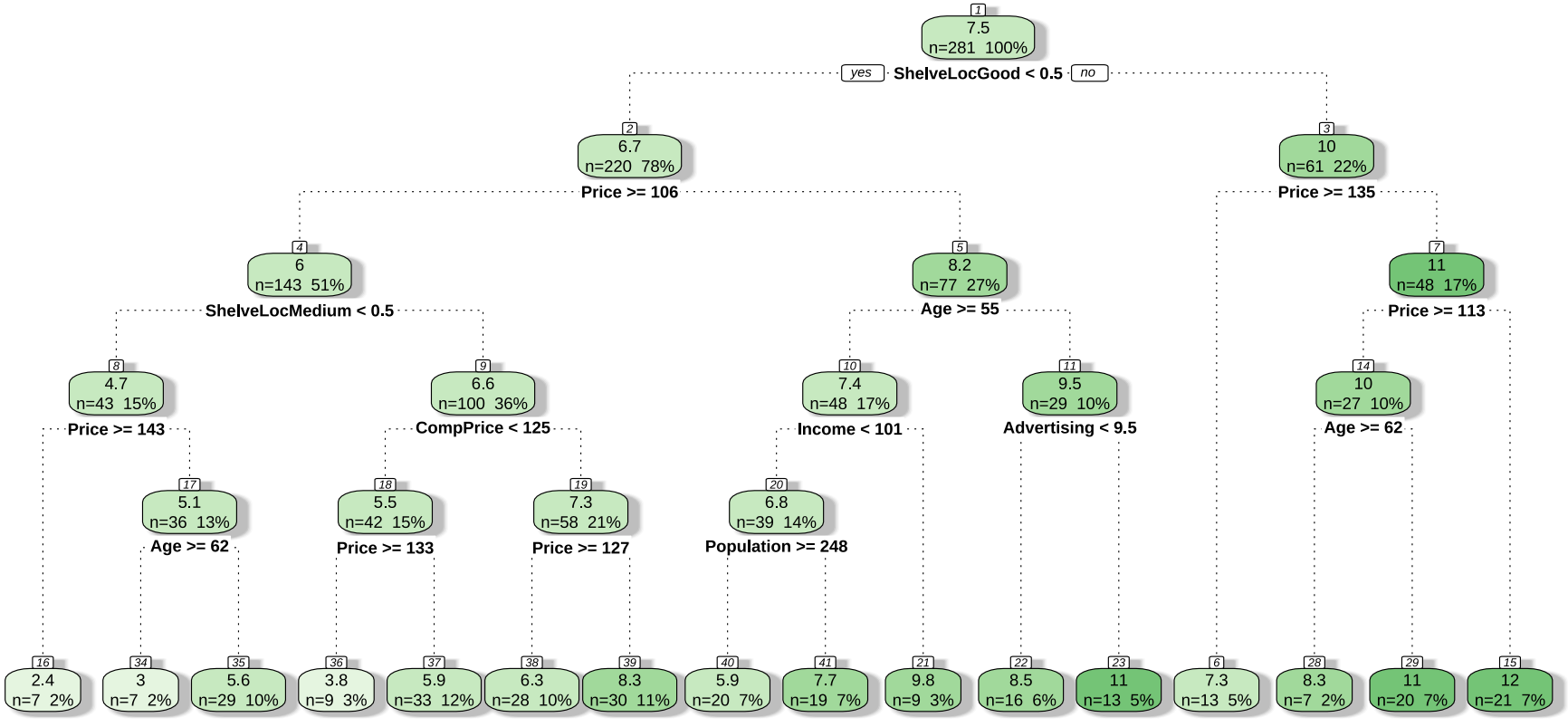
```

Do you wanna build a... tree?

```
fancyRpartPlot(mcv$finalModel, caption="")
```

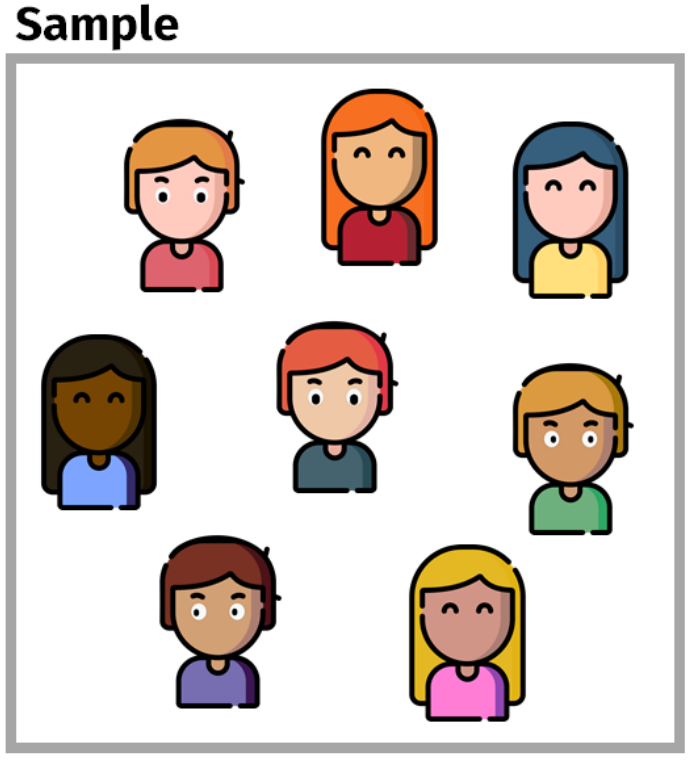


Seems a pretty complex tree... can we improve it?

Bagging

Introduction to Bagging

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



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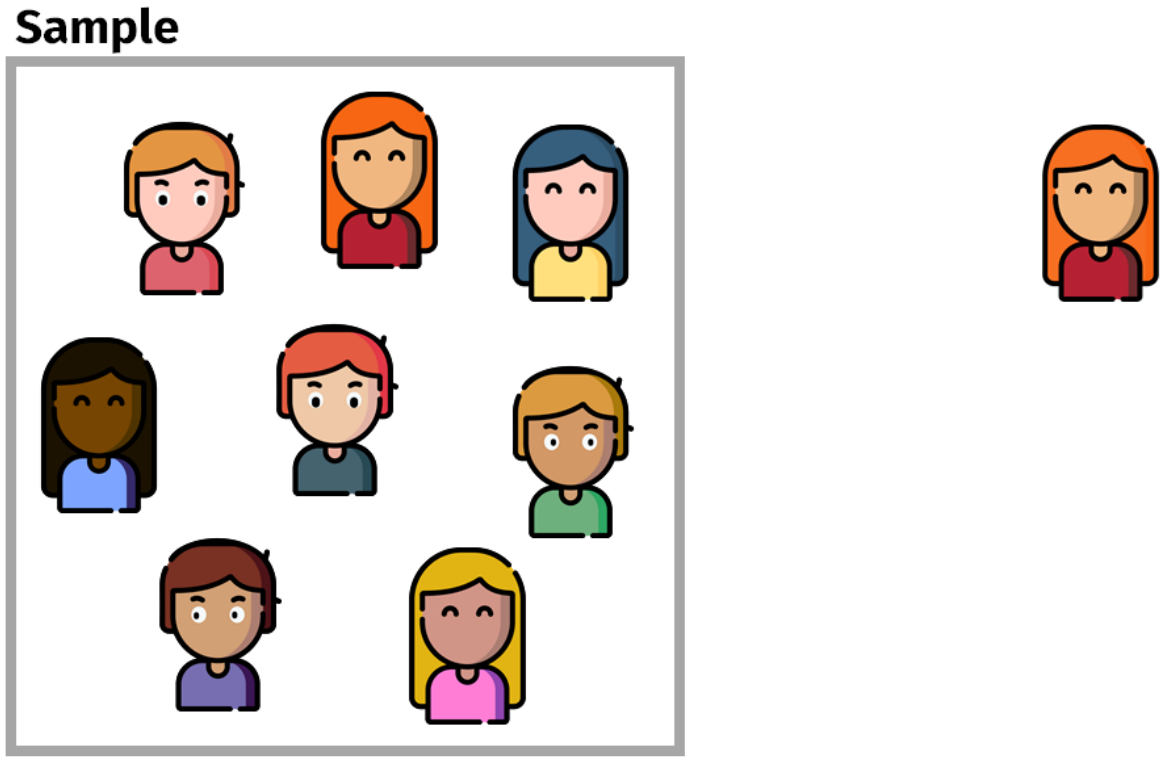

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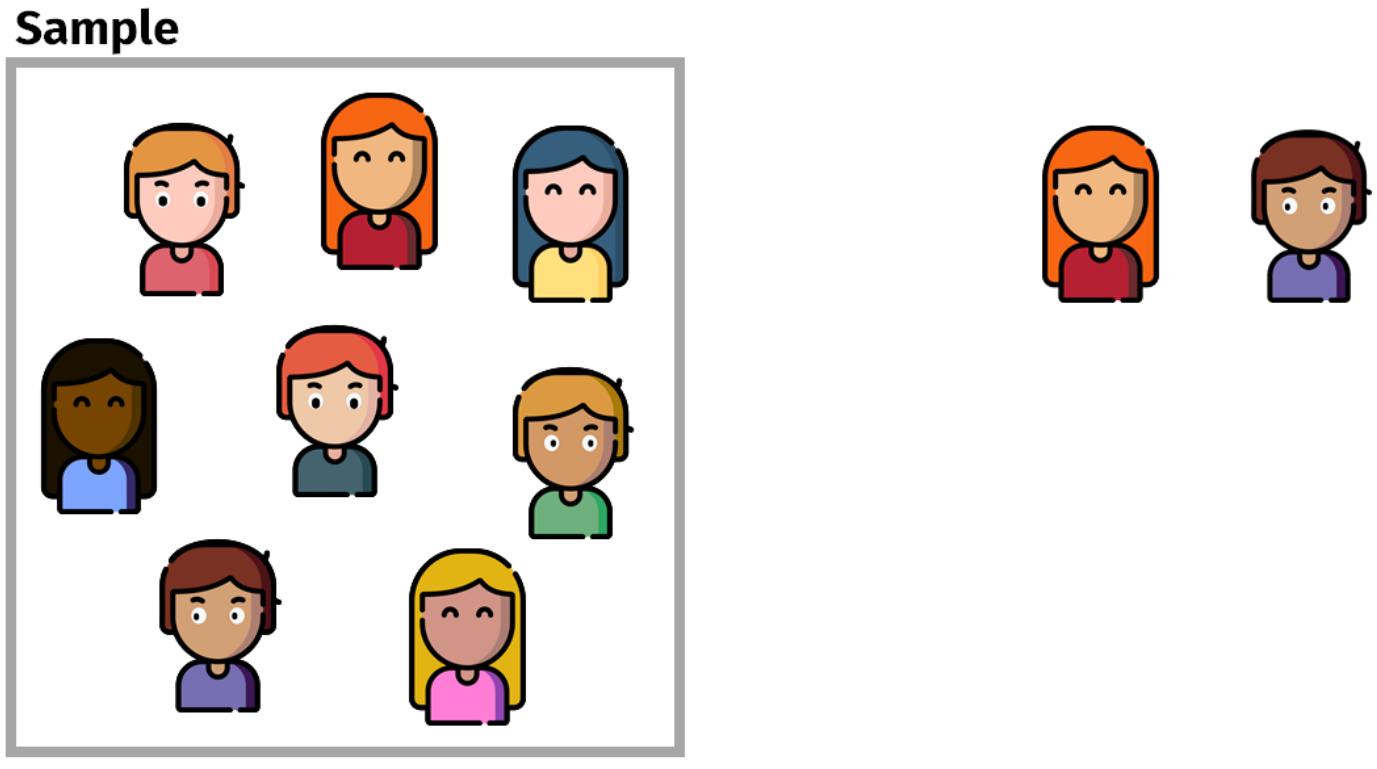

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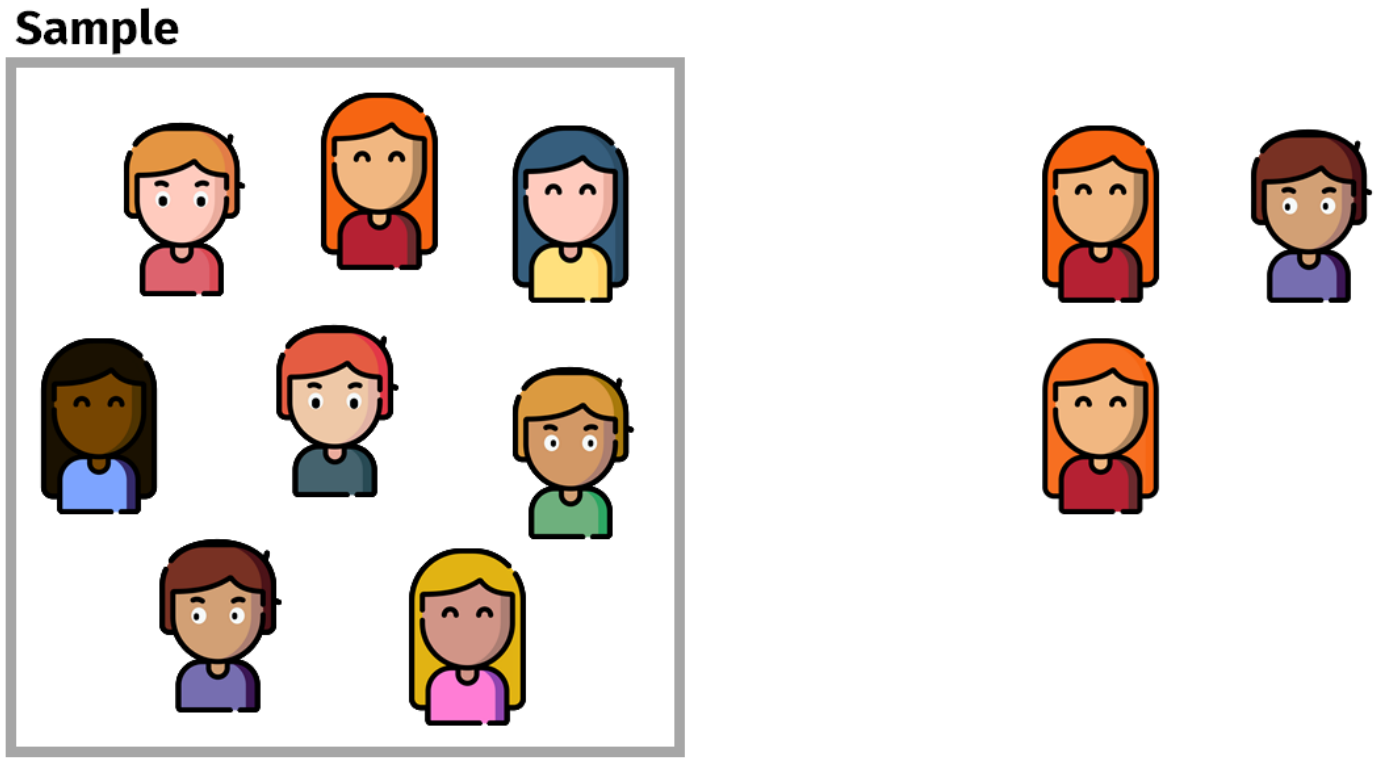

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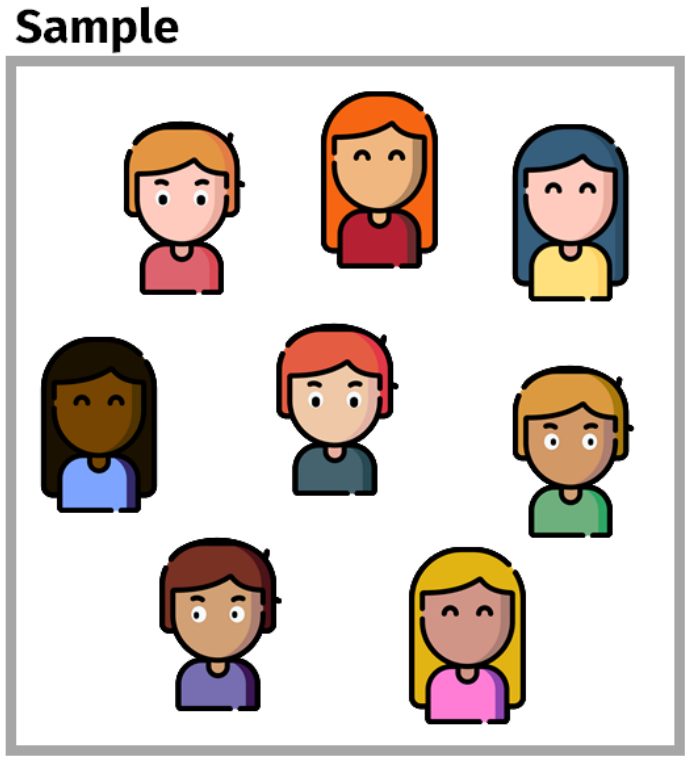
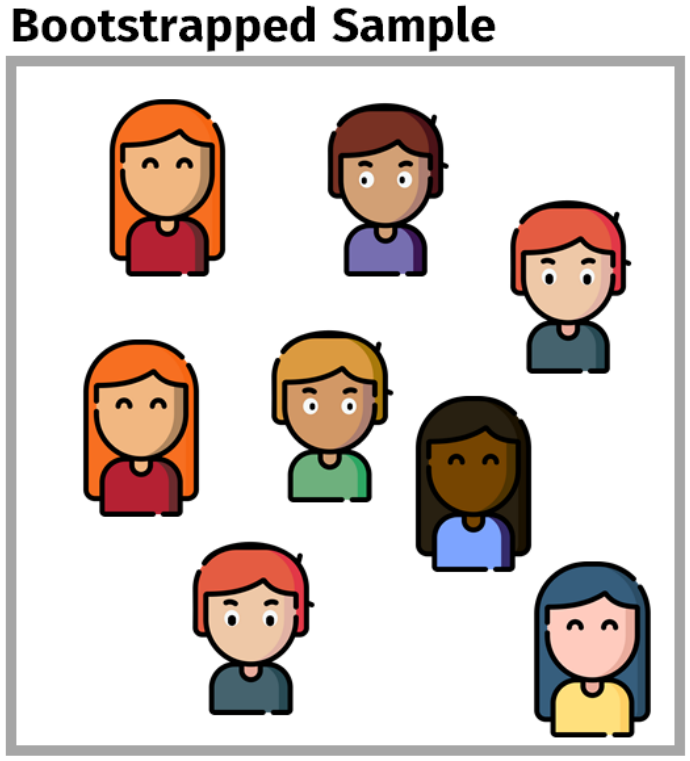


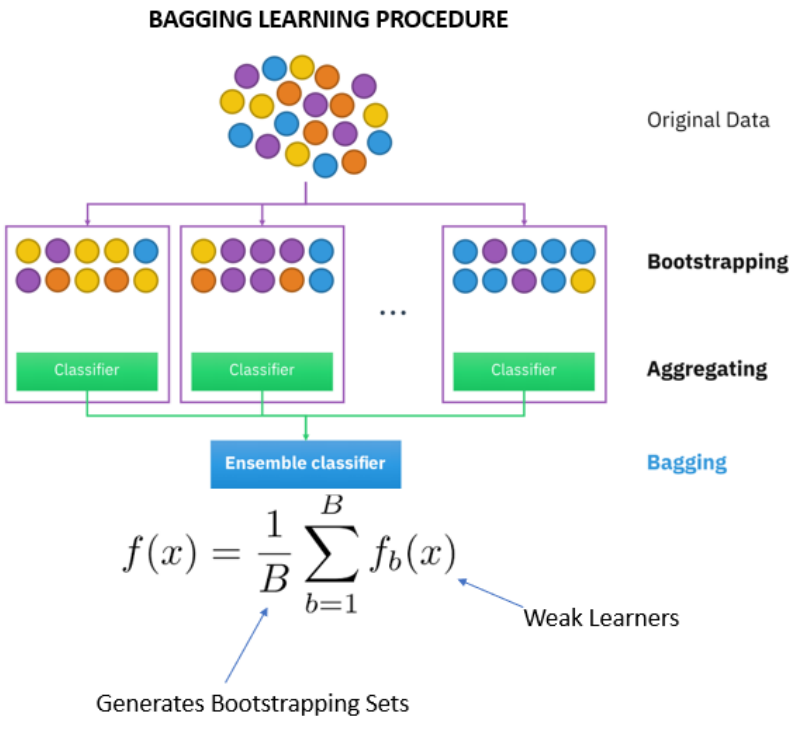


Bagging and Decision Trees

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:

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

Let's go back to our example

```
library(ipred)
library(rpart)

set.seed(100)

# train bagged model
b1 <- bagging(Sales ~ ., data = carseats.train,
              nbagg = 100,coob = TRUE,
              control = rpart.control(cp = 0))

b1
```

Let's go back to our example

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b1
```

Poll time

Why do we set cp=0?

Let's go back to our example

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set.seed(100)

# train bagged model
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              control = rpart.control(cp = 0))

b1
```

```
##
## Bagging regression trees with 100 bootstrap replications
##
## Call: bagging.data.frame(formula = Sales ~ ., data = carseats.train,
##     nbagg = 100, coob = TRUE, control = rpart.control(cp = 0))
##
## Out-of-bag estimate of root mean squared error:  1.7034
```

What is OOB RMSE?

- **OOB = Out of Bag**: It represents the RMSE for units that *were not used for building certain trees*.
- Example:
  - Bag 1 has units $\{1, 2, 2\}$, Bag 2 units $\{1, 2, 3\}$, and Bag 3 $\{2, 3, 3\}$
  - OOB RMSE would be estimating using RMSE for **unit 1 in Bag 3** and **unit 3 in Bag 1**.

No need for cross-validation!

Poll time

What is the main objective of bagging?

How does it compare to the best pruned decision tree?

Let's see!

Best DT vs Bagging

```
library(caret)

set.seed(100)

tuneGrid <- expand.grid(cp = seq(0.002, 0.004, 0.000001))

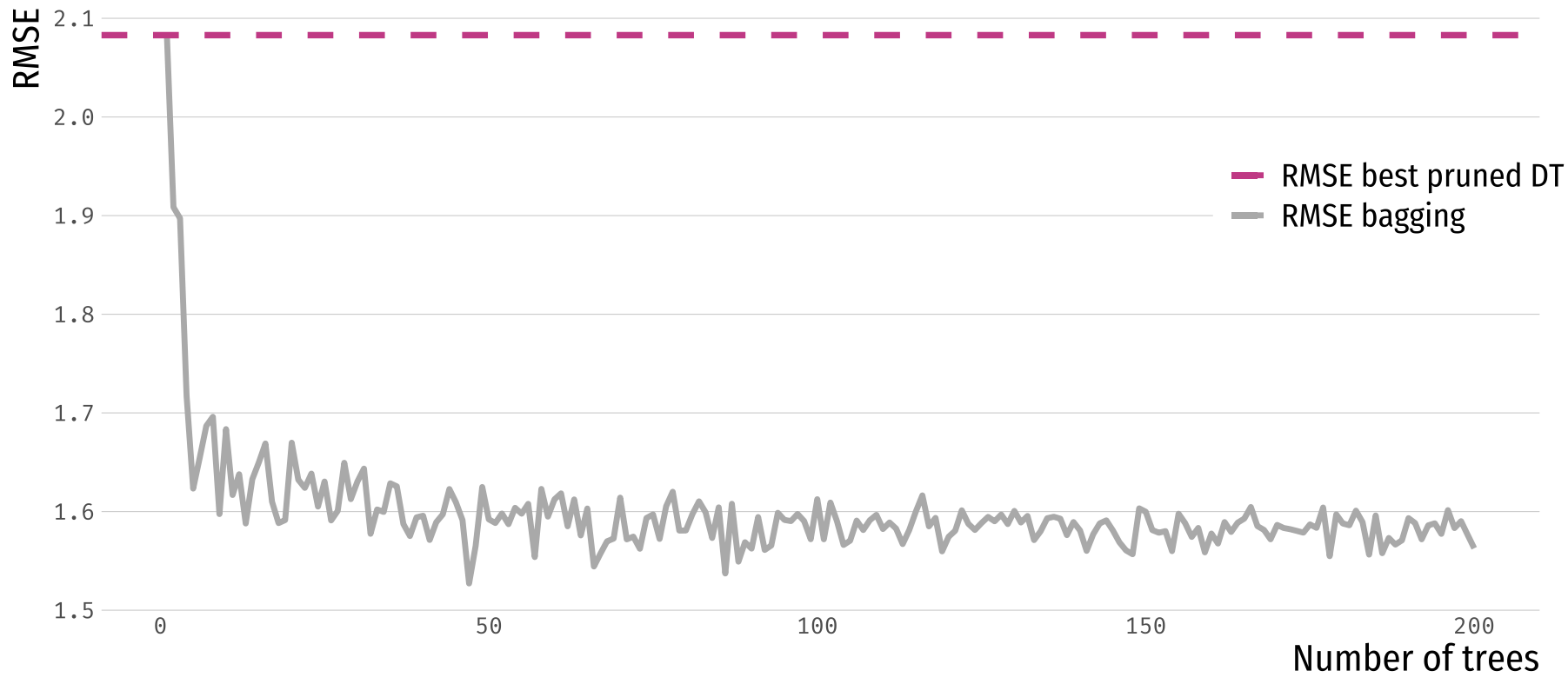
mcv <- train(Sales ~ ., data = carseats.train,
             method = "rpart", trControl = trainControl("cv", number = 10),
             tuneGrid = tuneGrid)

pred.mcv <- mcv %>% predict(carseats.test)

RMSE(pred.mcv, carseats.test$Sales)
```

```
## [1] 2.082905
```

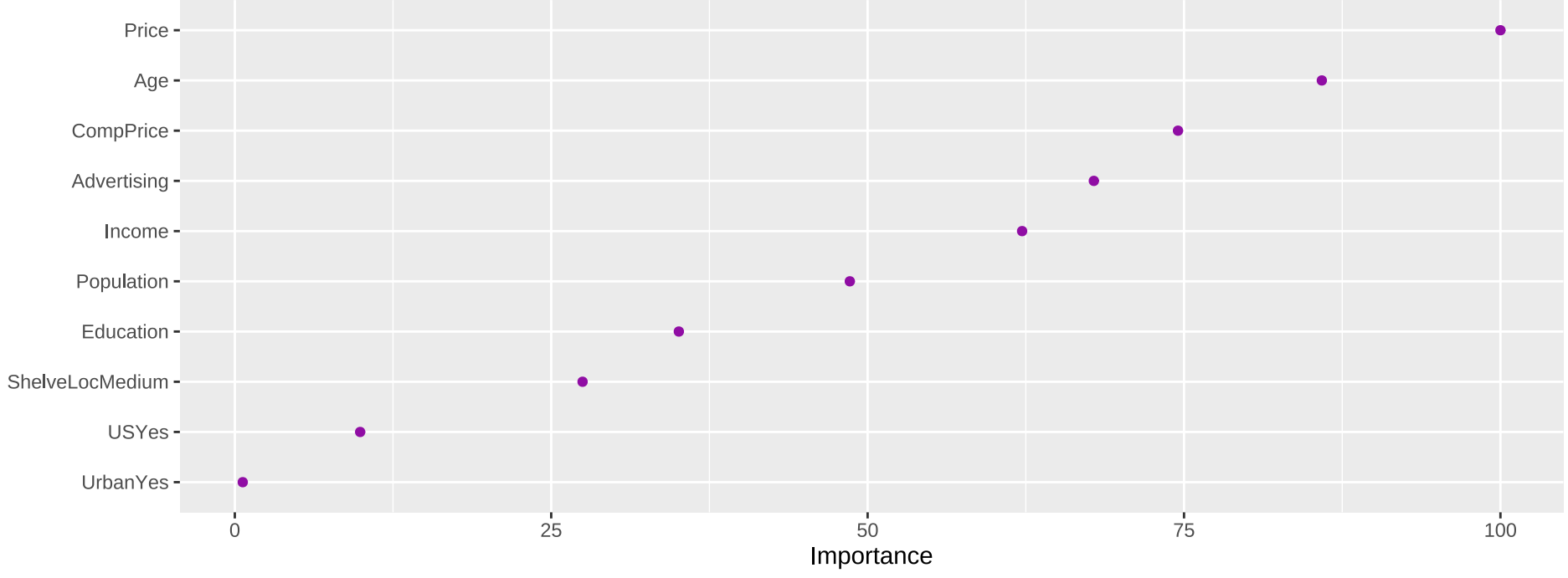
Best DT vs Bagging



Interpretability?

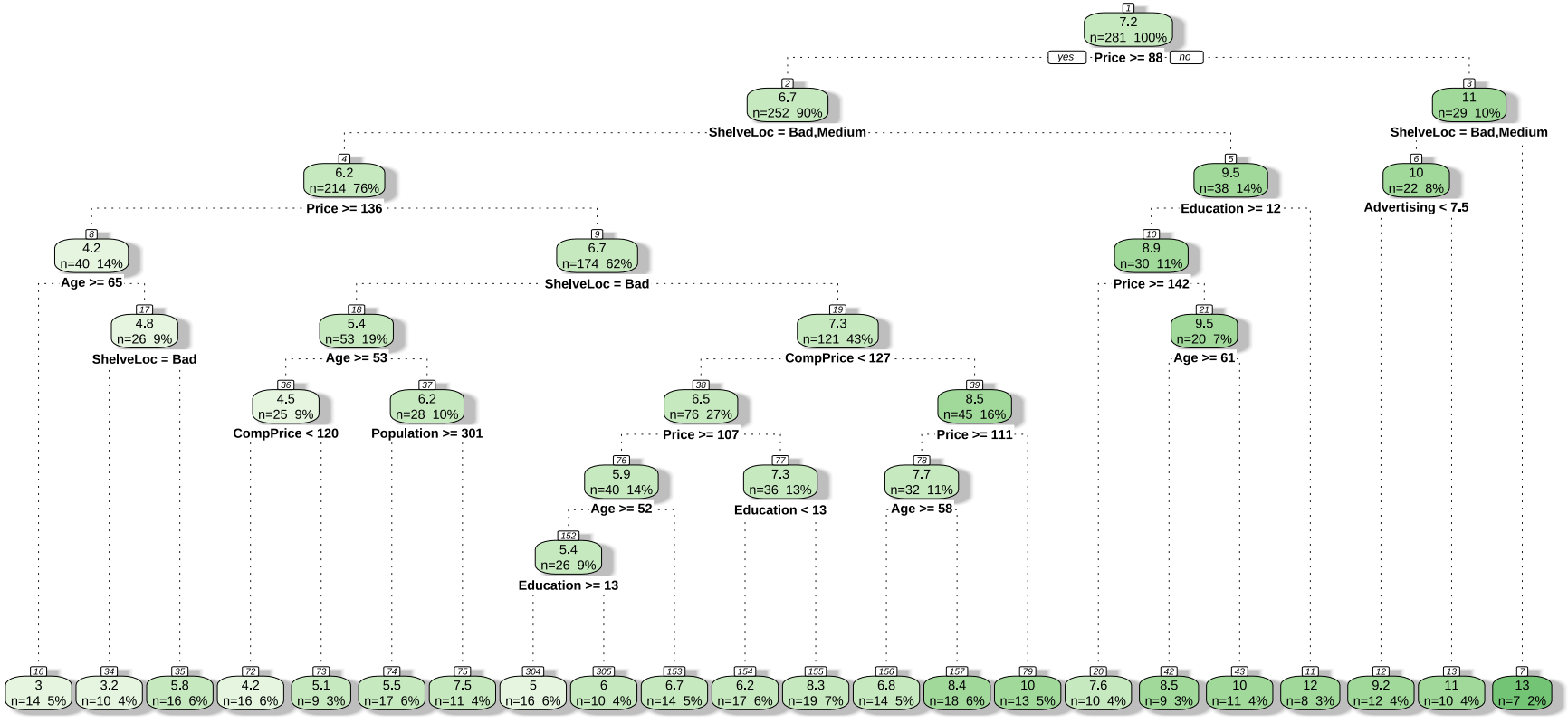
```
library(vip)
bt <- train(Sales ~ ., data = carseats.train, method = "treebag", trControl = trainControl("cv", nur
            nbagg = 100, control = rpart.control(cp = 0))

vip::vip(bt, num_features = 10, geom = "point")
```



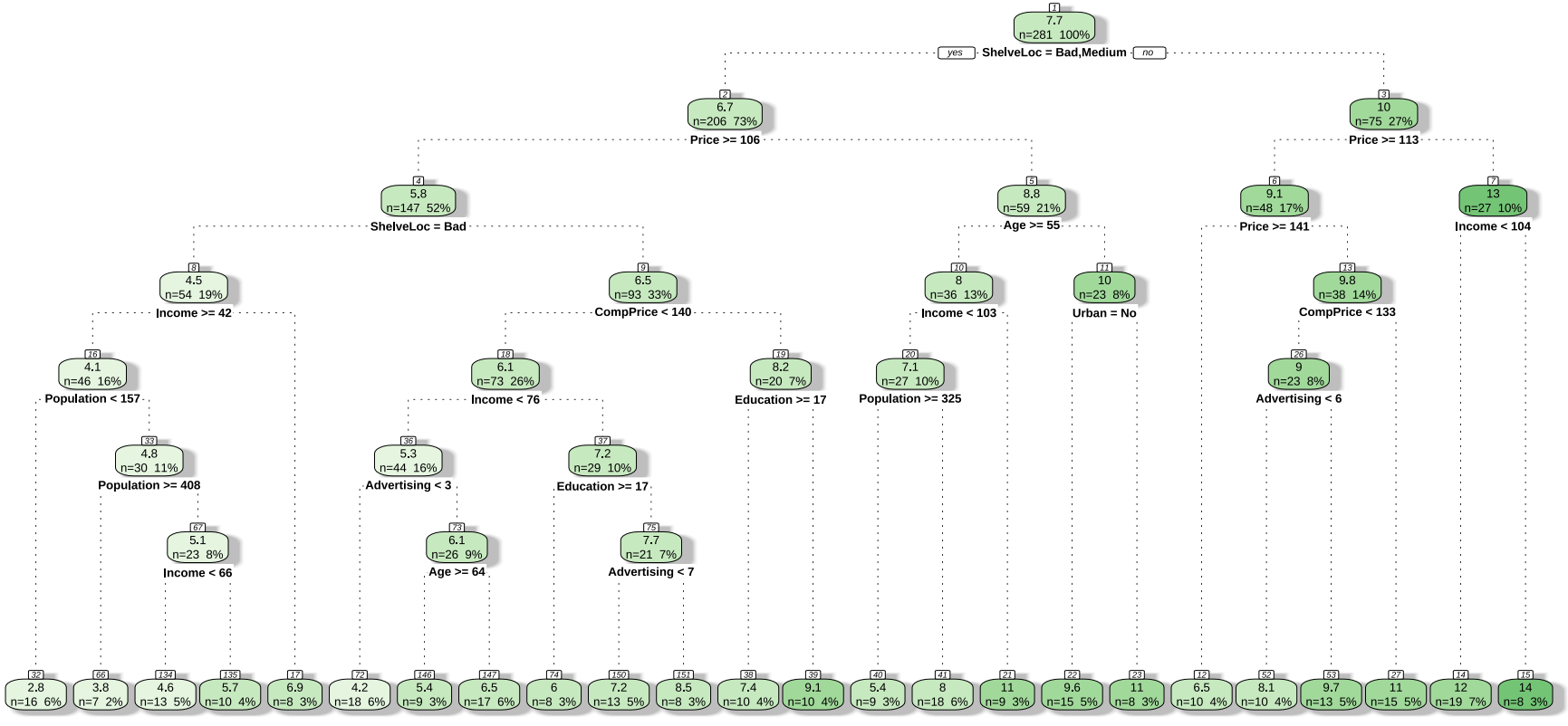
Disadvantages of bagged trees? (Tree 2)

```
fancyRpartPlot(b1$mtrees[[2]]$btree, caption="") #There are 100 trees!
```



Disadvantages of bagged trees? (Tree 3)

```
fancyRpartPlot(b1$mtrees[[3]]$btree, caption="") #There are 100 trees!
```



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

De-correlation: Vary *p* dimension

- 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
```

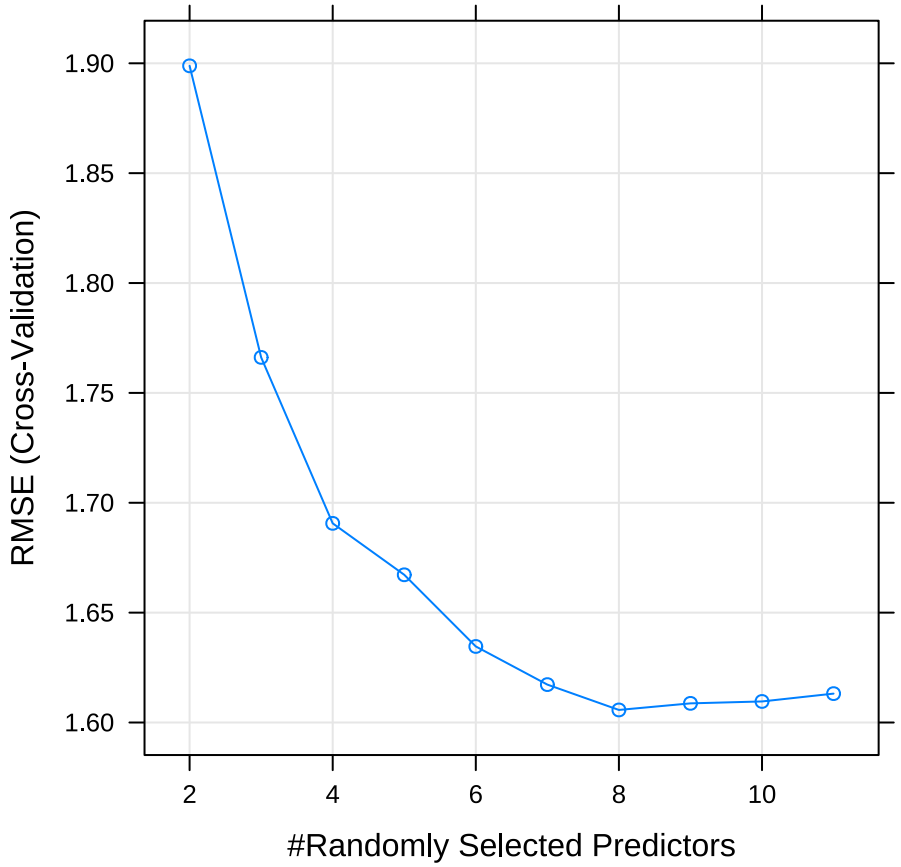
Source: Boehmke & Greenwell (2020)

Back to our example!

```
set.seed(100)

rfcv <- train(Sales ~ ., data = carseats.train
              method = "rf",
              trControl = trainControl("cv", nur
              tuneLength = 10)

plot(rfcv)
```



Our dataset has 11 variables (1 outcome + 10 predictors)... why do the predictors go from 2 to 11?

We need to look at the model.matrix

```
head(model.matrix(Sales ~ ., data = carseats.train))
```

```
##    (Intercept) CompPrice Income Advertising Population Price ShelveLocGood
## 1            1       138     73          11        276   120             0
## 2            1       111     48          16        260    83             1
## 4            1       117    100           4        466    97             0
## 5            1       141     64           3        340   128             0
## 7            1       115    105           0         45   108             0
## 11           1       121     78           9        150   100             0
##    ShelveLocMedium Age Education UrbanYes USYes
## 1                0  42        17        1     1
## 2                0  65        10        1     1
## 4                1  55        14        1     1
## 5                0  38        13        1     0
## 7                1  71        15        1     0
## 11               0  26        10        0     1
```

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

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

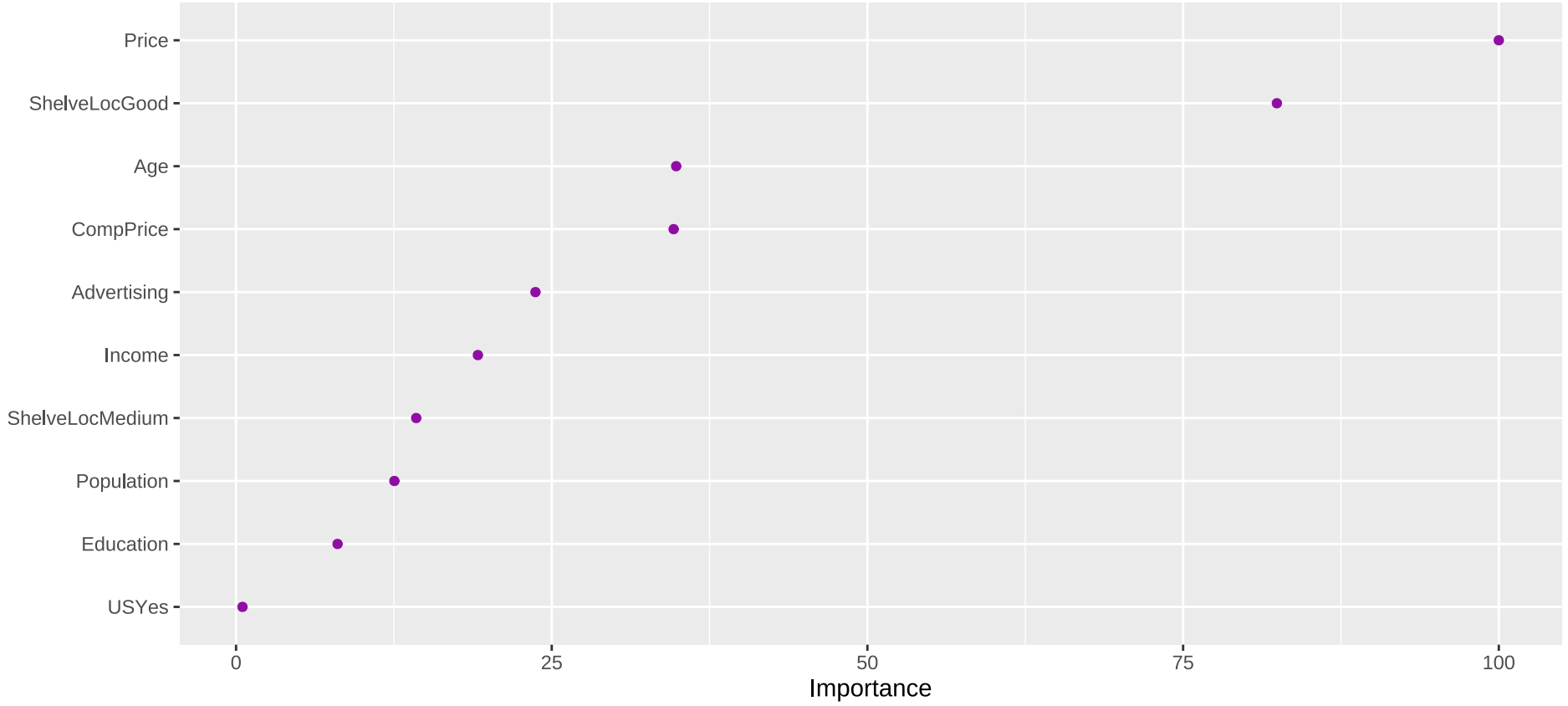
set.seed(100)

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

stopCluster(cl)
registerDoSEQ()
```

Covariance importance?

```
vip::vip(rfcv, num_features = 10, geom = "point")
```



Poll time

In a Random Forest, a higher number of trees will yield an...

Let's compare our models:

```
# Pruned tree
RMSE(mcv %>% predict(carseats.test), carseats.test$Sales)
```

```
## [1] 2.082905
```

```
# Bagged trees
RMSE(bt %>% predict(carseats.test), carseats.test$Sales)
```

```
## [1] 1.604022
```

```
# Random Forest
RMSE(rfcv %>% predict(carseats.test), carseats.test$Sales)
```

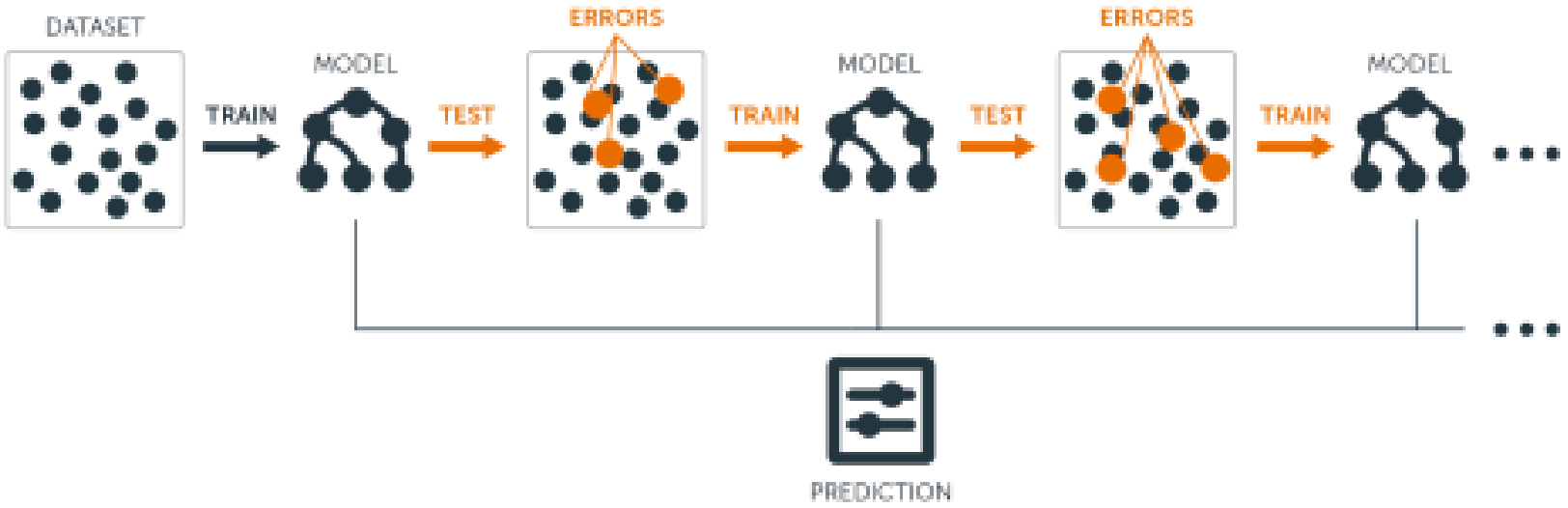
```
## [1] 1.50476
```

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**



Basic Algorithm for Gradient Boosting

```
1.  Set f=0 and r_i=y_i for all i in the training dataset
2.  Select number of trees to build (n_trees)
3.  for oosting = 1 to n_trees do
4.  |  Fit a tree f^b with d splits to the training data (X,r)
5.  |  Update f by adding a shrunken version of the new tree
6.  |  f(x) <-- f(x) + \lambda f^b(x)
7.  |  Update the residuals
8.  |  r_i <-- r_i - \lambda f^b(x_i)
9.  end
10. Output the boosted model
11. f(x) = \sum_{b=1}^B\lambda f^b(x)
```

Source: ISLR (2015)

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)

Poll time

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

Poll time

In boosting, a higher number of trees will yield an...

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

```
set.seed(100)

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

Gradient Boosting in R

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

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

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

```
##   n.trees interaction.depth shrinkage n.minobsinnode
## 7     350                 1       0.1             10
```

Let's do a comparison!

```
# Pruned tree
RMSE(mcv %>% predict(carseats.test), carseats.test$Sales)
```

```
## [1] 2.082905
```

```
# Bagged trees
RMSE(bt %>% predict(carseats.test), carseats.test$Sales)
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```
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```

```
# Random Forest
RMSE(rfcv %>% predict(carseats.test), carseats.test$Sales)
```

```
## [1] 1.50476
```

```
# Gradient Boosting
RMSE(gbm %>% predict(carseats.test), carseats.test$Sales)
```

```
## [1] 1.201098
```


COMEDY
CENTRAL

Poll time

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)

Next week

- **Text data**: Scrape and analyze different type of data.
- We will also **bring everything together**: Causal inference + prediction.
- No readings for next week, only a **small task** (*there will still be a JITT!*)

Final class!

Tips for the final project

- You can **transform variables** any way you want, or use **model selection methods**.
- You can **combine any sort of learner we have seen**.
- "Hands-On Machine learning" (on Bookmarks section).
- To test your code, **use smaller samples!**

References

- Boehmke, B. & B. Greenwell. (2020). "Hands-on Machine Learning with R"
- James, G. et al. (2013). "Introduction to Statistical Learning with Applications in R". *Springer. Chapter 8.*
- Singhal, G. (2020). "Ensemble methods in Machine Learning: Bagging vs. Boosting"