# Model Creation and Validation for the Social Vulnerability Index
# Training and Building Traditional Random Forest Models

Thesis for a Master of Public Health, Epidemiology

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## Contents

*Note: the table of contents acts as in-document hyperlinks*

## Statement of Purpose

The purpose of the file is to build is to build a multiple traditional random forest model (RF) and determine the best preforming model. The hyperparameters of the best model will then be used in a geographically weighted random forest model (GWFRF), which is preformed in the upsequent file. The following two sentence provide a overarching description of the two models. In a RF model, each tree in the forest is built from a different bootstrap sample of the training data, and at each node, a random subset of predictors (features) is considered for splitting, rather than the full set of predictors. A GWRF model expands on this concept by incorporating spatial information by weighting the training samples based on their geographic proximity to the prediction location. The splitting process in a RF model is determined by the mean squared error and in a GWRF is influenced by the spatial weights (i.e., weighted mean squared error), which adjust the contribution of each sample based on its geographic distance. Lastly, the feature importance plots will be generated for the final, and local feature importance plots will also be created.

### Defining Hyperparameters

In James et al 2021, Ch 8.2.2 Random Forests, James et al 2023, Ch 15.2 Definition of Random Forests and Garson 2021, Ch 5 Random Forest, the hyperparameters that are shared between the traditional RF and the geographically-weighted RF models include:

- **Number of randomly selected predictors**: This is the number of predictors (p) considered for splitting at each node. It controls the diversity among the trees. A smaller m leads to greater diversity, while a larger m can make the trees more similar to each other.
  - for regression this defaults to $p/3$, where $p$ is the total of predictor variables
- **Number of trees**: This is the total number of decision trees in the forest (m). More trees generally lead to a more stable and accurate model, but at the cost of increased computational resources and time.
  - for the `randomForest::randomForest()`, this defaults to 500

Additionally, GWRF involves an extra tuning spatial parameters:

- **Bandwidth parameter**: This controls the influence of spatial weights, determining how quickly the weight decreases with distance. A smaller bandwidth means only very close samples have significant influence, while a larger bandwidth allows more distant samples to also contribute to the model.

### Defining: `SpatialML`

Georganos et al (2019) created the `package(SpatialML)`, and subsequently the tuning is made possible by the `SpatialML::grf.bw()` function. The function uses an exhaustive approach (i.e., it tests sequential nearest neighbor bandwidths within a range and with a user defined step, and returns a list of goodness of fit statistics).

### Defining: Out of Bag Mean Error Rate

In Garson 2021, Ch 5 Random Forest, Garson teaches Random Forest Models by using `randomForest::randomForest()`, and in chapter 5.5.9 (pg. 267), he provides methods for tuning both of these parameters simultaneously using the Out of Bag MSE Error Rates. This value is a measure of the prediction error for data points that were not used in training each tree, hence this value is unique to ensemble methods. It is mathematically expressed as OOB Error Rate $= \frac{1}{n}\Sigma_{i=1}^{N}(y_i - \hat{y}_i^{\mathrm{OOB}})^2$ . $\hat{y}_i^{\mathrm{OOB}}$ is the OOB prediction for the i-th observation, which is obtained by averaging the predictions from only those trees that did not include i in their bootstrap sample. To provide a high-level summary, since each tree in a Random Forest is trained on a bootstrap sample (a random sample with replacement) of the data, approximately one-third of the data is not used for training each tree. This subset of data is referred to as the "out-of-bag" data for that tree, and this value is calculated using the data points that were not included in the bootstrap sample used to build each tree. The code in this file has been modified so that cross validation is implemented to ensure consistency across the models, and as such the only difference across models is the metric and the type of nested cross validation being used.

## Defining: Partially Spatial Nest-Cross Validation Method

All models will be validated and tuned with a nested cross-validation, a technique used to assess the performance of a model and tuning hyperparameters. It helps to avoid over fitting and provides an unbiased estimate of model performance. A spatial nested cross-validation is a two-level cross-validation procedure designed to evaluate a model's performance and tune its hyperparameters simultaneously. A nested cross-validation is a method that revolves around an outer and liner loop. An example of the workflow include:

- Split the data into "outer_k" folds defined by spatial hierarchical clustering.
- For each fold in the outer loop:
  - Use "outer_k - 1" folds for training.
  - Apply the inner cross-validation on this training set to tune hyperparameters.
  - Evaluate the performance of the model with the selected hyperparameters on the held-out test fold.
- Average the performance metrics across all outer folds to get an overall estimate

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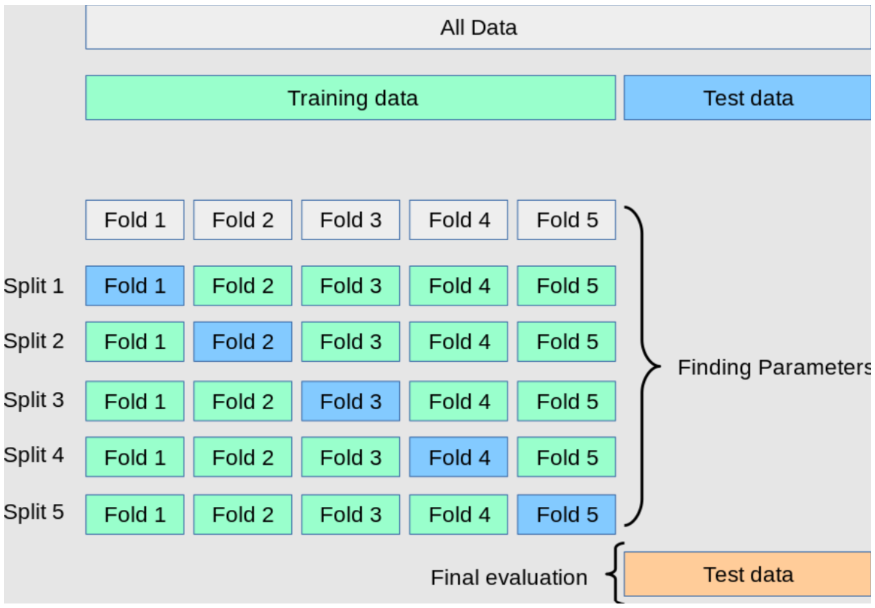
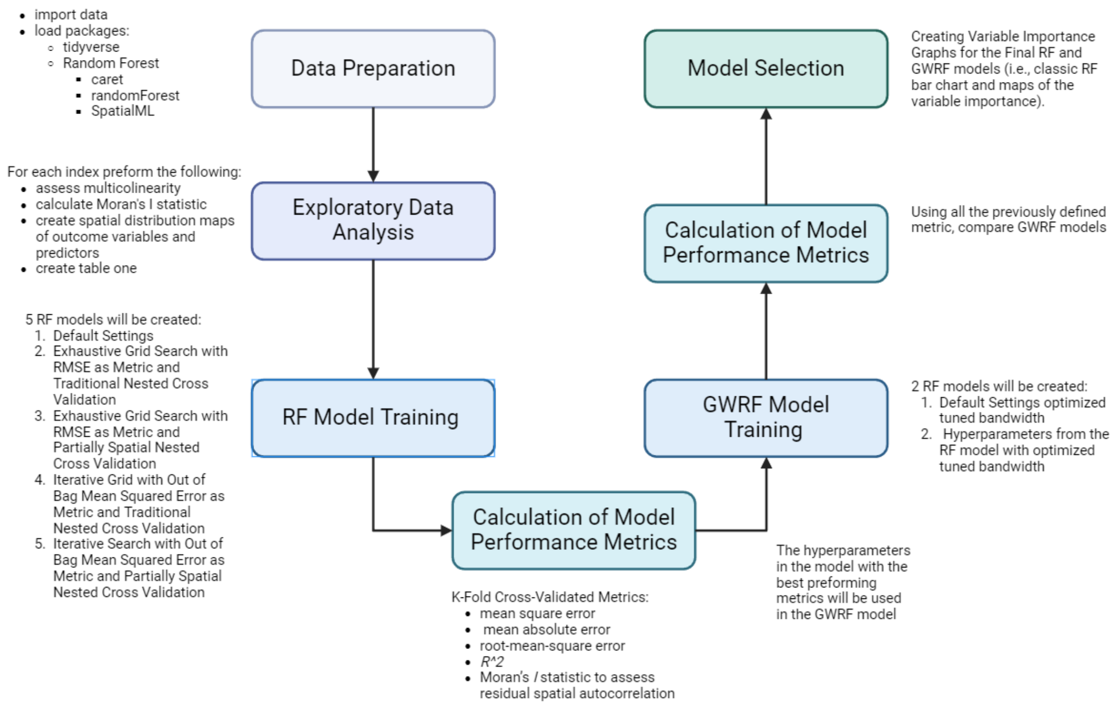
A visual description of the method, which can be in Jian et al (2022) - Rapid Analysis of Cylindrical Bypass Flow Field Based on Deep Learning Model.



- Outer Cross-Validation Loop:
  - Purpose: To estimate the model's performance on unseen data and provide a more reliable measure of how well the model generalizes to new data.
  - Procedure: The data set is divided into several folds (e.g., 5 or 10). In each iteration, one fold is used as the test set, and the remaining folds are used for training and hyper parameter tuning. Folds are defined by hierarchical clustering. This process is repeated for each fold, ensuring that every data point is used for testing exactly once.
- Inner Cross-Validation Loop:
  - Purpose: To select the best hyperparameters for the model.
  - Procedure: Within each training set from the outer loop, a further cross-validation is performed. This involves splitting the training data into additional folds (e.g., 3 or 5). The model is trained with various hyper parameter combinations on these inner folds, and the performance is evaluated to choose the optimal set of hyperparameters.

## Outline of Model Building Process

5 RF models will be built, and they differ based on the different hyperparameters: (1) default settings; (2) Exhaustive Grid Search with RMSE as Metric and Traditional Nested Cross Validation, (3) Exhaustive Grid Search with RMSE as Metric and Partially Spatial Nested Cross Validation, (4)Iterative Grid with Out of Bag Mean Squared Error as Metric and Traditional Nested Cross Validation (i.e., Modified Code from Garson 2021), (5) Iterative Search with Out of Bag Mean Squared Error as Metric and Partially Spatial Nested Cross Validation. For each model, MAE, RMSE, and $R^2$ will be calculated and the hyperparameters of the best model will continue onto the GWRF. To provide points of comparison in the GWRF, two additional models will be created. Thus, two GWRF models will be created: (1) default *mtry* and *ntrees* with optimized *bandwidth parameter*, and (2) using the previously defined best hyperparameters. The same model evaluation metrics will be compared in addition to calculating the residual autocorrelation.


Data Preparation
Exploratory Data Analysis
RF Model Training
Calculation of Model Performance Metrics
GWRF Model Training
Calculation of Model Performance Metrics
Model Selection

- import data
- load packages:
  - tidyverse
  - Random Forest
    - caret
    - randomForest
    - SpatialML

For each index preform the following:
- assess multicolinearity
- calculate Moran's I statistic
- create spatial distribution maps of outcome variables and predictors
- create table one

5 RF models will be created:
1. Default Settings
2. Exhaustive Grid Search with RMSE as Metric and Traditional Nested Cross Validation
3. Exhaustive Grid Search with RMSE as Metric and Partially Spatial Nested Cross Validation
4. Iterative Grid with Out of Bag Mean Squared Error as Metric and Traditional Nested Cross Validation
5. Iterative Search with Out of Bag Mean Squared Error as Metric and Partially Spatial Nested Cross Validation

K-Fold Cross-Validated Metrics:
- mean square error
- mean absolute error
- root-mean-square error
- *R^2*
- Moran's *I* statistic to assess residual spatial autocorrelation

The hyperparameters in the model with the best preforming metrics will be used in the GWRF model

2 RF models will be created:
1. Default Settings optimized tuned bandwidth
2. Hyperparameters from the RF model with optimized tuned bandwidth

Using all the previously defined metric, compare GWRF models

Creating Variable Importance Graphs for the Final RF and GWRF models (i.e., classic RF bar chart and maps of the variable importance).

## Traditional Random Forest Model

### Model Training and Hyperparameter Tuning

Models will be created and compared at the end of the section.

#### RF Model 1 - Default Settings

**Background**: The default settings for the RF model is $mtry$ = p/3, and ntrees = 500, where $p$ is the number of predictors. Nested cross validation is not preformed because the hyperparameters have already been predefined by default.

```
##
## Call:
##  randomForest(x = x, y = y, ntree = 500, mtry = param$mtry, importance = TRUE)
##                Type of random forest: regression
##                      Number of trees: 500
## No. of variables tried at each split: 5
##
##           Mean of squared residuals: 0.01881214
##                     % Var explained: 77.61
```

**Model 2 - Exhaustive Grid Search with RMSE as Metric and Traditional Nested Cross Validation**

**Background**: To preform an exhaustive Grid Search, Brownlee (2020) created a custom function that preforms the grid search. This function checks every combination of *mtry* and *ntree* values determines the final values with RMSE.

Table 1: Model 2 - Traditional Cross Validation: Hyperparametyer Tuning and Performance Metrics

| Fold | Tuned_mtry | Tuned_ntree | RMSE | MAE | R_squared |
|---|---|---|---|---|---|
| 1 | 11 | 100 | 0.161 | 0.130 | 0.710 |
| 2 | 5 | 100 | 0.137 | 0.110 | 0.788 |
| 3 | 5 | 150 | 0.151 | 0.122 | 0.759 |
| 4 | 5 | 950 | 0.158 | 0.125 | 0.726 |
| 5 | 3 | 350 | 0.169 | 0.139 | 0.722 |

Model 2 has hyperparameters set to $mtry = 5$, and $ntrees = 100$.

### Model 3 - Exhaustive Grid Search with RMSE as Metric and Partially Spatial Nested Cross Validation

**Background**: Preforms the same task as model 2 (i.e., tune hyperparameters with an exhaustive grid search), however where this model differs is occurs based on the nested cross validation. The outer loop is defined by `ClustGeo` package, which implements hierarchical clustering with soft contiguity constraint. The main arguments of the function are:

- a matrix D0 with the dissimilarities in the "feature space" (here socio-economic variables for instance).
- a matrix D1 with the dissimilarities in the "constraint" space (here a matrix of geographical dissimilarities).
- a mixing parameter alpha between 0 an 1. The mixing parameter sets the importance of the constraint in the clustering procedure.
- a scaling parameter scale with a logical value. If TRUE the dissimilarity matrices D0 and D1 are scaled between 0 and 1 (that is divided by their maximum value).

For more information on the package and the code implement please visit the following link Introduction to ClustGeo.

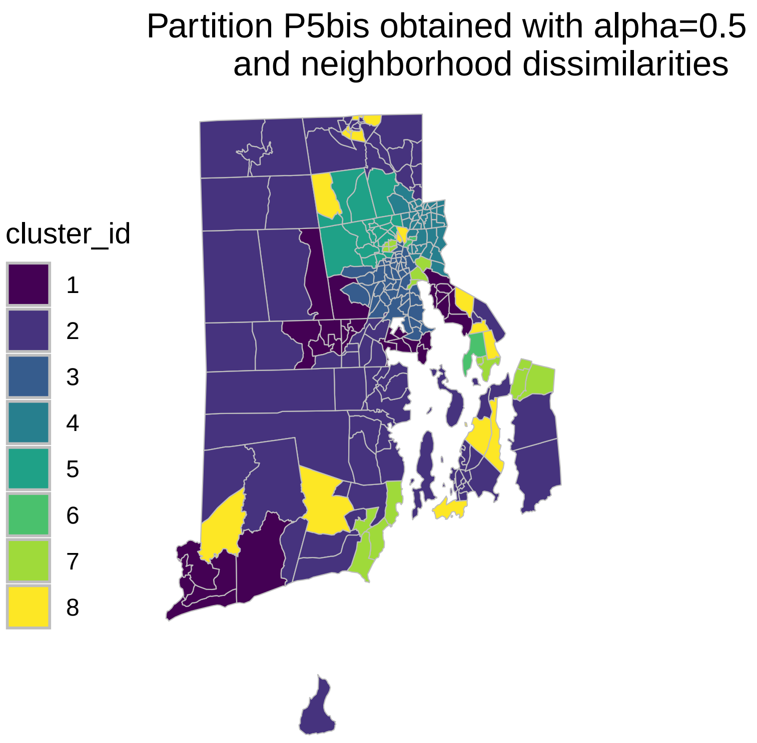

Partition P5bis obtained with alpha=0.5
and neighborhood dissimilarities
cluster_id
1
2
3
4
5
6
7
8

Table 2: Model 3 - Partially Spatial Cross Validation: Hyperparametyer Tuning and Performance Metrics

| Fold | Tuned_mtry | Tuned_ntree | RMSE | MAE | Rsquared |
|---|---|---|---|---|---|
| 1 | 10 | 250 | 0.122 | 0.105 | 0.871 |
| 2 | 8 | 600 | 0.142 | 0.118 | 0.845 |
| 3 | 15 | 200 | 0.147 | 0.108 | 0.735 |
| 4 | 10 | 150 | 0.132 | 0.106 | 0.755 |
| 5 | 14 | 350 | 0.129 | 0.092 | 0.788 |
| 6 | 15 | 150 | 0.132 | 0.101 | 0.821 |
| 7 | 14 | 300 | 0.145 | 0.105 | 0.719 |
| 8 | 5 | 200 | 0.128 | 0.106 | 0.754 |

Model 3 has hyperparameters set to $mtry = 10$, and $ntrees = 250$.

**Model 4 - Iterative Grid with Out of Bag Mean Squared Error as Metric and Traditional Nested Cross Validation**

This code snippet is designed to optimize the hyperparameters *mtry* and *ntree* in a Random Forest model and by examining the OOB MSE across these combinations, the code identifies which parameters yield the lowest error, helping to optimize the Random Forest model. Here's how the code meets this objective:

- Iterative Search for *mtry*: The `mtry_iter` function generates an iterable sequence of *mtry* values, starting from 1 up to the number of predictors, incremented by a step factor. This allows the code to explore different numbers of predictors used at each split in the trees.
- Specification of *ntree* Values: A predefined vector *vntree* contains different values for the number of trees to be grown in the forest. This allows the code to assess how the number of trees impacts the model performance.
- Error Calculation Across Hyperparameter Combinations: The tune function performs a grid search over the specified *mtry* values and the maximum number of trees specified in *vntree.* For each combination, the function trains a Random Forest model and calculates the OOB error rate, MSE since y is continuous.
- Result Aggregation: The results are combined into a data frame, which can then be analyzed to identify the optimal combination of *mtry* and *ntree* that minimizes the OOB error rate.

Table 3: Model 4 - Traditional Cross Validation: Hyperparametyer Tuning and Performance Metrics

| Fold | Best_mtry | Best_ntree | Test_Error | RMSE | MAE | R_squared |
|---|---|---|---|---|---|---|
| 1 | 6 | 500 | 0.021 | 0.146 | 0.111 | 0.743 |
| 2 | 15 | 750 | 0.020 | 0.141 | 0.112 | 0.783 |
| 3 | 13 | 200 | 0.021 | 0.143 | 0.113 | 0.750 |
| 4 | 7 | 200 | 0.019 | 0.138 | 0.106 | 0.769 |
| 5 | 16 | 550 | 0.012 | 0.110 | 0.086 | 0.851 |

Model 4 has hyperparameters set to *mtry* = 16, and *ntrees* = 550.

**Model 5 - Iterative Search with Out of Bag Mean Squared Error as Metric and Partially Spatial Nested Cross Validation**

Table 4: Model 5 - Partially Spatial Cross Validation: Hyperparametyer Tuning and Performance Metrics

| Fold | Best_mtry | Best_ntree | Test_Error | RMSE | MAE | R_squared |
|---|---|---|---|---|---|---|
| 1 | 11 | 100 | 0.015 | 0.121 | 0.097 | 0.822 |
| 2 | 11 | 650 | 0.015 | 0.122 | 0.098 | 0.784 |
| 3 | 8 | 100 | 0.020 | 0.142 | 0.117 | 0.761 |
| 4 | 9 | 200 | 0.018 | 0.135 | 0.110 | 0.810 |
| 5 | 4 | 550 | 0.020 | 0.142 | 0.115 | 0.766 |
| 6 | 6 | 100 | 0.027 | 0.165 | 0.125 | 0.670 |
| 7 | 8 | 150 | 0.019 | 0.140 | 0.111 | 0.793 |
| 8 | 15 | 1000 | 0.027 | 0.163 | 0.130 | 0.626 |

Model 5 has hyperparameters set to $mtry = 11$, and $ntrees = 100$.

## RF Model Evaluation

The relatively low MSE and RMSE values across the models indicate that the predictions are generally close to the actual values. The high R-Squared values suggest that each model explains a significant portion of the variance in the target variable. However, since model 5 produced code that is lowest RMSE, and second highest R-squared value (off only by 0.014%), these are the parameters that will be head contains for the GWRF.

- Mean Absolute Error (MAE):$\frac{1}{n}\Sigma_{i=1}^{n}|y_i - \hat{y}_i|$
- Mean Squared Error (MSE): $\frac{1}{n}\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2$
- Root Mean Squared Error (RMSE):$\sqrt{\frac{1}{n}\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2}$
- R-Squared Value: $\frac{\Sigma(y-\hat{y})^2}{\Sigma(y-\bar{y})^2}$

Table 5: Performance Metrics for Each Model

| Model | Best_mtry | Best_ntree | Test_Error | RMSE | MAE | R_squared |
|---|---|---|---|---|---|---|
| 1 | 5 | 500 | NA | 0.137 | 0.111 | 0.787 |
| 2 | 5 | 100 | NA | 0.137 | 0.110 | 0.788 |
| 3 | 10 | 250 | NA | 0.122 | 0.105 | 0.871 |
| 4 | 16 | 550 | 0.012 | 0.110 | 0.086 | 0.851 |
| 5 | 11 | 100 | 0.015 | 0.121 | 0.097 | 0.822 |

## Code Appendix

```
knitr::opts_chunk$set(warning = FALSE, message = FALSE, echo = FALSE)
knitr::opts_chunk$set(fig.width=6, fig.height=4)
options(tigris_use_cache = TRUE)
options(repos = c(CRAN = "https://cran.r-project.org"))
knitr::include_graphics("/Users/diazg/Documents/GitHub/MPH-Thesis_GeographicalRandomForest/Nes
knitr::include_graphics("/Users/diazg/Documents/GitHub/MPH-Thesis_GeographicalRandomForest/Met
#####################
#### Preparation ####
#####################

### importing packages
# define desired packages
library(tidyverse)    # general data manipulation
library(knitr)        # Rmarkdown interactions
library(here)         # define top level of project folder
                          # this allows for specification of where
                          # things live in relation to the top level
library(foreach)      # parallel execution
# spatial tasks
library(tigris)       # obtain shp files
library(spdep)        # exploratory spatial data analysis
# random forest
library(caret)        # machine learning model training
library(rsample)      # splitting testing/training data
library(randomForest) # traditional RF model
library(SpatialML)    # spatial RF model
# others
library(doParallel)   # parallel processing
library(foreach)      # parallel processing
library(ggpubr)       # arrange multiple graphs
library(ClustGeo)

### setting seed
set.seed(926)

### loading data
svi_df = read_csv(here::here("01_Data", "svi_df.csv")) %>%
  mutate(fips = as.character(fips)) %>%
  select(-...1)

### obtaining SPH files for RI tracts
tracts = tracts(state = "RI", year = 2022, cb = TRUE)

### joining data
map = inner_join(tracts, svi_df, by = c("GEOID" = "fips")) %>%
```

```r
  select(rpl_themes, starts_with("e_"))
# keep a copy for later
map_map = map

### defining analytical coordinates and df
df_coords = map %>%
  mutate(
    # redefines geometry to be the centroid of the polygon
    geometry = st_centroid(geometry),
    # pulls the lon and lat for the centroid
    lon = map_dbl(geometry, ~st_point_on_surface(.x)[[1]]),
    lat = map_dbl(geometry, ~st_point_on_surface(.x)[[2]])) %>%
  # removes geometry, coerce to data.frame
  st_drop_geometry() %>%
  # only select the lon and lat
  select(lon, lat)

# only obtain response and predictor variables
df = svi_df %>%
  st_drop_geometry() %>%
  select(rpl_themes, starts_with("e_"))

unregister_dopar <- function() {
    env <- foreach:::.foreachGlobals
    rm(list=ls(name=env), pos=env)
}
####################
##### RF Mod 1 #####
####################

### setting seed
set.seed(926)

# obtain the number of predictors
pred_num = svi_df %>%
  st_drop_geometry() %>%
  select(starts_with("e_")) %>%
  colnames() %>%
  length()
# determine the default number of predictors
mtry = round(pred_num / 3)

# creating the first model
# cross validated evaluation
cl = makeCluster(detectCores() - 1)  # Use one less core than available
registerDoParallel(cl)
```

```r
rf_mod1 = train(rpl_themes ~ e_pov150 + e_unemp + e_hburd +
    e_nohsdp + e_uninsur + e_age65 + e_age17 +
    e_disabl + e_sngpnt + e_limeng + e_minrty +
    e_munit + e_mobile + e_crowd + e_noveh + e_groupq,
                 data = df,
                 method = "rf",
                 trControl = trainControl(method = "cv", number = 10, allowParallel = TRUE ),
                 tuneGrid = expand.grid(mtry = mtry),
                 ntree = 500,
                 importance = TRUE)

stopCluster(cl)
unregister_dopar()

# Print the results
rf_mod1$finalModel

Best_mtry = 5
Best_ntree = 500
Test_Error = NA
RMSE = rf_mod1$results$RMSE
MAE  = rf_mod1$results$MAE
R_squared =  rf_mod1$results$Rsquared

model1_table = data.frame(Best_mtry, Best_ntree, Test_Error, RMSE, MAE, R_squared)
####################
##### RF Mod 2 #####
####################

### setting seed
set.seed(926)

### creating the custom function
customRF <- list(type = "Regression", library = "randomForest", loop = NULL)
customRF$parameters <- data.frame(parameter = c("mtry", "ntree"), class = rep("numeric", 2), la
customRF$grid <- function(x, y, len = NULL, search = "grid") {}
customRF$fit <- function(x, y, wts, param, lev, last, weights, classProbs, ...) {
  randomForest(x, y, mtry = param$mtry, ntree=param$ntree, ...)
}
customRF$predict <- function(modelFit, newdata, preProc = NULL, submodels = NULL)
   predict(modelFit, newdata)
customRF$prob <- function(modelFit, newdata, preProc = NULL, submodels = NULL)
   predict(modelFit, newdata, type = "prob")
customRF$sort <- function(x) x[order(x[,1]),]
customRF$levels <- function(x) x$classes
### defining the outer folds
outer_folds = createFolds(df$rpl_themes, k = 5)
```

```r
df = df %>%
  mutate(outer_fold_id = case_when(
    row_number() %in% outer_folds$Fold1 ~ 1,
    row_number() %in% outer_folds$Fold2 ~ 2,
    row_number() %in% outer_folds$Fold3 ~ 3,
    row_number() %in% outer_folds$Fold4 ~ 4,
    row_number() %in% outer_folds$Fold5 ~ 5,
    TRUE ~ 999
  ))

nested_cv = function(form, data, response_var, method, trControl, tuneGrid, k) {

  # Initialize the list to store nested cross-validation results
  model_results = list()

  # Perform the nested cross-validation
  for (i in seq_len(k)) {
    train_data = data %>% filter(outer_fold_id == i)
    test_data = data %>% filter(outer_fold_id != i)

    # Perform inner cross-validation with parallel processing
    inner_model = train(
      form = form,
      data = train_data,
      method = method,
      trControl = trControl,
      tuneGrid = tuneGrid,
      importance = TRUE
    )

    # Evaluate the model on the outer test data
    predictions = predict(inner_model, newdata = test_data)
    performance_metric = postResample(pred = predictions, obs = test_data[[response_var]])

    # Store the results
    model_results[[i]] = list(
      model = inner_model,
      performance = performance_metric
    )
  }

  return(model_results)
}
### define arguments
grid = expand.grid(.mtry = c(1:16),
                   .ntree = c(100, 150, 200, 250,
                              300, 350, 400, 450,
                              500, 550, 600, 650,
                              700, 750, 800, 850,
                              900, 950, 1000))

ctrl = trainControl(method = "cv", number = 10)

k = length(outer_folds)

model2_results = nested_cv(
  form = rpl_themes ~ e_pov150 + e_unemp + e_hburd +
    e_nohsdp + e_uninsur + e_age65 + e_age17 +
    e_disabl + e_sngpnt + e_limeng + e_minrty +
    e_munit + e_mobile + e_crowd + e_noveh + e_groupq,
  response_var = "rpl_themes",
  data = df,
  method = customRF,
  trControl = ctrl,
  tuneGrid = grid,
  k = k
)

unregister_dopar()
Fold = c(1:5)

Tuned_mtry = c(as.numeric(model2_results[[1]]$model$bestTune[1]),
               as.numeric(model2_results[[2]]$model$bestTune[1]),
               as.numeric(model2_results[[3]]$model$bestTune[1]),
               as.numeric(model2_results[[4]]$model$bestTune[1]),
               as.numeric(model2_results[[5]]$model$bestTune[1]))

Tuned_ntree = c(as.numeric(model2_results[[1]]$model$bestTune[2]),
               as.numeric(model2_results[[2]]$model$bestTune[2]),
               as.numeric(model2_results[[3]]$model$bestTune[2]),
               as.numeric(model2_results[[4]]$model$bestTune[2]),
               as.numeric(model2_results[[5]]$model$bestTune[2]))

RMSE = c(as.numeric(model2_results[[1]]$performance[[1]]),
         as.numeric(model2_results[[2]]$performance[[1]]),
         as.numeric(model2_results[[3]]$performance[[1]]),
         as.numeric(model2_results[[4]]$performance[[1]]),
         as.numeric(model2_results[[5]]$performance[[1]]))

MAE = c(as.numeric(model2_results[[1]]$performance[[3]]),
         as.numeric(model2_results[[2]]$performance[[3]]),
         as.numeric(model2_results[[3]]$performance[[3]]),
         as.numeric(model2_results[[4]]$performance[[3]]),
         as.numeric(model2_results[[5]]$performance[[3]]))
```

```r
R_squared = c(as.numeric(model2_results[[1]]$performance[[2]]),
         as.numeric(model2_results[[2]]$performance[[2]]),
         as.numeric(model2_results[[3]]$performance[[2]]),
         as.numeric(model2_results[[4]]$performance[[2]]),
         as.numeric(model2_results[[5]]$performance[[2]]))

tab = data.frame(Fold, Tuned_mtry, Tuned_ntree, RMSE, MAE, R_squared)

Best_mtry = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Tuned_mtry)

Best_ntree = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Tuned_ntree)

Test_Error = NA

RMSE = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(RMSE)

MAE  = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(MAE)

R_squared = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(R_squared)

Best_Fold = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Fold)

# access the model information by preforming the following function: model2_results[[Best_Fold

model2_table = data.frame(Best_mtry, Best_ntree, Test_Error, RMSE, MAE, R_squared)

kable(tab, caption = "Model 2 - Traditional Cross Validation: Hyperparametyer Tuning and Perfo
      digits = 3,
      align = c("lllccc"))

####################
##### RF Mod 3 #####
####################

### this code c
```

```r
D0 <- dist(df)
tree <- hclustgeo(D0)

"
You cut the dendrogram horizontally at a level that
represents a reasonable trade-off between the
number of clusters and the within-cluster similarity, with
the goal to  Look for large vertical gaps between
successive merges. The idea is to cut the dendrogram at
a height where the gap between clusters is largest,
indicating that merging clusters beyond that point would
result in combining distinct groups.

I am going to continue with k = 8 because
the large cluster found in k = 4 graphs
colored in red contains the branch that is less homogeneous or
the distance between clsutesr within the branch is smaller.
Additionally since the the gaol is cross validation
obtaining

Graphs 4 are illustrated to should the largest vertical
distance, while 8 was choosen to emphasis the equal groups
"

# k=4
plot(tree, hang = -1, label = FALSE,
     xlab = "", sub = "",
     main = "Ward Dendrogram with D0 only")
rect.hclust(tree ,k = 4, border = c(1:4))
legend("topright", legend = paste("cluster", 1:4),
       fill=1:5, bty="n", border = "white")
# k=8
plot(tree, hang = -1, label = FALSE,
     xlab = "", sub = "",
     main = "Ward Dendrogram with D0 only")
rect.hclust(tree ,k = 8, border = c(1:8))
legend("topright", legend = paste("cluster", 1:8),
       fill=1:5, bty="n", border = "white")

# taking geographical and neighorhood constraints into account
list.nb = poly2nb(map, queen=TRUE) #list of neighbours of each city
A = nb2mat(neighbours = list.nb,style="B", zero.policy = TRUE)
D1 = as.dist(1-A)
# choice of mixing parameter
range.alpha = seq(0,1,0.1)
K = 8
cr = choicealpha(D0, D1,
                 range.alpha,
                 K,
                 graph=FALSE)

# normalization if required given the characteristics
# geographic distances with other data, normalization
# might be required to balance the contributions of
# geographic and non-geographic distances. This ensures
# that neither component disproportionately influences
# the clustering result.

plot(cr, norm = TRUE)

# here the plot seggust to choose alpha = 0.2
tree = hclustgeo(D0,D1,alpha=0.2)
P5bis = cutree(tree,8)
map$cluster_id = as.factor(P5bis)
df_coords$cluster_id = as.factor(P5bis)
# graph produced by clustering method
ggplot(data = map) +
  geom_sf(aes(fill = cluster_id), color = "grey") +
  scale_fill_viridis_d(name = "cluster_id") +
  labs(title = "Partition P5bis obtained with alpha=0.5
         and neighborhood dissimilarities") +
  theme_void() +
  theme(legend.position = "left")
# This function performs nested cross-validation with parallel processing
spatial_nested_cv = function(form, data, method, trControl, tuneGrid, cluster_col, k) {
  outer_folds = createFolds(data[[cluster_col]], k = length(unique(data[[cluster_col]])), retu

  outer_results = foreach(i = seq_along(outer_folds), .packages = c('caret', 'randomForest'),
    train_indices = outer_folds[[i]]
    train_data = data[train_indices, ]
    test_data = data[-train_indices, ]

    # Perform inner cross-validation
    inner_model = train(
      form = form,
      data = train_data,
      method = method,
      trControl = trControl,
      tuneGrid = tuneGrid,
      importance = TRUE
    )

    # Evaluate the model on the outer test data
    predictions <- predict(inner_model, newdata = test_data)
    performance_metric <- postResample(pred = predictions, obs = test_data$rpl_themes)

    list(
      model = inner_model,
      performance = performance_metric
    )
  }

  stopCluster(cl)  # Stop the parallel backend

  return(outer_results)
}
# implementing an exhaustive search
map = map %>% st_drop_geometry()

# Register parallel backend
num_cores <- detectCores() - 1
cl <- makeCluster(num_cores)
registerDoParallel(cl)

model3_results = spatial_nested_cv(
  form = rpl_themes ~ e_pov150 + e_unemp + e_hburd +
    e_nohsdp + e_uninsur + e_age65 + e_age17 +
    e_disabl + e_sngpnt + e_limeng + e_minrty +
    e_munit + e_mobile + e_crowd + e_noveh + e_groupq,
  data = map,
  method = customRF,
  trControl = ctrl,
  tuneGrid = grid,
  cluster_col = "cluster_id",
  k = 10)

unregister_dopar()
Fold = c(1:8)

Tuned_mtry = c(as.numeric(model3_results[[1]]$model$bestTune[1]),
               as.numeric(model3_results[[2]]$model$bestTune[1]),
               as.numeric(model3_results[[3]]$model$bestTune[1]),
               as.numeric(model3_results[[4]]$model$bestTune[1]),
               as.numeric(model3_results[[5]]$model$bestTune[1]),
               as.numeric(model3_results[[6]]$model$bestTune[1]),
               as.numeric(model3_results[[7]]$model$bestTune[1]),
               as.numeric(model3_results[[8]]$model$bestTune[1]))

Tuned_ntree = c(as.numeric(model3_results[[1]]$model$bestTune[2]),
               as.numeric(model3_results[[2]]$model$bestTune[2]),
               as.numeric(model3_results[[3]]$model$bestTune[2]),
               as.numeric(model3_results[[4]]$model$bestTune[2]),
               as.numeric(model3_results[[5]]$model$bestTune[2]),
               as.numeric(model3_results[[6]]$model$bestTune[2]),
               as.numeric(model3_results[[7]]$model$bestTune[2]),
               as.numeric(model3_results[[8]]$model$bestTune[2]))

RMSE = c(as.numeric(model3_results[[1]]$performance[[1]]),
         as.numeric(model3_results[[2]]$performance[[1]]),
         as.numeric(model3_results[[3]]$performance[[1]]),
         as.numeric(model3_results[[4]]$performance[[1]]),
         as.numeric(model3_results[[5]]$performance[[1]]),
         as.numeric(model3_results[[6]]$performance[[1]]),
         as.numeric(model3_results[[7]]$performance[[1]]),
         as.numeric(model3_results[[8]]$performance[[1]]))

Rsquared = c(as.numeric(model3_results[[1]]$performance[[2]]),
         as.numeric(model3_results[[2]]$performance[[2]]),
         as.numeric(model3_results[[3]]$performance[[2]]),
         as.numeric(model3_results[[4]]$performance[[2]]),
         as.numeric(model3_results[[5]]$performance[[2]]),
         as.numeric(model3_results[[6]]$performance[[2]]),
         as.numeric(model3_results[[7]]$performance[[2]]),
         as.numeric(model3_results[[8]]$performance[[2]]))

MAE = c(as.numeric(model3_results[[1]]$performance[[3]]),
         as.numeric(model3_results[[2]]$performance[[3]]),
         as.numeric(model3_results[[3]]$performance[[3]]),
         as.numeric(model3_results[[4]]$performance[[3]]),
         as.numeric(model3_results[[5]]$performance[[3]]),
         as.numeric(model3_results[[6]]$performance[[3]]),
         as.numeric(model3_results[[7]]$performance[[3]]),
         as.numeric(model3_results[[8]]$performance[[3]]))

tab = data.frame(Fold, Tuned_mtry, Tuned_ntree, RMSE, MAE, Rsquared)

Best_mtry = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Tuned_mtry)

Best_ntree = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Tuned_ntree)

Test_Error = NA

RMSE = tab %>%
  filter(RMSE == min(RMSE)) %>%
```

```r
  pull(RMSE)

MAE  = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(MAE)

R_squared = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Rsquared)

Best_Fold = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Fold)

# access the model information by preforming the following function: model3_results[[Best_Fold

model3_table = data.frame(Best_mtry, Best_ntree, Test_Error, RMSE, MAE, R_squared)

kable(tab, caption = "Model 3 - Partially Spatial Cross Validation: Hyperparametyer Tuning and
      digits = 3,
      align = c("lllccc"))
####################
##### RF Mod 4 #####
####################

# create an interaction function to search over different values of mtry
mtry_iter = function(from, to, stepFactor = 1.05){
  nextEl = function(){
    if (from > to) stop('StopIteration')
    i = from
    from <<- ceiling(from * stepFactor)
    i
  }
  obj = list(nextElem = nextEl)
  class(obj) = c('abstractiter', 'iter')
  obj
}

# Define the function to calculate RMSE, MAE, and R-squared
calculate_metrics <- function(predictions, actuals) {
  residuals <- predictions - actuals
  mse <- mean(residuals^2)
  rmse <- sqrt(mse)
  mae <- mean(abs(residuals))
  r_squared <- 1 - sum(residuals^2) / sum((actuals - mean(actuals))^2)

  return(c(RMSE = rmse, MAE = mae, R2 = r_squared))
```

```
}


# Nested cross-validation function with random forest
nested_cv_tune <- function(x, y, ntree = c(51, 101, 501, 1001, 1501), num_folds = 5) {

  # Create outer cross-validation folds
  outer_folds <- createFolds(y, k = num_folds, returnTrain = TRUE)

  # Initialize list to store outer fold results
  outer_results <- list()

  # Initialize list to store final models
  final_models <- list()

  # Iterate over each outer fold
  for (i in seq_along(outer_folds)) {
    train_index <- outer_folds[[i]]
    x_train <- x[train_index, ]
    y_train <- y[train_index]
    x_test <- x[-train_index, ]
    y_test <- y[-train_index]

    # Inner cross-validation for hyperparameter tuning
    inner_results <- foreach(mtry = mtry_iter(1, ncol(x_train)), .combine = 'rbind', .packages
      model <- randomForest(x_train, y_train, ntree = max(ntree), mtry = mtry, keep.forest = F
      if (is.factor(y)) {
        errors <- data.frame(ntree = ntree, mtry = mtry, error = model$err.rate[ntree, 1])
      } else {
        errors <- data.frame(ntree = ntree, mtry = mtry, error = model$mse[ntree])
      }
      return(errors)
    }

    # Find the best hyperparameters based on the inner fold results
    best_params <- inner_results[which.min(inner_results$error), ]

    # Train the final model on the entire outer training set using the best hyperparameters
    final_model <- randomForest(x_train, y_train, ntree = best_params$ntree, mtry = best_param

    # Store the final model in the list
    final_models[[i]] <- final_model

    # Test the final model on the outer test set
    final_pred <- predict(final_model, x_test)

    # Calculate performance metrics
```

```r
    if (is.factor(y)) {
      test_error <- mean(final_pred != y_test)
      rmse <- NA
      mae <- NA
      rsquared <- NA
    } else {
      test_error <- mean((final_pred - y_test)^2)
      rmse <- sqrt(mean((final_pred - y_test)^2))
      mae <- mean(abs(final_pred - y_test))
      rsquared <- 1 - (sum((final_pred - y_test)^2) / sum((y_test - mean(y_test))^2))
    }

    # Store the results
    outer_results[[i]] <- data.frame(
      Fold = i,
      Best_mtry = best_params$mtry,
      Best_ntree = best_params$ntree,
      Test_Error = test_error,
      RMSE = rmse,
      MAE = mae,
      R_squared = rsquared
    )
  }

  # Combine all outer fold results
  final_results <- do.call(rbind, outer_results)

  # Stop the parallel backend
  stopCluster(cl)

  # Return both the results and the models
  return(list(Results = final_results, Models = final_models))
}

# create a vector of ntree values of interest
vntree = c(100, 150, 200, 250,
           300, 350, 400, 450,
           500, 550, 600, 650,
           700, 750, 800, 850,
           900, 950, 1000)

# specify the predictor (x) and outcome (y) object
x = df %>% select(starts_with("e_"))
y = df %>% pull(rpl_themes)

# Register parallel backend
num_cores <- detectCores() - 1
```

```r
cl <- makeCluster(num_cores)
registerDoParallel(cl)

# call the custom function
model4_results = nested_cv_tune(x, y, ntree = vntree, num_folds = 5)

unregister_dopar()

model4_models = model4_results$Models
model4_results = model4_results$Results
Best_mtry = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Best_mtry)

Best_ntree = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Best_ntree)

Test_Error = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Test_Error)

RMSE = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(RMSE)

MAE  = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(MAE)

R_squared = model4_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(R_squared)

Best_Fold = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Fold)

# access the model information by preforming the following function: model4_models[[Best_Fold]

model4_table = data.frame(Best_mtry, Best_ntree, Test_Error, RMSE, MAE, R_squared)

kable(model4_results, caption = "Model 4 - Traditional Cross Validation: Hyperparametyer Tunin
      digits = 3,
      align = c("lllcccc"))
####################
##### RF Mod 5 #####
```

```r
####################

# Nested cross-validation function with random forest
spatial_nested_cv_tune <- function(formula, data, response_var, cluster_col, num_predictors, n

  # Create outer cross-validation folds
  outer_folds <- createFolds(data[[cluster_col]], k = length(unique(data[[cluster_col]])), retu

  # Initialize list to store outer fold results and models
  outer_results <- list()
  final_models <- list()

  # Iterate over each outer fold
  for (i in seq_along(outer_folds)) {
    train_index <- outer_folds[[i]]
    train_data <- data[train_index, ]
    test_data <- data[-train_index, ]

    # Inner cross-validation for hyperparameter tuning
    inner_results <- foreach(mtry = mtry_iter(1, num_predictors), .combine = 'rbind', .package
      model <- randomForest(formula, data = train_data, ntree = max(ntree), mtry = mtry, keep.i
      if (is.factor(train_data[[response_var]])) {
        errors <- data.frame(ntree = ntree, mtry = mtry, error = model$err.rate[ntree, 1])
      } else {
        errors <- data.frame(ntree = ntree, mtry = mtry, error = model$mse[ntree])
      }
      return(errors)
    }

    # Find the best hyperparameters based on the inner fold results
    best_params <- inner_results[which.min(inner_results$error), ]

    # Train the final model on the entire outer training set using the best hyperparameters
    final_model <- randomForest(formula, data = train_data, ntree = best_params$ntree, mtry = 

    # Store the final model
    final_models[[i]] <- final_model

    # Test the final model on the outer test set
    final_pred <- predict(final_model, test_data)

    # Calculate performance metrics using response_var
    y_test <- test_data[[response_var]]
    if (is.factor(y_test)) {
      test_error <- mean(final_pred != y_test)
      rmse <- NA
      mae <- NA
      rsquared <- NA
    } else {
      test_error <- mean((final_pred - y_test)^2)
      rmse <- sqrt(mean((final_pred - y_test)^2))
      mae <- mean(abs(final_pred - y_test))
      rsquared <- 1 - (sum((final_pred - y_test)^2) / sum((y_test - mean(y_test))^2))
    }

    # Store the results
    outer_results[[i]] <- data.frame(
      Fold = i,
      Best_mtry = best_params$mtry,
      Best_ntree = best_params$ntree,
      Test_Error = test_error,
      RMSE = rmse,
      MAE = mae,
      R_squared = rsquared
    )
  }

  # Combine all outer fold results
  final_results <- do.call(rbind, outer_results)

  # Stop the parallel backend
  stopCluster(cl)


  return(list(Results = final_results, Models = final_models))
}
# create a vector of ntree values of interest
vntree = c(100, 150, 200, 250,
           300, 350, 400, 450,
           500, 550, 600, 650,
           700, 750, 800, 850,
           900, 950, 1000)

# specify the predictor (x) and outcome (y) object
cluster_id = map %>% select(cluster_id) %>% st_drop_geometry()
x = map %>% select(starts_with("e_")) %>% st_drop_geometry()
y = map %>% pull(rpl_themes) %>% st_drop_geometry()

# Register parallel backend
num_cores <- detectCores() - 1
cl <- makeCluster(num_cores)
registerDoParallel(cl)

# call the custom function
```

```r
model5_results = spatial_nested_cv_tune(
  form = rpl_themes ~ e_pov150 + e_unemp + e_hburd +
    e_nohsdp + e_uninsur + e_age65 + e_age17 +
    e_disabl + e_sngpnt + e_limeng + e_minrty +
    e_munit + e_mobile + e_crowd + e_noveh + e_groupq,
  data = map,
  response_var = "rpl_themes",
  num_predictors = 16,
  cluster_col = "cluster_id", ntree = vntree)

unregister_dopar()

model5_models = model5_results$Models
model5_results = model5_results$Results
Best_mtry = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Best_mtry)

Best_ntree = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Best_ntree)

Test_Error = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(Test_Error)

RMSE = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(RMSE)

MAE  = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(MAE)

R_squared = model5_results %>%
  filter(Test_Error == min(Test_Error)) %>%
  pull(R_squared)

Best_Fold = tab %>%
  filter(RMSE == min(RMSE)) %>%
  pull(Fold)

# access the model information by preforming the following function: model5_models[[Best_Fold]

model5_table = data.frame(Best_mtry, Best_ntree, Test_Error, RMSE, MAE, R_squared)

kable(model5_results, caption = "Model 5 - Partially Spatial Cross Validation: Hyperparametyer
      digits = 3,
      align = c("lllcccc"))
####################
##### RF Models ####
####################
# make a list of all the model objects
rf_model_1 = rf_mod1$finalModel
rf_model_2 = model2_results[[Best_Fold]]$model$finalModel
rf_model_3 = model3_results[[Best_Fold]]$model$finalModel
rf_model_4 = model4_models[[Best_Fold]]
rf_model_5 = model5_models[[Best_Fold]]

final_model_lst = list(rf_model_1, rf_model_2,
                      rf_model_3, rf_model_4,
                      rf_model_5)


# Create a data frame with the results
results_rf = rbind(model1_table, model2_table,
                   model3_table, model4_table,
                   model5_table)

Model = c(1, 2, 3, 4, 5)

results_rf = cbind(as.data.frame(Model), results_rf)

# Print the results using kable
kable(results_rf, caption = "Performance Metrics for Each Model",
      digits = 3, align = c("l", "c", "c", "c", "c", "c", "c"))

# Export the results_rf as csv file
write.csv(results_rf, "results_rf.csv", row.names = FALSE)


save(rf_model_1, file = "rf_model_1.RData")
save(rf_model_2, file = "rf_model_2.RData")
save(rf_model_3, file = "rf_model_3.RData")
save(rf_model_4, file = "rf_model_4.RData")
save(rf_model_5, file = "rf_model_5.RData")
```