Machine Learning with Tree-Based Models in R

Your Name Here

Last modified on April 25, 2025 09:14:50 Eastern Daylight Time

Table of contents

Preface 3

1 Classification Trees 4

Welcome to the course! - (video) . . . 4
1.1 Why tree-based methods? . . . 4
1.2 Specify that tree . . . 4
Instructions . . . 5
1.3 Train that model . . . 6
Instructions . . . 6
How to grow your tree - (video) . . . 9
1.4 Train/test split . . . 9
Instructions . . . 9
1.5 Avoiding class imbalances . . . 10
Instructions . . . 10
1.6 From zero to hero . . . 12
Instructions . . . 12
Predict and evaluate - (video) . . . 15
1.7 Make predictions . . . 15
Instructions . . . 15
1.8 Crack the matrix . . . 16
Instructions . . . 16
1.9 Are you predicting correctly? . . . 18
Instructions . . . 18

References 21

Preface

This material is from the DataCamp course Machine Learning with Tree-Based Models in R by Sandro Raabe.

Course Description: Tree-based machine learning models can reveal complex non-linear relationships in data and often dominate machine learning competitions. In this course, you'll use the tidymodels package to explore and build different tree-based models—from simple decision trees to complex random forests. You'll also learn to use boosted trees, a powerful machine learning technique that uses ensemble learning to build high-performing predictive models. Along the way, you'll work with health and credit risk data to predict the incidence of diabetes and customer churn.

Reminder to self: each `*.qmd` file contains one and only one chapter, and a chapter is defined by the first-level heading `#`.

1 Classification Trees

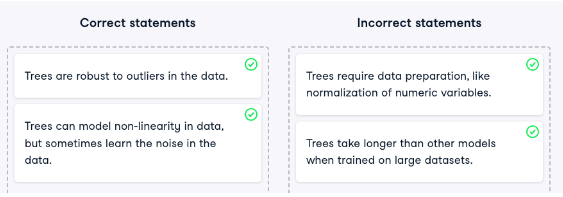
Ready to build a real machine learning pipeline? Complete step-by-step exercises to learn how to create decision trees, split your data, and predict which patients are most likely to suffer from diabetes. Last but not least, you'll build performance measures to assess your models and judge your predictions.

Welcome to the course! - (video)

1.1 Why tree-based methods?

Tree-based models are one class of methods used in machine learning. They are superior in many ways, but also have their drawbacks.

Which of these statements are true and which are false?



Correct statements	Incorrect statements
Trees are robust to outliers in the data. ✓	Trees require data preparation, like normalization of numeric variables. ✓
Trees can model non-linearity in data, but sometimes learn the noise in the data. ✓	Trees take longer than other models when trained on large datasets. ✓

1.2 Specify that tree

In order to build models and use them to solve real-world problems, you first need to lay the foundations of your model by creating a model specification. This is the very first step in every machine learning pipeline that you will ever build.

You are going to load the relevant packages and design the specification for your classification tree in just a few steps.

A magical moment, enjoy!

Instructions

- Load the `tidymodels` package.

```r
library(tidymodels)
```

- Pick a model class for decision trees, save it as `tree_spec`, and print it.

```r
# Pick a model class
tree_spec <- decision_tree()

# Print the result
tree_spec
```

```
Decision Tree Model Specification (unknown mode)

Computational engine: rpart
```

- Set the engine to `"rpart"` and print the result.

```r
# Pick a model class
tree_spec <- decision_tree() |>
  # Set the engine
  set_engine("rpart")

# Print the result
tree_spec
```

```
Decision Tree Model Specification (unknown mode)

Computational engine: rpart
```

- Set the mode to `"classification"` and print the result.

```r
# Pick a model class
tree_spec <- decision_tree() |>
  # Set the engine
  set_engine("rpart") |>
  # Set the mode
  set_mode("classification")
```

```
# Print the result
tree_spec
```

```
Decision Tree Model Specification (classification)

Computational engine: rpart
```

> Note
>
> You created a decision tree model class, used an `rpart` engine, and set the mode to `"classification"`. Remember, you will need to perform similar steps every time you design a new model. Come back anytime if you need a reminder!

1.3 Train that model

A model specification is a good start, just like the canvas for a painter. But just as a painter needs color, the specification needs data. Only the final model is able to make predictions:

Model specification + data = model

In this exercise, you will train a decision tree that models the risk of diabetes using health variables as predictors. The response variable, `outcome`, indicates whether the patient has diabetes or not, which means this is a binary classification problem (there are just two classes). The dataset also contains health variables of patients like `blood_pressure`, `age`, and `bmi`.

For the rest of the course, the `tidymodels` package will always be pre-loaded. In this exercise, the `diabetes` dataset is also available in your workspace.

```
diabetes <- read_csv("./data/diabetes_tibble.csv")
# Change character outcome to a factor
diabetes <- diabetes |>  mutate_if(is.character, as.factor)
```

Instructions

- Create `tree_spec`, a specification for a decision tree with an `rpart` engine.

```
# Create the specification
tree_spec <- decision_tree() |>
  set_engine("rpart") |>
  set_mode("classification")
```

- Train a model `tree_model_bmi`, where the `outcome` depends only on the `bmi` predictor by fitting the `diabetes` dataset to the specification.

```
# Train the model
tree_model_bmi <- tree_spec |>
  fit(outcome ~ bmi, data = diabetes)
```

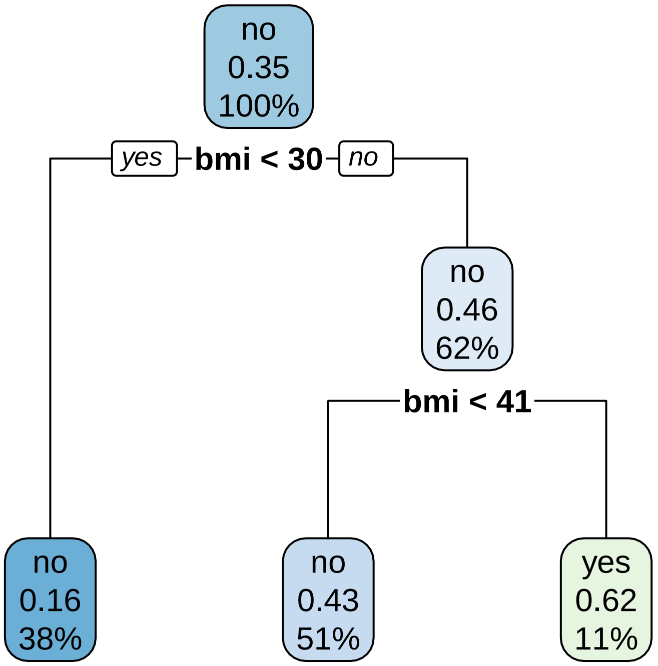
- Print the model to the console.

```
# Print the model
tree_model_bmi
```

```
parsnip model object

n= 768

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 768 268 no (0.6510417 0.3489583)
  2) bmi< 29.85 291  47 no (0.8384880 0.1615120) *
  3) bmi>=29.85 477 221 no (0.5366876 0.4633124)
    6) bmi< 40.85 392 168 no (0.5714286 0.4285714) *
    7) bmi>=40.85 85  32 yes (0.3764706 0.6235294) *
```

- Graph the model with `rpart.plot()`

```
tree_model_bmi |>
  extract_fit_engine() |>
  rpart.plot::rpart.plot()
```



Tip

Each node shows:

- the predicted class (`no` or `yes` diabetes),
- the predicted probability of diabetes,
- the percentage of observations in the node.

Note

You have defined your model with `decision_tree()` and trained it to predict outcome using `bmi` like a professional coach! Printing the model displays useful information, such as the training time, the model formula used during training, and the node details. Remember, to fit a model to data is just a different phrase for training it. Don't worry about the precise output too much, you'll cover that later!

How to grow your tree - (video)

1.4 Train/test split

In order to test your models, you need to build and test the model on two different parts of the data - otherwise, it's like cheating on an exam (as you already know the answers).

The data split is an integral part of the modeling process. You will dive into this by splitting the diabetes data and confirming the split proportions.

The `diabetes` data from the last exercise is pre-loaded in your workspace.

Instructions

- Split the `diabetes` tibble into `diabetes_split`, a split of 80% training and 20% test data.

```r
set.seed(123)
# Create the split
diabetes_split <- initial_split(diabetes, prop = 0.80)
```

- Print the resulting object.

```r
# Print the data split
diabetes_split
```

```
<Training/Testing/Total>
<614/154/768>
```

- Extract the training and test sets and save them as `diabetes_train` and `diabetes_test`.

```r
# Extract the training and test set
diabetes_train <- training(diabetes_split)
diabetes_test  <- testing(diabetes_split)
```

- Verify the correct row proportion in both datasets compared to the `diabetes` tibble.

```r
# Verify the proportions of both sets
round(nrow(diabetes_train) / nrow(diabetes), 2) == 0.80
```

```
[1] TRUE
```

```
round(nrow(diabetes_test) / nrow(diabetes), 2) == 0.20
```

```
[1] TRUE
```

> Note
>
> Using `training()` and `testing()` after the split ensures that you save your working datasets.

1.5 Avoiding class imbalances

Some data contains very imbalanced outcomes - like a rare disease dataset. When splitting randomly, you might end up with a very unfortunate split. Imagine all the rare observations are in the test and none in the training set. That would ruin your whole training process!

Fortunately, the `initial_split()` function provides a remedy. You are going to observe and solve these so-called class imbalances in this exercise.

There is already code provided to create a split object `diabetes_split` with a 75% training and 25% test split.

```
# Preparation
set.seed(9888)
diabetes_split <- initial_split(diabetes, prop = 0.75)
```

Instructions

- Count the proportion of `"yes"` outcomes in the training and test sets of `diabetes_split`.

```
# Proportion of 'yes' outcomes in the training data
counts_train <- table(training(diabetes_split)$outcome)
prop_yes_train <- counts_train["yes"] / sum(counts_train)

# Proportion of 'yes' outcomes in the test data
counts_test <- table(testing(diabetes_split)$outcome)
prop_yes_test <- counts_test["yes"] / sum(counts_test)

paste("Proportion of positive outcomes in training set:", round(prop_yes_train, 2))
```

```
[1] "Proportion of positive outcomes in training set: 0.31"
```

```r
paste("Proportion of positive outcomes in test set:", round(prop_yes_test, 2))
```

```
[1] "Proportion of positive outcomes in test set: 0.46"
```

- Redesign `diabetes_split` using the same training/testing proportion, but with the `outcome` variable being equally distributed in both sets. Count the proportion of `yes` outcomes in both datasets.

```r
set.seed(123)
# Create a split with a constant outcome distribution
diabetes_split <- initial_split(diabetes, strata = outcome)

# Proportion of 'yes' outcomes in the training data
counts_train <- table(training(diabetes_split)$outcome)
prop_yes_train <- counts_train["yes"] / sum(counts_train)

# Proportion of 'yes' outcomes in the test data
counts_test <- table(testing(diabetes_split)$outcome)
prop_yes_test <- counts_test['yes'] / sum(counts_test)

paste("Proportion of positive outcomes in training set:", round(prop_yes_train, 2))
```

```
[1] "Proportion of positive outcomes in training set: 0.35"
```

```r
paste("Proportion of positive outcomes in test set:", round(prop_yes_test, 2))
```

```
[1] "Proportion of positive outcomes in test set: 0.35"
```

Note

Impressive - from 31% vs. 46% positive outcomes to 35% in both sets. This was a tough one, but now you know how simple it is to avoid class imbalances! This is even more important in a large dataset with a very imbalanced target variable.

1.6 From zero to hero

You mastered the skills of creating a model specification and splitting the data into training and test sets. You also know how to avoid class imbalances in the split. It's now time to combine what you learned in the preceding lesson and build your model using only the training set!

You are going to build a proper *machine learning pipeline*. This is comprised of creating a model specification, splitting your data into training and test sets, and last but not least, fitting the training data to a model. Enjoy!

Instructions

- Create `diabetes_split`, a split where the training set contains three-quarters of all diabetes rows and where training and test sets have a similar distribution in the outcome variable.

```r
set.seed(9)
# Create the balanced data split
diabetes_split <- initial_split(diabetes,
                                prop = 0.75,
                                strata = outcome)
```

- Build a decision tree specification for your model using the `rpart` engine and save it as `tree_spec`.

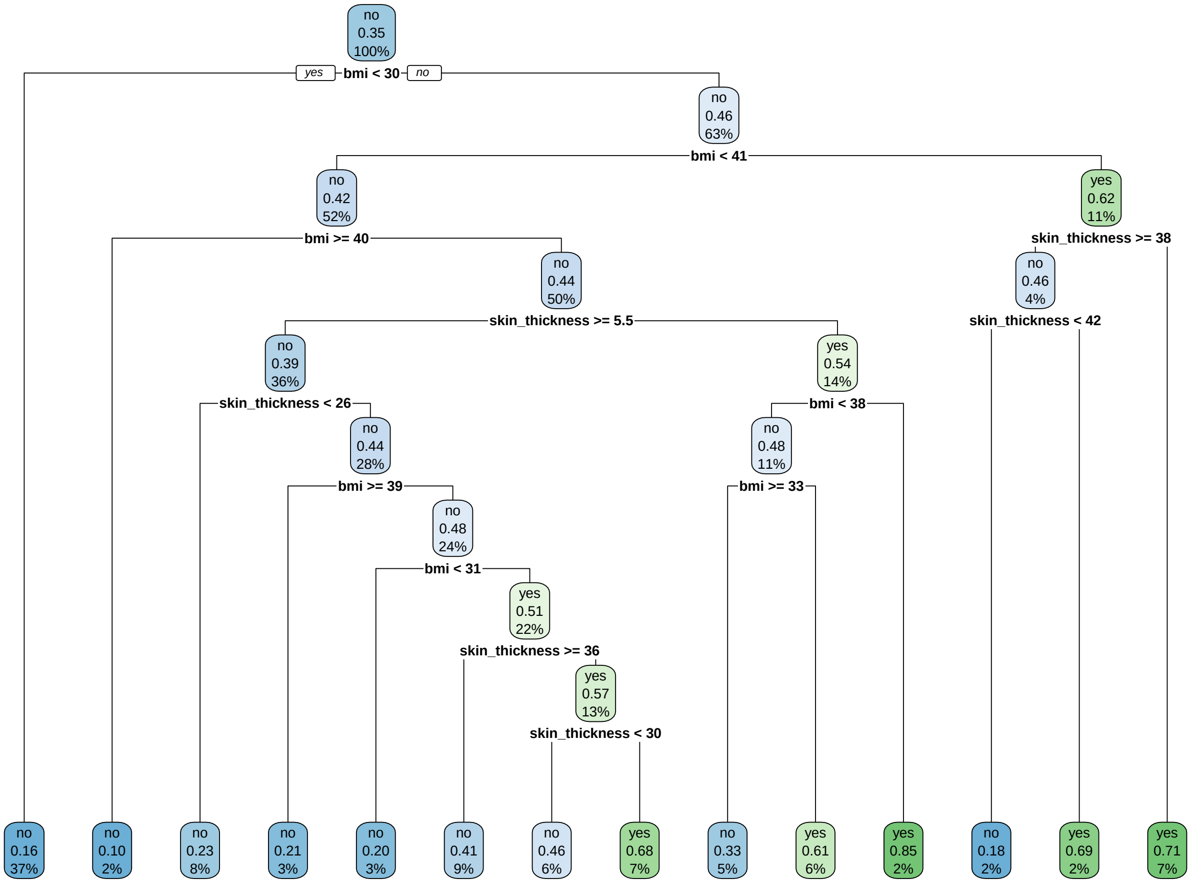
```r
# Build the specification of the model
tree_spec <- decision_tree() |>
  set_engine("rpart") |>
  set_mode("classification")
```

- Fit a model `model_trained` using the training data of `diabetes_split` with `outcome` as the target variable and `bmi` and `skin_thickness` as the predictors.

```r
# Train the model
model_trained <- tree_spec |>
  fit(outcome ~ bmi + skin_thickness,
      data = training(diabetes_split))

model_trained
```

```
parsnip model object

n= 576 

node), split, n, loss, yval, (yprob)
      * denotes terminal node

  1) root 576 201 no (0.6510417 0.3489583)  
    2) bmi< 29.85 213  34 no (0.8403756 0.1596244) *
    3) bmi>=29.85 363 167 no (0.5399449 0.4600551)  
      6) bmi< 40.85 297 126 no (0.5757576 0.4242424)  
       12) bmi>=40.05 10   1 no (0.9000000 0.1000000) *
       13) bmi< 40.05 287 125 no (0.5644599 0.4355401)  
         26) skin_thickness>=5.5 208  82 no (0.6057692 0.3942308)  
           52) skin_thickness< 25.5 48  11 no (0.7708333 0.2291667) *
           53) skin_thickness>=25.5 160  71 no (0.5562500 0.4437500)  
            106) bmi>=38.8 19   4 no (0.7894737 0.2105263) *
            107) bmi< 38.8 141  67 no (0.5248227 0.4751773)  
              214) bmi< 30.85 15   3 no (0.8000000 0.2000000) *
              215) bmi>=30.85 126  62 yes (0.4920635 0.5079365)  
                430) skin_thickness>=35.5 51  21 no (0.5882353 0.4117647) *
                431) skin_thickness< 35.5 75  32 yes (0.4266667 0.5733333)  
                  862) skin_thickness< 29.5 37  17 no (0.5405405 0.4594595) *
                  863) skin_thickness>=29.5 38  12 yes (0.3157895 0.6842105) *
         27) skin_thickness< 5.5 79  36 yes (0.4556962 0.5443038)  
           54) bmi< 37.65 66  32 no (0.5151515 0.4848485)  
            108) bmi>=33.05 30  10 no (0.6666667 0.3333333) *
            109) bmi< 33.05 36  14 yes (0.3888889 0.6111111) *
           55) bmi>=37.65 13   2 yes (0.1538462 0.8461538) *
      7) bmi>=40.85 66  25 yes (0.3787879 0.6212121)  
       14) skin_thickness>=37.5 24  11 no (0.5416667 0.4583333)  
         28) skin_thickness< 41.5 11   2 no (0.8181818 0.1818182) *
         29) skin_thickness>=41.5 13   4 yes (0.3076923 0.6923077) *
       15) skin_thickness< 37.5 42  12 yes (0.2857143 0.7142857) *
```

```r
# Graph the model
model_trained |>
  extract_fit_engine() |>
  rpart.plot::rpart.plot()
```



Tip

Each node shows:

- the predicted class (`no` or `yes` diabetes),
- the predicted probability of diabetes,
- the percentage of observations in the node.

Note

That pipeline was perfectly handcrafted!f Let's head over to the engine room to check your model's performance.

Predict and evaluate - (video)

1.7 Make predictions

Making predictions with data is one of the fundamental goals of machine learning. Now that you know how to split the data and fit a model, it's time to make predictions about unseen samples with your models.

You are going to make predictions about your test set using a model obtained by fitting the training data to a tree specification.

Available in your workspace are the datasets that you generated previously (`diabetes_train` and `diabetes_test`) and a decision tree specification `tree_spec`, which was generated using the following code:

```
tree_spec <- decision_tree() |>
  set_engine("rpart") |>
  set_mode("classification")
diabetes_train <- training(diabetes_split)
diabetes_test <- testing(diabetes_split)
```

Instructions

- Fit your specification to the training data using `outcome` as the target variable and all predictors to create model.

```
# Train your model
model <- tree_spec |>
  fit(outcome ~ ., data = diabetes_train)
```

- Use your `model` to predict the outcome of diabetes for every observation in the test set and assign the result to `predictions`.

```
# Generate predictions
predictions <- predict(model,
                       new_data = diabetes_test,
                       type = "class")
```

- Add the true test set outcome to `predictions` as a column named `true_class` and save the result as `predictions_combined`.

```
# Add the true outcomes
predictions_combined <- predictions |>
  mutate(true_class = diabetes_test$outcome)
```

- Use the `head()` function to print the first rows of the result.

```
# Print the first  6 lines of the result
predictions_combined |>
  head() |>
  kable()
```

.pred_class	true_class
no	yes
no	no
no	yes
no	no
no	yes
no	yes

Note

Now every predicted `.pred_class` has its `true_class` counterpart. The natural next step would be to compare these two and see how many are correct. You are about to find out in the next exercise.

1.8 Crack the matrix

Visual representations are a great and intuitive way to assess results. One way to visualize and assess the performance of your model is by using a confusion matrix. In this exercise, you will create the confusion matrix of your predicted values to see in which cases it performs well and in which cases it doesn't.

The result of the previous exercise, `predictions_combined`, is still loaded.

Instructions

- Calculate the confusion matrix of the `predictions_combined` tibble and save it as `diabetes_matrix`. Print the result to the console.

```
# The confusion matrix
diabetes_matrix <- conf_mat(predictions_combined,
                            truth = true_class,
                            estimate = .pred_class)

# Print the matrix
diabetes_matrix
```

```
          Truth
Prediction no yes
       no  99  36
       yes 26  31
```

```
# Print metrics
diabetes_matrix |>
  summary() |>
  kable()
```

.metric	.estimator	.estimate
accuracy	binary	0.6770833
kap	binary	0.2638219
sens	binary	0.7920000
spec	binary	0.4626866
ppv	binary	0.7333333
npv	binary	0.5438596
mcc	binary	0.2657016
j_index	binary	0.2546866
bal_accuracy	binary	0.6273433
detection_prevalence	binary	0.7031250
precision	binary	0.7333333
recall	binary	0.7920000
f_meas	binary	0.7615385

- Out of all true `no` outcomes, what percent did your model correctly predict?

```
99/(99 + 26)
```

```
[1] 0.792
```

```
sens(predictions_combined,
     truth = true_class,
     estimate = .pred_class) -> M1
M1
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 sens    binary         0.792
```

> Note
>
> Your model found 79.2% of all positive (`no` diabetes) outcomes. This measure is called ***sensitivity***.

1.9 Are you predicting correctly?

Your model should be as good as possible, right? One way you can assess this is by counting how often it predicted the correct classes compared to the total number of predictions it made. As discussed in the video, we call this performance measure accuracy. You can either calculate this manually or by using a handy shortcut. Both obtain the same result.

The confusion matrix `diabetes_matrix` and the tibble `predictions_combined` are loaded.

Instructions

- Print `diabetes_matrix` to the console and use its entries to directly calculate `correct_predictions`, the number of correct predictions. Save the total number of predictions to `all_predictions`. Calculate and the accuracy, save it to `acc_manual`, and print it.

```
diabetes_matrix
```

```
          Truth
Prediction no yes
       no  99  36
       yes 26  31
```

```
# Calculate the number of correctly predicted classes
correct_predictions <- 99 + 31

# Calculate the number of all predicted classes
all_predictions <- 99 + 36 + 26 + 31

# Calculate and print the accuracy
acc_manual <- correct_predictions / all_predictions
acc_manual
```

```
[1] 0.6770833
```

- Calculate the accuracy using a `yardstick` function and store the result in `acc_auto`. Print the accuracy estimate.

```
# The accuracy calculated by a function
acc_auto <- accuracy(predictions_combined,
                     truth = true_class,
                     estimate = .pred_class)
acc_auto$.estimate
```

```
[1] 0.6770833
```

- Accuracy is very intuitive but also has its limitations. Imagine we have a naive model that always predicts `no`, regardless of the input. What would the accuracy be for that model?

```
HDF <- data.frame(true_class = diabetes_test$outcome,
                  .pred_class = factor(rep("no", 192),
                                       levels = c("no", "yes")))

accuracy(HDF, truth = true_class, estimate = .pred_class)
```

```
# A tibble: 1 x 3
  .metric  .estimator .estimate
  <chr>    <chr>          <dbl>
1 accuracy binary         0.651
```

For the naive model, it would be accurate 65.1% of the time.

Note

A naive model always predicting no is almost as good as our model. Luckily there are more useful performance metrics which we'll cover later in the course. Stay tuned for Chapter 3!

References