Welcome to the course!

MACHINE LEARNING WITH TREE-BASED MODELS IN R

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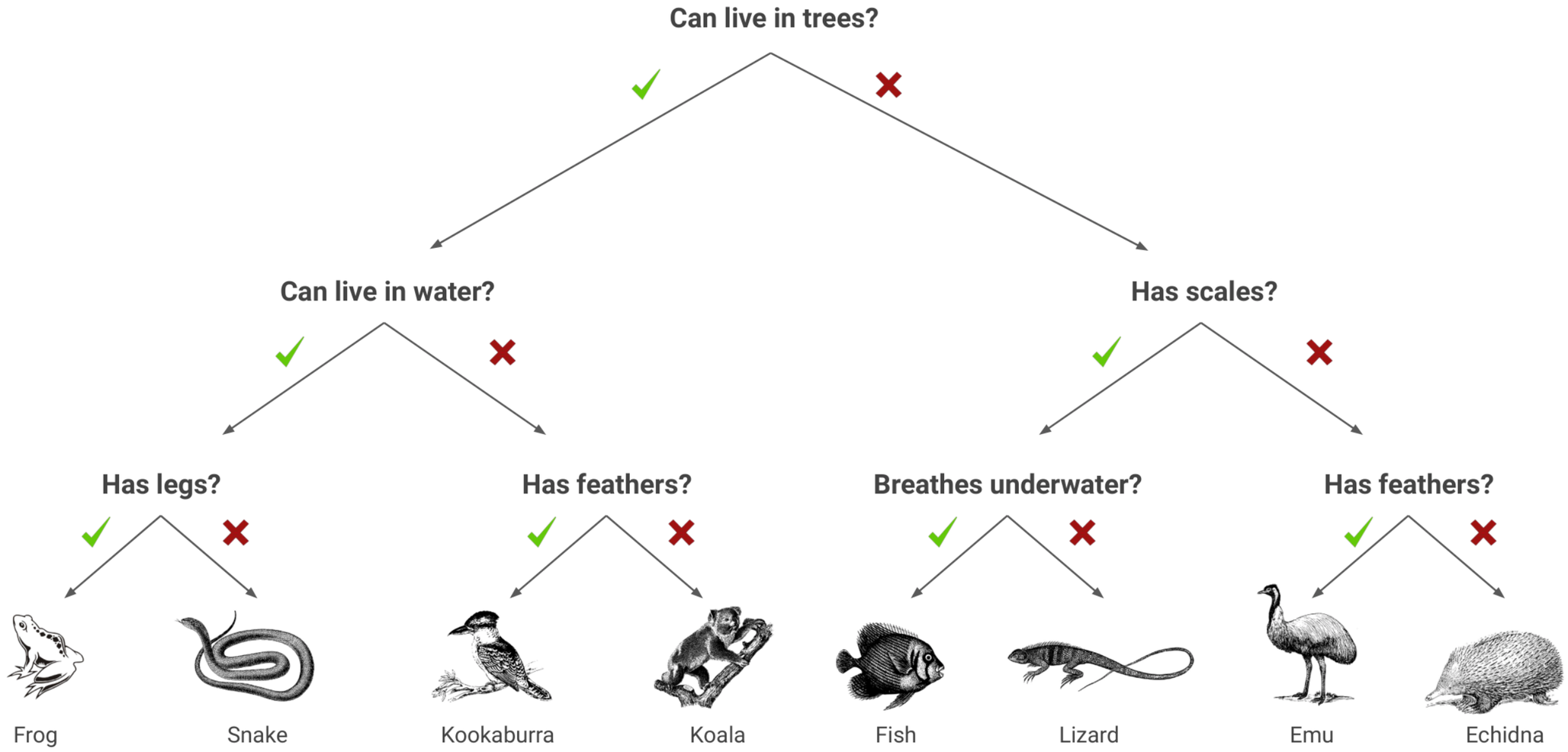
Course overview

- **Chapter 1**: Classification trees
- **Chapter 2**: Regression trees, cross-validation, bias-variance tradeoff
- **Chapter 3**: Hyperparameter tuning, bagging, random forests
- **Chapter 4**: Boosted trees

Decision trees are flowcharts



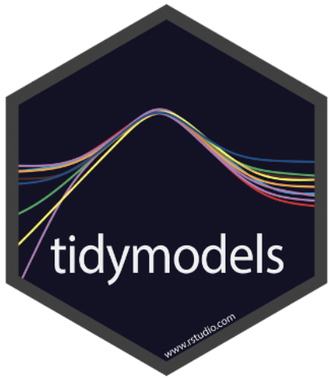
[1] https://aca.edu.au/resources/decision-trees-classifying-animals/decision-trees.pdf

Advantages of tree-based models

- Easy to explain and understand
- Possible to capture non-linear relationships
- Require no normalization or standardization of numeric features
- No need to create dummy indicator variables
- Robust to outliers
- Fast for large datasets

Disadvantages of tree-based models

- Hard to interpret if large, deep, or ensembled
- High variance, complex trees are prone to overfitting



Splitting data

Preprocessing

Model specifications

Model performance

View models and metrics in a tidy way

Make modeling workflow

Tune hyperparameters and get performance metrics

Tune hyperparameters

The tidymodels package

```
library(tidymodels)
```

```
-- Attaching packages --------------------- tidymodels 0.1.2 --
v parsnip   0.1.4       v rsample   0.0.8
v dplyr     1.0.2       v tibble    3.0.4
v yardstick 0.0.7       v tune      0.1.2
```

Create a decision tree

Specification / functional design

1. Pick a model class

```
library(tidymodels)


decision_tree()
```

```
Decision Tree Model Specification (unknown)
```

Create a decision tree

2. Set the engine that powers your model

```
library(tidymodels)


decision_tree() %>%
    set_engine("rpart")
```

```
Decision Tree Model Specification (unknown)


Computational engine: rpart
```

Create a decision tree

3. Set the mode (classification or regression)

```
library(tidymodels)

decision_tree() %>%
     set_engine("rpart") %>%
     set_mode("classification")
```

```
Decision Tree Model Specification (classification)

Computational engine: rpart
```

From a model specification to a real model

Specification is a skeleton and needs data to be trained with

```
library(tidymodels)
tree_spec <- decision_tree() %>%
               set_engine("rpart") %>%
               set_mode("classification")
```

```
# A model specification is fit using a formula to training data
tree_spec %>%
  fit(formula = outcome ~ age + bmi,
      data = diabetes)
```

```
parsnip model object
Fit time: 19 ms
n = 652
```

Let's build a model!

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How to grow your tree

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Diabetes dataset

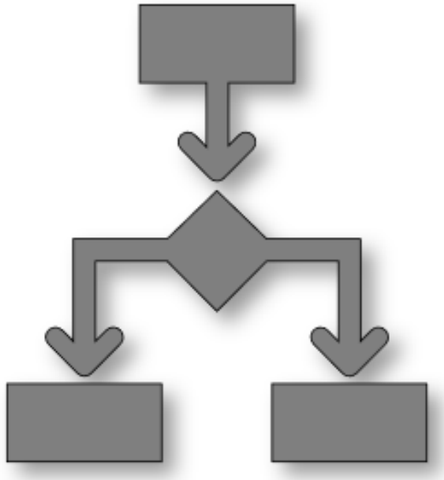
```
head(diabetes)
```

```
# A tibble: 6 x 9
  outcome pregnancies glucose blood_pressure skin_thickness insulin   bmi    age
  <fct>         <int>   <int>          <int>          <int>   <int> <dbl>  <int>
1 yes               6     148             72             35       0  33.6     50
2 no                1      85             66             29       0  26.6     31
3 yes               8     183             64              0       0  23.3     32
```

Using the whole dataset

- Used all your data for training - no data left to test the model

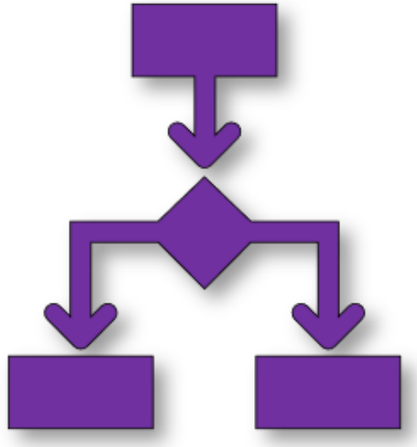
Decision tree



Performance check

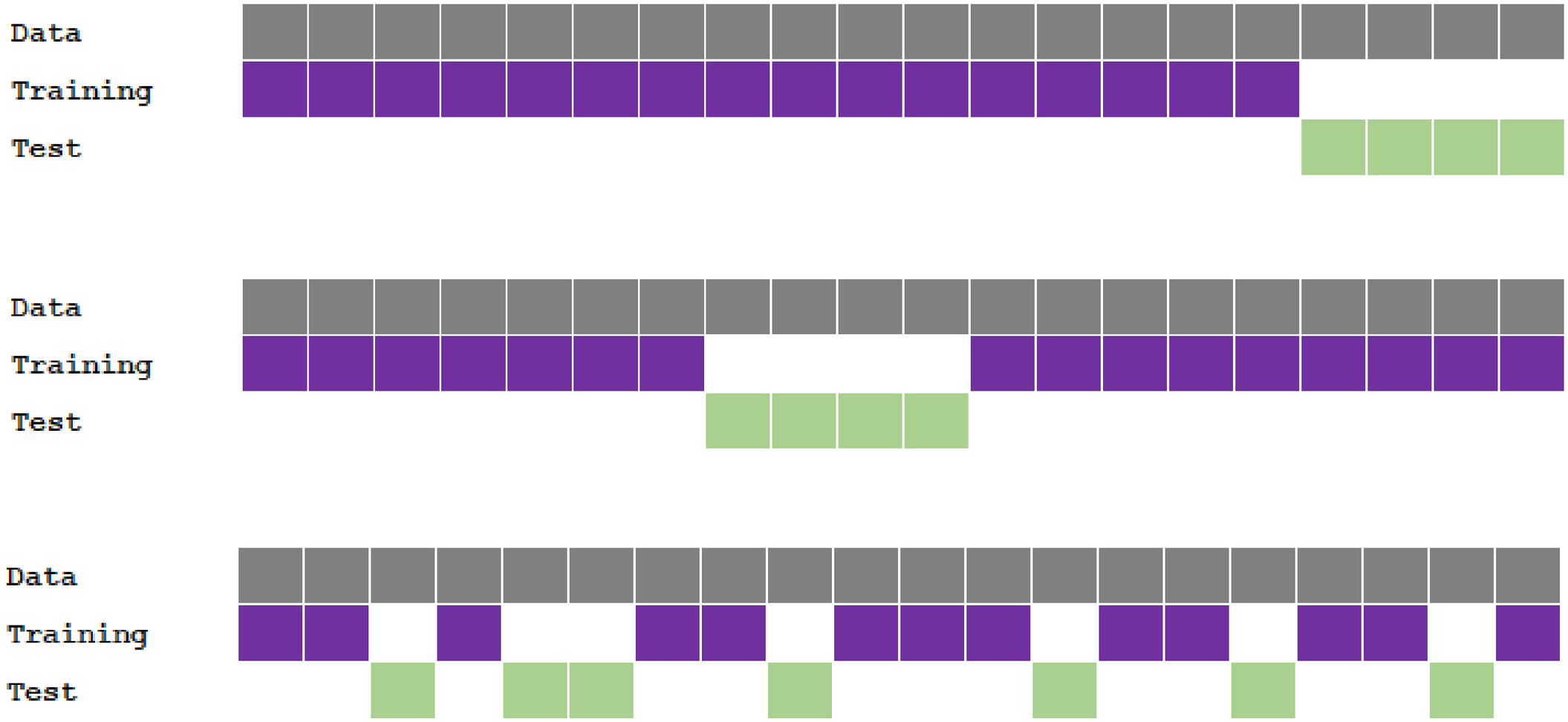
Data split

Decision tree



Performance check

Splitting methods



The initial_split() function

- Splits data randomly into single training and single test set

```
# Split data proportionally (default: 0.75)
diabetes_split <- initial_split(diabetes, prop = 0.9)
diabetes_split
```

```
<Analysis/Assess/Total>
<692/76/768>
```

[1] from the rsample package

Functions training() and testing()

- Extract training and test sets from a data split

```
diabetes_train <- training(diabetes_split)
diabetes_test  <- testing(diabetes_split)
```

- Verification:

```
nrow(diabetes_train)/nrow(diabetes)
```

```
[1] 0.9007812
```

[1] from rsample

Avoid class imbalances

```
# Training count of 'yes' and 'no' outcomes
counts_train <- table(diabetes_train$outcome)
counts_train
```

```
 no yes
490 86
```

```
# Test data count of 'yes' and 'no' outcomes
counts_test <- table(diabetes_test$outcome)
counts_test
```

```
 no yes
 28  48
```

```
# Training proportion of 'yes' outcome
prop_yes_train <- counts_train["yes"]/
                  sum(counts_train)
prop_yes_train
```

```
0.15
```

```
# Test data proportion of 'yes' outcome
prop_yes_test <- counts_test["yes"]/
                     sum(counts_test)
prop_yes_test
```

```
0.63
```

Solution - enforce similar distributions

```
initial_split(diabetes,
              prop = 0.9,
              strata = outcome)
```

- Ensures random split with similar distribution of `outcome` variable

Let's split!

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Predict and evaluate

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Predicting on new data

General call:

```
predict(model, new_data, type)
```

Arguments:

1. Trained model
2. Dataset to predict on
3. Prediction type: labels or probabilities

Predicting on new data

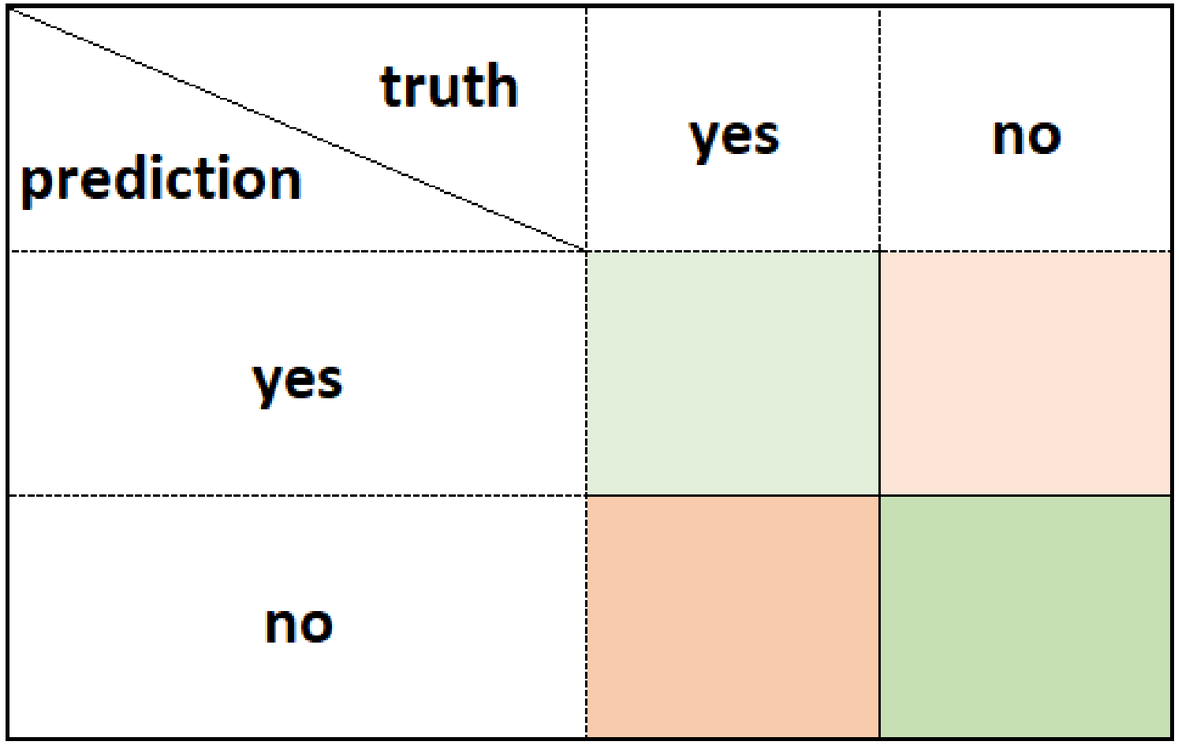
```
predict(model, new_data = test_data,
                type = "class")
```

```
  .pred_class
  <fct>
1 no
2 no
3 yes
4 no
```

```
predict(model, new_data = test_data,
                type = "prob")
```

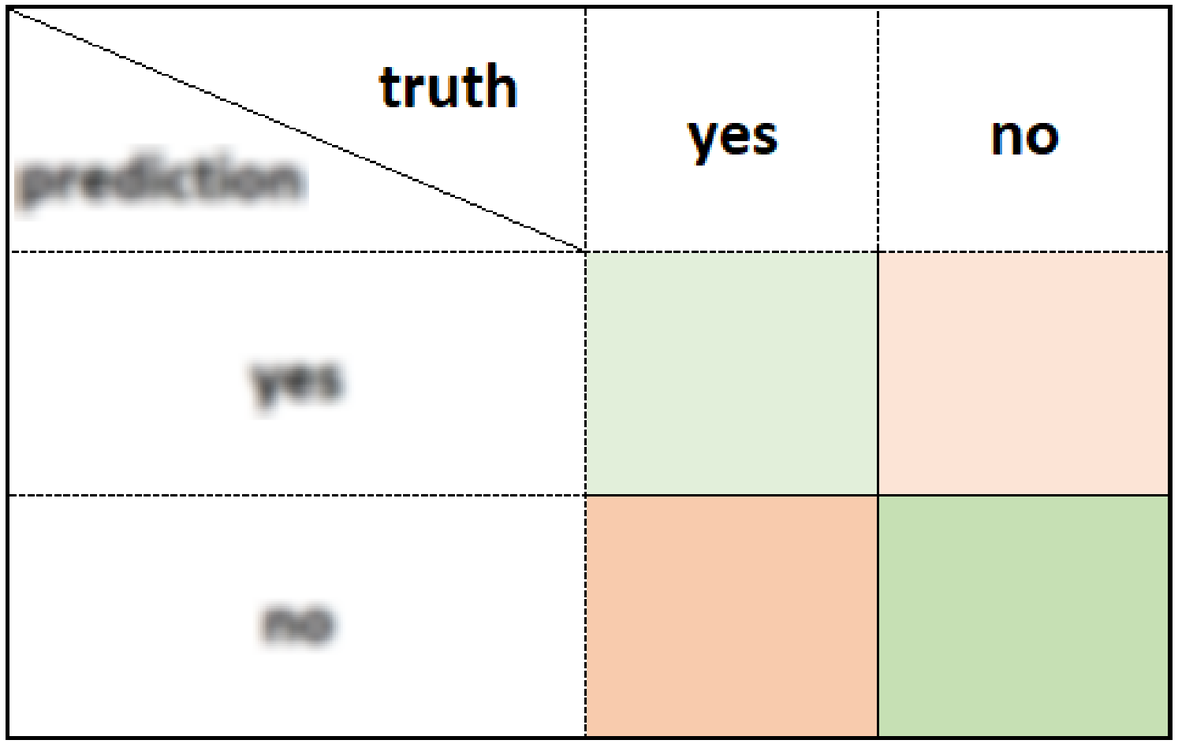
```
     .pred_no  .pred_yes
     <dbl>     <dbl>
1    0.866     0.134
2    0.956     0.044
3    0.672     0.328
4    0.877     0.123
```

Confusion matrix

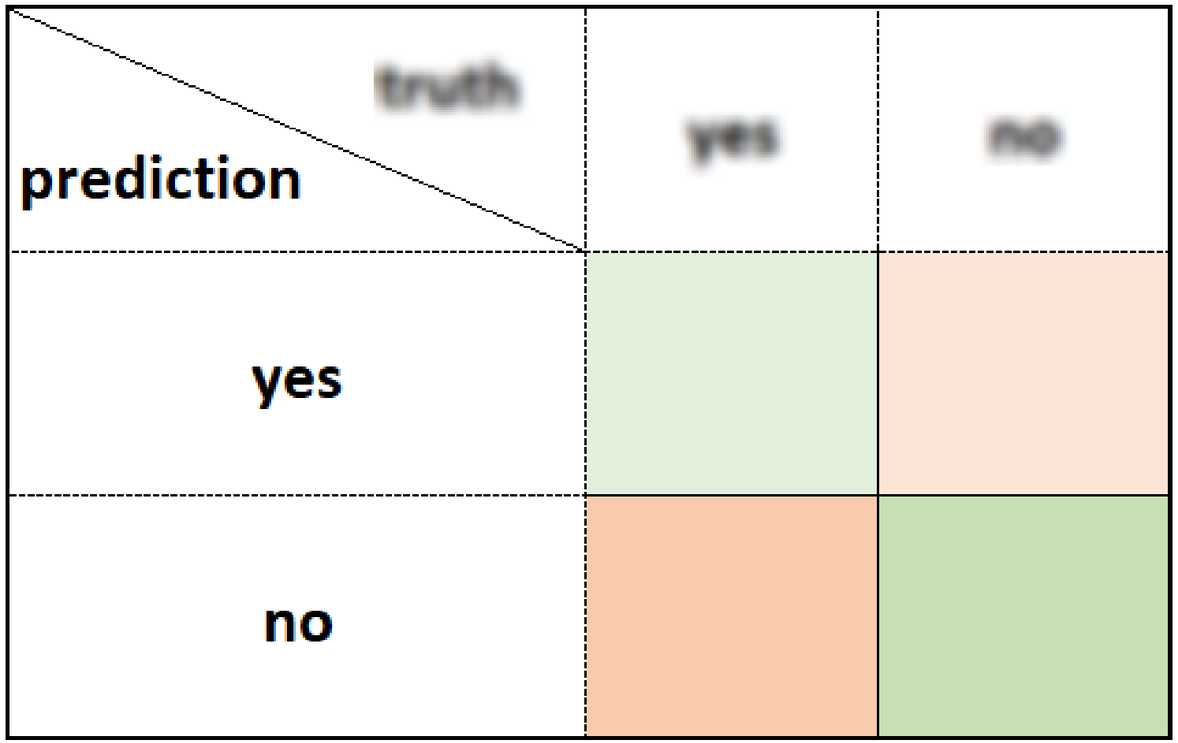


- Reveals how confused a model is

Confusion matrix



Confusion matrix



Confusion matrix

prediction \ truth	yes	no
yes	378	8
no	2	132

- Diagonal: correct predictions
- Off-diagonal: incorrect predictions

Confusion matrix

- **TP**: prediction is **yes**, truth is **yes**
- **TN**: prediction is **no**, truth is **no**
- **FP**: prediction is **yes**, truth is **no**
- **FN**: prediction is **no**, truth is **yes**

prediction \ truth	yes	no
yes	TP	FP
no	FN	TN

Create the confusion matrix

```
# Combine predictions and truth values
pred_combined <- predictions %>%
   mutate(true_class = test_data$outcome)

pred_combined
```

```
  .pred_class  true_class
  <fct>        <fct>
1 no           no
2 no           yes
3 no           no
4 yes          yes
```

```
# Calculate the confusion matrix
conf_mat(data = pred_combined,
         estimate = .pred_class,
         truth = true_class)
```

```
            Truth
Prediction    no   yes
       no    116    31
      yes     12    40
```

Accuracy

$$\text{accuracy} = \frac{\text{n of correct predictions}}{\text{n of total predictions}}$$

- Function name: `accuracy()`
- Same arguments as `conf_mat()`
  - `data`, `estimate` and `truth`
  - Common structure in `yardstick`

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

```
  .metric     .estimate
  <chr>           <dbl>
1 accuracy        0.708
```

Let's evaluate!

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