Model Creation: Enviornmental Justice 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 (GWFRF). 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.

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 others highlight shared parameters between the RF and GWRF models:

- 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 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, three GWRF models will be created: (1) default mtry and ntrees with optimized bandwidth parameter, (2) using the previously defined best hyperparameters, (3) using the optimized bandwidth parameter in step one, then tuning mtry, with ntrees set to default. The method for GWRF Model 3 uses Out of Bag Error Rate as the Metric. 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.

Preparation

Traditional Random Forest Model

Model Training and Hyperparameter Tuning

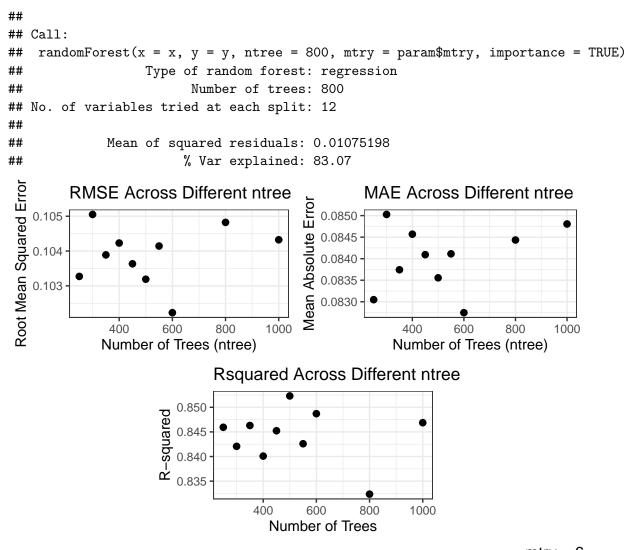
Models will be created and compared at the end of the section.

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.

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, preforming 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.



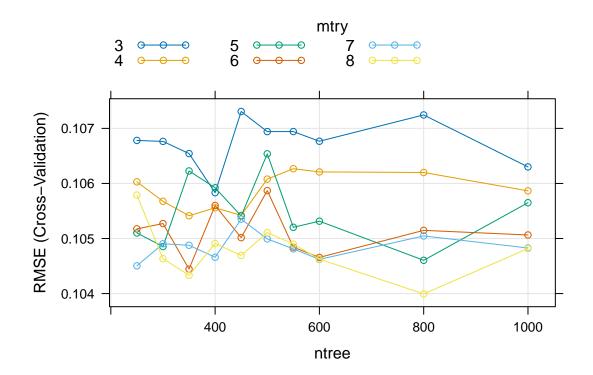
mtry = 6

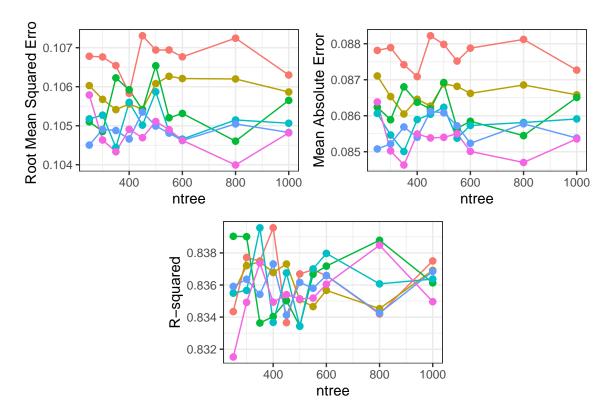
The second model hyperparameters have been set to mtry = 12, and ntrees = 800.

Model 3 - Exhaustive Grid Search with RMSE as Metric

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.

```
##
## Call:
## randomForest(x = x, y = y, ntree = param$ntree, mtry = param$mtry, importance = TRUE)
## Type of random forest: regression
## No. of variables tried at each split: 8
##
## Mean of squared residuals: 0.01074548
## % Var explained: 83.08
```





The final values used for the model were mtry = 8 and ntree = 800. 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.

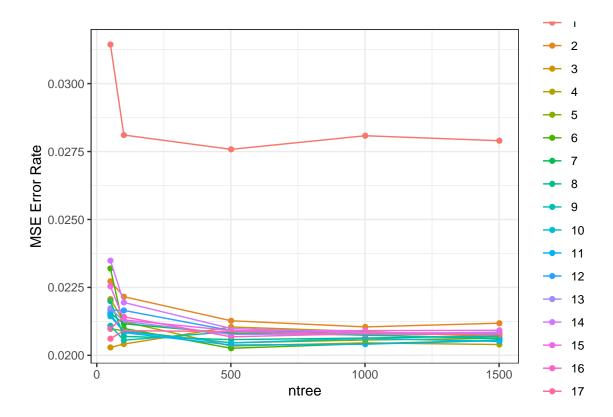
This approach ensures that both hyperparameters are tuned simultaneously, leading to a more efficient model optimization process. The final model hyperparameters have been set to m = 9, and ntrees = 501. The graph below illustrates that the errors across the hyperparameters used with this method are very similar.

```
# 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)</pre>
  }
  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_eji)
# 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 = FA
    if (is.factor(y)) {
     errors = data.frame(ntree = ntree, mtry = mtry, error = model$err.rate[ntree, 1])
     errors = data.frame(ntree = ntree, mtry = mtry, error = model$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 Preformance Metrics", digits = 4, align = c("l", "l", "c"))
```

Table 1: Model 4 Preformance Metrics

ntree	mtry	MSE
501	6	0.0203
51	3	0.0203
501	4	0.0203
501	11	0.0204
1501	4	0.0204
1001	11	0.0204



```
##
## Call:
## randomForest(x = x, y = y, ntree = ..1, mtry = param$mtry, importance = TRUE)
## Type of random forest: regression
## No. of variables tried at each split: 6
##
## Mean of squared residuals: 0.01104803
## % Var explained: 82.6
```

The final model hyperparameters have been set to mtry = 6, 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	12	500	0.085	0.105	0.835
Model 2	12	550	0.083	0.103	0.844
Model 3	8	540	0.086	0.105	0.836
Model 4	6	501	0.085	0.105	0.842

Training a Geographically Weighted Random Forest Model

GWRF Model 1

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

```
## Ranger result
##
## Call:
## ranger(rpl_eji ~ e_ozone + e_pm + e_dslpm + e_totcr + e_npl +
                                                                    e_tri + e_tsd + e_rmp +
##
## Type:
                                   Regression
                                   500
## Number of trees:
## Sample size:
                                   240
## Number of independent variables:
                                   36
## Mtry:
                                   12
## Target node size:
                                   5
## Variable importance mode:
                                   impurity
## Splitrule:
                                   variance
## 00B prediction error (MSE):
                                   0.01061433
## R squared (00B):
                                   0.8335626
##
      e ozone
                             e_dslpm
                     e_pm
                                         e_totcr
                                                      e_npl
                                                                  e_tri
## 0.04468540 0.30852189 0.21565943
                                      1.33741723 0.17726889 1.96279490
##
        e_tsd
                              {	t e}_{	t coal}
                                          e_lead
                                                      e_park
                                                               e_houage
                    e_rmp
##
  ##
     e_{wlkind}
                   {\tt e\_rail}
                              e_{	extbf{road}}
                                        e_airprt
                                                    e_impwtr
                                                              ep_minrty
   0.11227869 \quad 0.57724027 \quad 0.20292897 \quad 0.11768580 \quad 0.11070844 \quad 0.77473053
##
    ep_pov200
               ep_nohsdp
                                                   ep_houbdn
                                                             ep_uninsur
##
                            ep_unemp
                                      ep_renter
  0.83559929 1.10849097 0.10344450 0.87337408 0.24156240
##
                                                             0.16052974
##
     ep_noint
                 ep_age65
                            ep_age17
                                      ep_disabl ep_limeng
                                                              ep_mobile
  0.51251325  0.09177855  0.08898825  0.21740933  1.22067357
##
                                                             0.05030199
                           ep_asthma
##
    ep_groupq
                ep_bphigh
                                       ep_cancer
                                                    ep_mhlth ep_diabetes
  ##
              1st Qu.
                         Median
##
       Min.
                                    Mean
                                           3rd Qu.
                                                       Max.
## -0.253629 -0.070803 0.001584 0.003669 0.071375 0.316642
        Min.
                1st Qu.
                           Median
                                        Mean
                                                3rd Qu.
                                                             Max.
## -3.863e-02 -3.135e-03 4.204e-05 5.830e-05 4.502e-03 2.329e-02
##
                      Min
                                 Max
                                           Mean
## e_ozone
              0.000000e+00 0.16657977 0.01166416 0.026373238
## e_pm
              1.627322e-03 0.47345524 0.03212233 0.059937163
## e_dslpm
              2.396070e-03 0.79956503 0.04733299 0.098673361
## e_totcr
              1.966467e-03 1.07312138 0.09164882 0.189239347
## e_npl
              0.000000e+00 0.43877849 0.02837049 0.071846153
## e_tri
              1.539254e-04 0.47476457 0.09407893 0.115816166
## e_tsd
              0.000000e+00 0.05233505 0.00450023 0.007861019
## e_rmp
              3.445814e-05 0.28235947 0.03991593 0.056364100
              0.000000e+00 0.00000000 0.00000000 0.000000000
## e_coal
## e lead
              0.000000e+00 0.00000000 0.00000000 0.000000000
## e_park
              0.000000e+00 0.15076461 0.01144035 0.017145026
```

```
## e_houage
               3.005441e-03 0.17551236 0.02523248 0.023476700
## e_wlkind
               4.775245e-03 0.18024159 0.02018668 0.022363100
## e_rail
               8.706061e-04 0.45194974 0.03523789 0.064190025
## e_road
               2.949998e-05 0.30995353 0.03423681 0.048140191
## e_airprt
               0.000000e+00 0.26025327 0.02327458 0.052681604
## e_impwtr
               2.805287e-03 0.13521078 0.02259338 0.022197326
## ep minrty 5.905723e-03 0.29238514 0.06513552 0.049927779
## ep_pov200
              9.197471e-03 0.45906601 0.13195498 0.111725501
## ep nohsdp
              1.322510e-02 0.47373983 0.13495005 0.105650122
## ep_unemp
               3.943823e-03 0.16508108 0.02620598 0.028528941
## ep_renter
               5.409651e-03 0.58838003 0.10014596 0.085300880
## ep_houbdn
               7.083068e-03 0.35046171 0.06751131 0.055193361
## ep_uninsur 3.893328e-03 0.24840528 0.03383773 0.031639436
## ep_noint
               5.965929e-03 0.45348962 0.12575910 0.113320837
## ep_age65
               2.182992e-03 0.13800869 0.01937324 0.023311159
## ep_age17
              3.108043e-03 0.15401943 0.03134260 0.031446758
## ep_disabl
               6.137318e-03 0.36984917 0.06056298 0.061305564
## ep_limeng
              4.142503e-03 0.36895952 0.06785540 0.059552523
## ep_mobile
             5.503401e-06 0.04987863 0.00990896 0.010889849
## ep_groupq
              2.408794e-03 0.06868492 0.01556478 0.009585813
## ep_bphigh
             4.544709e-03 0.38436169 0.06286123 0.078786554
## ep asthma
              8.226793e-03 0.43963538 0.08033395 0.106647229
## ep_cancer
               2.194027e-03 0.06714326 0.01277356 0.011041326
## ep_mhlth
               4.473070e-03 0.31947635 0.08074732 0.091290628
## ep_diabetes 1.444889e-02 0.52508913 0.13682725 0.088253480
```

The final model hyperparameters have been set to bandwidth = 49, mtry = 12, and ntrees = 500.

GWRF Model 2

This model contains the hyperparameters defined in the RF building section.

```
## Ranger result
##
## Call:
   ranger(rpl_eji ~ e ozone + e pm + e_dslpm + e_totcr + e npl +
                                                                 e_tri + e_tsd + e_rmp +
##
## Type:
                                  Regression
                                  800
## Number of trees:
                                  240
## Sample size:
## Number of independent variables:
                                  36
## Mtry:
## Target node size:
## Variable importance mode:
                                  impurity
## Splitrule:
                                  variance
## 00B prediction error (MSE):
                                  0.01071509
## R squared (00B):
                                  0.8319826
##
      e_ozone
                                                    e_npl
                    e_pm
                            e_dslpm
                                       e_totcr
                                                               e_tri
##
   ##
        e_tsd
                   e_rmp
                             e_coal
                                        e_lead
                                                   e_park
                                                             e_houage
                                    0.00000000 0.05552358 0.11281819
   0.02514420
                         0.00000000
##
              0.31598480
##
     e_{wlkind}
                  e_rail
                             e_road
                                      e_airprt
                                                 e_impwtr
                                                            ep_minrty
## 0.12064289
              0.57352822 0.21782886 0.08956095 0.12463339
                                                          0.69339834
##
    ep_pov200
               ep_nohsdp
                           ep_unemp
                                     ep_renter
                                                ep_houbdn
                                                           ep_uninsur
              ##
  0.85506604
                                                           0.19069234
##
     ep_noint
                ep_age65
                           ep_age17
                                     ep_disabl
                                                ep_limeng
                                                            ep_mobile
##
  0.54539434
              0.09710374
                        0.09483521 0.23049902 1.18096697
                                                           0.04770333
##
                          ep_asthma
                                     ep_cancer
                                                 ep_mhlth ep_diabetes
    ep_groupq
               ep_bphigh
                         0.66219145
                                    0.12382942 0.26530645
                                                           1.68080758
##
   0.12268079
              0.24307777
##
       Min.
              1st Qu.
                       Median
                                   Mean
                                         3rd Qu.
                                                     Max.
## -0.261473 -0.075487 0.005867 0.001862 0.068819 0.315302
                                              3rd Qu.
##
        Min.
               1st Qu.
                          Median
                                      Mean
                                                           Max.
                                                      0.0288374
## -0.0308604 -0.0033013 0.0005673 0.0001896 0.0043426
##
                     Min
                                Max
                                          Mean
## e_ozone
             0.000000000 0.18117006 0.014457231 0.029591942
             0.0020986042 0.43497196 0.036860523 0.059503875
## e_pm
             0.0043000119 \ 0.60718261 \ 0.048764918 \ 0.083467206
## e_dslpm
## e_totcr
             0.0037681251 0.79656877 0.079992166 0.139964135
             0.0000000000 \ 0.33642448 \ 0.025479229 \ 0.056979475
## e_npl
             0.0004295002 \ 0.39486178 \ 0.086727932 \ 0.097596941
## e_tri
## e_tsd
             0.000000000 0.05997935 0.005102481 0.008682967
## e_rmp
             0.0005180813 0.23197652 0.040274236 0.051471239
## e coal
             ## e_lead
             ## e park
             0.0000000000 \ 0.18186292 \ 0.013271870 \ 0.020353617
## e_houage
             0.0044427244 0.16969165 0.029361122 0.025969413
```

```
## e_wlkind
               0.0059190365 \ 0.18448696 \ 0.024183604 \ 0.023122595
               0.0010441108 \ 0.38315748 \ 0.037020544 \ 0.058193155
## e_rail
## e_road
               0.0003097620 \ 0.26639724 \ 0.035553062 \ 0.044888112
## e_airprt
               0.0000000000 \ 0.21988199 \ 0.021976896 \ 0.047143529
## e impwtr
               0.0045507812 0.13915360 0.024447494 0.021721302
## ep_minrty
               0.0077163066 0.30599237 0.074127225 0.052014263
## ep_pov200
               0.0122693081 0.42102764 0.120422876 0.080974172
## ep_nohsdp
               0.0192753275 0.35645576 0.123197239 0.077726424
## ep_unemp
               0.0054092285 0.13739037 0.031304983 0.027806488
## ep_renter
               0.0083628798 0.38783979 0.097605599 0.065222796
## ep_houbdn
               0.0129528340\ 0.24972488\ 0.073733332\ 0.047111214
## ep_uninsur
               0.0049589407 \ 0.27540449 \ 0.040950802 \ 0.033101485
## ep_noint
               0.0131526456\ 0.35762103\ 0.114012543\ 0.084757083
## ep_age65
               0.0031540796 0.13477704 0.022595917 0.025079364
               0.0040455006 0.13526952 0.034623467 0.027153301
## ep_age17
## ep_disabl
               0.0102541315 0.26847837 0.061347662 0.051174821
## ep_limeng
               0.0034557730 0.34994150 0.072440951 0.053672203
## ep_mobile
               0.0001481956 \ 0.05435700 \ 0.010857069 \ 0.011991083
## ep_groupq
               0.0031971931 0.05634757 0.017101618 0.009872093
## ep bphigh
               0.0071042942 0.32160118 0.064237818 0.068223728
## ep_asthma
               0.0091518792 0.34923752 0.077563560 0.080063952
## ep_cancer
               0.0035182091 0.08225959 0.017028374 0.013449289
## ep_mhlth
               0.0058690834 0.27665581 0.077878924 0.074813617
## ep_diabetes 0.0176545623 0.44690265 0.127320112 0.071652368
```

The final model hyperparameters have been set to bandwidth = 49, mtry = 6, and ntrees = 501.

GWRF Model Evaluation

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

Table 3: Performance Metrics for Each Model

Model	bw	mtry	ntree	MAE	RMSE	R_Squared
Model 5		5	500	0.082	0.103	0.833
Model 6	49	9	501	0.083	0.104	0.831

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.

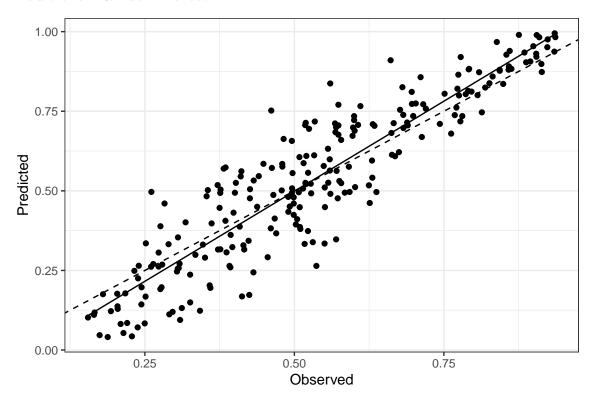
Model 4 (Traditional Random Forest) outperforms Model 6 (Geographically Weighted Random Forest) in terms of accuracy and explained variance. However, Model 6 is still valuable because it accounts for spatial dependencies. Model 6 might be more appropriate despite its lower overall performance metrics, 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

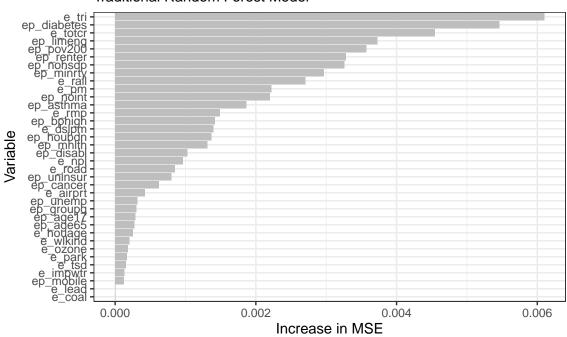
	Model	bw	mtry	ntree	MAE	RMSE	R_Squared
4	Model 4	-	6	501	0.085	0.105	0.842
2	Model 6	49	9	501	0.083	0.104	0.831

Graphs for the Final Models

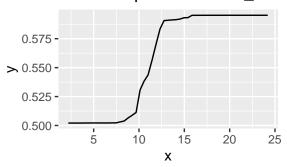
Traditional Random Forest



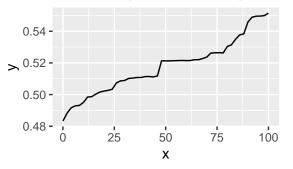
Variable Importance (Increase in %IncMSE)
Traditional Random Forest Model



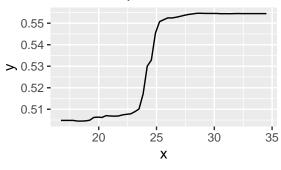
Partial Dependence of e_tri



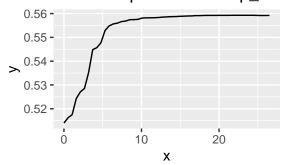
Partial Dependence of ep_diak



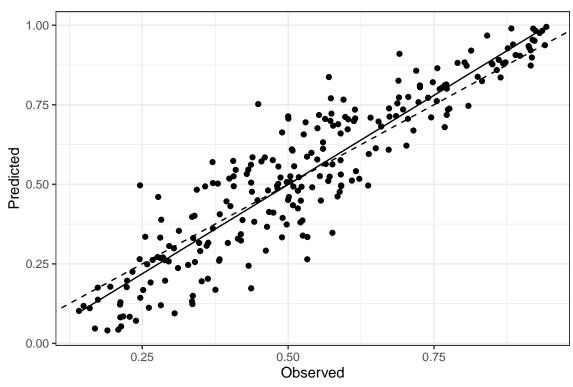
Partial Dependence of e_totcr

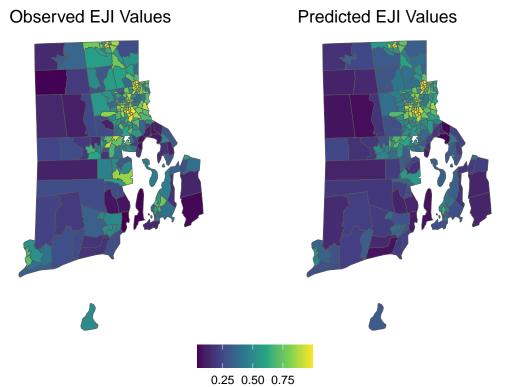


Partial Dependence of ep_lime



Geographically Weighted Random Forest





Variable Importance (Increase in %IncMSE)

Traditional Random Forest Model

