Minicourse II Introduction to Statistical Learning with tidymodels

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Course description

Introduce students to the main concepts in statistical learning focusing on supervised techniques for classification and regression problems such as decision trees, random forest among others.

All the methods will be implemented using tidymodels R package. This mini-course will be interactive with some hands-on practice. To take most of the course, students should use R at basic or intermediate level and it is recommended some previous contact with tidyverse R package.









Topics for today

- Intro to statistical learning
- Assessing Model Accuracy
- Classification and regression decision trees.
- Focused on CART algorithm
- Introduction to tidymodels
- Example with tidymodels







Type of Statistical learning methods

General context

- We observe a quantitative response Y and a set of p different predictors $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_p)$
- We are interested in the relationship between Y and X such that:

$$Y = f(\mathbf{X}) + \varepsilon$$

Where f is some fixed but unknown function of $(\mathbf{x}_1, \mathbf{x}_2, \dots \mathbf{x}_p)$ and represents the systematic information that \mathbf{X} provides about \mathbf{Y} . ε is a random error term. Which is independent of \mathbf{X} and has mean zero.









Type of Statistical learning methods

We are interested to study the relationship between Y y \mathbf{X}

$$Y = f(\mathbf{X}) + \varepsilon$$

Type of problems:

- Supervised, the response variable y_i it is available For each observation of the predictor variable(s) x_i . Regression problems (y_i is quantitative) or classification (y_i is qualitative)
- Unsupervised, for every observation we observe a vector of measurements
 x_i but no associated response y_i
- Semi supervise, y_i available for some x_i

It is important to identify the type of problem we have to explore and select possible methods to apply.

Model evaluation

- There is not a statistical method that is the best for all the possible problems.
- Some methods works really well in some problems but not in others.
- We need to decide for each problem which method works better.
- Selecting the best approach can be one of the most challenging parts of performing statistical learning in practice.









Example: Polynomial linear model

Regression problem

- we observe a predictor variable $x \in R$.
- Objective is to predict $y \in R$.
- In general $y = f(x) + \varepsilon$.
- Supose we know the data generating process, where $f(x) = sin(2 * \pi * x)$ plus a random noise (N(10,0,3)), (exemple PRML-Bishop).
- Let x equidistant in the interval [0,1].

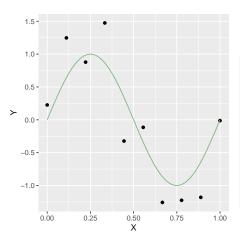








Scatter plot of simulated data (training). Green curve is $f(x) = sin(2 * x * \pi)$.





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- Simulate the data in this way allows us to capture properties from real data with certain regularity we want to learn.
- Observations are twisted by a random noise we don't control.
- The objective is to explore the training set to predict y values for new x values without knowing the true f.









A simple curve aproximation can be done using polynomial function such that:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_k x^k = \sum_{k=0}^K \beta_k x^k$$

Where K is the polynomial degree, it is a linear model because is linear in its parameters.

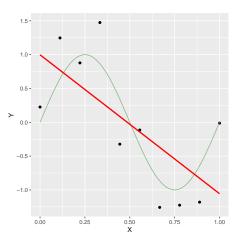






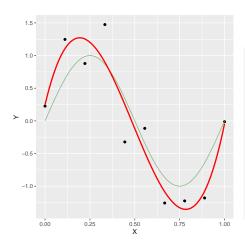


Example: with K=1



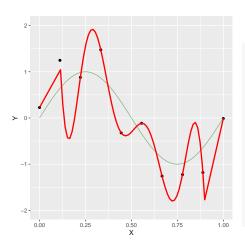
```
d \leftarrow tibble(x = seq(0,1,length.out = 20),
             f=sin(2*pi*x),
      y = f + rnorm(20, sd = 0.3))
p \leftarrow ggplot(d, aes(x = x, y = y)) +
  geom_point() +
  xlab("X") + ylab("Y")
f <- function(x){sin(2*pi*x)}</pre>
p1 <- p +
  geom_function(fun = f, color = '#7FB77E'
p1 + stat_smooth(method = 'lm',
formula = y ~ poly(x, 1, raw=TRUE),
se = FALSE, colour="red")
```

Example: with K=3



```
d \leftarrow tibble(x = seq(0,1,length.out = 10),
             f=sin(2*pi*x),
       y = f + rnorm(10, sd = 0.3))
p \leftarrow ggplot(d, aes(x = x, y = y)) +
  geom_point() +
  xlab("X") + ylab("Y")
f <- function(x){sin(2*pi*x)}</pre>
p1 <- p + geom_function(fun = f, color =
 p1 + stat_smooth(method = 'lm',
formula = y ~ poly(x, 3, raw=TRUE),
se = FALSE, colour="red")
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```

Example: with K=9



```
d \leftarrow tibble(x = seq(0,1,length.out = 10),
             f=sin(2*pi*x),
      y = f + rnorm(10, sd = 0.3))
p \leftarrow ggplot(d, aes(x = x, y = y)) +
  geom_point() +
  xlab("X") + ylab("Y")
f <- function(x){sin(2*pi*x)}</pre>
p1 <- p +
  geom_function(fun = f, color = '#7FB77E'
 p1 + stat_smooth(method = 'lm',
formula = y ~ poly(x, 9, raw=TRUE),
se = FALSE, colour="red")
```

How to elect the model?

A polynomial with K = 9 overfits, presents a samall error but is not a good approximation of f()

- To evaluate a statistical learning model in a data set, we need a measure of how well the predictions match the observed data.
- Quantify how close is the response predicted value of an observaation respect to the true response.
- In regression problem the most common measure is la medida mean square error (MSE).









How to select the model?

- $Tr = \{(y_i, \mathbf{x_i})\}_{i=1}^n$: training data set use to fit the model and estimate f.
- Most common accuracy measure Training MSEs.

$$MSE_{Tr} = Ave_{i \in Tr}[y_i - \hat{f}(\mathbf{x_i})]^2 = \frac{1}{n} \sum_{i=1}^{n} [y_i - \hat{f}(\mathbf{x_i})]^2$$









How to select the model?

- $Te = \{(y_i, \mathbf{x_i})\}_{i=1}^m$: test data set, observations to compute de accuracy, where not used to estimate f.
- A better accuracy measure is used based on the test set. Testing MSEe testeo.

$$MSE_{Te} = Ave_{i \in Te}[y_i - \hat{f}(\mathbf{x_i})]^2 = \frac{1}{m} \sum_{i=1}^{m} [y_i - \hat{f}(\mathbf{x_i})]^2$$

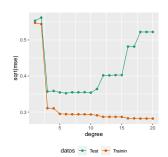








$RMSE_{Tr}$, vs $RMSE_{Te}$



```
d \leftarrow tibble(x = seq(0.1, length, out = 200),
            f=sin(2*pi*x).
      v = f + rnorm(200, sd = 0.3))
train.id <-sample(1:200,100)
err <- matrix(NA, ncol = 2, nrow = 20 )
for(k in 1:20) {
  m \leftarrow lm(y \sim poly(x, k, raw = TRUE),
            data = d[train.id,c('x','y')])
  pp <- predict(m, newdata = d[-train.id, c('x','y')] )
  err.ts <- mean((d$y[-train.id]-pp)^2)
  err.tr <-mean((d$y[train.id]-fitted(m))^2)
  err[k, ] <- cbind(err.tr, err.ts)
dt.err <- data.frame(grado=1:20, err) %>%
  set_names(nm = c('degree', 'Training', 'Test') ) %>%
  pivot_longer(cols = 2:3, values_to='mse', names_to='datos')
ggplot( dt.err, aes(x=degree, y= sqrt(mse), color=datos)) +
  geom_point() + geom_line() +
  scale color brewer(palette = 'Dark2')+
    theme(legend.position = 'bottom')
```

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- We are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen test data.
- Test data: the set of observations reserved to compute accuracy of the model for new data. Not used to estimate f. We can compute MSE_te
- The generalized performance of a statistical learning method is related with its predictive prformance computed with the testing data set.









Generally, training error will be smaller than test error Because the training data is used to fit the model, by design the error will be small relative to the error when the model is used on new data.









Bias-variance, trade-off

There are two competing forces that govern the choice of learning method: bias and variance.

- Bias is the error that is introduced by modeling a complicated problem by a simpler problem.
- Variance refers to how much your estimate would change if you had different training data. Its measuring how much your model depends on the data you have, to the neglect of future data.

The decide on the best model, from a range with different flexibility, you choose based on average test MSE at the bia-variance trade-off, where both are minimised.



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Decision trees

- Fifty Years of Classification and Regression Trees (Loh, 2014). Paper link.
- Tree algorithms can be used for classification or regession problems.
- First regression tree (Automatic Interaction Detection, AID) Morgan , 1963. There are a wide variety of tree methods and software to implemented them which increases its popularity.
- We will focused on CART algorithm (Breiman, 1984).









Decision trees

- Tree based methods consist in a nested partition squence which divide the predictor space, within these partitions, a model is used to predict the outcome.
- Then tree based models consist of one or more of nested if-then statements for the predictors that partition the data
- In theory regions defined by trees can be with different shapes. However we select methods where the predictor space is dividen in hight dimensional rectangles.





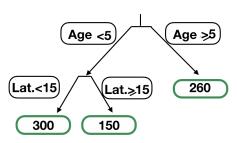




Regression trees (CART), examples

- Response: Appartment prices in thousands of USD in Montevideo
- Predictor variales: Construction age, latitude.
- Trees are composed with nodes, brunches and leaft.
- First node is the root node.
- Terminal nodes are leaves

Tree structure



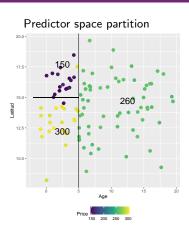








Regression tree regions



- First split Age= 5, region Age< 5 splits into Lat = 15 two regions are defined Lat > 15 and Lat < 15.
- This process defines 3 non overlap regions (R_1, R_2, R_3) .

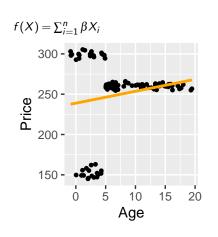


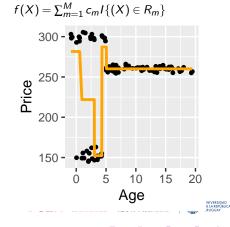






Lineal regression vs Regression Tree, housing example





Algorithm: growing a tree

- All observations in a single set
- Sort values on first variable
- Compute split criteria for all possible splits into two sets
- 4 Choose the best split on this variable
- Repeat 2-4 for all other variables
- 6 Choose the best split among all variables. Your data is now in two sets.
- Repeat 1-6 on each subset.
- Stop when stopping rule is achieved.









Main idea

Main idea is segmenting the predictor space into a number of simple regions, in each region a simple models is fitted.

The set of rules to partition the predictor space can be sumarized in a *decision* tree

f(X) estimate:

Regression Mean response in each leaft
Classification most frequent class on the leaf









The objective will be to define regions $R_1, R_2 \dots R_M$ such that minimize RSS

$$RSS = \sum_{m=1}^{M} \sum_{i \in R_m} (y_i - \hat{y}_{R_m})^2$$

 \hat{y}_{R_m} response variable mean in the training data set in R_m region.

This is computationally unfeasible since we would have to consider all possible partitions of the predictor space into M boxes.









Algorithm construction

Let (x_i, y_i) for i = 1, ... N con $x_i = (x_{i1}, x_{i2}, ... x_{ip})$, regression tree constructions consists in tree basic steps:

- Begin with all the training data.
- Select X_i and s which defines the partition $\{X_i < s\}$. This is based on gready algorithms, select the best partition in each step.
- The data are divided in two 'sons': $R_1(i,s) = \{X | X_i \le s\}$ y $R_2(j,s) = \{X | X_i > s\}$
- Repeat the procedure until reach the stoping rule criteria. Example: less than 5 observation per leaft.







How to find the best partition

In each step, find the best partition:

$$\bullet \ \left\{ X_j < s \right\} \ \text{divide the data in} \ R_1(j,s) = \left\{ X | X_j \le s \right\} \ \text{y} \ R_2(j,s) = \left\{ X | X_j > s \right\}$$

• Select the variable *j* the cut point *s* such tha minimizes:

$$min_{j,s} \left[\sum_{x_i \in R_1(j,s)} (y_i - \bar{y}_{R_1})^2 + \sum_{x_i \in R_2(j,s)} (y_i - \bar{y}_{R_2})^2 \right]$$

- \bar{y}_{R_1} y \bar{y}_{R_2} mean response in each region.
- Repeat the same procedure for all the regions until the stoping rule is met.

If Y is categorical, the evaluation have to change X recursors consistently the establishment of the standard of the stan







How long do I let the tree grow?

The tree size is a tunning parameter and governs the tree complexity.

- Very big, overfit (more complex, less bias)
- Very small, can not capture important patterns in the data (simpler, smaller variance)

Different stoping rules

- Not reduction in test error
- Small number of data in the leaf

Prefered method is to grow a big tree (T_0) with some stoping rule and *pruning* T_0 based on some cost-complexity penalty.



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Pruning - Cost-complexity criteria

For a subtree T, define $Q_m(T) = \frac{1}{N_m} \sum_{i \in R_m} (y_i - \bar{y}_m)^2$, R_m are leaves and |T|number of terminal nodes in the tree. Then,

$$C_{\alpha}(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

- Let T_0 complete tree, without pruning.
- $lpha \geq 0$ controls the balance between tree size and controla el balance entre el tamaño del árbol and goodness of fit to the data.
- Big values of α results in samll trees, big size penality.
- If $\alpha = 0$ then T_0 , not size penalization







Regression tree, Example

- Objective: Predict asking price for Montevideo Apartments
- Datos: Apartments sales February 2018- January 2019. Data from Mercado libre







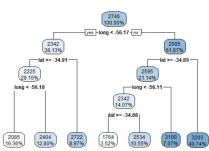


rpart R package

Los datos están en el objeto dat_apt , ajustamos un árbol SIN podar.

```
# Divide data in training and test
intrain <- sample(x = 1:nrow(dat_apt), size = nrow(dat_apt)*.8)
training <- dat_apt[intrain,]</pre>
testing <- dat_apt[-intrain,]</pre>
# rpart to fit the tree
# Two arguments: formula and data
# Just to describe the problem use lat and long as predictors
tree_apto <- rpart(precio_apt ~ lat + long, data = training)</pre>
# resulting tree structure
rpart.plot(tree_apt, digits = (-5))
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```

Regression tree, apartments price in MVD



- Mean price sqm in USD, percentage obs.
- Average apartment price in all the sample USD 2.746 per sqm.
- First partition on long (-56,17), at west the average price is USD 2.342 while east USD 2.995.

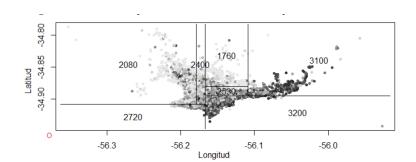








Regression tree











Some characteristics

- Simple to use and interprete.
- Trees can handle a mix of predictor types, categorical and quantitative.
- Incorporates interactions and monotonic transformations atomatically.
- Trees efficiently operate when there are missing values in the predictors.

Some problems

- Can be unestable in particular if are not pruned
- In genral the predictive error is bigger than other ML methods.
- Predicts a finite number of values, even when Y is continuous.









Classification

- The response variable have values in $\{1, ..., K\}$.
- Tree construction similar to regression.
- We need to modify:
 - f(X) estimation
 - Criterio to node spliting and prune the tree









f(X) estimate

Let \hat{p}_{mk} the proportion of observations in the classs k in the nodo m,

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

The observations in node m are classified based on **majority vote**,

$$k(m) = \operatorname{argmax}_k \hat{p}_{mk}$$

majority class in node m.







Partition criterio for nodo m

Several measures $Q_m(T)$ to evaluate the partitions. Impurity measures for node m:

- Classification error: $\frac{1}{N_m}\sum_{i\in R_m}I(y_i\neq k(m))=1-\max_k(\hat{p}_{mk}(m))$ proportions of observations in the region R_m which are not from the majority class.
- Gini index: $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^K \hat{p}_{mk} (1 \hat{p}_{mk})$ is small if all the \hat{p}_{mk} are close to 0 or 1, this means if the node has predominant observations from only one class (pure node).
- Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} log \hat{p}_{mk}$ small value is the node m is pure.

Any of these measures can be used to guide the pruning of the tree having into account the cost-complexity, in general the classification error is used.



Other tree algorithms

- CHAID, C4.5, FACT, QUEST, CRUISE, GUIDE, CTREE, PPtree, etc.
- Main differences between them are the node partition method.
- Some use kernel methods, nearest neighbor, lineal partitions in a subset of selected variables.
- Can be bibary trees or multipole partitions.
- Trees which use only one variable in each node partition generate partitions orthogonal to the axes. When more variables are used, partitions are obliques to the axes.











- Collection of packages for modeling and machine learning using tidyverse principles.
- install.packages("tidymodels")
- library(tidymodels) load the core packages and make them available in your current R session.











- rsample provides infrastructure for efficient data splitting and resampling
- parsnip is a tidy, unified interface for models which provides a fluent and standardized interface for a variety of different models.
- recipes recipes is a tidy interface to data pre-processing tools for feature engineering.
- tune helps you optimize the hyperparameters of your model and pre-processing steps.
- yardstick measures the effectiveness of models using performance metrics
- ...









Tree based methods, Lab

In this lab we will see different methods based on trees and explore how the model parameters changes. Also we will see how to change the hyperparameters to improve the predictive performance

- parsnip for model fitting
- recipes and workflows for transformatiosn and tune and dials to hyperparameter tunning
- rpart.plot to visualiza decition trees based on rpart package es engine.
- vip to visualize variable importance.









Apartment values in Montevideo

apt_redu data set contains information from one neighborhood in Montevideo (Pocitos) with apartments asking prices and some apartment characteristics. Regression problem, response variable log price in sqm (lpreciom2) the rest are used as predictor variables.

```
library(tidyverse)
library(here)
library(tidymodels)
library(rpart.plot)
library(vip)
data <- read_csv(here("Minicourse/apt_redu.csv"))</pre>
```



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Data splitting

- The primary approach for empirical model validation is to split the existing pool of data into two distinct sets, the training set and the test set.
- This training set is usually the majority of the data
- The other portion of the data is placed into the test set
- This is held in reserve until one or two models are chosen as the methods most likely to succeed









First we set the random number stream with set.seed() to be able to reproduce the results

Save the split information for an 80/20 split of the data (80% training and 20% test)

```
set.seed(2023)
data_split <- initial_split(data, prop = 0.80)
data_split
## <Training/Testing/Total>
## <12280/3070/15350>
```

The printed information denotes the amount of data in the training set







- The object data_split is an rsplit object and contains only the partitioning information
- To get the resulting data sets, we apply two more functions, training and test

```
data_train <- training(data_split)
data_test <- testing(data_split)

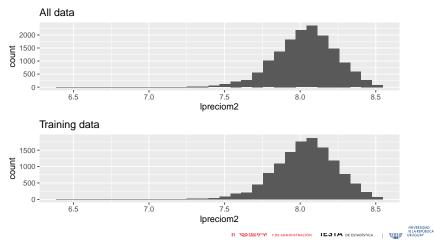
dim(data_train)
## [1] 12280 11</pre>
```







Distribution response in all data and training data



Fitting Models with parsnip

- 1. **Pick a model:** Specify the type of model based on its mathematical structure
- 2. **Set the engine:**, Most often this reflects the software package that should be used
- 3. **Set the mode (if needed):**, The mode reflects the type of prediction outcome. For numeric outcomes, the mode is regression; for qualitative outcomes, it is classification









Linear regression

set_mode() is note needed because we specify the model in the first step.







There are different ways to specify a linear regression selecting different engines We can see the possible engines availables

```
show_engines("linear_reg")
    A tibble: 7 x 2
##
    engine mode
    <chr> <chr>
##
##
    ٦m
       regression
  2 glm regression
##
    glmnet regression
##
  4 stan
         regression
##
  5 spark regression
##
    keras
          regression
## 7 brulee regression
```







Once the details of the model have been specified, the model estimation can be done with either the fit()function (to use a formula) or the fit_xy() function (when your data are already pre-processed).









```
lm_form_fit <-
  lm_mod %>%
  fit(lpreciom2 ~ lsup_constru + long, data = data)

lm_xy_fit <-
  lm_mod %>%
  fit_xy(
    x = data %>% select(lsup_constru, long),
    y = data %>% select(lpreciom2)
)
```







```
lm_form_fit
## parsnip model object
##
##
## Call:
## stats::lm(formula = lpreciom2 ~ lsup_constru + long, data = data)
##
## Coefficients:
## (Intercept) lsup_constru long
## 135.1762 -0.1666 2.2520
```







Decision tree

Link parsnip decision tree.

These tree specification can be used to create a classification tree. We can see the parsnip flexibility to create different models

```
tree_mod <- decision_tree() %>%
  set_engine("rpart")
```









With the model especification and the data we can fit the model

```
tree_fit <- tree_mod %>%
    set_mode("regression") %>%
fit(lpreciom2 ~ ., data = data_train)
```







```
tree fit
## parsnip model object
##
##
  n = 12280
##
  node), split, n, deviance, yval
##
         * denotes terminal node
##
    1) root 12280 512.62880 8.031064
##
##
      2) lsup_constru>=3.906998 8192 330.21000 7.980633
##
        4) lsup_constru>=4.620047 2261 92.79654 7.897630
          8) lsup_constru>=5.389061 154 10.65301 7.716920 *
##
##
          9) lsup_constru< 5.389061 2107 76.74693 7.910838 *
        5) lsup_constru< 4.620047 5931 215.89820 8.012275
##
##
         10) garage=No 3816 143.90470 7.978957 *
         11) garage=Si 2115 60.11451 8.072389 *
##
##
      3) lsup_constru< 3.906998 4088 119.83370 8.132123
##
        6) lsup_constru>=3.481122 3078 92.45661 8.103078
```

```
tree fit %>%
  extract_fit_engine() %>%
  summary()
## Call:
  rpart::rpart(formula = lpreciom2 ~ ., data = data)
##
    n = 12280
##
##
             CP nsplit rel error
                                                  xstd
                                     xerror
   1 0.12208652
                     0 1.0000000 1.0000572 0.01668184
   2 0.04197041
                     1 0.8779135 0.8781177 0.01556716
  3 0.02317277
                     2 0.8359431 0.8392745 0.01498730
  4 0.02050192
                     3 0.8127703 0.8156918 0.01493354
  5 0.01129189
                     4 0.7922684 0.7943303 0.01474401
  6 0.01052729
                     6 0.7696846 0.7617377 0.01449786
## 7 0.01000000
                     7 0.7591573 0.7606741 0.01450776
##
## Variable importance
## lsup constru dormitorios
                                              lexpensas
                                     banos
```

When the tree has to many nodes is more complex to read the original output. The rpart.plot package has some usefult functions to visualize the tree structure in a simple way. Only works for tree objects fitted with rpart

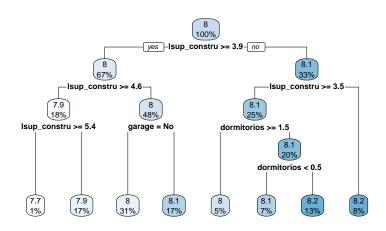
```
tree_fit %>%
  extract_fit_engine() %>%
  rpart.plot(roundint=FALSE)
```













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Predictions

augment will add column(s) for predictions to the given data

```
augment(tree_fit , new_data = data_test) %>%
  select(1, 12, 13)
     A tibble: 3,070 x 3
##
##
      lpreciom2 .pred .resid
##
          <dbl> <dbl> <dbl> <dbl>
           7.98 8.07 -0.0885
##
##
           8.24 8.16 0.0774
##
           8.33 8.16 0.175
##
           7.85 7.98 - 0.125
##
    5
           8.07 8.07 -0.00322
##
           8.09 8.16 -0.0720
##
           8.04
                 8.02 0.0205
##
           8.26
                 8.02 0.237
##
           8.23
                 7.91
                        0.319
           7.72
                 7.98 - 0.262
   10
```

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```
predict(tree_fit, new_data = data_test)
     A tibble: 3,070 x 1
##
##
      .pred
      <dbl>
##
       8.07
##
    1
##
       8.16
    3
       8.16
##
##
      7.98
    5
       8.07
##
##
    6
       8.16
##
    7
       8.02
##
    8
       8.02
    9
       7.91
##
   10
       7.98
##
  # ... with 3,060 more rows
```











How to check all possible engines for decision trees?

```
show_engines("decision_tree")

## # A tibble: 5 x 2

## engine mode

## <chr> <chr>
## 1 rpart classification

## 2 rpart regression

## 3 C5.0 classification

## 4 spark classification

## 5 spark regression
```









Your turn!

- To the complete data set, create a new response variable lpreciom2_c, categorical variable with two levels, high if lpreciom2 is bigger or equal than the mean of lpreciom2 and low if lpreciom2 is smaller than its mean value. Save the data in an object called new_data
- ② In the new_data set select all the variables but lpreciom2 because it is a perfect predictor for lpreciom2_c
- 3 Divide in training and test the new_data
- Using the object tree_mod fit a classification tree with the new variable









Part 1







Part 2

```
set.seed(2023)
data_split_c <- initial_split(new_data)

data_train_c <- training(data_split_c)
data_test_c <- testing(data_split_c)</pre>
```







Part 3

```
tree_fit_cl <- tree_mod %>%
  set_mode("classification") %>%
  fit(lpreciom2_c ~ ., data = data_train_c)
```







Your turn!

- Plot the tree structure
- 2 Compute the accuracy in the test set









```
tree_fit_cl %>%
  extract_fit_engine() %>%
  rpart.plot(roundint=FALSE)
```







