

# STA 235H - Classification and Regression Trees (CART)

Fall 2023

McCombs School of Business, UT Austin

# Announcements

- Next week will be the **last class with new material**.
- The final week of class will be for a **review session**.
  - Final Trivia!
- You need to choose a topic for **Homework 6**
  - Remember that this homework cannot be dropped.
  - All tasks have the same difficulty.
  - You will only be competing with people that choose your same dataset.

# Where we've been...

- Talking about **bias vs variance** trade-off.
- **Linear models, model selection and regularization:**
  - Linear regressions.
  - Stepwise selection.
  - Ridge and Lasso regression.



# ... and where we're going.



- Continue on our **prediction** journey:
  - **Decision Trees**: Classification and Regression Trees (CART)
  - **Activity in R**: Remember to try to complete it before the end of the class!

# Before we start... knowledge check!

- Ridge and lasso regression **add bias to a linear model to reduce variance**:
  - Remember that when we fit a ridge or lasso regression, we use all the predictors we have in our data!
- $\lambda$  represents the **ridge/lasso penalty**: The larger the  $\lambda$  the smaller the (sum of) coefficients, e.g.  $\sum_k \beta_k^2$  or  $\sum_k |\beta_k|$ .
  - We "mute" or decrease the relation between predictors and outcome.

**Q1: What is the main difference (in terms of the final model) between Ridge and Lasso regression?**

Trees, trees everywhere!

**From the videos/readings, how would you explain to someone what a decision tree is?**

# Idea behind Decision Trees

- Create a **flow chart** for making decisions
  - *How do we classify an individual or what value do we assign to an observation?*
- ... But there are **many** decisions!
  - How many variables do we use?
  - How do we sort them? In what order do we place them?
  - How do we split them?
  - How deep do we go?

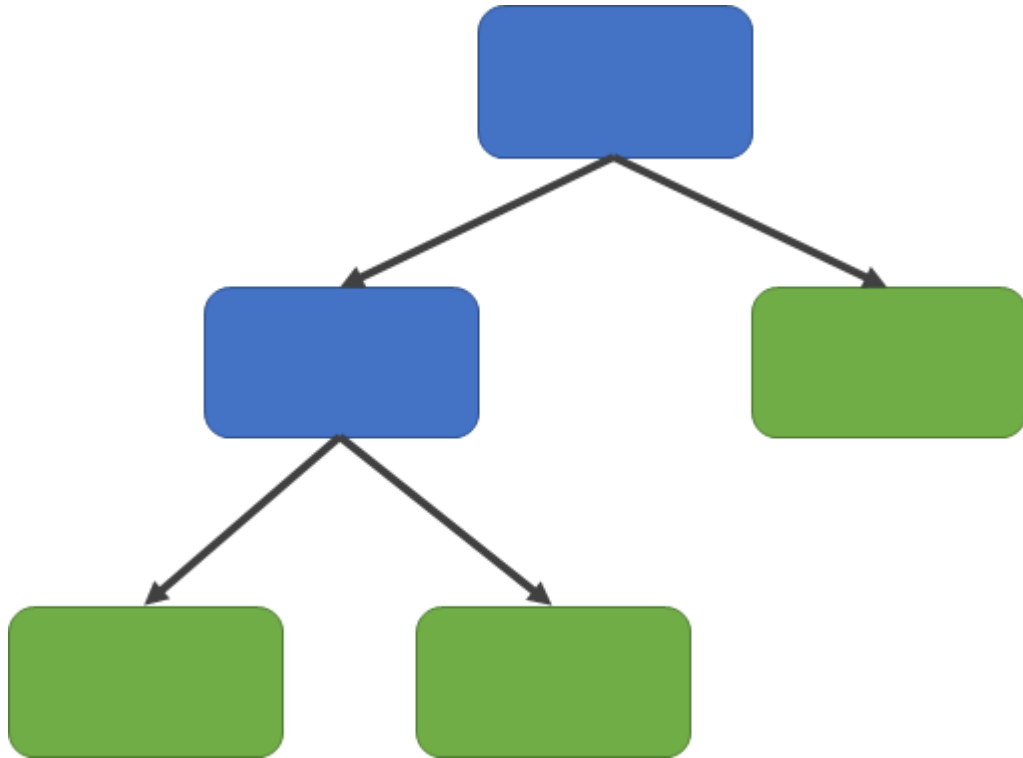


**Q2: What is the main disadvantage of a shallower tree (compared to a deeper tree)?**

**a) Higher variance**

**b) Higher bias**

# Structure of Decision Trees



## Structure:

- Root node
- Internal nodes
- Leaves

# Why do we like/not like Decision Trees?

## Main advantages

Simple interpretation

Mirror human decision-making

Graphic displays!

Handle categorical variables

## Main disadvantages

Overfitting

Not very accurate/not very robust

# Let's start with a simple example

Remember our Hbo Max example?

Predict who will cancel their subscription

We have some **information**:

- `city`: Whether the customer lives in a big city or not
- `female`: Whether the customer is female or not
- `age`: Customer's age (in years)
- `logins`: Number of logins to the platform in the past week.
- `succession`: Whether the person has watched the Succession or not.
- `unsubscribe`: Whether they canceled their subscription or not.

# The prediction task: Classification

- Our outcome is **binary**, so this is a **classification task**.
- Let's start looking at **two variables**:

## City & Succession

- Which one do you think should be at the top of the tree?

# How do we decide?

- **Recursive Binary Splitting:**
  - Divide regions of covariates in two (recursively).
  - This works both for continuous and categorical/binary variables
- We test out every covariate and see **which one reduces the error the most** in our predictions
  - In **regression tasks**, we can use RMSE.
  - In **classification tasks**, we can use accuracy/classification error rate, Gini Index, or entropy

$$G = \sum_{k=0}^1 \hat{p}_{mk}(1 - \hat{p}_{mk})$$

where  $\hat{p}_{mk}$  is the proportion of obs. in the  $m$  region for class  $k$ .

# How do we decide?

In our HBO Max example:

- $k$  represents the **different values that the outcome** can take (e.g.  $Unsubscribe \in \{0, 1\}$ ), and
- $m$  represents the **values that the predictor takes** (e.g.  $Succession = 0$ ).

E.g.:

- $p_{mk} = p_{00}$ : The proportion of people who are subscribed (Unsubscribed = 0) and that have not watched *Succession* (Succession = 0)
- $p_{mk} = p_{01}$ : The proportion of people who are unsubscribed (Unsubscribed = 1) and that have not watched *Succession* (Succession = 0)
- Usually, you want the Gini index to be **small**!

**Q3: According to the Gini Index, is it better or worse to have a high  $p_{mk}$  (i.e. closer to 1)?**

$$G = \sum_k^K \hat{p}_{mk}(1 - \hat{p}_{mk})$$



# Choosing predictors

- From the previous exercise, we can see that **using succession yields a lower Gini compared to city** (0.428 vs. 0.482)

**But we have more variables**

**How do we choose?**

# Basic Algorithm

1) Start at the root node

2) Split the parent node at covariate  $x_i$  to minimize the sum of child node impurities

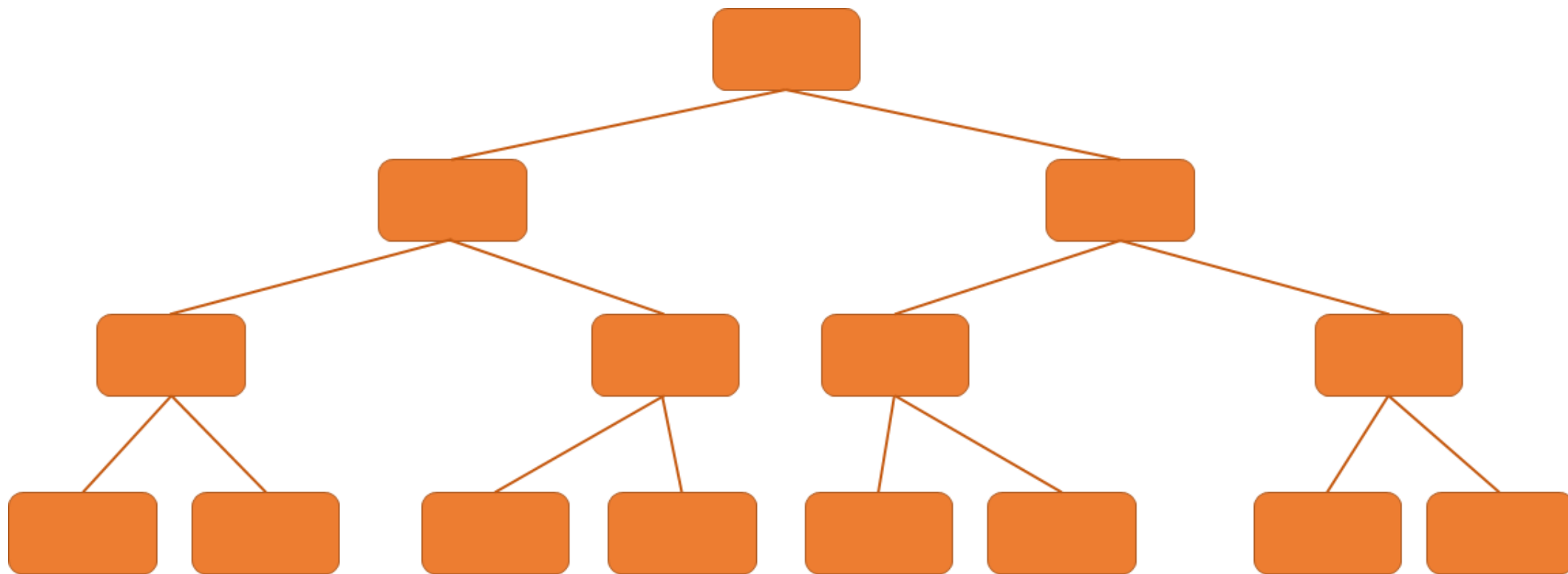
3) Stop if leaves are pure or early stopping criteria is satisfied, else repeat step (1) and (2) for each new child nodes

4) Prune your tree according to a complexity parameter (cp)

5) Assign the average outcome (regression) or the majority (classification) in each leaf.

Adapted from "Machine Learning FAQs" (Raschka, 2021)

# Grow full tree and prune it



# Hyper-parameter: Complexity parameter

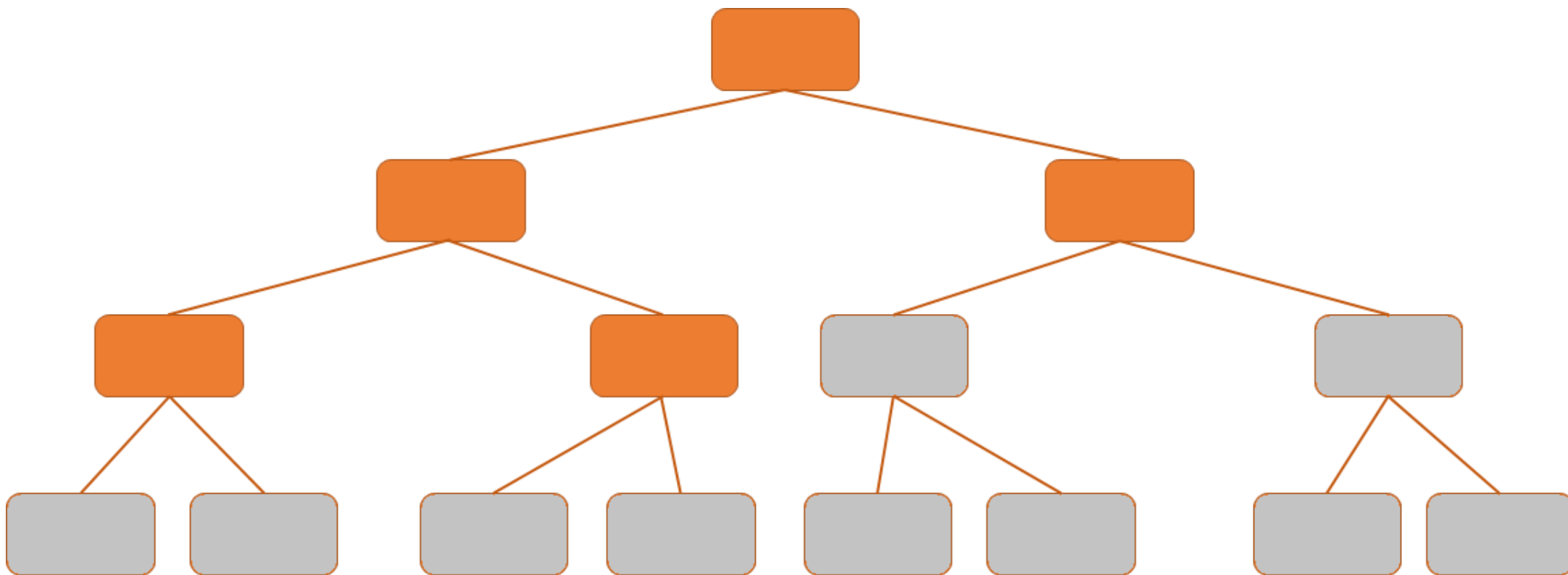
- Measure of how much a split should **improve prediction** for it to be worth it.

$$\sum_{m=1}^{|T|} \sum_{i:i \in R_m} (y_i - \hat{y}_i)^2 + \alpha |T|$$

- $|T|$ : Number of terminal nodes or leaves (e.g. size of the tree)
- $R_m$ : Predictor space of the  $m$ th leaf
- $\alpha$ : Tuning parameter

What happens if  $\alpha = 0$ ?

# Only attempt a split if it's worth it



# Let's see how to do it in R!

```
library(caret)
```

```
set.seed(100)
```

```
ct = train(  
  factor(unsubscribe) ~ . - id, data = hbo.train, #remember your outcome needs to be a factor!  
  method = "rpart", # The method is called rpart  
  trControl = trainControl("cv", number = 10),  
  tuneLength = 15  
)
```

# Let's see how to do it in R!

```
library(caret)

set.seed(100)

ct = train(
  factor(unsubscribe) ~ . - id, data = hbo.train, #remember your outcome needs to be a factor!
  method = "rpart",
  trControl = trainControl("cv", number = 10),
  tuneLength = 15
)
```

# Let's see how to do it in R!

```
library(caret)

set.seed(100)

ct = train(
  factor(unsubscribe) ~ . - id, data = hbo.train, #remember your outcome needs to be a factor!
  method = "rpart",
  trControl = trainControl("cv", number = 10),
  tuneLength = 15
)
```

- tuneLength is useful when you don't want to pass a specific grid (usually it might not be enough though!)



# We could also provide a grid of complexity parameters

```
library(rpart)

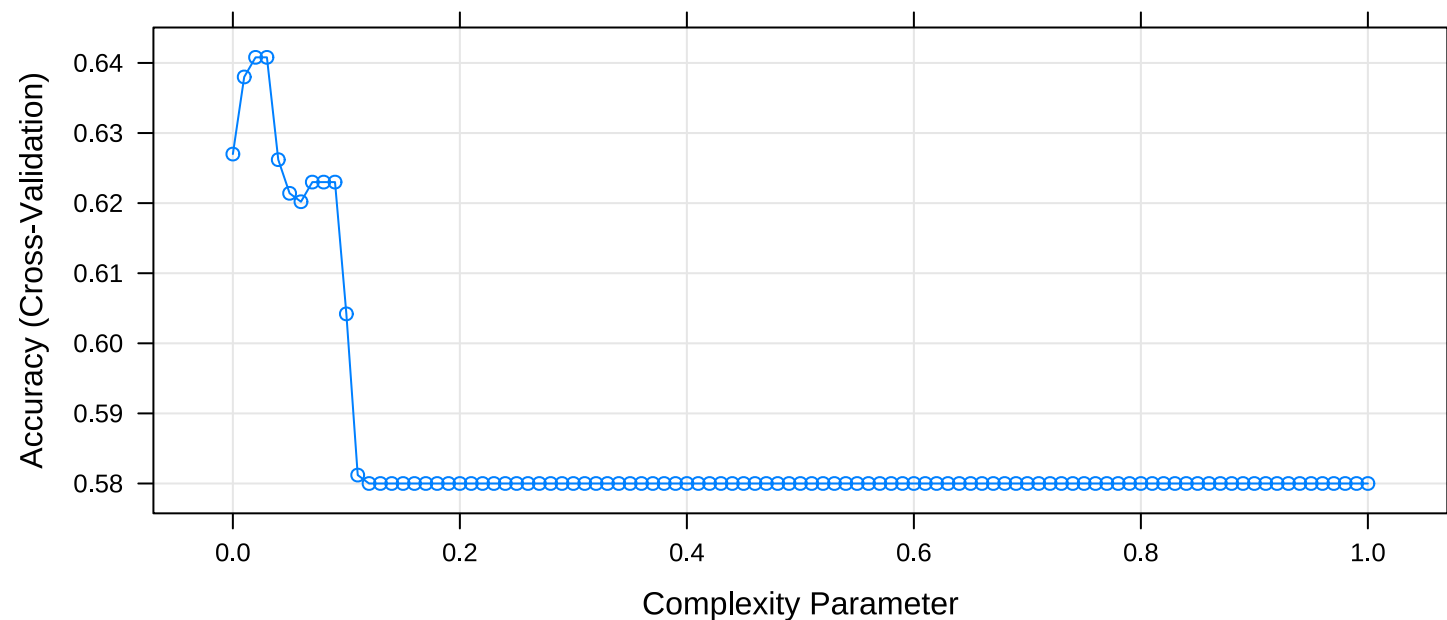
set.seed(100)

ct = train(
  factor(unsubscribe) ~ . - id, data = hbo.train,
  method = "rpart",
  trControl = trainControl("cv", number = 10),
  tuneGrid = expand.grid(cp = seq(0,1, by = 0.01)),
  control = rpart.control(minsplit = 20)
)
```

- cp: Complexity parameter
  - Split must decrease the overall lack of fit by a factor of cp, or is not attempted.
  - Parameter for **pruning the tree**.
  - Higher cp, smaller the tree!
- minsplit: Min. number of obs in a node to attempt a split.

# This works similarly to the penalty term in regularization...

```
plot(ct)
```

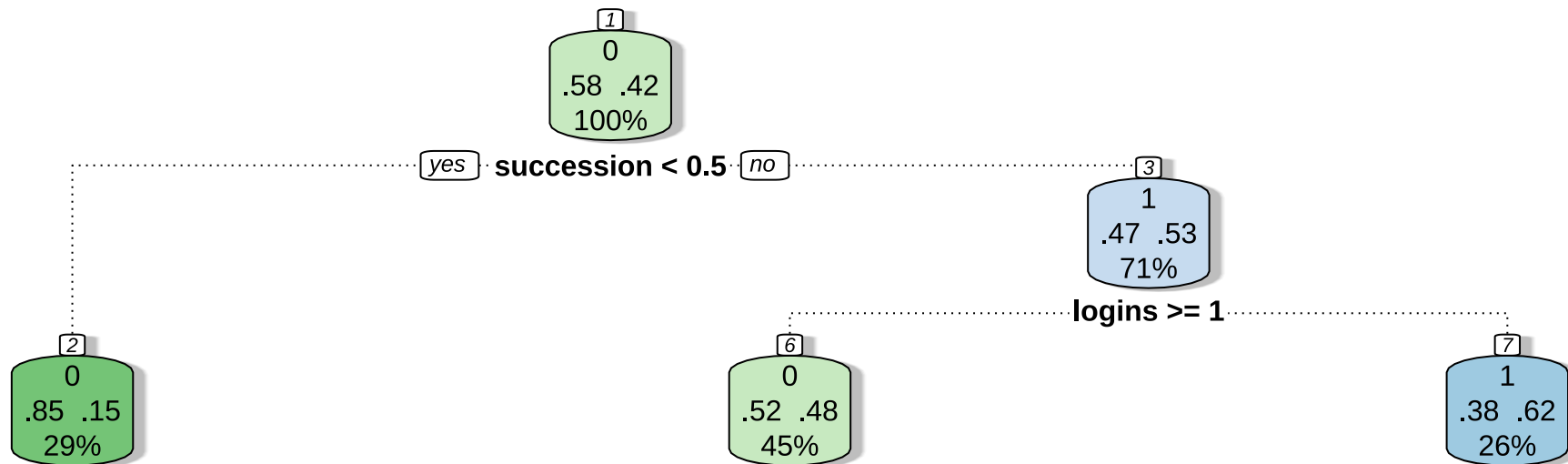


```
ct$bestTune
```

```
##      cp  
## 4 0.03
```

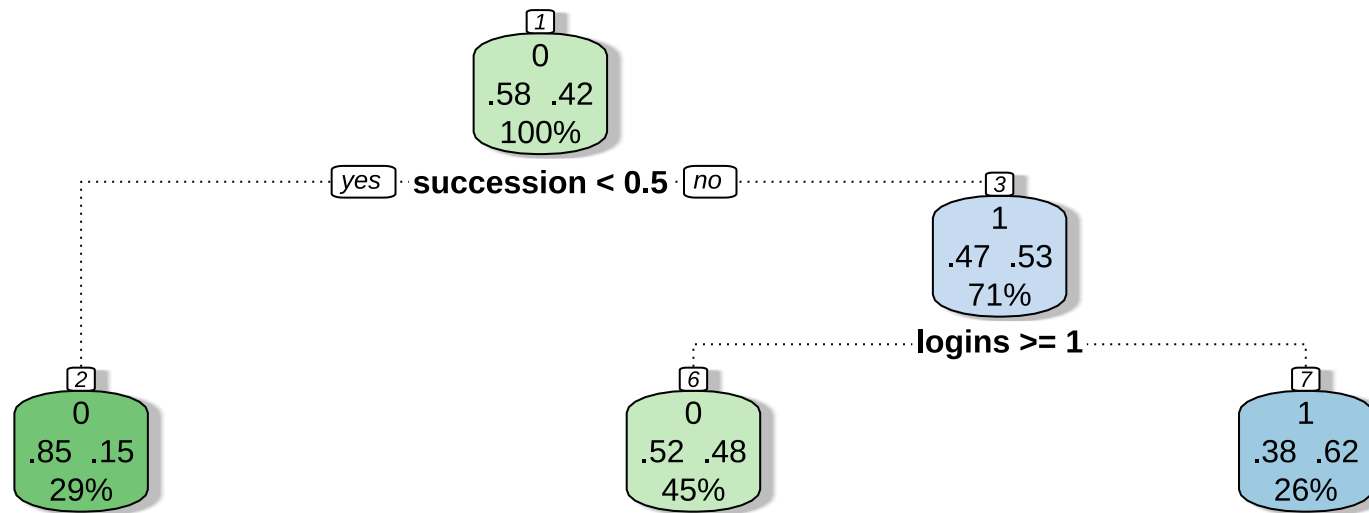
# ... And we can also plot the tree!

```
library(rattle)
fancyRpartPlot(ct$finalModel, caption = "Classification tree for Unsubscribe")
```



Classification tree for Unsubscribe

# What do you think the percentages in the leaves represent?



Classification tree for Unsubscribe

# Regression Trees

# Regression Trees

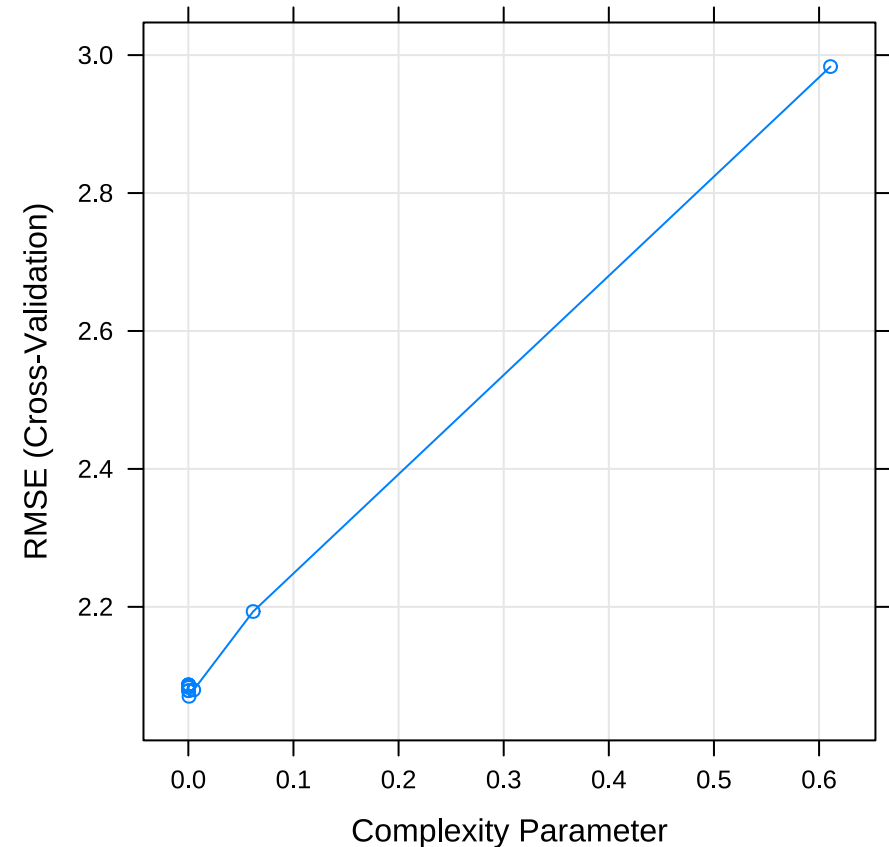
- Outcome is **continuous**
- Very similar to what we have seen with **classification trees**:
  - Predicted outcome is the **mean outcome for the leaf/region**.

# In R is basically the same

```
set.seed(100)

rt = train(
  logins ~. - unsubscribe - id, data = hbo.train,
  method = "rpart",
  trControl = trainControl("cv", number = 10),
  tuneLength = 20
)

plot(rt)
```



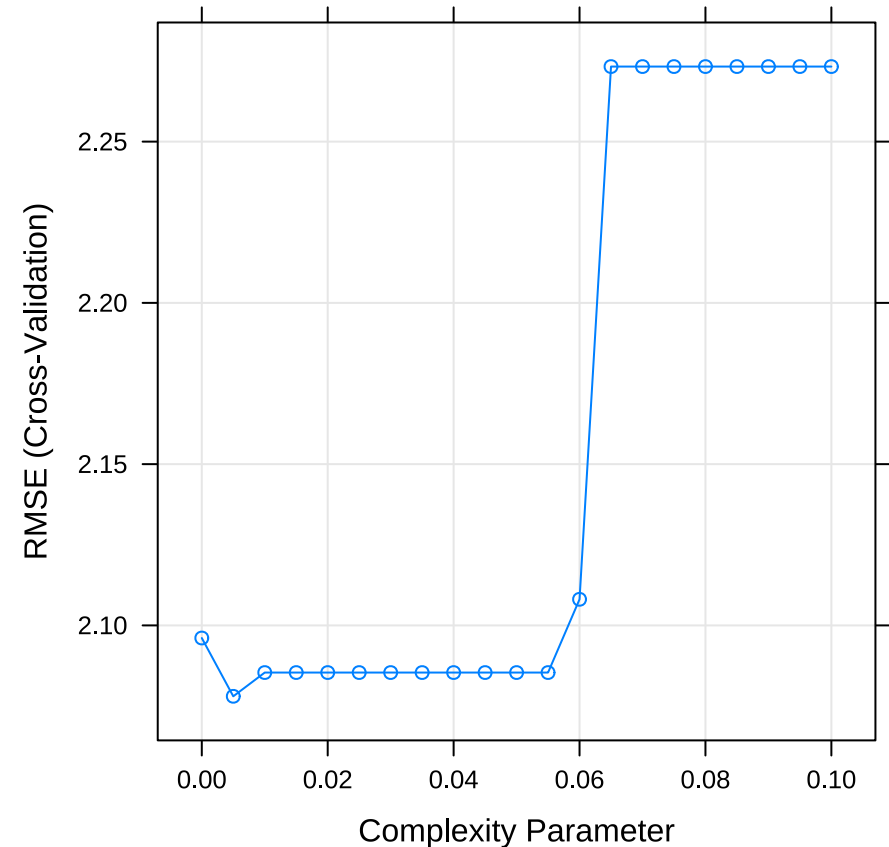
# Providing a specific grid for cp

```
set.seed(100)

tuneGrid = expand.grid(cp = seq(0, 0.1, by = 0.01))

rt = train(
  logins ~. - unsubscribe - id, data = hbo.train,
  method = "rpart",
  trControl = trainControl("cv", number = 10),
  tuneGrid = tuneGrid
)

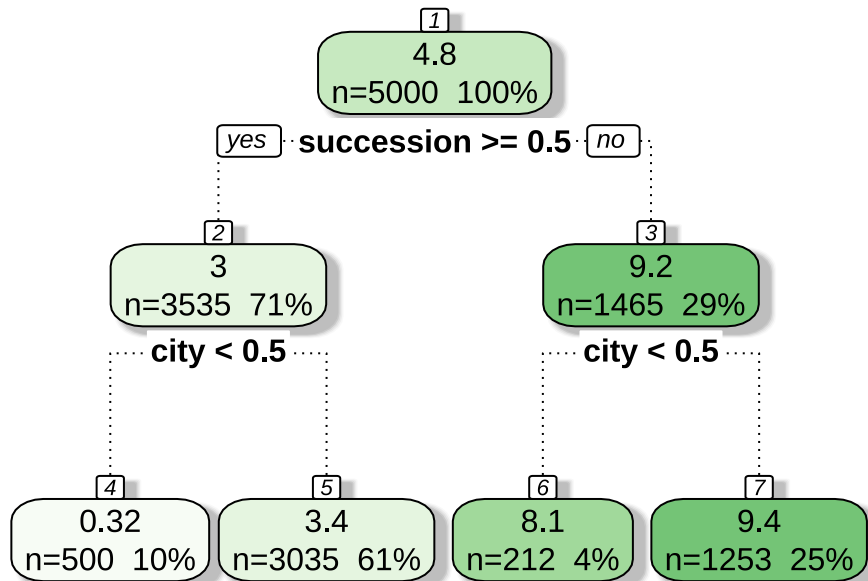
plot(rt)
```





# Plot the tree

```
fancyRpartPlot(rt$finalModel, caption="Regress:
```

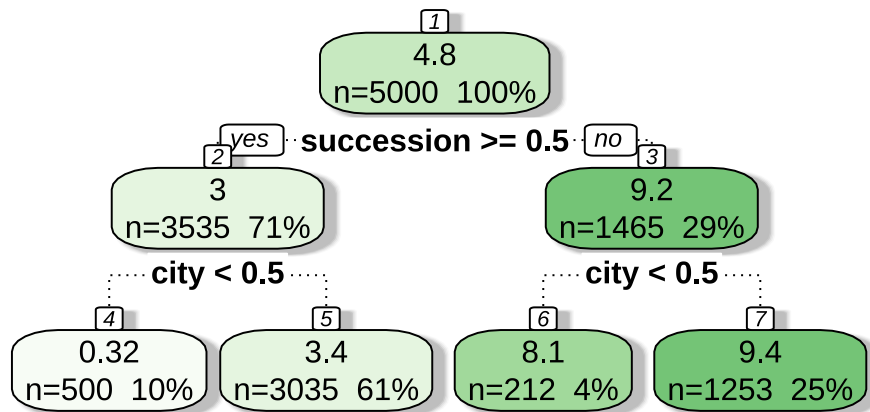


```
rt$finalModel
```

```
## n= 5000
##
## node), split, n, deviance, yval
##      * denotes terminal node
##
## 1) root 5000 66387.3700 4.806800
##    2) succession>=0.5 3535 24633.5000 2.973409
##      4) city< 0.5 500 517.1580 0.322000 *
##      5) city>=0.5 3035 20022.2800 3.410214 *
##    3) succession< 0.5 1465 1200.0180 9.230717
##      6) city< 0.5 212 132.2028 8.061321 *
##      7) city>=0.5 1253 728.8571 9.428571 *
```

## Q4: What would the predicted value be for a customer who hasn't watched GOT and lives in a city?

```
fancyRpartPlot(rt$finalModel, caption="Regress:
```



Regression Tree for Login

```
rt$finalModel
```

```
## n= 5000
##
## node), split, n, deviance, yval
##      * denotes terminal node
##
## 1) root 5000 66387.3700 4.806800
##    2) succession>=0.5 3535 24633.5000 2.973409
##      4) city< 0.5 500 517.1580 0.322000 *
##      5) city>=0.5 3035 20022.2800 3.410214 *
##    3) succession< 0.5 1465 1200.0180 9.230717
##      6) city< 0.5 212 132.2028 8.061321 *
##      7) city>=0.5 1253 728.8571 9.428571 *
```

# Main takeaways of decision trees



## Main advantages:

- Easy to interpret and explain (you can plot them!)
- Mirrors human decision-making.
- Can handle qualitative predictors (without need for dummies).

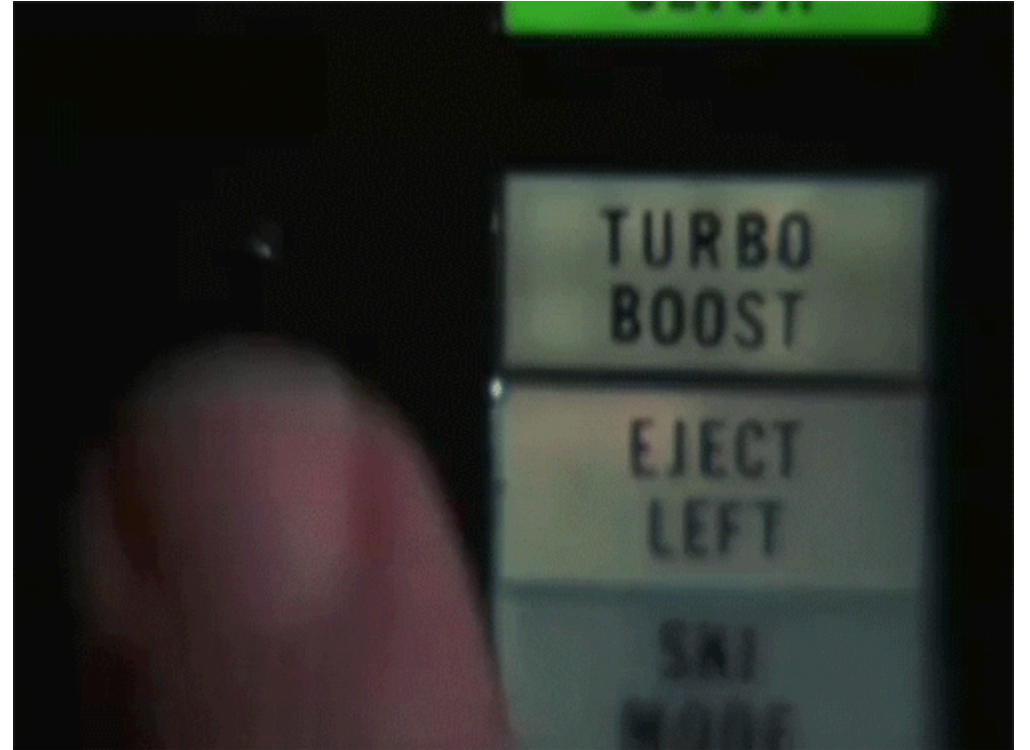
## Main disadvantages:

- Accuracy not as high as other methods
- Very sensitive to training data (e.g. overfitting)

# Next class

Use of decision trees as building blocks for **more powerful prediction methods!**

- Bagging
- Random Forests
- Boosting



# References

- James, G. et al. (2021). "Introduction to Statistical Learning with Applications in R". *Springer. Chapter 8*
- Starmer, J.. (2018). "Decision Trees". *Video materials from StatQuest (YouTube)*.
- STDHA. (2018). "CART Model: Decision Tree Essentials"