# **Topics in Computational Social Science - Lab 2**

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# **Lab 2: Machine Learning and Prediction**

In this lab, we will cover the basics of fitting and assessing supervised machine learning algorithms. Specifically, we will cover fitting a random forest model, sample splitting, and model performance metrics. As discussed in lecture, these machine learning methods are being increasingly applied in the social sciences. For an overview on applications of machine learning in sociology and best practices, please see:

- Molina, Mario, and Filiz Garip. 2019. 'Machine Learning for Sociology'. Annual Review of Sociology 45(1):27–45. doi: 10.1146/annurev-soc-073117-041106.
- Kapoor, Sayash, Emily Cantrell, Kenny Peng, Thanh Hien Pham, Christopher A. Bail, Odd Erik Gundersen, Jake M. Hofman, Jessica Hullman, Michael A. Lones, Momin M. Malik, Priyanka Nanayakkara, Russell A. Poldrack, Inioluwa Deborah Raji, Michael Roberts, Matthew J. Salganik, Marta Serra-Garcia, Brandon M. Stewart, Gilles Vandewiele, and Arvind Narayanan. 2023. 'REFORMS: Reporting Standards for Machine Learning Based Science'. doi: 10.1126/sciadv.adk3452.

### **Exercise 1**

In exercise 1, we'll simulate some data and practice fitting and assessing the performance of models. We'll fit an ordinary least squares (OLS) regression model and random forest model (one of the most popular machine learning algorithms).

Simulating data can be a helpful way of building intuition for machine learning and statistical concepts. When we simulate data, we can control the specific relationship between the features/predictors and the outcome. By generating data with known relationships between features (predictors) and the outcome, we can assess how well different algorithms recover these relationships. Since we know the true underlying relationships in simulated data, we can directly compare the estimated results to the ground truth.

Here, we'll investigate the (hypothetical) association between coffee consumption in cups and reported average stress level for a day. Before we get started, we'll load in all the packages we need for our analysis.

```
— Conflicts -
                                                       - tidyverse_conflicts() —
* dplyr::filter() masks stats::filter()
* dplyr::lag()
                 masks stats::lag()
i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts
to become errors
library(tidymodels)
                      ## machine learning package
— Attaching packages -
                                                            - tidymodels 1.1.1 —
                                         1.2.0
✓ broom
               1.0.5
                          ✓ rsample

✓ dials

              1.2.1

✓ tune

                                         1.1.2
✓ infer
               1.0.6
                          ✓ workflows
                                         1.1.4
                          ✓ workflowsets 1.0.1

✓ modeldata

              1.3.0
                                         1.3.1
✓ parsnip
              1.2.0
                          ✓ yardstick
✓ recipes
               1.0.10
— Conflicts -
                                                     – tidymodels_conflicts() —
* scales::discard() masks purrr::discard()
* dplyr::filter() masks stats::filter()
* recipes::fixed() masks stringr::fixed()
* dplyr::lag() masks stats::lag()
* yardstick::spec() masks readr::spec()
* recipes::step() masks stats::step()
• Learn how to get started at https://www.tidymodels.org/start/
 library(cowplot)
                       ## pretty plots
```

Attaching package: 'cowplot'

The following object is masked from 'package:lubridate':

stamp

```
library(ranger) ## ranger

## set seed for reproducibility
set.seed(47)
```

We also set a seed for this analysis. This ensures that our results are reproducible. A **seed** is an initial value used by a random number generator to produce a sequence of pseudo-random numbers. Setting a seed ensures that the same sequence of random numbers is generated every time the code is run, making results reproducible and consistent across different runs.

# Simulating data

To simulate the data, we'll use a few helpful functions:

- runif generates n draws from uniform distribution between a given min and max value
- rnorm generates n draws with a given mean and standard deviation

We'll create a predictor variable (in machine learning language, a "feature") called coffee. This will correspond to cups of coffee consumed in a given day.

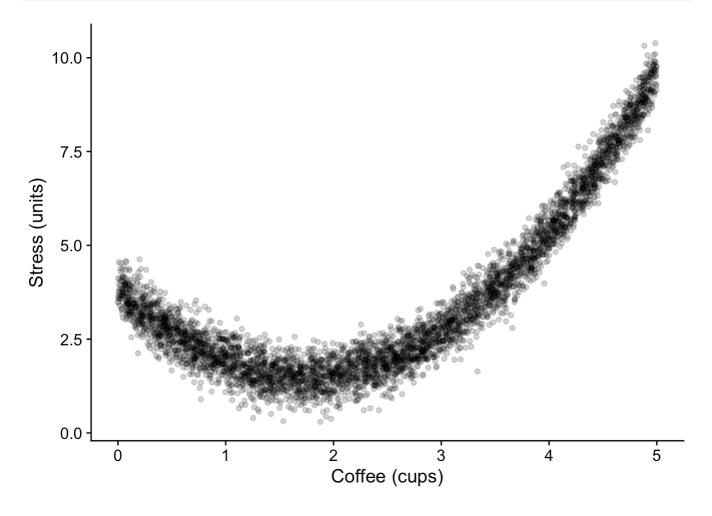
We'll then create an outcome variable stress that is related to coffee in a non-linear fashion. We'll combine these two variables together into one data.frame.

```
## non-linear data
coffee = runif(n = 5000, min = 0, max = 5)
stress = ((2 * coffee^2) - (7 * coffee) + 10 + rnorm(n = 5000, mean = 0, sd = 1))/2.6

## create a data frame with columns coffee and stress
sim_data <- data.frame(coffee, stress)</pre>
```

## **Exploratory data analysis**

The first thing that you want to do when you get new data is exploratory data analysis. The primary goal of exploratory data analysis is to take a first pass at detecting patterns, spot anomalies/outliers, and summarize key characteristics. The best way to start is often through **visualization**.



In machine learning, sample splitting is a key step to ensure that models generalize well to unseen data. The simplest sample splitting is a test-train split. Recall from lecture:

- The training set is used to fit the model
- The testing set evaluates how well the model performs on unseen data

This helps prevent overfitting, where a model performs well on training data but poorly on new data.

To split the sample, we can use the initial\_split() function from the rsample package. The rsample package is part of the tidymodels framework.

This function will automatically randomly split the data into a training partition and a test partition according to the proportions we provide as an argument to the function.

```
## split into two folds (partitions)
sim_data_split <- initial_split(sim_data, prop = .75)

## split into a train-test sample
sim_data_train <- training(sim_data_split)
sim_data_test <- testing(sim_data_split)</pre>
```

# Simple Ordinary Least Squares (OLS) Regression Model

First, we'll try fitting an OLS regression model (linear regression). Simple models like OLS are easy to interpret and are generally a good starting place for the modeling process. We'll fit a model of the form:

$$\hat{Y} = \beta_0 + \beta_1 X + \varepsilon$$

Where:

- $\hat{Y}$  represents the predicted *stress*
- $\beta_0$  is the intercept
- $\beta_1$  is the coefficient for *cups of coffee*
- X is the \texttt{coffee} variable,
- $\varepsilon$  represents the error term

They can also serve as a helpful benchmark to help you understand how much better more complex machine learning algorithms are doing than a simple model.

```
# Fit models
model_linear <- lm(stress ~ coffee, data = sim_data_train)
## print out summary of linear model
summary(model_linear)</pre>
```

```
Call:
```

lm(formula = stress ~ coffee, data = sim\_data\_train)

#### Residuals:

```
Min
         10 Median
                      3Q
                           Max
-2.832 -1.222 -0.362 1.111 4.030
```

#### Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.65581 0.04789 13.69 <2e-16 ***
coffee
          1.14323
                     0.01667 68.58 <2e-16 ***
```

Signif. codes: 0 '\*\*\* 0.001 '\*\* 0.01 '\* 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.472 on 3748 degrees of freedom Multiple R-squared: 0.5565, Adjusted R-squared: 0.5564 F-statistic: 4703 on 1 and 3748 DF, p-value: < 2.2e-16

```
# Predict on the test datasets
predicted_stress <- predict(model_linear, sim_data_test)</pre>
```

Understanding check: What is the intercept telling us? What is the coefficient for coffee telling us? Are the coefficients significant? Do significant coefficients tell us anything about model performance?

### **Model Performance Metrics**

To assess the performance of our model, we'll use several different model performance metrics.

### Mean Absolute Error (MAE)

MAE measures the average absolute differences between actual and predicted values:

$$ext{MAE} = rac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

It provides an intuitive measure of the magnitude of error, treating all deviations equally.

### Root Mean Squared Error (RMSE)

RMSE squares the errors before averaging, making it more sensitive to large deviations. It then takes the square root of the mean squared errors to bring the error units back to the original scale of the dependent variable, making it easier to interpret compared to Mean Squared Error (MSE):

$$ext{RMSE} = \sqrt{rac{1}{n}\sum_{i=1}^n (y_i - \hat{y}_i)^2}$$

This metric is widely used and penalizes large errors more than smaller ones.

# R-squared ( $R^2$ )

 ${\mathbb R}^2$  quantifies how well the model explains variance in the dependent variable:

$$R^2 = 1 - rac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - ar{y})^2}$$

where  $\bar{y}$  is the mean of the observed values. Higher values indicate a better fit, with  $R^2=1$  representing a perfect model and  $R^2=0$  representing a model doing no better than predicing mean of outcome variable.

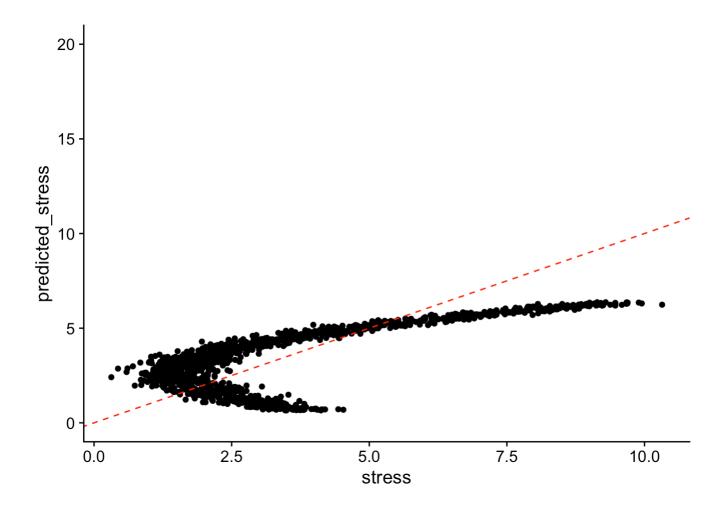
Each metric provides different information. MAE is simple to interpret, RMSE places a larger penalty on larger errors (why might we want this?), and  $R^2$  provides a simple metric of overall model fit.

To assess model performance, we'll need to add our predictions onto our test data.

```
## add predictions onto test (hold-out) data
sim_data_test_w_predictions <- sim_data_test %>%
mutate(predicted_stress = predicted_stress)
```

Now, let's visualize our errors in a calibration plot, which allows us to directly compare the predicted vs. actual values and analyze residuals.

```
sim_data_test_w_predictions %>%
  ggplot(aes(x = stress, y = predicted_stress)) +
  geom_point() +
  theme_cowplot() +
  ylim(0, 20) +
  geom_abline(color = "red", linetype = "dashed")
```



If our predictions were perfect, they would lie along the red dashed line at 45 degrees. Here, we see lots of deviations away from this line... based on this visual check, it looks like our model could be improved!

# Calculate model performance metrics

To more formally assess the performance of our model, we'll calculate the three error metrics introduced above. We'll write functions to calculate these error metrics—in general, if you anticipate reusing code more than once, it can be helpful to write a function. Spend a little bit of time following the logic of each function and ensuring it's correct.

```
# Function to compute Mean Absolute Error (MAE)
mae <- function(actual, predicted) {
    mean(abs(actual - predicted))
}

# Function to compute Root Mean Squared Error (MSE)
rmse <- function(actual, predicted) {
    sqrt(mean((actual - predicted)^2))
}

# Function to compute R-squared (R²)
r_squared <- function(actual, predicted) {
    ss_total <- sum((actual - mean(actual))^2)
    ss_residual <- sum((actual - predicted)^2)</pre>
```

```
1 - (ss_residual / ss_total)
}
```

Let's use the functions we just created to calculate model performance metrics for our linear model:

```
rmse mae r_squared
1 1.490971 1.271684 0.5504965
```

The model is doing moderately well — the  $\mathbb{R}^2$  value tells us that 56% of the variance is explained by the model (but 44% is not).

# Machine learning - random forest

Random forest is an ensemble learning method that improves prediction accuracy by combining multiple decision trees.

At a high level, random forest works by:

- 1. Creating multiple decision trees using different random subsets of the training data
- 2. Averaging predictions across trees (for regression) to make a final prediction
- 3. Reducing overfitting by ensuring that individual trees don't rely too heavily on any single feature or pattern in the data

Random Forest is particularly useful for handling nonlinear relationships (like ours!), high-dimensional datasets (many features), and noisy data. We'll use it to model the relationship between coffee and stress and evaluate whether it outperforms our linear model. We picked random forest because of its popularity and versatility.

To fit the model, we'll use the tidymodel <u>package</u>. This is a well-maintained modern framework in R for streamlining machine learning workflows. It's similar to the tidyverse in that it contains multiple core packages and adheres to tidyverse principles.

We'll first need to define the random forest model we want to fit. We'll start by specifying the *hyperparameters* for our random forest model. Hyperparameters are configurable settings that control a model's learning process; they have to be specified in advance and not learned from the data. Here's the hyperparameters we'll use:

- mtry = 1: Only one predictor is considered for each split (we only have 1 predictor).
- trees = 500: The model builds 500 decision trees for better averaging.
- min\_n = 5: Each terminal node must have at least 5 observations.

We'll set the engine to Ranger, which is a fast implementation of random forest. We'll also need to specify that this is a regression problem (predicting a continuous outcome) and not a classification problem (predicting a categorical or binary outcome).

```
# Define a random forest model specification
rf_spec <- rand_forest(mtry = 1, trees = 500, min_n = 5) %>%
    set_engine("ranger") %>%
    set_mode("regression")

# Train the Random Forest model
rf_fit <- rf_spec %>%
    fit(stress ~ coffee, data = sim_data_train)
```

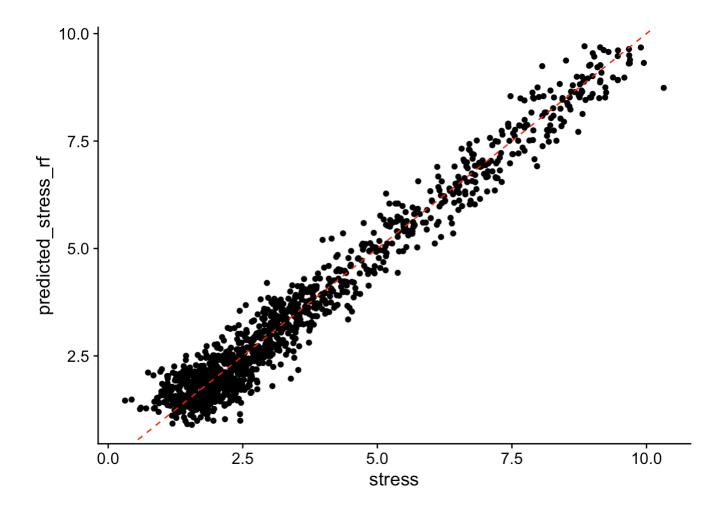
Next, we'll use our random forest model to make predictions in our *test* dataset.

```
## make predictions
sim_data_test_rf <- predict(rf_fit, new_data = sim_data_test)

# Rename predicted column
sim_data_test_rf_predictions <- sim_data_test_rf %>%
bind_cols(sim_data_test) %>%  # Add actual values for comparison
rename(predicted_stress_rf = .pred) # Rename predictions to be normal
```

Let's make a calibration plot to compare how well our random forest predictions are doing out-of-sample.

```
sim_data_test_rf_predictions %>%
  ggplot(aes(x = stress, y = predicted_stress_rf)) +
  geom_point() +
  theme_cowplot() +
  geom_abline(color = "red", linetype = "dashed")
```



This quick visual inspection suggests that our random forest model is performing much better than our linear regression! There is much higher agreement between our true, observed stress and our predicted stress. Let's investigate this more formally...

# **Exercise 1 questions:**

- **1.1** Using our model performance functions from above, calculate for the random forest algorithm's predictions in the *test* data:
  - i. Mean Absolute Error (MAE)
  - ii. Root Mean Squared Error (RMSE)
  - iii.  $\mathbb{R}^2$  (Coefficient of Determination)
- **1.2** Does the random forest model or linear regression model have better predictive accuracy? Compare their MAE, RMSE, and  $\mathbb{R}^2$ . Does it matter which error metric we use?
- **1.3** Bias in machine learning refers to the systematic deviation of model predictions from the true values. A model is considered biased if it consistently overestimates or underestimates the actual values. To formally assess bias, we compute the average prediction error (mean residual):

$$ext{Bias} = rac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_{ ext{true},i})$$

Write a function to calculate bias (hint: modify the mean absolute error function). Apply this function

to predictions from both the linear model and random forest model. Do either of the models systematically over- or under-predict?

# **Exercise 2 - Predicting Subnational Internet Adoption**

In exercise 2, we will train and evaluate a random forest model to predict internet adoption among women aged 15–49 at the first administrative level (e.g., state). Unlike previous exercises, we will use real-world data rather than simulated data.

Our dataset includes various subnational features, such as:

- The weighted proportion of men and women on Facebook
- Geospatial indicators, such nightlight intensity

To assess how well our model generalizes, we will use two different cross-validation strategies.

### Read in real data

Download the css\_lab2\_subnational\_internet.csv file from the canvas page and read it in using the read\_csv package.

```
## read in data
## you'll need to updat this path
internet_df <- read_csv("~/Downloads/css_lab2_subnational_internet.csv")</pre>
```

```
Rows: 570 Columns: 14

— Column specification —
Delimiter: ","
chr (2): gid_1, country
dbl (12): perc_used_internet_past12months_wght_age_15_to_49_wom, perc_used_i...

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

### **Feature Definitions**

It's important to understand what each variable (feature) in your dataset is telling you. Often there is a codebook or some other documentation available that provides descriptions of features along with other helpful information. This is a good place to start—sometime variables (features) aren't actually capturing what you would expect!

Here's the descriptions of the features we have available in our dataset:

- gid\_1: Subnational administrative unit identifier (from GADM, a global administrative boundaries database).
- country: Name of the country corresponding to the administrative unit.
- perc\_used\_internet\_past12months\_wght\_age\_15\_to\_49\_wom: Percentage of women (ages 15–49) who used the internet in the past 12 months, weighted.
- perc\_used\_internet\_past12months\_wght\_age\_15\_to\_49\_fm\_ratio: Female-to-male ratio of internet usage among individuals aged 15–49, weighted.

- hdi\_national: National-level composite measure of health, education, and standard of living.
- gdi\_national: National-level Gender Development Index (GDI), measuring inequality with respect to life expectancy at birth, education, and expected years of schooling
- subnational\_gdi: Subnational-level Gender Development Index
- subnational\_hdi\_females: Subnational composite measure of health, education, and standard of living for women
- subnational\_hdi\_males: Subnational composite measure of health, education, and standard of living for men
- nl\_mean\_zscore: Z-score of nighttime lights intensity, often used as a proxy for economic activity.
- pop\_density\_zscore: Z-score of population density, normalizing population per unit area.
- fb\_pntr\_18p\_female: Facebook penetration rate among women aged 18+ (percentage of women on Facebook in the last month relative to population).
- fb\_pntr\_18p\_male: Facebook penetration rate among men aged 18+ (percentage of women on Facebook in the last month relative to population).

# Fit machine learning model

First, we'll split our data into a test and a training partition, just like we did in exercise 1.

```
## sgenerate train and test folds (partitions)
internet_df_split <- initial_split(internet_df, prop = .75)

## split into a train-test sample
internet_df_train <- training(internet_df_split)
internet_df_test <- testing(internet_df_split)

## check number of observations in each dataset
nrow(internet_df_train)/nrow(internet_df)</pre>
```

### [1] 0.7491228

```
nrow(internet_df_test)/nrow(internet_df)
```

#### [1] 0.2508772

Now we'll fit a random forest model again. We'll keep the same number of trees and tree depth as above (these are standard), but we'll now use 3 features in each decision tree (mtry = 3).

For this model, we'll start with just three features:

- 1. Night lights data (nl\_mean\_zscore) a proxy for economic activity and overall development
- 2. Facebook penetration among women (fb\_pntr\_18p\_female) an indicator of digital access
- 3. Subnational Human Development Index for females (subnational\_hdi\_females) subnational composite measure of health, education, and standard of living for women

```
# Define a random forest model specification
rf_spec <- rand_forest(mtry = 3, trees = 500, min_n = 5) %>%
    set_engine("ranger") %>%
```

Just to help build intuition, let's check our model performance metrics on the *training* data.

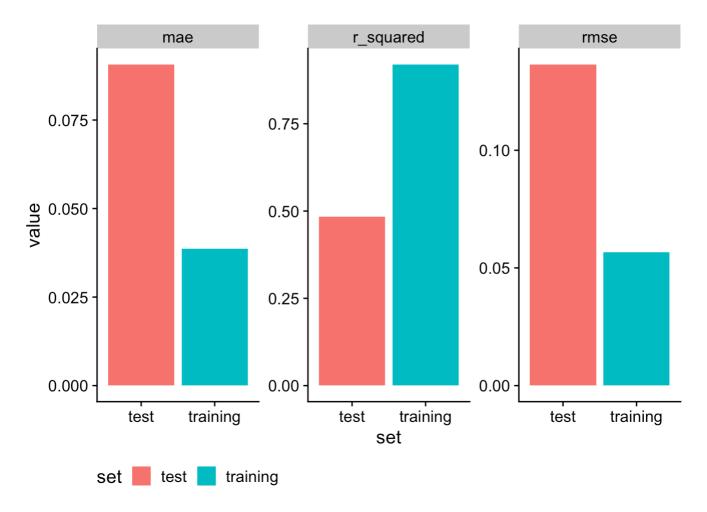
Our model performance here is amazing! So good, in fact, that we should be suspicious...remember, assessing model performance on the data we trained is highly misleading! A model can just memorize patterns in the training data.

Let's check how things look when we assess model performance in the test data:

Let's visualize the difference in model performance metrics.

```
model_performance_combined <- model_performance_metrics_training %>%
    mutate(set = "training") %>%
    bind_rows(model_performance_metrics_test %>% mutate(set = "test")) %>%
    pivot_longer(cols = -set, names_to = "metric", values_to = "value")

model_performance_combined %>%
    ggplot(aes(x = set, y = value, fill = set)) +
    geom_col() +
    facet_wrap(~metric, scales = "free") +
    theme_cowplot() +
    theme(legend.position = "bottom")
```



Does our model perform better in the test dataset or the training dataset? Is this consistent across all three metrics?

## **Cross-validation**

In traditional train-test splitting, a common limitation is that not all data points are used for both training and testing — this can lead to less efficient/reliable model evaluations. Cross-validation addresses this by ensuring that each observation is used in both training and validation phases, providing a more comprehensive assessment of the model's performance.

The most common method is k-fold cross-validation, where the data is split into k parts (folds). The model is trained on k-1 folds and tested on the remaining fold. This process repeats k times, with each fold used for testing once. The results are averaged to the overall performance metric.

That's what we'll do here. First, we'll use the vfold\_cv function to randomly split our dataset into 10 separate folds. For k-fold cross-validation, 10 is a fairly standard choice for the number of folds—but there may be settings where want to use a different number of folds.

We'll use our full dataset (we are using cross-validation instead of doing a test/train split).

```
## create folds
folds <- vfold_cv(internet_df, v = 10)
folds</pre>
```

```
# 10-fold cross-validation
# A tibble: 10 \times 2
   splits
                    id
   <list>
                    <chr>
 1 <split [513/57]> Fold01
 2 <split [513/57]> Fold02
 3 <split [513/57]> Fold03
 4 <split [513/57]> Fold04
 5 <split [513/57]> Fold05
 6 <split [513/57] > Fold06
 7 <split [513/57]> Fold07
 8 <split [513/57] > Fold08
 9 <split [513/57] > Fold09
10 <split [513/57] > Fold10
```

Like in the other examples, we need to define our random forest model. After we've defined our model, the key function we want to use for cross-validation is fit\_resamples(), which evaluates the model's performance using k-fold cross-validation. The function will fit the model to multiple subsets of the data and assesses its performance on corresponding test sets.

We'll also have the function automatically calculate the three model performance metrics we're interested in. We will need to manually specify the error metrics in the fit\_resamples() function from the yardstick package. We'll use mean absolute error (MAE), root mean squared error (RMSE), and  $\mathbb{R}^2$ .

```
# Define a random forest model specification (same as above)
rf_spec <- rand_forest(mtry = 3, trees = 500, min_n = 5) %>%
set_engine("ranger") %>%
set_mode("regression")

## Define a random forest specification
rf_res <- fit_resamples(
    rf_spec,
    perc_used_internet_past12months_wght_age_15_to_49_wom ~ fb_pntr_18p_female + subnati    resamples = folds,
    metrics = metric_set(yardstick::rmse, yardstick::mae, yardstick::rsq)
)</pre>
```

To access the error metric that were calculated by the fit\_resamples() function, we can use the collect\_metrics() function.

```
## get error metrics
error_metrics_10fold <- collect_metrics(rf_res)

## print out error metrics
error_metrics_10fold %>%
   mutate(cv_method = "10-fold")
```

```
# A tibble: 3 \times 7
  .metric .estimator mean
                           n std err .config
                                                         cv method
 <chr>
        <chr> <dbl> <int>
                                <dbl> <chr>
                                                         <chr>
1 mae
         standard 0.0897 10 0.00326 Preprocessor1_Model1 10-fold
2 rmse
                            10 0.00502 Preprocessor1 Model1 10-fold
         standard 0.130
3 rsq
         standard
                   0.669
                            10 0.0211 Preprocessor1_Model1 10-fold
```

Here, we're interested in the mean of the performance error metrics across the 10 different folds. Our model appears to be performing well, explaining 66% of the variation in internet adoption using only three features.

# **Exercises 2 - questions**

In our lab, we used standard 10-fold cross-validation. But perhaps we want to know how well our model would perform in countries we had no training data at all (e.g., not one of the 34 countries in our dataset).

To replicate this scenario, we can employ leave-one-country-out cross-validation. In this approach, we iteratively exclude all subnational units from one country, train the model on subnational units from the remaining countries, and then assess its performance on the excluded country's subnational units. This method evaluates the model's ability to generalize to unseen countries (assuming they are similar to the countries we have in our dataset).

**2.1** Test the performance of our model using leave-one-country-out cross-validation. Here, we'll split into folds based on country (rather than random). Calculate MAE, RMSE, and  $\mathbb{R}^2$ .

```
## hint: make new folds
folds <- group_vfold_cv(internet_df_train, group = country)
folds</pre>
```

- 10 <split [391/36] > Resample10
- # i 24 more rows
- **2.2** When we use leave-one-country-out cross-validation, does the model perform better or worse? Is this consistent across all three error metrics? Why might this be?
- **2.3** Create a calibration plot with our observed (x-axis) and predicted (y-axis) values for both 10-fold cross-validation and leave-one-country-out cross-validation predictions.

## **Bonus** exercises

- How can we improve our model's performance? Try playing around with (i) adding additional features and (ii) changing the hyperparameters. What helped the most? Assess performance using 10-fold cross-validation.
- With your best algorithm, what's the difference in  $\mathbb{R}^2$  as assessed using leave-one-country-out cross-validation vs. standard 10-fold cross-validation? Does this match your intuition?
- What real world data availability scenarios do leave-one-country-out cross-validation and 10fold cross-validation correspond to?
- What other features not in our model would you want to include to help improve the model's performance?