

**Model Creation and Validation for the Social
Vulnerability Index
Training Random Forest and Geographically Weighted
Random Forest Models**

Thesis for a Master of Public Health, Epidemiology

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Statement of Purpose

The purpose of the file is to build two final models: a traditional random forest model (RF) and a geographically weighted random forest model (GWRF). The following two sentences provide an 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.

Overview of Hyperparameters Definitions

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.

Outline of Hyper-parameter Tuning Process

4 RF models will be built, and they differ based on the different hyperparameters: (1) default settings, (2) first tune p , and subsequently tune, then m while keeping p constant, (3) simultaneously tune m and p with a grid search, (4) tuned with Out of Bag MSE Error Rates as described by Garson 2021. Two metrics will be implemented in the tuning process: Root Mean Squared Error and Out of Bag Error Rate.

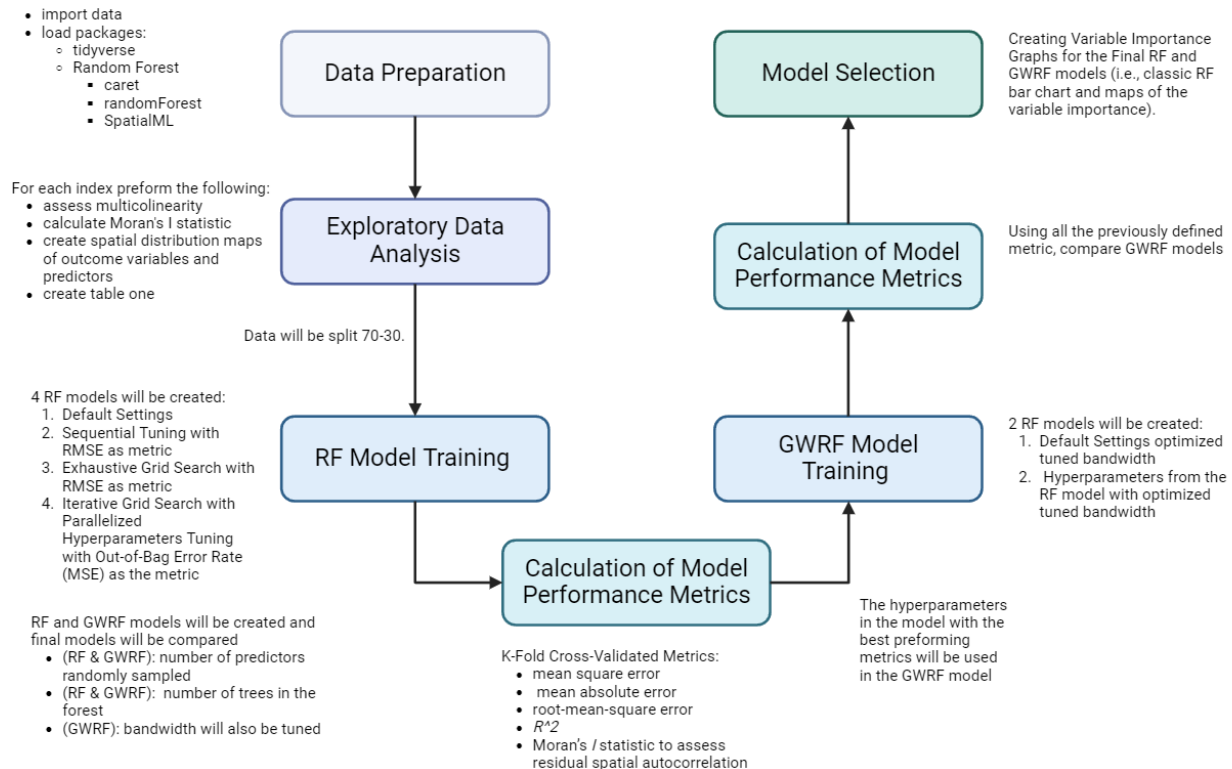
In Garson 2021, Ch 5 Random Forest, Garson teaches Random Forest Models by using `randomForest::randomForest()`, and in chapter 5.5.9 (pg. 267), he provides methods for tuning both of these parameters simultaneously using the Out of Bag MSE Error Rates. This value is a measure of the prediction error for data points that were not used in training each tree, and it can be written as $\text{OOB Error Rate} = \frac{1}{n} \sum_{i=1}^N (y_i - \hat{y}_i^{\text{OOB}})^2$. \hat{y}_i^{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.

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).

4 RF models will be built, and they differ based on the different hyperparameters: (1) default settings; (2) tuned by first tuning *mtry*, with *ntrees* set to default, and subsequently tuning then *ntrees* while keeping the newly defined *mtry* constant and both methods use RMSE as the metric; (3) tuned both *mtry* and *ntrees* with an Exhaustive Grid Search and both methods use RMSE as the metric, (4) tune tuned with Out of Bag MSE Error Rates as described by Garson 2021. For each model, MAE, MSE, 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.

Lastly, the feature importance plots will be generated for the final, and local feature importance plots will also be created.



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.

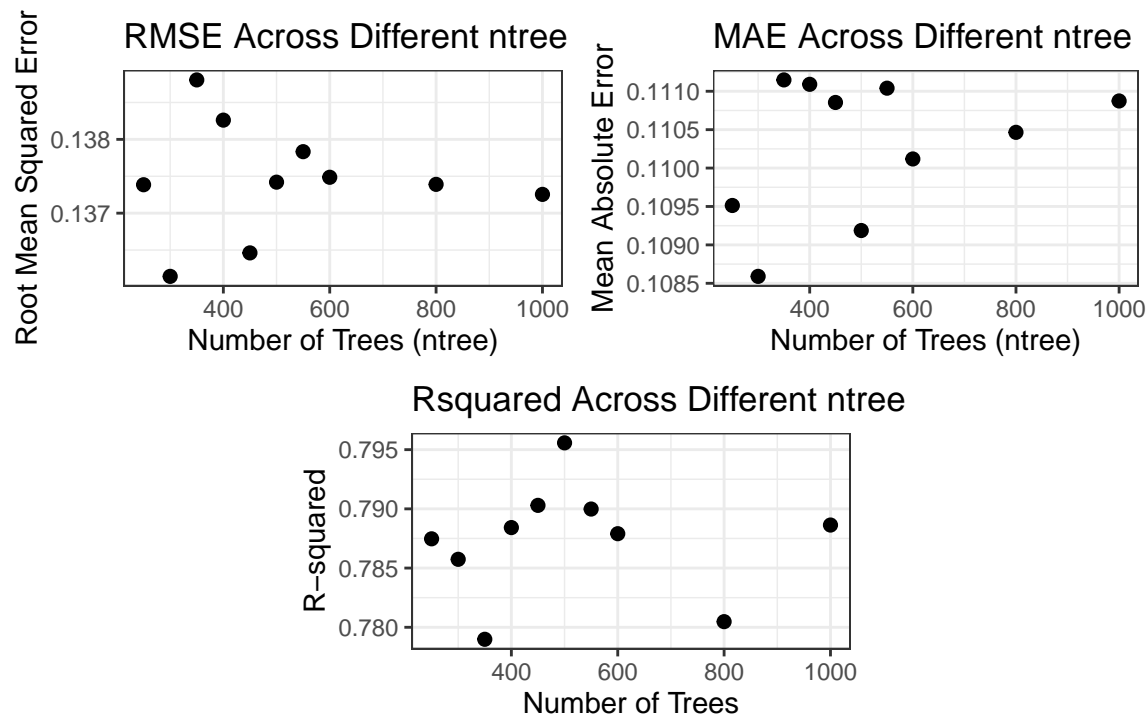
```
##
## Call:
##  randomForest(x = x, y = y, ntree = 500, mtry = param$mtry, importance = TRUE)
##              Type of random forest: regression
##              Number of trees: 500
## No. of variables tried at each split: 5
##
##              Mean of squared residuals: 0.01921465
##              % Var explained: 77.13
```

RF Model 2 - Sequential Processing With RMSE Metric

Background: This model training process uses a combination of sequential processing and cross-validation. First, tuning the `mtry` parameter by using cross-validation to find the best value for each iteration. The model runs 10 times (i.e., the for loop) because given the nature of the building random forest models, the value of `m` within the loop changes. Therefore, performing the function 10 times and taking the average of the most optimal `mtry` value it calculates and prints the average of the best `mtry` values. During the second step, the `ntree` is changing and cross-validated while `mtry` is held constant.

```
##
## Call:
## randomForest(x = x, y = y, ntree = 300, mtry = param$mtry, importance = TRUE)
##               Type of random forest: regression
##               Number of trees: 300
## No. of variables tried at each split: 6
##
##               Mean of squared residuals: 0.01867418
##               % Var explained: 77.78
```

The following graph illustrates performance metrics across different values of `ntree`, and the selection for the final `ntree` value stems from having the lowest RMSE/MAE and the highest R-Squared Value.



`mtry = 6`

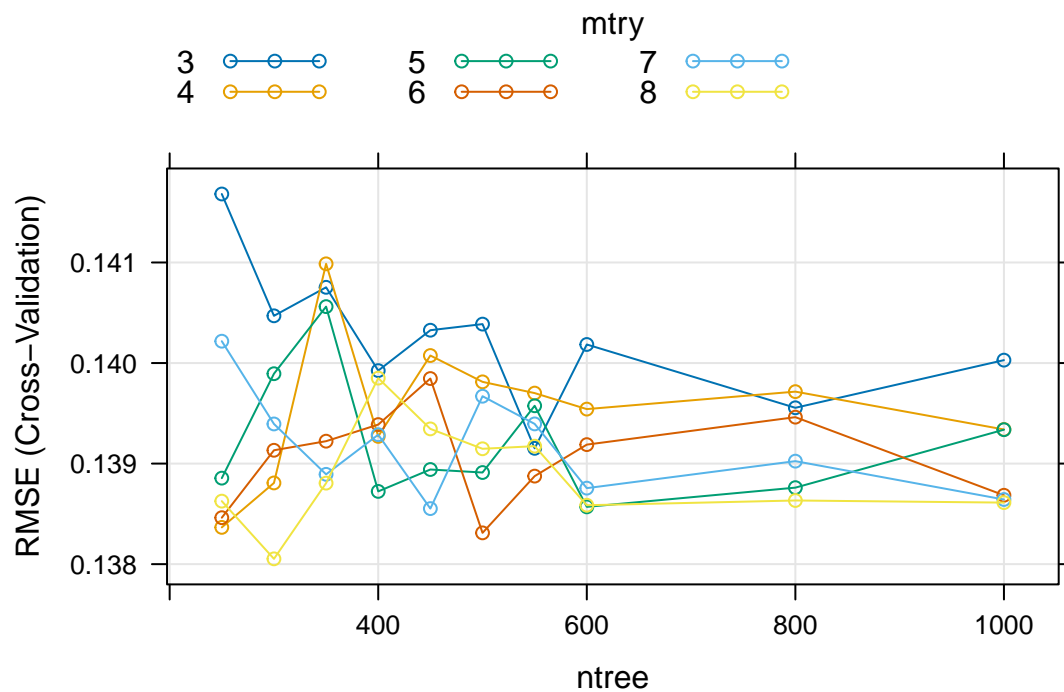
The second model hyperparameters have been set to `mtry = 6`, and `ntrees = 300`.

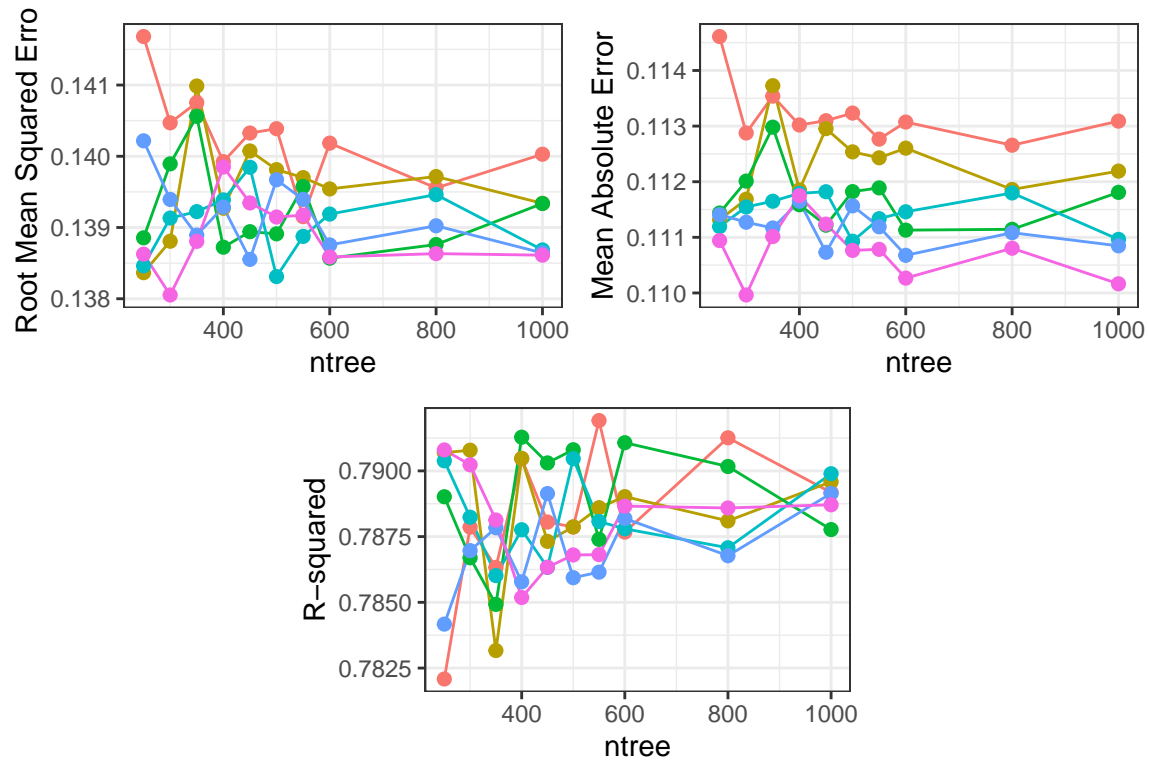
Model 3 - Exhaustive Grid Search with RMSE as Metric

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

```
##  
## Call:  
## randomForest(x = x, y = y, ntree = param$ntree, mtry = param$mtry,      importance = TRUE)  
##           Type of random forest: regression  
##           Number of trees: 300  
## No. of variables tried at each split: 8  
##  
##           Mean of squared residuals: 0.01880437  
##           % Var explained: 77.62
```

The following graph illustrates performance metrics across different values of *ntree*, and the selection for the final *ntree* value stems from having the lowest RMSE/MAE and the highest R-Squared Value.





The final values used for the model were $mtry = 8$ and $ntree = 300$. Note that the variation between each of the combinations is minimal.

Model 4

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 if *y* is continuous).
- Parallel Processing: The `foreach` loop with the `.dopar` argument allows for parallel execution of the grid search, which speeds up the computation.
- 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.

```
#####  
##### 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  
}  
  
# create a vector of ntree values of interest  
vntree = c(51, 101, 501, 1001, 1501)  
  
# specify the predictor (x) and outcome (y) object  
x = df %>% select(starts_with("e_")) %>% st_drop_geometry()  
y = df %>% pull(rpl_themes)  
  
# Create a function to get random forest error information for different mtry values  
tune = function(x, y, ntree = vntree, mtry = NULL, keep.forest = FALSE, ...) {
```

```

# Define the combination function to aggregate results
comb = function(a, b) {
  if (is.null(a)) return(b)
  rbind(a, b)
}
results = foreach(mtry = mtry_iter(1, ncol(x)), .combine = comb, .packages = 'randomForest')
  model = randomForest::randomForest(x, y, ntree = max(ntree), mtry = mtry, keep.forest = FALSE)
  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)
}
return(results)
}

# running the tuning
results = tune(x,y) %>%
  mutate(MSE = error) %>%
  select(-error)

# examinations of other hyperparameters
# table
temp = results %>%
  arrange(MSE) %>%
  head()

kable(temp, caption = "Model 4 Performance Metrics", digits = 4, align = c("l", "l", "c"))

```

Table 1: Model 4 Performance Metrics

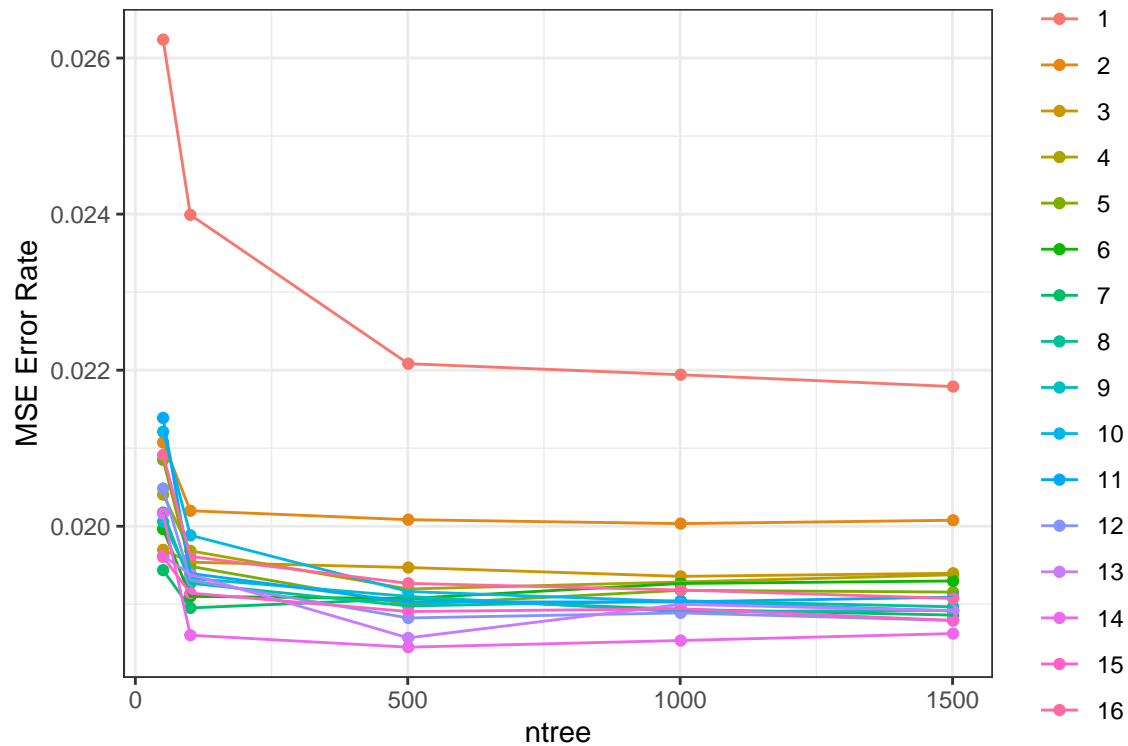
ntree	mtry	MSE
501	14	0.0184
1001	14	0.0185
501	13	0.0186
101	14	0.0186
1501	14	0.0186
1501	12	0.0188

```

# plot
ggplot(results, aes(y = MSE, x = ntree,
                    color = as.factor(mtry))) +
  geom_point() +
  geom_line() +
  theme_bw() +

```

```
labs(color = "mtry", y = "MSE Error Rate")
```



```
best_mtry = temp$mtry[[1]]
best_ntree = temp$ntree[[1]]

# creating the first model
rf_mod4 = train(rpl_themes ~.,
                data = df,
                method = "rf",
                trControl = trainControl(method = "cv", number = 10),
                tuneGrid = expand.grid(mtry = best_mtry),
                ntree = best_ntree,
                importance = TRUE)

# Print the results
rf_mod4$finalModel

##
## Call:
## randomForest(x = x, y = y, ntree = ..1, mtry = param$mtry, importance = TRUE)
##           Type of random forest: regression
##           Number of trees: 501
## No. of variables tried at each split: 14
##
##           Mean of squared residuals: 0.01908644
##           % Var explained: 77.29
```

The final model hyperparameters have been set to $mtry = 14$, and $ntrees = 501$. The graph below illustrates that the errors across the hyperparameters used with this method are very similar.

RF Model Evaluation

Despite variations in the m and $ntrees$ parameters across different models, the overall prediction performance remains consistent. 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 4 produced code that is lowest MSE and RMSE, and highest R-squared value, these are the parameters that will be head contains for the GWRF.

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

Table 2: Performance Metrics for Each Model

Model	mtry	ntree	MAE	RMSE	R_Squared
Model 1	5	500	0.111	0.139	0.790
Model 2	6	550	0.112	0.138	0.789
Model 3	8	540	0.112	0.139	0.788
Model 4	14	501	0.108	0.138	0.789

Training a Geographically Weighted Random Forest Model

GWRF Model 1

This model has hyperparameters defined with *mtry* and *trees* by the default, and optimized *bandwidth*.

```
## Ranger result
##
## Call:
## ranger(rpl_themes ~ e_pov150 + e_unemp + e_hburd + e_nohsdp + e_uninsur + e_age65 + e_age17,
##
## Type: Regression
## Number of trees: 500
## Sample size: 246
## Number of independent variables: 16
## Mtry: 5
## Target node size: 5
## Variable importance mode: impurity
## Splitrule: variance
## OOB prediction error (MSE): 0.01898519
## R squared (OOB): 0.774974
## e_pov150 e_unemp e_hburd e_nohsdp e_uninsur e_age65 e_age17
## 3.11886904 0.35103129 0.72168143 1.52655612 0.44640200 1.05723955 0.50747560
## e_disabl e_sngpnt e_limeng e_minrty e_munit e_mobile e_crowd
## 0.28549567 0.48836060 3.30680893 2.50852329 0.96675258 0.09114209 1.31459441
## e_noveh e_groupq
## 3.25499941 0.30207710
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## -0.407359 -0.109665 -0.005041 -0.006256 0.096517 0.501859
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## -0.0457386 -0.0068265 0.0000491 0.0009267 0.0079773 0.0614741
## Min Max Mean StD
## e_pov150 0.046156835 0.88564486 0.33982742 0.16187352
## e_unemp 0.014877945 0.31376208 0.08115051 0.04731030
## e_hburd 0.021651832 0.66255123 0.16761710 0.12182127
## e_nohsdp 0.038328814 1.14256174 0.25038711 0.20982340
## e_uninsur 0.020891089 0.22493313 0.07990350 0.04257707
## e_age65 0.014934781 0.79831976 0.14149547 0.18942335
## e_age17 0.015950759 0.24873496 0.07811220 0.04815336
## e_disabl 0.021494108 0.49258775 0.07935985 0.05388009
## e_sngpnt 0.020125384 0.52719856 0.11282993 0.08591079
## e_limeng 0.017820815 1.13352793 0.28145306 0.19524155
## e_minrty 0.028178321 0.89391507 0.22791211 0.18023411
## e_munit 0.016766064 0.94984198 0.20420939 0.18799483
## e_mobile 0.001055735 0.07820255 0.01465081 0.01209504
## e_crowd 0.019229361 0.91334070 0.20558264 0.14672485
## e_noveh 0.054622095 0.88894292 0.35680150 0.20188076
## e_groupq 0.021167695 0.18541030 0.06335931 0.02737005
```

The final model hyperparameters have been set to $bandwidth = 49$, $mtry = 5$, and $ntrees = 500$.

GWRF Model 2

This model has hyperparameters defined with *mtry* and *trees* by the default, and optimized *bandwidth*.

```
## Ranger result
##
## Call:
## ranger(rpl_themes ~ e_pov150 + e_unemp + e_hburd + e_nohsdp +          e_uninsur + e_age65 + e_
##
## Type:                      Regression
## Number of trees:           501
## Sample size:               246
## Number of independent variables: 16
## Mtry:                      14
## Target node size:          5
## Variable importance mode:   impurity
## Splitrule:                 variance
## OOB prediction error (MSE): 0.01883109
## R squared (OOB):           0.7768005
##   e_pov150   e_unemp   e_hburd   e_nohsdp   e_uninsur   e_age65   e_age17
## 4.10081279 0.31785849 0.31273405 0.88710876 0.30684484 1.15957328 0.47339192
##   e_disabl   e_sngpnt   e_limeng   e_minrty   e_munit   e_mobile   e_crowd
## 0.25058089 0.30080880 5.31853956 1.33509068 1.08804794 0.09666911 0.84673178
##   e_noveh   e_groupq
## 3.32078161 0.24738591
##      Min.    1st Qu.    Median      Mean    3rd Qu.      Max.
## -0.4601121 -0.1193271 -0.0009903 -0.0062199  0.1036436  0.4871807
##      Min.    1st Qu.    Median      Mean    3rd Qu.      Max.
## -0.0546891 -0.0064796 -0.0001545  0.0005713  0.0066960  0.0579278
##
##           Min           Max           Mean           StD
## e_pov150  0.0134565521 1.08182924 0.319395820 0.22224044
## e_unemp   0.0047098959 0.31425217 0.053719871 0.04439710
## e_hburd   0.0077887639 1.12829917 0.134592860 0.18749551
## e_nohsdp  0.0192541366 2.37289162 0.304738276 0.43303174
## e_uninsur 0.0100748366 0.20525875 0.052836979 0.04051624
## e_age65   0.0043546796 1.50395820 0.160254345 0.29791113
## e_age17   0.0067403201 0.34369630 0.057245864 0.06093593
## e_disabl  0.0077638674 0.38294912 0.037217133 0.03840158
## e_sngpnt  0.0064697490 0.75923053 0.086742849 0.11356979
## e_limeng  0.0080110778 2.47321868 0.261771262 0.29669757
## e_minrty  0.0091052206 1.30925511 0.207884201 0.24281671
## e_munit   0.0119653092 1.67699261 0.245406399 0.33357410
## e_mobile  0.0002019652 0.07982328 0.009813122 0.01180187
## e_crowd   0.0093362544 1.62490074 0.192861641 0.24326663
## e_noveh   0.0152481131 1.60799589 0.398805303 0.36846838
## e_groupq  0.0071932965 0.24371320 0.045329541 0.03001460
```

The final model hyperparameters have been set to *bandwidth* = 47, *mtry* = 14, and *ntrees* = 501.

GWRF Model Evaluation

The models both perform nearly identically because the hyperparameters perform nearly identically. Therefore, the model defined by the previous traditional random forest model.

Table 3: Performance Metrics for Each Model

Model	bw	mtry	ntree	MAE	RMSE	R_Squared
Model 5	49	5	500	0.110	0.138	0.774
Model 6	47	9	501	0.108	0.137	0.776

Random Forest Model Comparisons

Model 4 shows a lower MAE and MSE, indicating that it generally makes smaller errors in prediction. The RMSE is also relatively low, and the high R^2 value (0.791) suggests that this model explains a significant portion of the variance in the SVI. Overall, Model 4 performs well and is effective in predicting SVI using the selected predictors.

Model 6 has higher MAE and MSE values, indicating that it makes larger errors on average compared to Model 4. The RMSE is also higher, and the R^2 is lower (0.638), suggesting that Model 6 explains less variance in the SVI. This could mean that while the Geographically Weighted Random Forest accounts for spatial autocorrelation, it may not perform as well in terms of overall prediction accuracy as the traditional Random Forest.

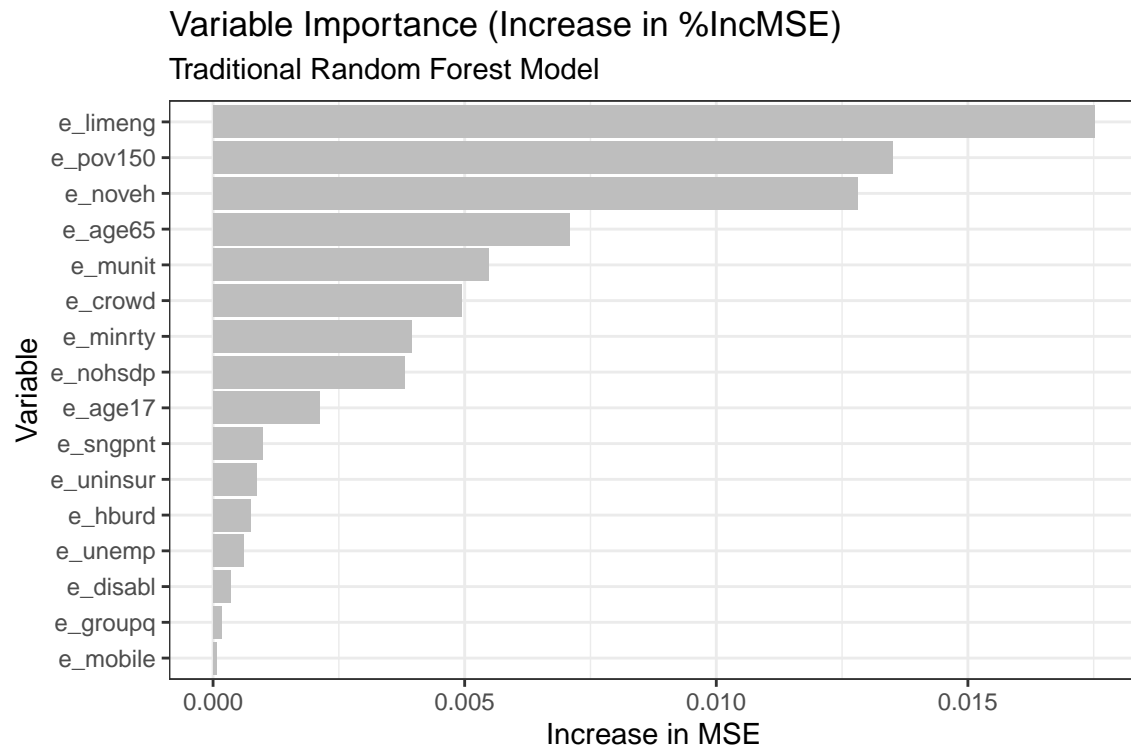
Model 4 (Traditional Random Forest) outperforms Model 6 (Geographically Weighted Random Forest) in terms of accuracy and explained variance. However, Model 6 is still valuable because it accounts for spatial dependencies. Model 6 might be more appropriate despite its lower overall performance metrics, particularly if the goal is to understand regional variations in the SVI. However, if the focus is purely on predictive accuracy, Model 4 appears to be the better choice.

Table 4: Performance Metrics for Each Model

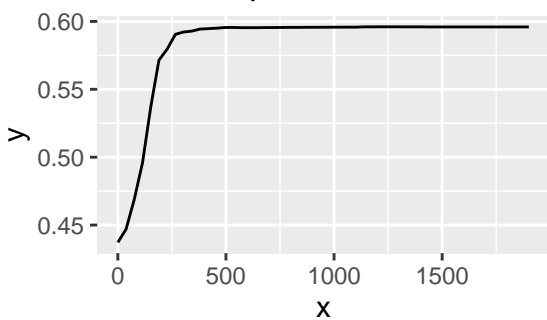
	Model	bw	mtry	ntree	MAE	RMSE	R_Squared
4	Model 4	-	14	501	0.108	0.138	0.789
2	Model 6	47	9	501	0.108	0.137	0.776

Graphs for the Final Models

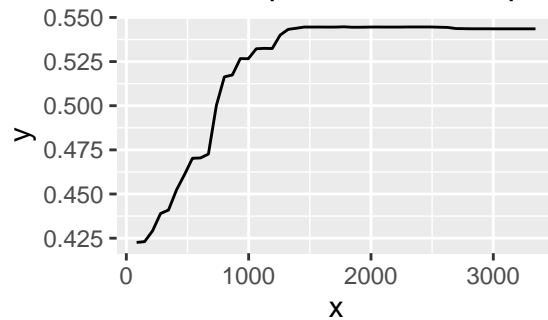
Traditional Random Forest



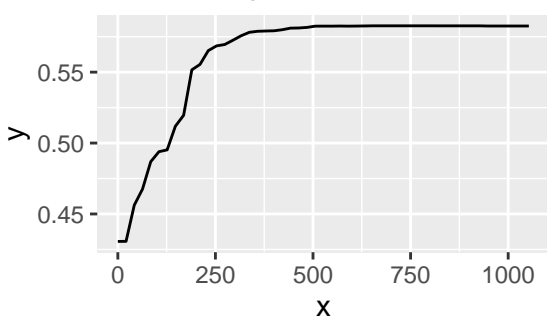
Partial Dependence of e_limer



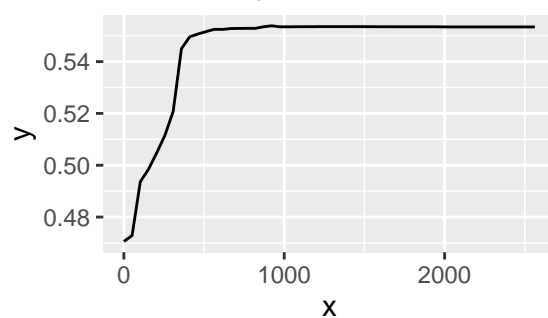
Partial Dependence of e_pov'



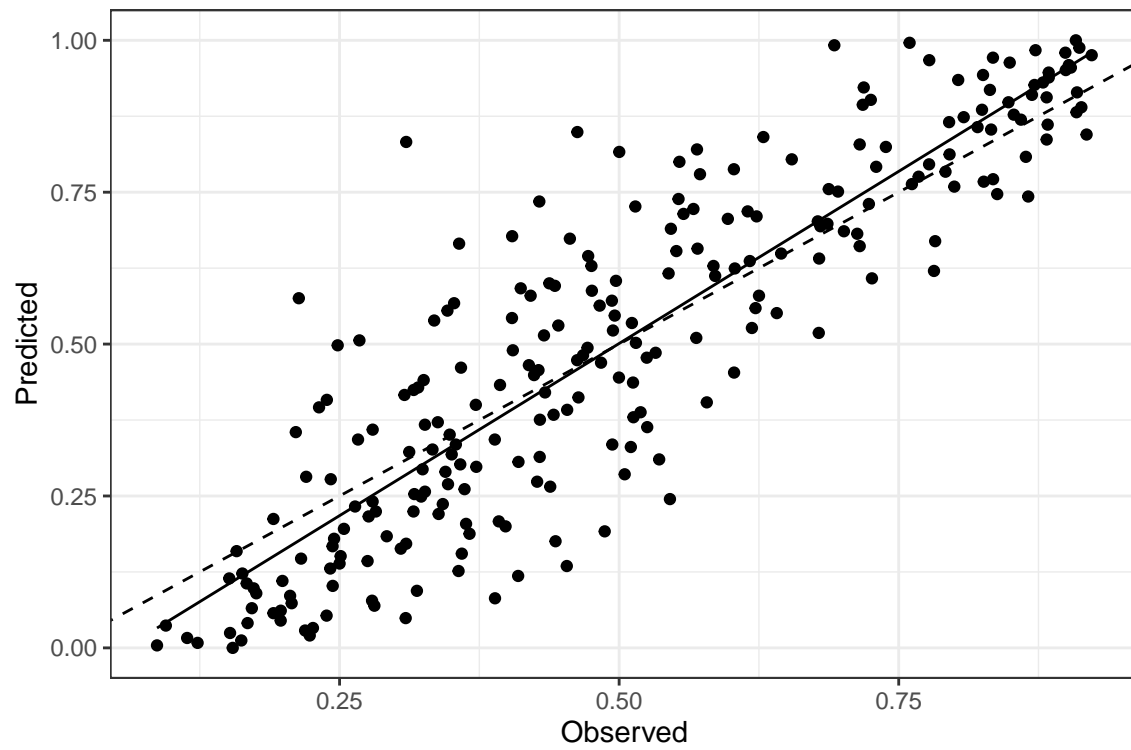
Partial Dependence of e_nove



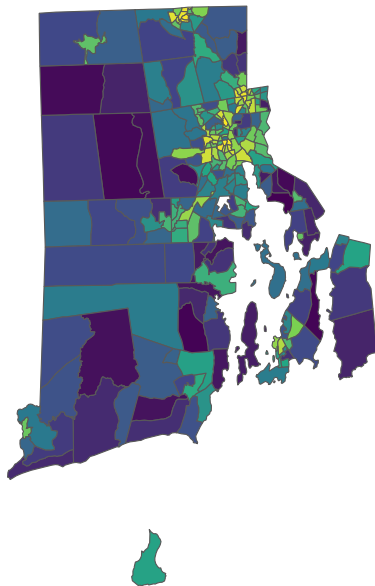
Partial Dependence of e_muni



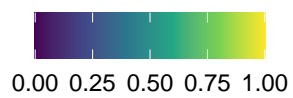
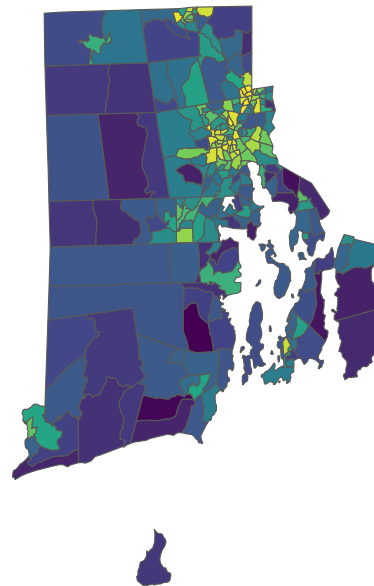
Geographically Weighted Random Forest



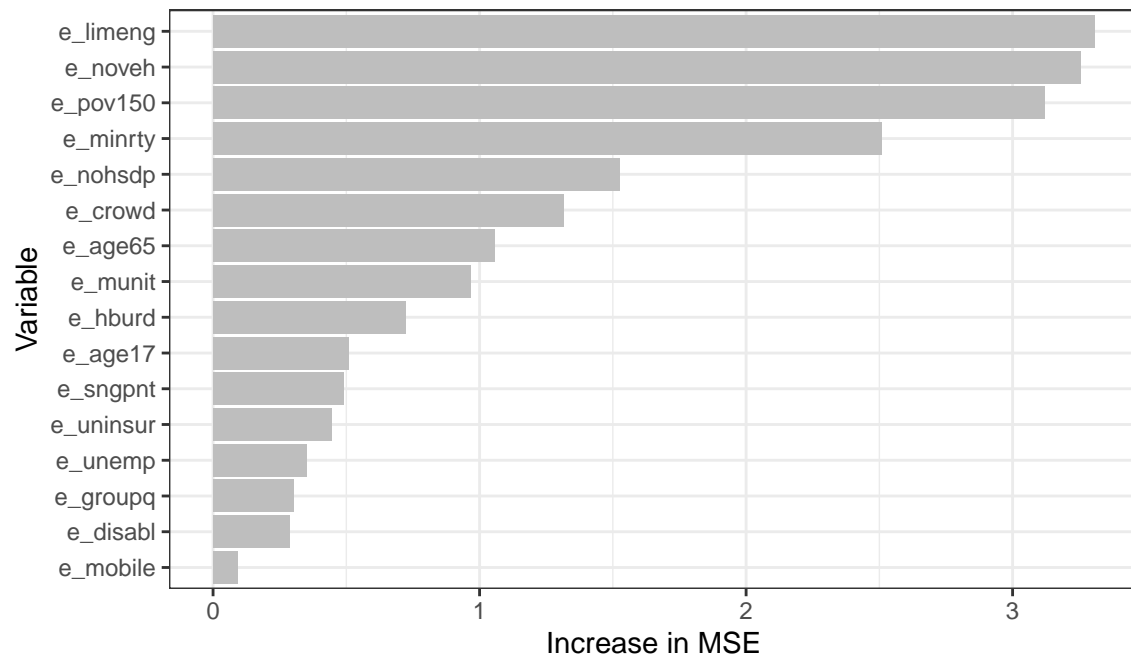
Observed SVI Values



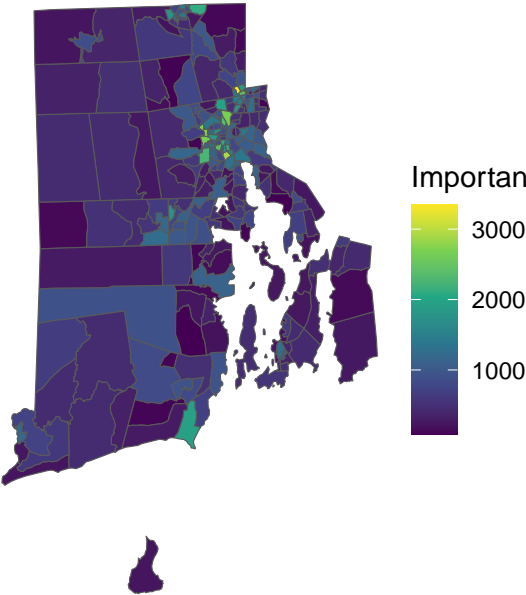
Predicted SVI Values



Variable Importance (Increase in %IncMSE)
Geographically Weighted Random Forest Model

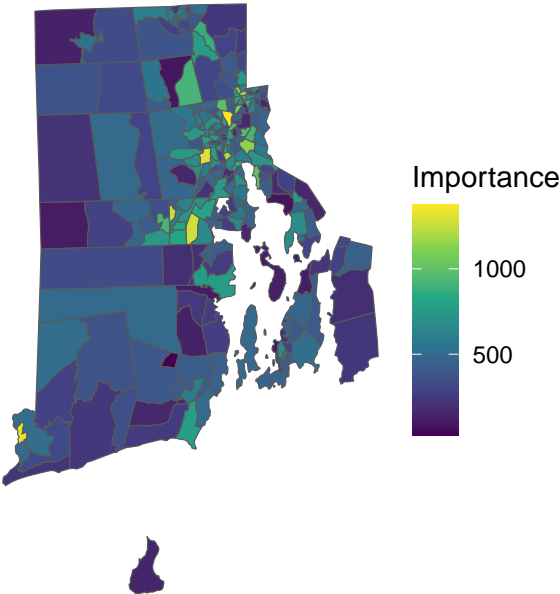


e_pov150

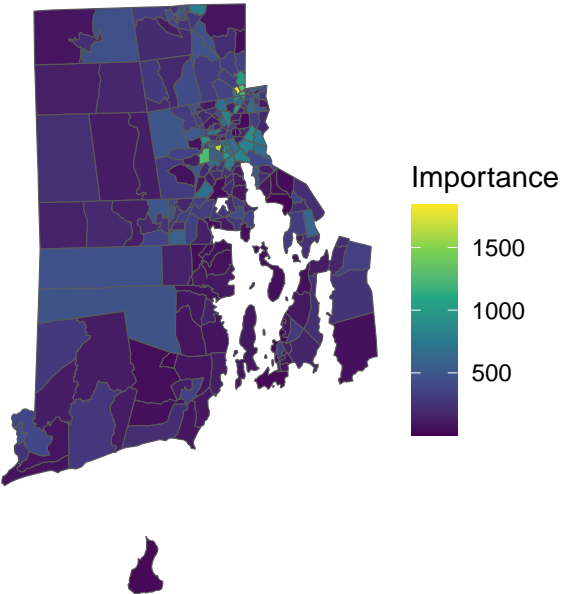


Local Variable Importance of SocioEconomic Status Variables

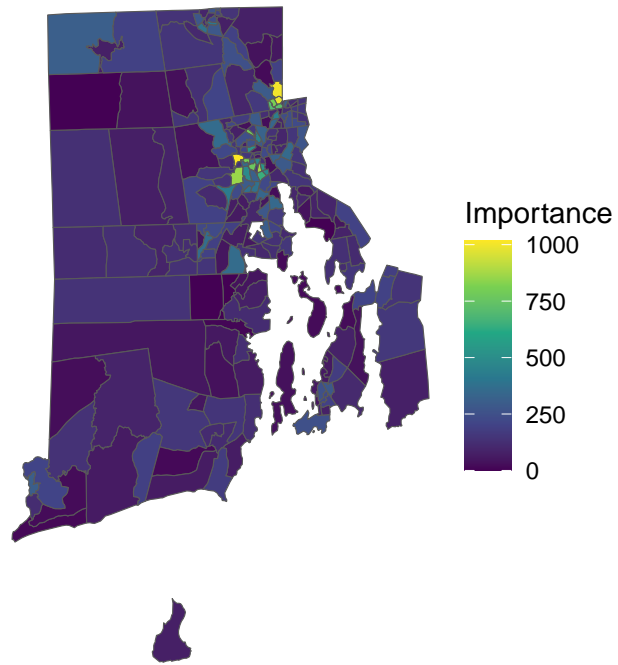
e_hburd



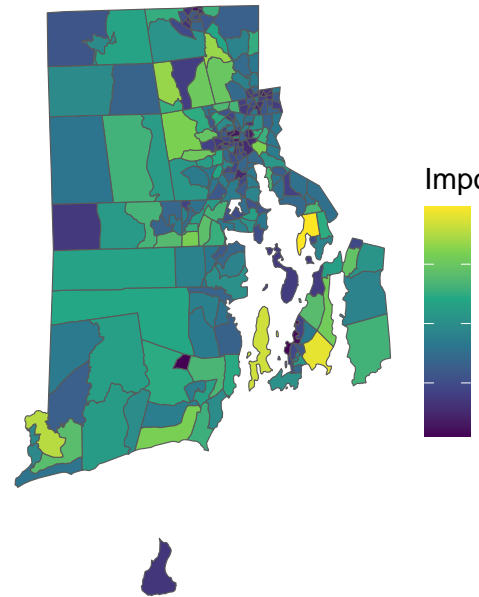
e_nohsdp



e_uninsur

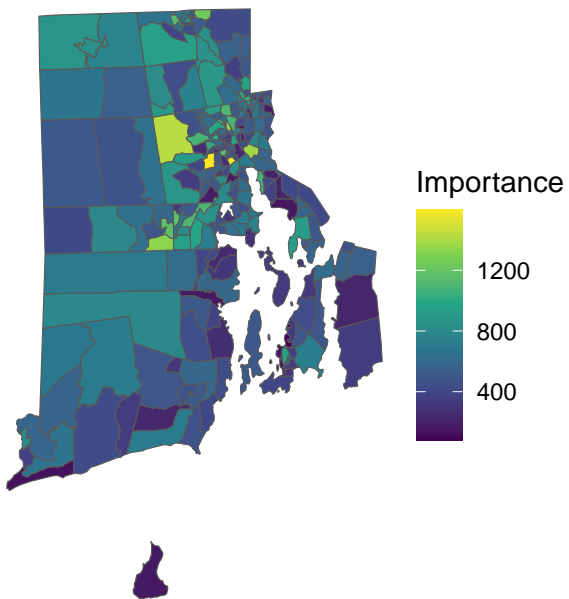


e_age65

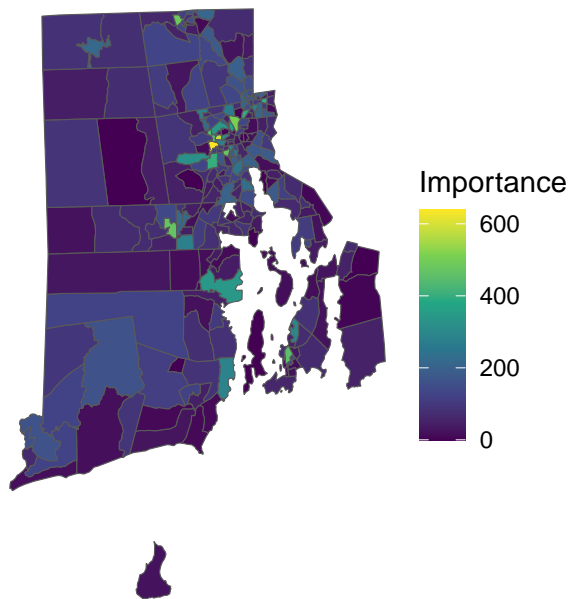


Local Variable Importance of Household Characteristics Variables

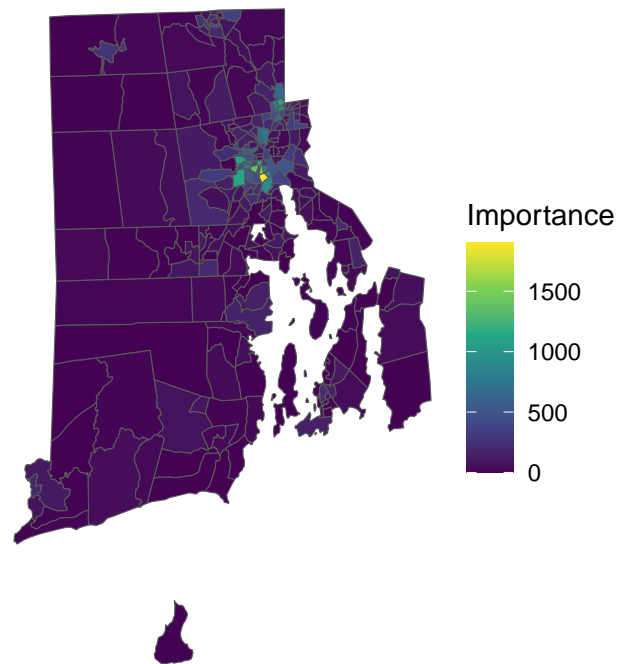
e_disabl



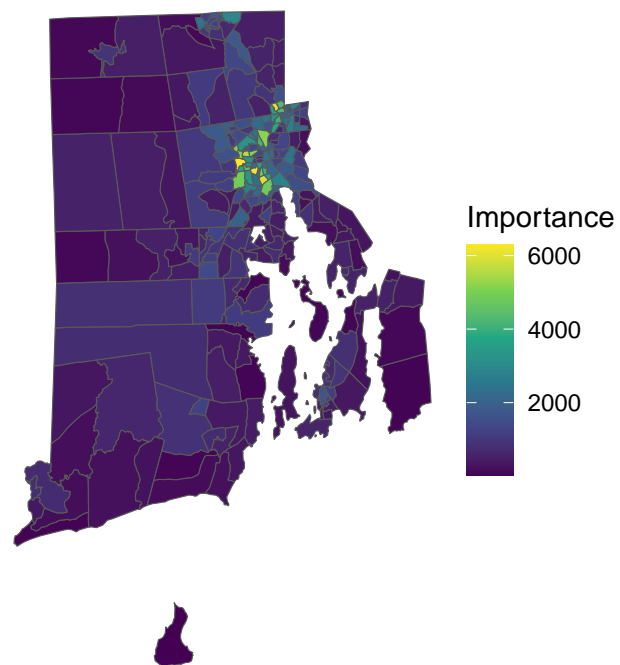
e_sngpnt



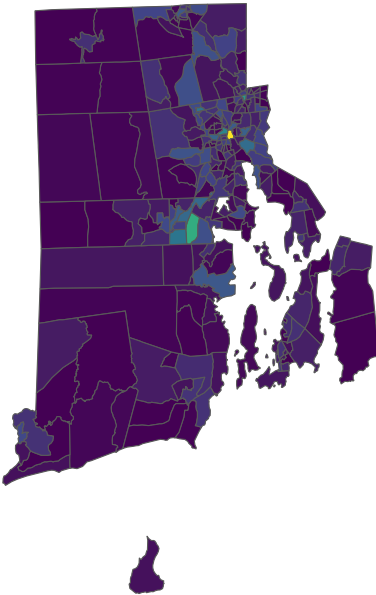
e_limeng



Local Variable Importance of Racial & Ethnic Minority Status Variables
e_minrty

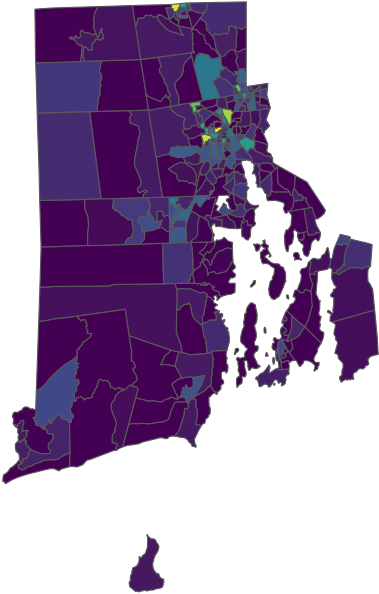


e_munit

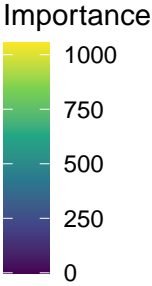
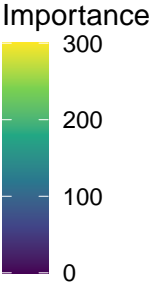
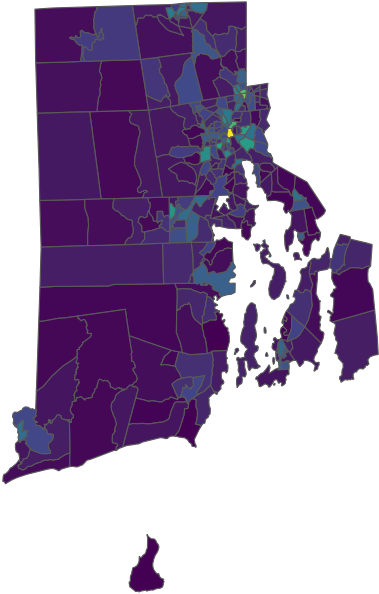


Local Variable Importance of Housing Type & Transportation Variables

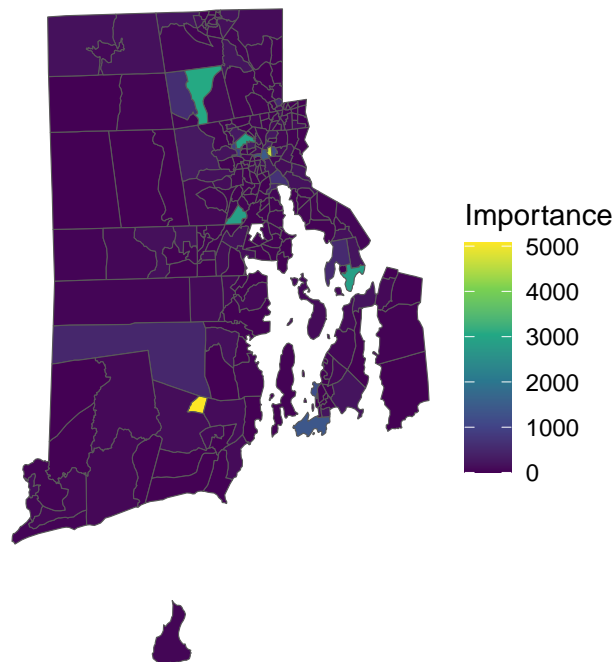
e_crowd



e_noveh



e_groupq



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"))
#####
#### 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(foreach)       # parrallel processing
library(ggpubr)        # arrange multiple graphs

### 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
svi_df = inner_join(tracts, svi_df, by = c("GEOID" = "fips"))

### defining analytical coordinates and df
df_coords = svi_df %>%
  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_"))
#####
##### 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
rf_mod1 = train(rpl_themes ~.,
                data = df,
                method = "rf",
                trControl = trainControl(method = "cv", number = 10),
                tuneGrid = expand.grid(mtry = mtry),
                ntree = 500,
                importance = TRUE)

# Print the results
rf_mod1$finalModel
#####
##### RF Mod 2 #####
#####

### setting seed
set.seed(926)

### Step 1: Find the best `mtry` value
# Create an empty list to store the results
results_list = vector("list", 10)
# Loop to repeat the code 10 times
for (i in 1:10) {
  # Train the random forest model with 10-fold cross-validation
  rf_mod2 = train(rpl_themes ~ ., data = df, method = "rf",
                  ntree = 500, # Start with a default number of trees
                  trControl = trainControl(method = "cv", number = 10),
                  tuneGrid = expand.grid(mtry = c(3:8)))

  # print model results
  # print(rf_mod2)
  plot(rf_mod2)

  # Extract the best number of predictors (mtry) from the model
  m = rf_mod2$bestTune$mtry

  # Store the result in the list
  results_list[[i]] = m
}

mean_mtry = round(mean(unlist(results_list)))

```

```

# Step 2: Find the best `ntree` value using cross-validation with the optimal `mtry`
store_maxtrees = list()
ntree_values = c(250, 300, 350, 400, 450, 500, 550, 600, 800, 1000) # List of `ntree` values to test

for (ntree in ntree_values) {
  rf_maxtrees = train(rpl_themes ~ ., data = df, method = "rf",
    tuneGrid = expand.grid(mtry = mean_mtry), # Use the fixed best `mtry`
    trControl = trainControl(method = "cv", number = 10),
    ntree = ntree)

  # print model results
  # print(rf_maxtrees)

  store_maxtrees[[as.character(ntree)]] <- rf_maxtrees
}

# 500 subjectively made
# summary(resamples(store_maxtrees))

# creating the first model
rf_mod2 = train(rpl_themes ~ .,
  data = df,
  method = "rf",
  trControl = trainControl(method = "cv", number = 10),
  tuneGrid = expand.grid(mtry = mean_mtry),
  ntree = 300,
  importance = TRUE)

# Print the results
rf_mod2$finalModel
# Initialize an empty data frame to store all metrics
metrics_df <- data.frame()

# Loop through each model in store_maxtrees
for (ntree in names(store_maxtrees)) {
  model <- store_maxtrees[[ntree]]

  # Extract metrics for the current model
  model_metrics <- data.frame(
    ntree = as.numeric(ntree), # Capture the ntree value
    RMSE = model$results$RMSE, # Extract RMSE
    MAE = model$results$MAE, # Extract MAE
    Rsquared = model$results$Rsquared, # Extract Rsquared
    mtry = model$bestTune$mtry # Capture the mtry value
  )

  # Append the metrics to the main data frame
  metrics_df <- rbind(metrics_df, model_metrics)
}

```

```

}

# Create the line graph
a=ggplot(metrics_df, aes(x = ntree, y = RMSE)) +
  geom_point(size = 2) +
  labs(title = "RMSE Across Different ntree",
       x = "Number of Trees (ntree)",
       y = "Root Mean Squared Error",
       shape = "ntree") +
  theme_bw()

b=ggplot(metrics_df, aes(x = ntree, y = MAE)) +
  geom_point(size = 2) +
  labs(title = "MAE Across Different ntree",
       x = "Number of Trees (ntree)",
       y = "Mean Absolute Error",
       shape = "ntree") +
  theme_bw()

c=ggplot(metrics_df, aes(x = ntree, y = Rsquared)) +
  geom_point(size = 2) +
  labs(title = "Rsquared Across Different ntree",
       x = "Number of Trees",
       y = "R-squared",
       shape = "ntree") +
  theme_bw()

blank = ggplot() + theme_void()

fig = ggarrange(
  ggarrange(a, b, blank, nrow = 1,
            widths = c(1, 1, 0), legend = "none"),
  ggarrange(blank, c, blank, nrow = 1,
            widths = c(0.5, 1, 0.5), legend = "none"),
  nrow = 2,
  legend = "none"
)

annotate_figure(fig, bottom = text_grob("mtry = 6", hjust = 1, x = 1))
#####
##### RF Mod 3 #####
#####

### setting seed
set.seed(926)

```

```

# Define the tuned parameter
grid = expand.grid(.mtry = c(3:8),
                  .ntree = c(250, 300, 350, 400, 450, 500, 550, 600, 800, 1000) )

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

# create custom
customRF <- list(type = "Regression", library = "randomForest", loop = NULL)
customRF$parameters <- data.frame(parameter = c("mtry", "ntree"), class = rep("numeric", 2), labels = c("mtry", "ntree"))
customRF$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

# creating the first model
rf_mod3 = train(rpl_themes ~.,
               data = df,
               method = customRF,
               trControl = ctrl,
               tuneGrid = grid,
               importance = TRUE)

# Print the results
rf_mod3$finalModel
plot(rf_mod3)

metrics_df = as.data.frame(rf_mod3$results)

# Create the line graph
a = ggplot(metrics_df, aes(x = ntree, y = RMSE, color = as.factor(mtry))) +
  geom_line() +
  geom_point(size = 2) +
  labs(y = "Root Mean Squared Error") +
  theme_bw()

b = ggplot(metrics_df, aes(x = ntree, y = MAE, color = as.factor(mtry))) +
  geom_line() +
  geom_point(size = 2) +
  labs(y = "Mean Absolute Error") +
  theme_bw()

```



```

c = ggplot(metrics_df, aes(x = ntree, y = Rsquared, color = as.factor(mtry))) +
  geom_line() +
  geom_point(size = 2) +
  labs(y = "R-squared") +
  theme_bw()

fig = ggarrange(
  ggarrange(a, b, blank, nrow = 1,
    widths = c(1, 1, 0), legend = "none"),
  ggarrange(blank, c, blank, nrow = 1,
    widths = c(0.5, 1, 0.5), legend = "none"),
  nrow = 2,
  legend = "none"
)
annotate_figure(fig)
#####
##### 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
}

# create a vector of ntree values of interest
vntree = c(51, 101, 501, 1001, 1501)

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

# Create a function to get random forest error information for different mtry values
tune = function(x, y, ntree = vntree, mtry = NULL, keep_forest = FALSE, ...) {

  # Define the combination function to aggregate results
  comb = function(a, b) {
    if (is.null(a)) return(b)
    rbind(a, b)
  }

```

```

results = foreach(mtry = mtry_iter(1, ncol(x)), .combine = comb, .packages = 'randomForest')
  model = randomForest::randomForest(x, y, ntree = max(ntree), mtry = mtry, keep.forest = FALSE)
  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)
}
return(results)
}

# running the tuning
results = tune(x,y) %>%
  mutate(MSE = error) %>%
  select(-error)

# examinations of other hyperparameters
# table
temp = results %>%
  arrange(MSE) %>%
  head()

kable(temp, caption = "Model 4 Performance Metrics", digits = 4, align = c("l", "l", "c"))

# plot
ggplot(results, aes(y = MSE, x = ntree,
                    color = as.factor(mtry))) +
  geom_point() +
  geom_line() +
  theme_bw() +
  labs(color = "mtry", y = "MSE Error Rate")

best_mtry = temp$mtry[[1]]
best_ntree = temp$ntree[[1]]

# creating the first model
rf_mod4 = train(rpl_themes ~.,
  data = df,
  method = "rf",
  trControl = trainControl(method = "cv", number = 10),
  tuneGrid = expand.grid(mtry = best_mtry,
    ntree = best_ntree,
    importance = TRUE)

# Print the results
rf_mod4$finalModel

```

```
#####
#### RF Models ####
#####

# Create a data frame with the results
results_rf = data.frame(
  Model = c("Model 1", "Model 2", "Model 3", "Model 4"),
  mtry = c(rf_mod1$results$mtry,
            rf_mod2$results$mtry,
            rf_mod3$bestTune[[1]],
            rf_mod4$results$mtry),
  ntree = c(500, 550, 540, 501),
  MAE = c(rf_mod1$results$MAE,
            rf_mod2$results$MAE,
            mean(rf_mod3$results$MAE),
            rf_mod4$results$MAE),
  RMSE = c(rf_mod1$results$RMSE,
            rf_mod2$results$RMSE,
            mean(rf_mod3$results$RMSE),
            rf_mod4$results$RMSE),
  R_Squared = c(rf_mod1$results$Rsquared,
                 rf_mod2$results$Rsquared,
                 mean(rf_mod3$results$Rsquared),
                 rf_mod4$results$Rsquared))

# 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"))
#####
#### GWRF Mod 1 ####
#####

# testing for optimal bandwidth
temp = SpatialML::grf.bw(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,
                          dataset = df,
                          kernel = "adaptive",
                          bw.min = 20,
                          bw.max = 50,
                          coords = df_coords,
                          trees = 500,
                          mtry = mtry,
                          step = 1, importance = "impurity")
best.bw_gwrf_mod1 = temp$Best.BW
```

```

# defining the spatial model with prior model hyparameters
gwr_mod1 = SpatialML::grf(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,
                          dframe = df,
                          kernel = "adaptive",
                          coords = df_coords,
                          bw = best.bw_gwr_mod1,
                          ntree = 500,
                          mtry = mtry,
                          importance = "impurity")

#####
#### GWR Mod 2 ####
#####

# testing for optimal bandwidth
temp = SpatialML::grf.bw(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,
                          dataset = df,
                          kernel = "adaptive",
                          bw.min = 20,
                          bw.max = 50,
                          coords = df_coords,
                          trees = best_ntree,
                          mtry = rf_mod4$results$mtry,
                          step = 1)

best.bw_gwr_mod2 = temp$Best.BW

# defining the spatial model with prior model hyparameters
gwr_mod2 = SpatialML::grf(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,
                          dframe = df,
                          kernel = "adaptive",
                          coords = df_coords,
                          bw = best.bw_gwr_mod2,
                          ntree = best_ntree,
                          mtry = rf_mod4$results$mtry,
                          importance.mode = "impurity") # this is a ranger argument
                                                         # specification of this value
                                                         # corrected errors that previously appeared

```

```

# no importance value specified

#####
#### GWRF Models ####
#####

# Model 5
predictions5 = gwr_mod1$Global.Model$predictions
mse5 = mean((df$rp1_themes - predictions5)^2)
rmse5 = sqrt(mse5)
mae5 = sum(abs(df$rp1_themes - predictions5))/length(predictions5)
r_squared5 = 1 - sum((df$rp1_themes - predictions5)^2) / sum((df$rp1_themes - mean(df$rp1_themes))^2)

# Model 6
predictions6 = gwr_mod2$Global.Model$predictions
mse6 = mean((df$rp1_themes - predictions6)^2)
rmse6 = sqrt(mse6)
mae6 = sum(abs(df$rp1_themes - predictions6))/length(predictions6)
r_squared6 = 1 - sum((df$rp1_themes - predictions6)^2) / sum((df$rp1_themes - mean(df$rp1_themes))^2)

# Create a data frame with the results
results_grf = data.frame(
  Model = c("Model 5", "Model 6"),
  bw = c(best.bw_gwr_mod1, best.bw_gwr_mod2),
  mtry = c(5, 9),
  ntree = c(500, 501),
  MAE = c(mae5, mae6),
  RMSE = c(rmse5, rmse6),
  R_Squared = c(r_squared5, r_squared6)
)

# Print the results using kable
kable(results_grf, caption = "Performance Metrics for Each Model",
      digits = 3, align = c("l", "c", "c", "c", "c", "c", "c"))
#####
#### All Models ####
#####
final_results = results_rf[4,] %>%
  mutate(bw = "-") %>%
  select(Model, bw, mtry, ntree, MAE, RMSE, R_Squared)

final_results = rbind(final_results, results_grf[2,])

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

```

```
#####

df = df %>%
  mutate(rf_pred = as.data.frame(rf_mod4$finalModel$predicted)[[1]])

# Predicted 1:1 Plot
#ggplot(df, aes(x = rf_pred, y = rpl_themes)) +
#  geom_point() +
#  theme_bw() +
#  geom_abline(slope=1, intercept=0, linetype="dashed", size=0.5) +
#  geom_smooth(method = "lm", se = FALSE, colour="black", size=0.5) +
#  labs(x="Observed", y = "Predicted")

# Variable Importance
temp = as.data.frame(rf_mod4$finalModel$importance)
colnames(temp) = c("IncMSE", "IncNodePurity")
temp = tibble::rownames_to_column(temp, "Variable")

ggplot(temp, aes(x = fct_reorder(Variable, IncMSE), y = IncMSE)) +
  geom_bar(stat = "identity", fill = "grey") +
  coord_flip() + # Flip coordinates for better readability
  labs(title = "Variable Importance (Increase in %IncMSE)",
       subtitle = "Traditional Random Forest Model",
       x = "Variable",
       y = "Increase in MSE") +
  theme_bw()

# Generate Partial Dependence Plots and store them as ggplot objects
a = as.data.frame(randomForest::partialPlot(rf_mod4$finalModel, df, e_limeng, plot = FALSE))
b = as.data.frame(randomForest::partialPlot(rf_mod4$finalModel, df, e_pov150, plot = FALSE))
c = as.data.frame(randomForest::partialPlot(rf_mod4$finalModel, df, e_noveh, plot = FALSE))
d = as.data.frame(randomForest::partialPlot(rf_mod4$finalModel, df, e_munit, plot = FALSE))

# Convert the base R plots to ggplot objects
plot_a <- ggplot(a, aes(x, y)) + geom_line() + labs(title = "Partial Dependence of e_limeng")
plot_b <- ggplot(b, aes(x, y)) + geom_line() + labs(title = "Partial Dependence of e_pov150")
plot_c <- ggplot(c, aes(x, y)) + geom_line() + labs(title = "Partial Dependence of e_noveh")
plot_d <- ggplot(d, aes(x, y)) + geom_line() + labs(title = "Partial Dependence of e_munit")

# Arrange the plots in a grid
gridExtra::grid.arrange(plot_a, plot_b, plot_c, plot_d, nrow = 2, ncol = 2)
#####
### GWR Results ###
#####

# Spatial Distribution of Prediction and Observation Summary Index Values
svi_df = svi_df %>%
```

```

mutate(grf_pred = gwr_mod1$Global.Model$predictions)

# Predicted 1:1 Plot
ggplot(svi_df, aes(x = grf_pred, y = rpl_themes)) +
  geom_point() +
  theme_bw() +
  geom_abline(slope=1, intercept=0, linetype="dashed", size=0.5) +
  geom_smooth(method = "lm", se = FALSE, colour="black", size=0.5) +
  labs(x="Observed", y = "Predicted")

a = ggplot(svi_df, aes(fill = rpl_themes)) +
  geom_sf() +
  theme_void() +
  scale_fill_viridis_c() +
  labs(title = "Observed SVI Values") +
  theme(legend.title=element_blank())

b = ggplot(svi_df, aes(fill = grf_pred)) +
  geom_sf() +
  theme_void() +
  scale_fill_viridis_c() +
  labs(title = "Predicted SVI Values") +
  theme(legend.title=element_blank())

ggarrange(a,b, ncol = 2, common.legend = TRUE, legend="bottom")

# Global Variable Importance
temp = as.data.frame(gwr_mod1$Global.Model$variable.importance)
colnames(temp) = c("IncMSE")
temp = tibble::rownames_to_column(temp, "Variable")
ggplot(temp, aes(x = reorder(Variable, IncMSE), y = IncMSE)) +
  geom_bar(stat = "identity", fill = "grey") +
  coord_flip() + # Flip coordinates for better readability
  labs(title = "Variable Importance (Increase in %IncMSE)",
       subtitle = "Geographically Weighted Random Forest Model",
       x = "Variable",
       y = "Increase in MSE") +
  theme_bw()

# Local Variable Importance
variable_names = colnames(gwr_mod1$Local.Variable.Importance)
plot_lst = list()

# Loop through the names and create maps
for (var_name in variable_names) {

  # Generate the map using ggplot2
  p <- ggplot(svi_df, aes_string(fill = var_name)) +

```

```

    geom_sf() +
    scale_fill_viridis_c() +
    labs(title = paste(var_name),
         fill = "Importance") +
    theme_void()

    # Save the plot or print it
    plot_lst[[var_name]] = p
  }

  ##### SES Variable
  ggarrange(plot_lst[["e_pov150"]], plot_lst[["e_unemp"]])
  ggarrange(plot_lst[["e_hburd"]], plot_lst[["e_nohsdp"]])
  plot_lst[["e_uninsur"]]
  ##### Household Characteristics
  ggarrange(plot_lst[["e_age65"]], plot_lst[["e_age17"]])
  ggarrange(plot_lst[["e_disabl"]], plot_lst[["e_sngpnt"]])
  plot_lst[["e_limeng"]]
  ##### Racial & Ethnic Minority Status
  plot_lst[["e_minrty"]]
  ##### Housing Type & Transportation
  ggarrange(plot_lst[["e_munit"]], plot_lst[["e_mobile"]])
  ggarrange(plot_lst[["e_crowd"]], plot_lst[["e_noveh"]])
  plot_lst[["e_groupq"]]

```