Exercise 2.2

2025-01-26

1. Data Analysis and Preprocessing

1.0 Load necessary libraries

```
## Loading required package: Matrix

## Loaded glmnet 4.1-8

## randomForest 4.7-1.2

## Type rfNews() to see new features/changes/bug fixes.

##
## Attaching package: 'randomForest'

## The following object is masked from 'package:ggplot2':
##
##     margin

## Type 'citation("pROC")' for a citation.

##
## Attaching package: 'pROC'

## The following objects are masked from 'package:stats':
##
##     cov, smooth, var

## corrplot 0.95 loaded
```

1.1 Open Dataset

```
## 'data.frame':    1096 obs. of  18 variables:
##  $ PM10     : int  12 15 25 33 23 14 20 15 22 28 ...
##  $ NO       : int  14 7 22 34 41 14 19 13 9 13 ...
##  $ NO2      : int  37 28 47 43 46 48 51 42 45 48 ...
##  $ SO2      : int  8 7 13 16 19 18 11 12 8 12 ...
##  $ T.min    : num  -0.6 -1.3 -4.2 -2.5 2.4 6.5 3 4.8 5.6 5.4 ...
##  $ T.max    : num  4.4 5.6 -0.7 4 7.7 9.1 8.8 9 10.4 11.7 ...
##  $ T.moy    : num  1.17 2.01 -2.93 1.52 5.03 ...
```

```
##  $ DV.maxvv : int  160 20 40 200 200 210 160 160 260 210 ...
##  $ DV.dom   : num  180 22.5 180 202.5 180 ...
##  $ VV.max   : int  8 7 3 4 5 6 7 9 10 7 ...
##  $ VV.moy   : num  5.35 4.96 2.25 2.71 3.25 ...
##  $ PL.som   : int  11 3 0 0 0 0 0 9 3 0 ...
##  $ HR.min   : int  93 78 63 86 91 87 74 85 74 82 ...
##  $ HR.max   : int  97 96 91 97 98 97 94 96 94 97 ...
##  $ HR.moy   : num  96.2 87.9 82.6 94 96.2 ...
##  $ PA.moy   : num  1011 1017 1024 1022 1022 ...
##  $ GTrouen  : num  0.7 -0.5 2.4 2.7 2.4 0.6 -0.1 0 -0.1 1.2 ...
##  $ GTlehavre: num  -0.3 0 0.1 -0.2 -0.2 -0.3 -0.5 NA -0.5 0.1 ...
```

1.2 Dataset summary

```
## Dataset structure:
```

```
## List of 2
##  $ X:'data.frame':   1096 obs. of  17 variables:
##   ..$ NO       : int [1:1096] 14 7 22 34 41 14 19 13 9 13 ...
##   ..$ NO2      : int [1:1096] 37 28 47 43 46 48 51 42 45 48 ...
##   ..$ SO2      : int [1:1096] 8 7 13 16 19 18 11 12 8 12 ...
##   ..$ T.min    : num [1:1096] -0.6 -1.3 -4.2 -2.5 2.4 6.5 3 4.8 5.6 5.4 ...
##   ..$ T.max    : num [1:1096] 4.4 5.6 -0.7 4 7.7 9.1 8.8 9 10.4 11.7 ...
##   ..$ T.moy    : num [1:1096] 1.17 2.01 -2.93 1.52 5.03 ...
##   ..$ DV.maxvv : int [1:1096] 160 20 40 200 200 210 160 160 260 210 ...
##   ..$ DV.dom   : num [1:1096] 180 22.5 180 202.5 180 ...
##   ..$ VV.max   : int [1:1096] 8 7 3 4 5 6 7 9 10 7 ...
##   ..$ VV.moy   : num [1:1096] 5.35 4.96 2.25 2.71 3.25 ...
##   ..$ PL.som   : int [1:1096] 11 3 0 0 0 0 0 9 3 0 ...
##   ..$ HR.min   : int [1:1096] 93 78 63 86 91 87 74 85 74 82 ...
##   ..$ HR.max   : int [1:1096] 97 96 91 97 98 97 94 96 94 97 ...
##   ..$ HR.moy   : num [1:1096] 96.2 87.9 82.6 94 96.2 ...
##   ..$ PA.moy   : num [1:1096] 1011 1017 1024 1022 1022 ...
##   ..$ GTrouen  : num [1:1096] 0.7 -0.5 2.4 2.7 2.4 0.6 -0.1 0 -0.1 1.2 ...
##   ..$ GTlehavre: num [1:1096] -0.3 0 0.1 -0.2 -0.2 -0.3 -0.5 NA -0.5 0.1 ...
##  $ Y: int [1:1096] 12 15 25 33 23 14 20 15 22 28 ...
```

```
##
## Feature matrix dimensions: 1096 17
```

```
##
## Response variable summary (numeric):
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
##    6.00   16.00   20.00   21.19   25.00   95.00      10
```

The dataset differs from the original as the response variable is numeric, not binary. Also now we have a much better dataset with just 17 variables and 1096 observations

1.3 Check for missing values

```
##
##
## Missing values check:
```

```
##
## Features missing values: 89
```

```
##
## Response missing values: 10
```

As the number of the missing values is insignificant, for the sake of simplicity we just delete them

```
## Removed rows: 64
```

```
## New dataset size: 1032 observations
```

Let's double check the missing values after we have deleted the rows with missing values

```
##
##
## Missing values check:
```

```
##
## Features missing values: 0
```

```
##
## Response missing values: 0
```

1.5 Check scaling need

```
##
##
## Scaling check:
```

```
##
## Feature mean range: 0.62 1017.62
```

```
##
## Feature SD range: 1.24 102.77
```

Obviously scaling is required. We will apply it on the subsequent steps.

1.6 Check for multicollinearity

```
##
##
## Highly correlated feature pairs (|r| > 0.8): 5
```

```
##
## Highly Correlated Feature Pair 1 :
## Feature 1: T.min
## Feature 2: T.max
## Correlation between T.min and T.max : 0.9
##
## Highly Correlated Feature Pair 2 :
## Feature 1: T.min
## Feature 2: T.moy
## Correlation between T.min and T.moy : 0.96
##
## Highly Correlated Feature Pair 3 :
## Feature 1: T.max
## Feature 2: T.moy
## Correlation between T.max and T.moy : 0.98
##
## Highly Correlated Feature Pair 4 :
## Feature 1: VV.max
## Feature 2: VV.moy
## Correlation between VV.max and VV.moy : 0.91
##
## Highly Correlated Feature Pair 5 :
## Feature 1: HR.min
## Feature 2: HR.moy
## Correlation between HR.min and HR.moy : 0.92
```

The analysis identified five highly correlated feature pairs within the temperature, wind, and humidity categories, each exhibiting correlation coefficients above 0.8. Specifically, the temperature features (T.min, T.max, T.moy), wind features (VV.max, VV.moy), and humidity features (HR.min, HR.moy) show strong interrelationships. Given this high multicollinearity, it may be tempting to retain only the average values for each category. However, the analysis will initially include all features and progressively address multicollinearity by eliminating redundant variables.

1.7 Summary of the data analysis

Summary of the New Dataset and Analysis Plan

1. **Moderate-Dimensional Data with Sufficient Observations**:
   - The feature matrix has dimensions of **1032 observations × 17 features**, making this dataset significantly different from the previous one. Unlike the earlier dataset, where the number of features far exceeded the number of observations (p > n), this dataset is well-suited for traditional statistical methods such as **Ordinary Least Squares (OLS) regression**. The ratio of observations to features (n=1032, p=17) ensures that the design matrix $ X'X $ is invertible, enabling reliable estimation of model coefficients.
   - Among the 17 features, **5 are multicollinear**, which introduces redundancy in the dataset. This multicollinearity is likely due to overlapping information across certain features, as some features

represent ranges or categories that could be summarized by averages. While it may be tempting to simplify the dataset by retaining only average values for each category, the analysis will initially include all features and progressively address multicollinearity through systematic elimination of redundant variables.

2. **Numeric Response Variable**:
   - Unlike the binary response variable in the previous dataset, the response variable in this dataset is **numeric**. This indicates a regression problem rather than a classification task.
3. **Scaling and Feature Standardization**:
   - Standardization will still be applied to ensure comparability and improve the performance of models sensitive to feature scaling, such as PCA and regularized regression. Scaling will also help mitigate potential issues arising from multicollinearity during model training.
4. **Modeling Approach**:
   - Given the improved characteristics of this dataset (sufficient observations and moderate dimensionality), we can now employ a broader range of modeling techniques. The analysis will proceed as follows:
     - **4.1 Start with OLS**: As the dataset satisfies the conditions for OLS (n > p and no singularities in $ X'X $), we will begin with a baseline linear regression model to establish a performance benchmark.
     - **4.2 Correlation Filtering**: To address multicollinearity, we will identify and remove highly correlated features based on pairwise correlation coefficients. This step will reduce redundancy while preserving interpretability.
     - **4.3 Apply Variance Inflation Factor (VIF)**: VIF will be used to assess and mitigate multicollinearity. Features with high VIF values (e.g., >10) will be removed iteratively until multicollinearity is sufficiently reduced.
     - **4.4 Stepwise Selection**: A stepwise feature selection approach (forward, backward, or hybrid) will be applied to identify the most relevant subset of features for predicting the response variable.
     - **4.5 Principal Component Analysis (PCA)**: PCA will be explored as a dimensionality reduction technique to capture the majority of variance in the data using fewer components. This will help address any residual multicollinearity and reduce noise in the dataset.
   - Following these preprocessing steps, we will proceed with the same suite of models used in the previous analysis:
     - **Regularized Models**: Lasso, Ridge, and Elastic Net will be evaluated for their ability to handle multicollinearity and perform implicit feature selection.
     - **Tree-Based Models**: CART and Random Forest will serve as robust alternatives, particularly for capturing nonlinear relationships and interactions among features. VSURF will again be used for feature selection within the Random Forest framework.
5. **Cross-Validation and Train-Test Split**:
   - Despite the larger dataset, **cross-validation** remains essential to ensure robust model evaluation and generalization. We will use **5-fold cross-validation** to maximize the use of the available data while minimizing variance in performance estimates.
   - The dataset will be split into **80% training** and **20% testing** subsets. Model performance will be evaluated on the test set using metrics appropriate for regression tasks, such as **Mean Squared Error (MSE)**, **Root Mean Squared Error (RMSE)**, and **R-squared ($ R^2 $)**. These metrics provide insights into prediction accuracy and the proportion of variance explained by the model.

2. Basic regression models

2.1 Basic LM

```
##
## === Linear Model Summary ===

##
## Call:
## lm(formula = Y ~ ., data = train_df)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.143  -3.413  -0.595   2.582  49.569
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 21.26182    0.19864 107.040  < 2e-16 ***
## NO           3.66921    0.32151  11.413  < 2e-16 ***
## NO2          1.36561    0.32519   4.199 2.97e-05 ***
## SO2          1.65814    0.25542   6.492 1.48e-10 ***
## T.min        3.62535    1.20365   3.012  0.00268 **
## T.max        5.99994    1.95246   3.073  0.00219 **
## T.moy       -7.21958    2.60193  -2.775  0.00565 **
## DV.maxvv    -0.40568    0.26198  -1.549  0.12189
## DV.dom      -0.53909    0.26921  -2.002  0.04557 *
## VV.max      -0.40471    0.51630  -0.784  0.43335
## VV.moy      -0.08347    0.53393  -0.156  0.87582
## PL.som      -0.57053    0.22945  -2.486  0.01310 *
## HR.min       1.43588    0.74140   1.937  0.05313 .
## HR.max      -0.60187    0.39285  -1.532  0.12590
## HR.moy      -1.57377    0.89052  -1.767  0.07756 .
## PA.moy       0.74323    0.24298   3.059  0.00230 **
## GTrouen      0.18567    0.37425   0.496  0.61996
## GTlehavre    1.06773    0.34076   3.133  0.00179 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.705 on 807 degrees of freedom
## Multiple R-squared:  0.5717, Adjusted R-squared:  0.5627
## F-statistic: 63.37 on 17 and 807 DF,  p-value: < 2.2e-16

##
## === Cross-Validation Results ===

##   Fold      MSE     RMSE        R2
## 1    1 61.79753 7.861140 0.4658901
## 2    2 37.00695 6.083334 0.6008507
## 3    3 24.98802 4.998802 0.5955907
## 4    4 24.20858 4.920221 0.5635860
## 5    5 24.57733 4.957553 0.4486567

##
## Mean CV MSE: 34.5157
```

```
##
## Mean CV RMSE: 5.7642
```

```
##
## Mean CV R-squared: 0.5349
```

```
##
## === Test Set Evaluation ===
```

```
## MSE: 27.9471
```

```
## RMSE: 5.2865
```

```
## R-squared: 0.4961
```

```
##
## === Model Coefficients ===
```

```
##        Feature Coefficient
## 1  (Intercept)     21.2618
## 2           NO      3.6692
## 3          NO2      1.3656
## 4          SO2      1.6581
## 5        T.min      3.6253
## 6        T.max      5.9999
## 7        T.moy     -7.2196
## 8     DV.maxvv     -0.4057
## 9       DV.dom     -0.5391
## 10      VV.max     -0.4047
## 11      VV.moy     -0.0835
## 12      PL.som     -0.5705
## 13      HR.min      1.4359
## 14      HR.max     -0.6019
## 15      HR.moy     -1.5738
## 16      PA.moy      0.7432
## 17     GTrouen      0.1857
## 18   GTlehavre      1.0677
```

```
##
## Number of coefficients (including intercept): 18
```

```
##
## Number of features (excluding intercept): 17
```

2.2 Correlation Filtering

```
##
## === Correlation Filtering ===
```

```
## Highly correlated feature pairs (|r| > 0.8): 5
```

```
##
## Removing features with high multicollinearity:
## [1] "T.max"  "T.moy"  "VV.moy" "HR.moy"
##
## Highly correlated pairs details:
## T.min          vs T.max         : r = 0.90
## T.min          vs T.moy         : r = 0.96
## T.max          vs T.moy         : r = 0.98
## VV.max         vs VV.moy        : r = 0.91
## HR.min         vs HR.moy        : r = 0.92
```

```
##
## === Linear Model Summary ===
```

```
##
## Call:
## lm(formula = Y ~ ., data = train_df)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.821  -3.473  -0.610   2.440  50.311
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  21.2618     0.1994 106.609  < 2e-16 ***
## NO            3.7271     0.3219  11.579  < 2e-16 ***
## NO2           1.4170     0.3204   4.422 1.11e-05 ***
## SO2           1.7053     0.2549   6.689 4.17e-11 ***
## T.min         2.0569     0.2695   7.633 6.43e-14 ***
## DV.maxvv     -0.4152     0.2597  -1.599  0.11018
## DV.dom       -0.6364     0.2678  -2.376  0.01774 *
## VV.max       -0.4760     0.2525  -1.885  0.05982 .
## PL.som       -0.5597     0.2264  -2.473  0.01361 *
## HR.min       -0.2854     0.2854  -1.000  0.31757
## HR.max       -0.9466     0.2516  -3.763  0.00018 ***
## PA.moy        0.7353     0.2411   3.049  0.00237 **
## GTrouen       0.4042     0.3438   1.176  0.24006
## GTlehavre     1.1842     0.3383   3.500  0.00049 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.728 on 811 degrees of freedom
## Multiple R-squared:  0.5661, Adjusted R-squared:  0.5592
## F-statistic:  81.4 on 13 and 811 DF,  p-value: < 2.2e-16
```

```
##
## === Cross-Validation Results ===
```

```
##   Fold      MSE     RMSE        R2
## 1    1 61.43289 7.837914 0.4690416
## 2    2 36.84339 6.069876 0.6026148
## 3    3 25.43862 5.043671 0.5882982
## 4    4 23.61515 4.859543 0.5742838
## 5    5 25.20303 5.020262 0.4346206
```

```
##
## Mean CV MSE: 34.5066
```

```
##
## Mean CV RMSE: 5.7663
```

```
##
## Mean CV R-squared: 0.5338
```

```
##
## === Test Set Evaluation ===
```

```
## MSE: 28.4852
```

```
## RMSE: 5.3372
```

```
## R-squared: 0.4864
```

```
##
## === Model Coefficients ===
```

```
##        Feature Coefficient
## 1  (Intercept)     21.2618
## 2           NO      3.7271
## 3          NO2      1.4170
## 4          SO2      1.7053
## 5        T.min      2.0569
## 6     DV.maxvv     -0.4152
## 7       DV.dom     -0.6364
## 8       VV.max     -0.4760
## 9       PL.som     -0.5597
## 10      HR.min     -0.2854
## 11      HR.max     -0.9466
## 12      PA.moy      0.7353
## 13     GTrouen      0.4042
## 14   GTlehavre      1.1842
```

```
##
## Number of coefficients (including intercept): 14
```

```
##
## Number of features (excluding intercept): 13
```

2.3 Variance Inflation Factor (VIF)

```
##
## === VIF Analysis ===
```

```
## Loading required package: carData
```

```
##
## -- VIF Iteration 1 --
## Removing feature: T.moy (VIF = 171.4 )
##
## -- VIF Iteration 2 --
## Removing feature: T.max (VIF = 21.2 )
##
## -- VIF Iteration 3 --
## Removing feature: HR.moy (VIF = 16.7 )
##
## -- VIF Iteration 4 --
```

```
##
## Final removed features by VIF: T.moy, T.max, HR.moy
```

```
##
## === Linear Model Summary ===
```

```
##
## Call:
## lm(formula = Y ~ ., data = train_df)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.833  -3.482  -0.597   2.433  50.341
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  21.2618     0.1996 106.548  < 2e-16 ***
## NO            3.7267     0.3221  11.571  < 2e-16 ***
## NO2           1.4053     0.3236   4.343 1.58e-05 ***
## SO2           1.7066     0.2551   6.690 4.17e-11 ***
## T.min         2.0558     0.2697   7.624 6.90e-14 ***
## DV.maxvv     -0.4263     0.2631  -1.620 0.105537
## DV.dom       -0.6311     0.2687  -2.349 0.019084 *
## VV.max       -0.3557     0.5157  -0.690 0.490525
## VV.moy       -0.1417     0.5297  -0.267 0.789201
## PL.som       -0.5699     0.2297  -2.481 0.013285 *
## HR.min       -0.2687     0.2923  -0.919 0.358261
## HR.max       -0.9622     0.2584  -3.724 0.000210 ***
## PA.moy        0.7313     0.2417   3.025 0.002562 **
## GTrouen       0.3960     0.3453   1.147 0.251790
## GTlehavre     1.1815     0.3387   3.489 0.000511 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.732 on 810 degrees of freedom
## Multiple R-squared:  0.5662, Adjusted R-squared:  0.5587
## F-statistic:  75.5 on 14 and 810 DF,  p-value: < 2.2e-16
```

```
##
## === Cross-Validation Results ===
```

```
##   Fold      MSE     RMSE        R2
## 1    1 61.81030 7.861953 0.4657797
## 2    2 36.84752 6.070215 0.6025704
## 3    3 25.48758 5.048523 0.5875057
## 4    4 23.63101 4.861173 0.5739980
## 5    5 25.20225 5.020184 0.4346380

##
## Mean CV MSE: 34.5957

##
## Mean CV RMSE: 5.7724

##
## Mean CV R-squared: 0.5329

##
## === Test Set Evaluation ===

## MSE: 28.457

## RMSE: 5.3345

## R-squared: 0.4869

##
## === Final Model Diagnostics ===

##
## Variance Inflation Factors (VIF):
##      Feature      VIF
## 1         NO 2.601794
## 2        NO2 2.626030
## 3        SO2 1.632406
## 4      T.min 1.823807
## 5   DV.maxvv 1.735874
## 6     DV.dom 1.811104
## 7     VV.max 6.671103
## 8     VV.moy 7.037325
## 9     PL.som 1.323062
## 10    HR.min 2.143153
## 11    HR.max 1.674314
## 12    PA.moy 1.465635
## 13   GTrouen 2.991305
## 14 GTlehavre 2.876678

##
## === Model Coefficients ===
```

```
##        Feature Coefficient
## 1  (Intercept)     21.2618
## 2           NO      3.7267
## 3          NO2      1.4053
## 4          SO2      1.7066
## 5        T.min      2.0558
## 6     DV.maxvv     -0.4263
## 7       DV.dom     -0.6311
## 8       VV.max     -0.3557
## 9       VV.moy     -0.1417
## 10      PL.som     -0.5699
## 11      HR.min     -0.2687
## 12      HR.max     -0.9622
## 13      PA.moy      0.7313
## 14     GTrouen      0.3960
## 15   GTlehavre      1.1815
```

```
##
## Number of coefficients (including intercept): 15
```

```
##
## Number of features (excluding intercept): 14
```

2.4 Stepwise Selection

```
##
## === Stepwise Selection ===
```

```
## Start:  AIC=2891.12
## Y ~ NO + NO2 + SO2 + T.min + T.max + T.moy + DV.maxvv + DV.dom +
##     VV.max + VV.moy + PL.som + HR.min + HR.max + HR.moy + PA.moy +
##     GTrouen + GTlehavre
##
##             Df Sum of Sq   RSS    AIC
## - VV.moy     1       0.8 26270 2889.2
## - GTrouen    1       8.0 26277 2889.4
## - VV.max     1      20.0 26289 2889.8
## <none>                   26269 2891.1
## - HR.max     1      76.4 26345 2891.5
## - DV.maxvv   1      78.1 26347 2891.6
## - HR.moy     1     101.7 26370 2892.3
## - HR.min     1     122.1 26391 2892.9
## - DV.dom     1     130.5 26399 2893.2
## - PL.som     1     201.3 26470 2895.4
## - T.moy      1     250.6 26519 2896.9
## - T.min      1     295.3 26564 2898.3
## - PA.moy     1     304.5 26573 2898.6
## - T.max      1     307.4 26576 2898.7
## - GTlehavre  1     319.6 26588 2899.1
## - NO2        1     574.1 26843 2907.0
## - SO2        1    1371.8 27641 2931.1
## - NO         1    4239.7 30508 3012.6
```

```
##
## Step:  AIC=2889.15
## Y ~ NO + NO2 + SO2 + T.min + T.max + T.moy + DV.maxvv + DV.dom +
##     VV.max + PL.som + HR.min + HR.max + HR.moy + PA.moy + GTrouen +
##     GTlehavre
##
##             Df Sum of Sq   RSS    AIC
## - GTrouen    1       8.4 26278 2887.4
## <none>                   26270 2889.2
## - HR.max     1      75.8 26345 2889.5
## - DV.maxvv   1      77.5 26347 2889.6
## - HR.moy     1     100.9 26371 2890.3
## - VV.max     1     115.5 26385 2890.8
## - HR.min     1     121.9 26391 2891.0
## + VV.moy     1       0.8 26269 2891.1
## - DV.dom     1     132.7 26402 2891.3
## - PL.som     1     202.0 26472 2893.5
## - T.moy      1     253.4 26523 2895.1
## - T.min      1     296.0 26566 2896.4
## - PA.moy     1     309.2 26579 2896.8
## - T.max      1     311.9 26582 2896.9
## - GTlehavre  1     320.9 26591 2897.2
## - NO2        1     586.4 26856 2905.4
## - SO2        1    1371.2 27641 2929.1
## - NO         1    4239.3 30509 3010.6
##
## Step:  AIC=2887.41
## Y ~ NO + NO2 + SO2 + T.min + T.max + T.moy + DV.maxvv + DV.dom +
##     VV.max + PL.som + HR.min + HR.max + HR.moy + PA.moy + GTlehavre
##
##             Df Sum of Sq   RSS    AIC
## <none>                   26278 2887.4
## - DV.maxvv   1      73.8 26352 2887.7
## - HR.max     1      75.4 26353 2887.8
## - HR.moy     1      99.6 26378 2888.5
## + GTrouen    1       8.4 26270 2889.2
## - HR.min     1     123.4 26401 2889.3
## - VV.max     1     124.4 26402 2889.3
## + VV.moy     1       1.2 26277 2889.4
## - DV.dom     1     131.9 26410 2889.5
## - PL.som     1     208.7 26487 2891.9
## - T.moy      1     253.4 26531 2893.3
## - T.min      1     288.6 26567 2894.4
## - PA.moy     1     305.7 26584 2894.9
## - T.max      1     343.4 26621 2896.1
## - GTlehavre  1     511.4 26789 2901.3
## - NO2        1     613.8 26892 2904.5
## - SO2        1    1369.0 27647 2927.3
## - NO         1    4422.5 30701 3013.7
```

```
## Selected features after stepwise selection: NO, NO2, SO2, T.min, T.max, T.moy, DV.maxvv, DV.dom, VV.r
```

```
##
## === Linear Model Summary ===
```

```
##
## Call:
## lm(formula = selected_formula, data = train_df)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.210  -3.440  -0.644   2.546  49.610
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  21.2618     0.1984 107.153  < 2e-16 ***
## NO            3.6960     0.3168  11.668  < 2e-16 ***
## NO2           1.3919     0.3202   4.347 1.56e-05 ***
## SO2           1.6554     0.2550   6.492 1.48e-10 ***
## T.min         3.4918     1.1714   2.981  0.00296 **
## T.max         6.2092     1.9098   3.251  0.00120 **
## T.moy        -7.2458     2.5941  -2.793  0.00534 **
## DV.maxvv     -0.3885     0.2577  -1.507  0.13208
## DV.dom       -0.5405     0.2682  -2.015  0.04421 *
## VV.max       -0.4899     0.2503  -1.957  0.05067 .
## PL.som       -0.5730     0.2261  -2.535  0.01144 *
## HR.min        1.4274     0.7323   1.949  0.05160 .
## HR.max       -0.5971     0.3919  -1.524  0.12799
## HR.moy       -1.5483     0.8842  -1.751  0.08031 .
## PA.moy        0.7415     0.2417   3.068  0.00223 **
## GTlehavre     1.1582     0.2919   3.968 7.89e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.699 on 809 degrees of freedom
## Multiple R-squared:  0.5716, Adjusted R-squared:  0.5636
## F-statistic: 71.95 on 15 and 809 DF,  p-value: < 2.2e-16
```

```
##
## === Cross-Validation Results ===
```

```
##   Fold      MSE     RMSE        R2
## 1    1 61.00122 7.810328 0.4727725
## 2    2 36.96371 6.079778 0.6013172
## 3    3 24.94626 4.994623 0.5962666
## 4    4 24.14199 4.913450 0.5647864
## 5    5 24.33609 4.933162 0.4540686
```

```
##
## Mean CV MSE: 34.2779
```

```
##
## Mean CV RMSE: 5.7463
```

```
##
## Mean CV R-squared: 0.5378
```

```
##
## === Test Set Evaluation ===
```

```
## MSE: 27.8327

## RMSE: 5.2757

## R-squared: 0.4981

##
## === Final Model Coefficients ===

##        Feature Coefficient
## 1  (Intercept)     21.2618
## 2           NO      3.6960
## 3          NO2      1.3919
## 4          SO2      1.6554
## 5        T.min      3.4918
## 6        T.max      6.2092
## 7        T.moy     -7.2458
## 8     DV.maxvv     -0.3885
## 9       DV.dom     -0.5405
## 10      VV.max     -0.4899
## 11      PL.som     -0.5730
## 12      HR.min      1.4274
## 13      HR.max     -0.5971
## 14      HR.moy     -1.5483
## 15      PA.moy      0.7415
## 16   GTlehavre      1.1582

##
## Number of coefficients (including intercept): 16

##
## Number of features (excluding intercept): 15
```

2.5 Principal Component Analysis (PCA)

```
##
## === PCA-Based Dimension Reduction ===

## Number of principal components selected: 9

##
## === Linear Model Summary ===

##
## Call:
## lm(formula = Y ~ ., data = train_pcs)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -14.847  -3.446  -0.500   2.512  48.563
##
```

```
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 21.26182    0.20286 104.808  < 2e-16 ***
## PC1          0.32908    0.09385   3.506 0.000479 ***
## PC2          2.89361    0.10497  27.567  < 2e-16 ***
## PC3         -0.24028    0.13511  -1.778 0.075711 .
## PC4         -0.66875    0.17303  -3.865 0.000120 ***
## PC5         -1.41473    0.18635  -7.592 8.63e-14 ***
## PC6         -2.08343    0.23939  -8.703  < 2e-16 ***
## PC7          0.33529    0.25491   1.315 0.188775
## PC8          2.03246    0.26107   7.785 2.11e-14 ***
## PC9          0.68843    0.29337   2.347 0.019183 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.827 on 815 degrees of freedom
## Multiple R-squared:  0.5489, Adjusted R-squared:  0.5439
## F-statistic: 110.2 on 9 and 815 DF,  p-value: < 2.2e-16
```

```
##
## === Cross-Validation Results ===
```

```
##   Fold      MSE     RMSE        R2
## 1    1 61.95678 7.871263 0.4645137
## 2    2 40.10189 6.332605 0.5674694
## 3    3 26.20795 5.119370 0.5758473
## 4    4 21.79691 4.668716 0.6070618
## 5    5 25.34140 5.034024 0.4315164
```

```
##
## Mean CV MSE: 35.081
```

```
##
## Mean CV RMSE: 5.8052
```

```
##
## Mean CV R-squared: 0.5293
```

```
##
## === Test Set Evaluation ===
```

```
## MSE: 44.5091
```

```
## RMSE: 6.6715
```

```
## R-squared: 0.1974
```

```
##
## === Final Model Coefficients (PCA) ===
```

```
##      Predictor Coefficient
## 1  (Intercept)     21.2618
## 2          PC1      0.3291
## 3          PC2      2.8936
## 4          PC3     -0.2403
## 5          PC4     -0.6688
## 6          PC5     -1.4147
## 7          PC6     -2.0834
## 8          PC7      0.3353
## 9          PC8      2.0325
## 10         PC9      0.6884
```

```
##
## Number of coefficients (including intercept): 10
```

```
##
## Number of principal components used (excluding intercept): 9
```

2.6 Conclusion

Model	CV_MSE	CV_RMSE	CV_R2	Test_MSE	Test_RMSE	Test_R2
OLS	34.5157	5.7642	0.5349	27.9471	5.2865	0.4961
Correlation Filtering	34.5066	5.7663	0.5338	28.4852	5.3372	0.4864
VIF	34.5957	5.7724	0.5329	28.4570	5.3345	0.4869
Stepwise Selection	34.2779	5.7463	0.5378	27.8327	5.2757	0.4981
PCA	35.0810	5.8052	0.5293	44.5091	6.6715	0.1974

```
## Summary of Y (Training):
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    6.00   16.00   20.00   21.26   25.00   95.00
```

```
##
## Range of Y (Training):  6 to 95
```

```
##
## Standard Deviation of Y (Training):  8.6276
```

```
## Model Test Metrics:
```

```
## Test MSE: 27.8327
```

```
## Test RMSE: 5.2757
```

```
## Test R-squared: 0.4981
```

```
## RMSE as a percentage of the response range:  5.93 %
```

```
## RMSE as a percentage of the response standard deviation:  61.15 %
```

Among the various modeling approaches evaluated, **only the stepwise selection method managed to improve the baseline OLS results**. In contrast, both the **correlation filtering** and **VIF-based approaches** resulted in slightly worse performance. Furthermore, the **PCA-based model** demonstrated the poorest performance by a significant margin. These findings suggest that simply deleting correlated features or reducing dimensionality through PCA does not necessarily lead to performance improvements; in fact, it may remove predictive information essential for model generalization.

Based on the results from OLS Test MSE: 27.8327 and Test RMSE: 5.2757 are relatively low when considered as a small percentage of the overall range (6%). However, since RMSE is about 61% of the standard deviation, there is still a considerable amount of prediction error relative to the natural variability in the response. An R^2 of 0.4981 indicates that OLS model explains about half the variance, which is moderate. This might be acceptable in many practical situations but also suggests there is room for improvement.

3. Regularized regression models

3.1 LASSO model

```
##
## === Model Fitting Summary ===

## GLMNET Cross-Validation Results:

## Best lambda (lambda.min): 0.002154435

## Number of lambda values tested: 10

## Fold count:

## Minimum MSE achieved: 34.5082

## Minimum RMSE achieved: 5.8744

## Maximum R-squared achieved: 0.5364

##
## Cross-Validation Performance:

##    Lambda   MSE  RMSE     R2    SD
##   1.00000 40.92 6.397 0.4502 9.025
##   0.46416 36.45 6.037 0.5103 8.101
##   0.21544 34.94 5.911 0.5306 7.602
##   0.10000 34.60 5.882 0.5352 7.403
##   0.04642 34.57 5.879 0.5356 7.329
##   0.02154 34.62 5.884 0.5349 7.319
##   0.01000 34.57 5.880 0.5355 7.271
##   0.00464 34.51 5.875 0.5363 7.251
##   0.00215 34.51 5.874 0.5364 7.242
##   0.00100 34.51 5.875 0.5364 7.238

##
## === Test Set Evaluation ===
```

```
## MSE: 27.9424
```

```
## RMSE: 5.2861
```

```
## R-squared: 0.4961
```

```
##
## === Non-Zero Coefficients ===
```

```
##      Feature Coefficient
##  (Intercept) 21.26181818
##           NO  3.67858361
##          NO2  1.37349145
##          SO2  1.66235517
##        T.min  3.19751770
##        T.max  5.23615144
##        T.moy -6.05471168
##     DV.maxvv -0.40658060
##       DV.dom -0.54989051
##       VV.max -0.39985701
##       VV.moy -0.08915399
##       PL.som -0.56635311
##       HR.min  1.24527992
##       HR.max -0.65177756
##       HR.moy -1.36718710
##       PA.moy  0.74016567
##      GTrouen  0.18347312
##    GTlehavre  1.07499920
```

```
##
## Non-zero coefficients (including intercept): 18
```

```
## Non-zero coefficients (excluding intercept): 17
```

3.2 RIDGE model

```
##
## === Model Fitting Summary ===
```

```
## GLMNET Cross-Validation Results:
```

```
## Best lambda (lambda.min): 0.4641589
```

```
## Number of lambda values tested: 10
```

```
## Fold count:
```

```
## Minimum MSE achieved: 34.4102
```

```
## Minimum RMSE achieved: 5.866
```

```
## Maximum R-squared achieved: 0.5377

##
## Cross-Validation Performance:

##    Lambda   MSE  RMSE     R2    SD
##   1.00000 34.43 5.868 0.5375 7.609
##   0.46416 34.41 5.866 0.5377 7.430
##   0.21544 34.47 5.871 0.5369 7.351
##   0.10000 34.51 5.875 0.5364 7.319
##   0.04642 34.51 5.875 0.5364 7.302
##   0.02154 34.49 5.873 0.5366 7.284
##   0.01000 34.49 5.873 0.5366 7.267
##   0.00464 34.50 5.874 0.5365 7.254
##   0.00215 34.51 5.874 0.5364 7.247
##   0.00100 34.51 5.875 0.5364 7.242

##
## === Test Set Evaluation ===

## MSE: 28.1332

## RMSE: 5.3041

## R-squared: 0.4927

##
## === Non-Zero Coefficients ===

##       Feature Coefficient
##   (Intercept)  21.2618182
##            NO   3.4000709
##           NO2   1.4526096
##           SO2   1.6424410
##         T.min   0.9640487
##         T.max   0.9200983
##         T.moy   0.1427990
##      DV.maxvv  -0.4251865
##        DV.dom  -0.5718161
##        VV.max  -0.3545431
##        VV.moy  -0.2002309
##        PL.som  -0.5377504
##        HR.min   0.2863261
##        HR.max  -0.8212215
##        HR.moy  -0.3682087
##        PA.moy   0.7398794
##       GTrouen   0.3668272
##     GTlehavre   1.0659635

##
## Non-zero coefficients (including intercept): 18

## Non-zero coefficients (excluding intercept): 17
```

3.3 Elastic Net model

```
##
## === Model Fitting Summary ===

## Best alpha: 0.5

## Best lambda (lambda.min): 0.001

## Number of lambda values tested: 10

## Fold count:

## Minimum MSE achieved: 33.753

## Minimum RMSE achieved: 5.8097

## Maximum R-squared achieved: 0.5466

##
## Cross-Validation Performance:

##  Alpha   Lambda   MSE  RMSE     R2    SD
##    0.2 1.000000 35.08 5.923 0.5288 7.912
##    0.2 0.464159 34.56 5.879 0.5357 7.542
##    0.2 0.215443 34.50 5.873 0.5366 7.381
##    0.2 0.100000 34.56 5.879 0.5357 7.334
##    0.2 0.046416 34.59 5.881 0.5353 7.304
##    0.2 0.021544 34.52 5.875 0.5363 7.284
##    0.2 0.010000 34.50 5.873 0.5365 7.266
##    0.2 0.004642 34.50 5.874 0.5365 7.254
##    0.2 0.002154 34.51 5.874 0.5364 7.247
##    0.2 0.001000 34.51 5.875 0.5364 7.243
##    0.5 1.000000 36.46 6.038 0.5102 2.634
##    0.5 0.464159 34.48 5.872 0.5368 2.460
##    0.5 0.215443 34.00 5.831 0.5433 2.386
##    0.5 0.100000 33.92 5.824 0.5443 2.351
##    0.5 0.046416 33.95 5.827 0.5439 2.336
##    0.5 0.021544 33.92 5.824 0.5443 2.301
##    0.5 0.010000 33.81 5.814 0.5458 2.288
##    0.5 0.004642 33.77 5.811 0.5464 2.286
##    0.5 0.002154 33.76 5.810 0.5465 2.285
##    0.5 0.001000 33.75 5.810 0.5466 2.284
##    0.8 1.000000 39.24 6.264 0.4729 2.770
##    0.8 0.464159 35.35 5.946 0.5251 1.953
##    0.8 0.215443 34.49 5.873 0.5366 1.620
##    0.8 0.100000 34.36 5.861 0.5385 1.463
##    0.8 0.046416 34.39 5.864 0.5380 1.379
##    0.8 0.021544 34.45 5.870 0.5371 1.342
##    0.8 0.010000 34.37 5.862 0.5383 1.290
##    0.8 0.004642 34.32 5.858 0.5390 1.281
##    0.8 0.002154 34.31 5.857 0.5391 1.280
##    0.8 0.001000 34.31 5.857 0.5391 1.279
```

```
##
## === Test Set Evaluation ===

## MSE: 27.9483

## RMSE: 5.2866

## R-squared: 0.496

##
## === Non-Zero Coefficients ===

##       Feature Coefficient
##   (Intercept) 21.26181818
##            NO  3.67502199
##           NO2  1.37125506
##           SO2  1.66204976
##         T.min  3.40397669
##         T.max  5.49549628
##         T.moy -6.51606874
##      DV.maxvv -0.40661471
##        DV.dom -0.54608713
##        VV.max -0.39907425
##        VV.moy -0.09031654
##        PL.som -0.56831050
##        HR.min  1.32020235
##        HR.max -0.62598822
##        HR.moy -1.46331245
##        PA.moy  0.74087827
##       GTrouen  0.19159128
##     GTlehavre  1.07341640

##
## Non-zero coefficients (including intercept): 18

## Non-zero coefficients (excluding intercept): 17
```

3.4 Conclusion

Model	Best_Lambda	Best_Alpha	CV_MSE	CV_RMSE	CV_R2	Test_MSE	Test_RMSE	Test_R2	NonZero_Coefficients
Lasso	0.0022	NA	34.5082	5.8744	0.5364	27.9424	5.2861	0.4961	17
Ridge	0.4642	NA	34.4102	5.8660	0.5377	28.1332	5.3041	0.4927	17
Elastic Net	0.0010	0.5	33.7530	5.8097	0.5466	27.9483	5.2866	0.4960	17

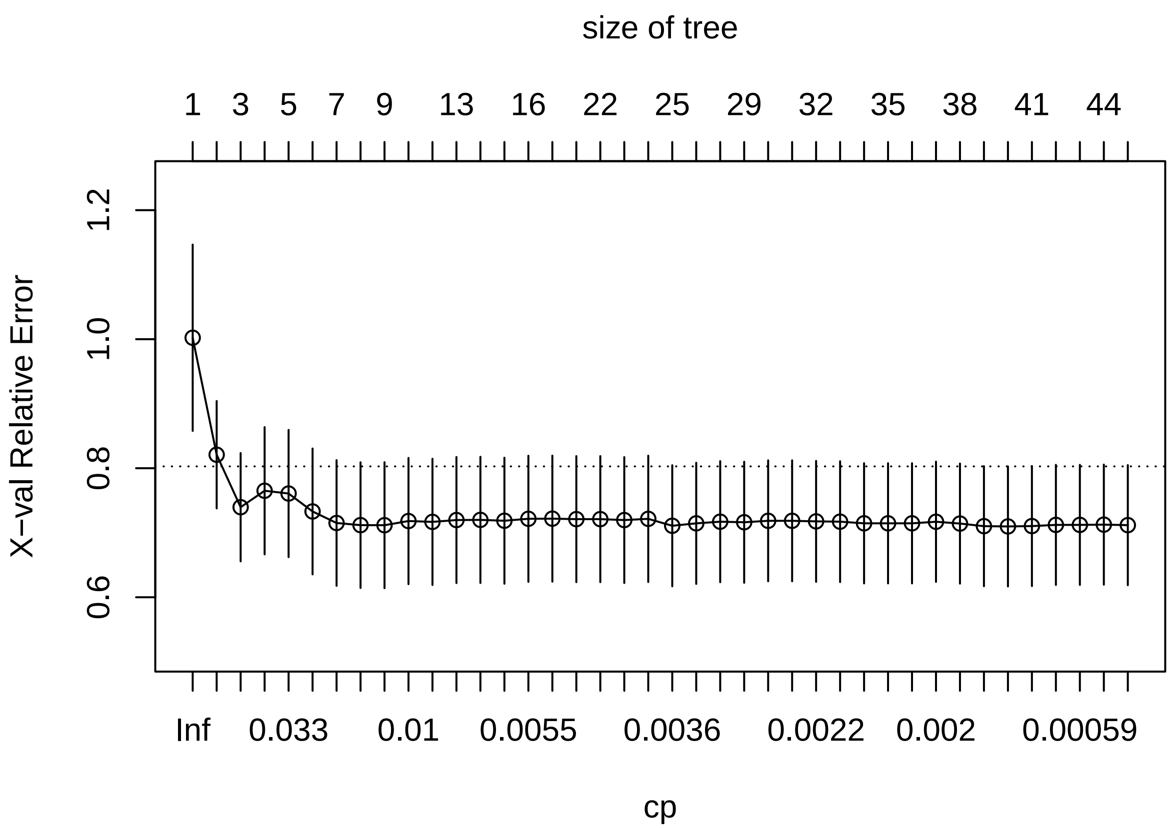
The results show that all three models (lasso, ridge, and elastic net) exhibit similar performance in terms of both cross-validation and test-set metrics. One particularly interesting observation is that neither lasso nor elastic net reduced the number of features: all models ended up with 17 non-zero predictors (excluding the intercept). In this case the chosen regularization parameters did not force any coefficients out of the model, suggesting that every predictor contributes meaningfully to the model's performance.

4. CART and Random Forest models

4.1 Basic RPART

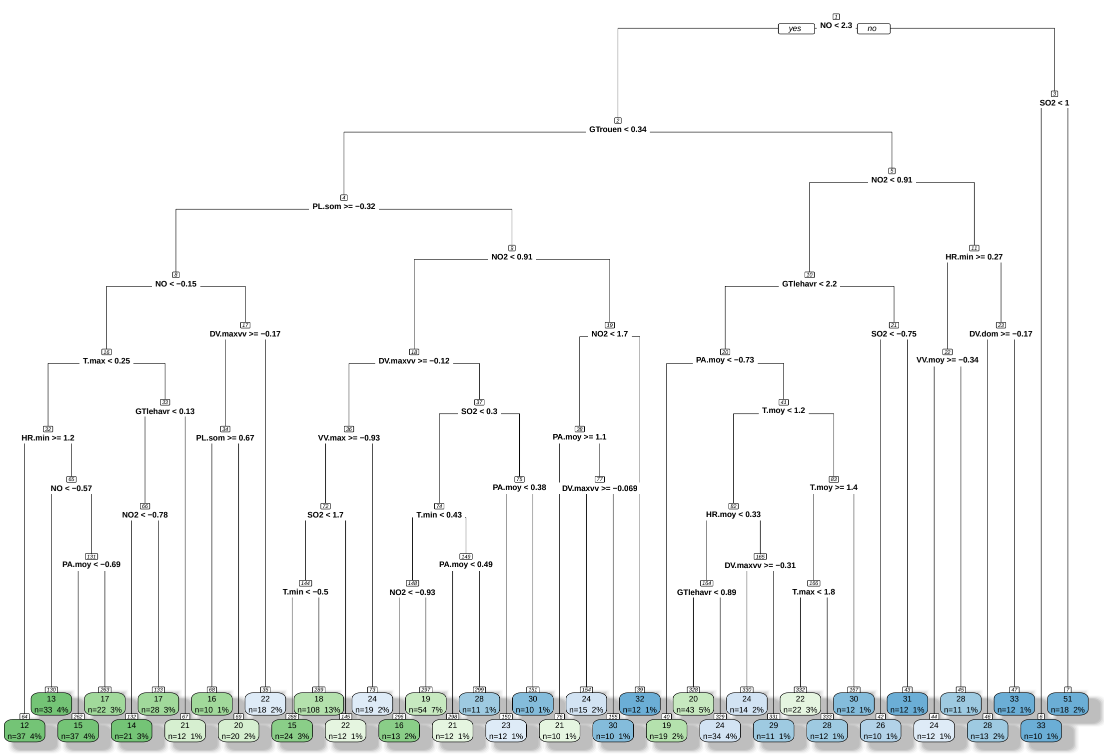
```
##
## === Cross-Validation Results ===

## Mean Cross-Validation MSE: 54.0182

## Mean Cross-Validation RMSE: 7.2328

## Mean Cross-Validation R-squared: 0.2399

##
## === RPART Model Summary ===

##
## Regression tree:
## rpart(formula = Y ~ ., data = train_df, method = "anova", control = rpart.control(xval = 5,
##     cp = 1e-04, minsplit = 5, minbucket = 10, maxdepth = 8))
##
## Variables actually used in tree construction:
##  [1] DV.dom    DV.maxvv  GTlehavre GTrouen   HR.max    HR.min    HR.moy
##  [8] NO        NO2       PA.moy    PL.som    SO2       T.max     T.min
## [15] T.moy     VV.max    VV.moy
##
## Root node error: 61335/825 = 74.346
##
## n= 825
##
##            CP nsplit rel error  xerror     xstd
## 1  0.25517987      0   1.00000 1.00223 0.144371
## 2  0.10154940      1   0.74482 0.82093 0.083245
## 3  0.04671272      2   0.64327 0.73958 0.083976
## 4  0.03412636      3   0.59656 0.76509 0.098611
## 5  0.03279346      4   0.56243 0.76077 0.098600
## 6  0.01844332      5   0.52964 0.73297 0.097577
## 7  0.01236063      6   0.51119 0.71509 0.097459
## 8  0.01061341      7   0.49883 0.71177 0.097428
## 9  0.01019291      8   0.48822 0.71168 0.097624
## 10 0.01001096      9   0.47803 0.71814 0.097851
## 11 0.00953867     10   0.46802 0.71685 0.097854
## 12 0.00737893     12   0.44894 0.71968 0.097695
## 13 0.00686223     13   0.44156 0.71992 0.097800
## 14 0.00656108     14   0.43470 0.71862 0.097659
## 15 0.00453895     15   0.42814 0.72163 0.097769
## 16 0.00416810     16   0.42360 0.72182 0.097697
## 17 0.00416002     17   0.41943 0.72110 0.097690
## 18 0.00397222     21   0.40270 0.72110 0.097690
## 19 0.00392595     22   0.39873 0.71965 0.097566
## 20 0.00363165     23   0.39481 0.72156 0.097943
## 21 0.00355867     24   0.39117 0.71079 0.093855
```

```
## 22 0.00292707     25   0.38762 0.71455 0.093875
## 23 0.00246573     27   0.38176 0.71714 0.093847
## 24 0.00239588     28   0.37930 0.71625 0.093830
## 25 0.00236303     29   0.37690 0.71849 0.093738
## 26 0.00233135     30   0.37454 0.71849 0.093738
## 27 0.00216728     31   0.37220 0.71760 0.093739
## 28 0.00214497     32   0.37004 0.71718 0.093652
## 29 0.00210625     33   0.36789 0.71461 0.093148
## 30 0.00209268     34   0.36579 0.71461 0.093148
## 31 0.00207391     35   0.36369 0.71461 0.093148
## 32 0.00187195     36   0.36162 0.71702 0.093181
## 33 0.00167796     37   0.35975 0.71423 0.093126
## 34 0.00135113     38   0.35807 0.71018 0.093115
## 35 0.00111350     39   0.35672 0.70978 0.093054
## 36 0.00064252     40   0.35561 0.71031 0.093051
## 37 0.00059767     41   0.35496 0.71217 0.093064
## 38 0.00057838     42   0.35437 0.71217 0.093064
## 39 0.00043124     43   0.35379 0.71257 0.093062
## 40 0.00010000     44   0.35336 0.71180 0.093061
```




```
##
## Optimal Complexity Parameter (CP): 0.001113502

## Final Tree Size: 79 nodes

##
## === Test Set Evaluation ===
```

```
## MSE: 39.0057

## RMSE: 6.2455

## R-squared: 0.2967

##
## === Variable Importance ===

##          NO        NO2   GTrouen        SO2 GTlehavre      T.max      T.moy     PL.som
## 18440.100  9201.996  6530.975  4794.136  4708.561  4554.848  4142.218  3398.593
##     VV.moy     HR.min     HR.moy     PA.moy      T.min   DV.maxvv     DV.dom     VV.max
##   3125.636  3004.276  2886.841  2252.807  2200.831  1567.724  1298.321  1221.588
##     HR.max
##    190.127

##
## === Decision Tree Structure ===
```

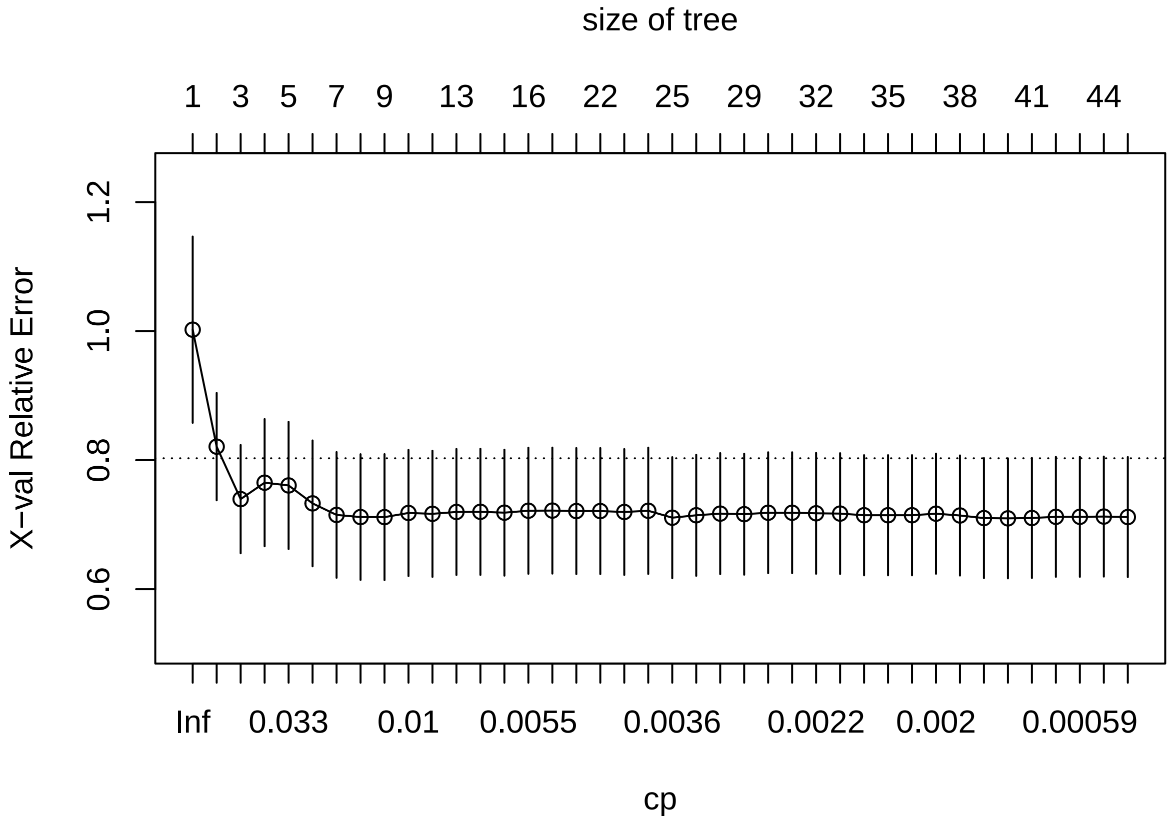


4.2 Fine-tuned RPART

```
##
## === Cross-Validation Results ===

## Mean Cross-Validation MSE: 54.0182

## Mean Cross-Validation RMSE: 7.2328
```

```
## Mean Cross-Validation R-squared: 0.2399

##
## === RPART Model Summary ===

##
## Regression tree:
## rpart(formula = Y ~ ., data = train_df, method = "anova", control = rpart.control(xval = 5,
##     cp = 1e-04, minsplit = 5, minbucket = 10, maxdepth = 8))
##
## Variables actually used in tree construction:
##  [1] DV.dom    DV.maxvv  GTlehavre GTrouen   HR.max    HR.min    HR.moy
##  [8] NO        NO2       PA.moy    PL.som    SO2       T.max     T.min
## [15] T.moy     VV.max    VV.moy
##
## Root node error: 61335/825 = 74.346
##
## n= 825
##
##            CP nsplit rel error  xerror     xstd
## 1  0.25517987      0   1.00000 1.00223 0.144371
## 2  0.10154940      1   0.74482 0.82093 0.083245
## 3  0.04671272      2   0.64327 0.73958 0.083976
## 4  0.03412636      3   0.59656 0.76509 0.098611
## 5  0.03279346      4   0.56243 0.76077 0.098600
## 6  0.01844332      5   0.52964 0.73297 0.097577
## 7  0.01236063      6   0.51119 0.71509 0.097459
## 8  0.01061341      7   0.49883 0.71177 0.097428
## 9  0.01019291      8   0.48822 0.71168 0.097624
## 10 0.01001096      9   0.47803 0.71814 0.097851
## 11 0.00953867     10   0.46802 0.71685 0.097854
## 12 0.00737893     12   0.44894 0.71968 0.097695
## 13 0.00686223     13   0.44156 0.71992 0.097800
## 14 0.00656108     14   0.43470 0.71862 0.097659
## 15 0.00453895     15   0.42814 0.72163 0.097769
## 16 0.00416810     16   0.42360 0.72182 0.097697
## 17 0.00416002     17   0.41943 0.72110 0.097690
## 18 0.00397222     21   0.40270 0.72110 0.097690
## 19 0.00392595     22   0.39873 0.71965 0.097566
## 20 0.00363165     23   0.39481 0.72156 0.097943
## 21 0.00355867     24   0.39117 0.71079 0.093855
## 22 0.00292707     25   0.38762 0.71455 0.093875
## 23 0.00246573     27   0.38176 0.71714 0.093847
## 24 0.00239588     28   0.37930 0.71625 0.093830
## 25 0.00236303     29   0.37690 0.71849 0.093738
## 26 0.00233135     30   0.37454 0.71849 0.093738
## 27 0.00216728     31   0.37220 0.71760 0.093739
## 28 0.00214497     32   0.37004 0.71718 0.093652
## 29 0.00210625     33   0.36789 0.71461 0.093148
## 30 0.00209268     34   0.36579 0.71461 0.093148
## 31 0.00207391     35   0.36369 0.71461 0.093148
## 32 0.00187195     36   0.36162 0.71702 0.093181
## 33 0.00167796     37   0.35975 0.71423 0.093126
## 34 0.00135113     38   0.35807 0.71018 0.093115
```

```
## 35 0.00111350     39   0.35672 0.70978 0.093054
## 36 0.00064252     40   0.35561 0.71031 0.093051
## 37 0.00059767     41   0.35496 0.71217 0.093064
## 38 0.00057838     42   0.35437 0.71217 0.093064
## 39 0.00043124     43   0.35379 0.71257 0.093062
## 40 0.00010000     44   0.35336 0.71180 0.093061
```




```
##
## One Standard Error Optimal Complexity Parameter (CP): 0.04671272
```

```
## Final Tree Size: 5 nodes
```

```
##
## === Test Set Evaluation ===
```

```
## MSE: 45.6268
```

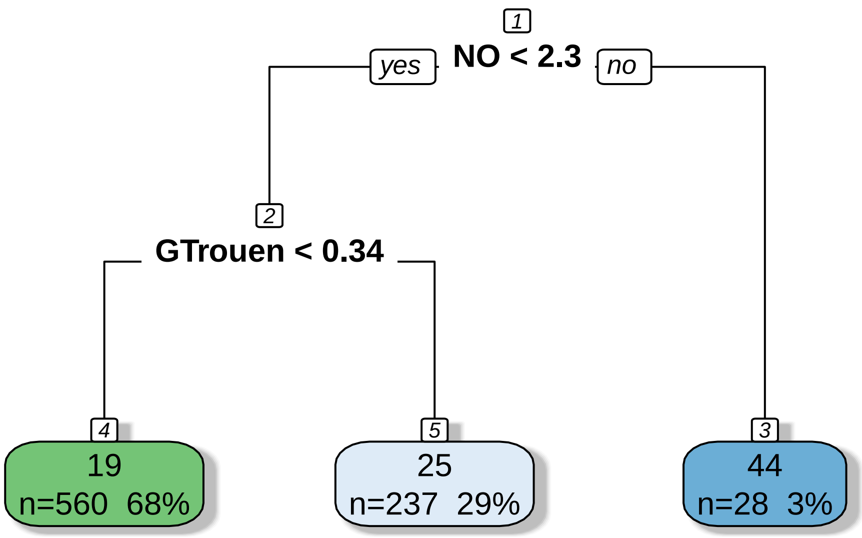
```
## RMSE: 6.7548
```

```
## R-squared: 0.1773
```

```
##
## === Variable Importance ===
```

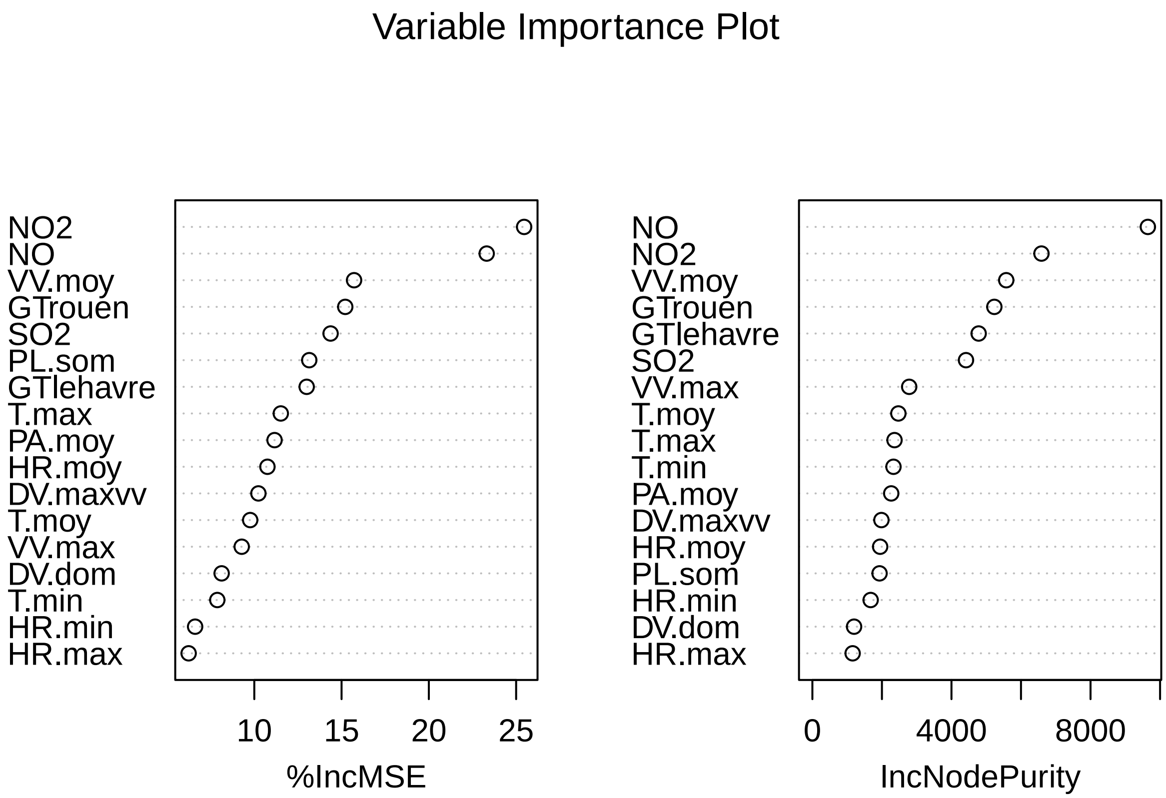
```
##          NO     GTrouen         NO2  GTlehavre       T.max      HR.min         SO2
## 15651.5715   6228.5780   3912.8929  2890.9012   1760.8216   1208.9223   1117.9694
##     VV.moy       T.moy      HR.moy
##  1117.9694   1103.7986    893.5513
```

```
##
## === Decision Tree Structure ===
```



4.3 Basic Random forest

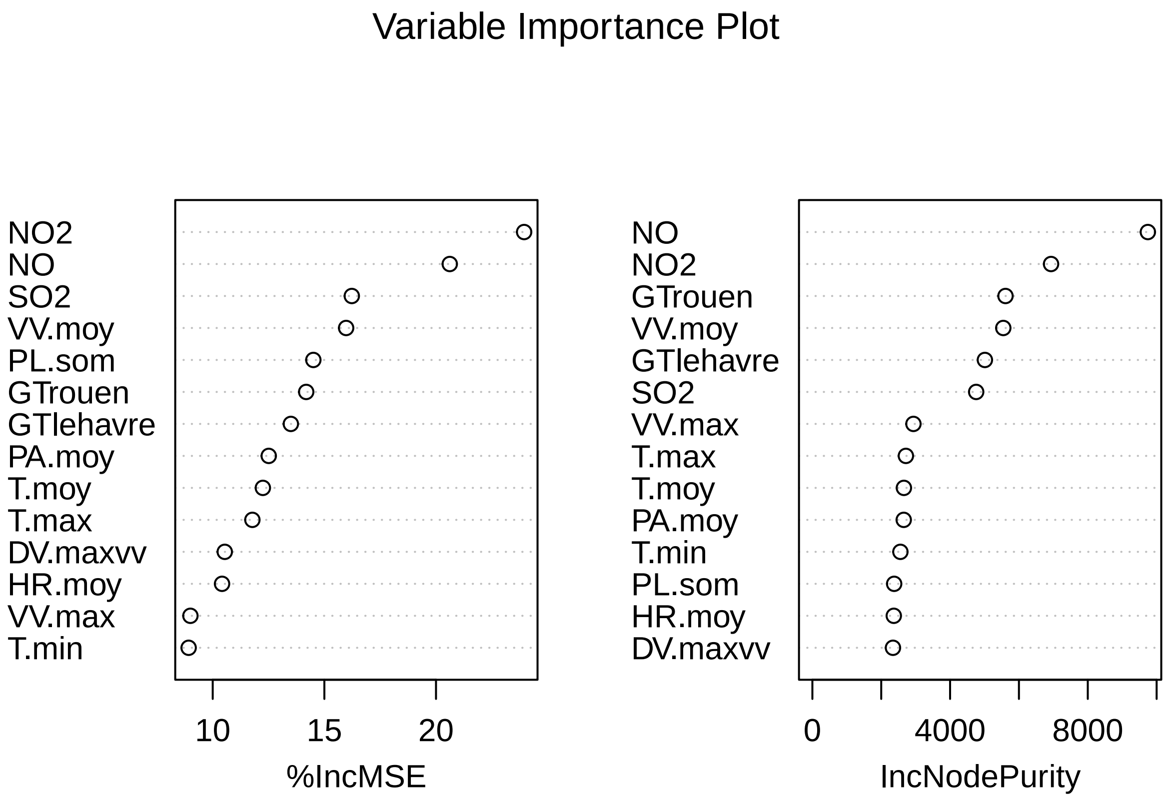
```
##
## === Cross-Validation Results (Regression) ===

## Mean CV MSE: 32.168

## Mean CV RMSE: 5.5379

## Mean CV R-squared: 0.5766

##
## === Test Set Evaluation (Regression) ===

## Test MSE: 26.388

## Test RMSE: 5.1369

## Test R-squared: 0.5242

##
## === Variable Importance ===
```



4.4 Random forest with VSURF

```
##
## === Cross-Validation Results (Regression) ===


## Mean MSE: 32.168


## Mean RMSE: 5.5379


## Mean R-squared: 0.5766


## Thresholding step
## Estimated computational time (on one core): 25.8 sec.
##
## Interpretation step (on 17 variables)
## Estimated computational time (on one core): between 8.5 sec. and  34 sec.
##
## Prediction step (on 14 variables)
## Maximum estimated computational time (on one core): 26.6 sec.
##   |                                                                              |


##
## === Test Set Evaluation (Regression) ===


## Test MSE: 26.5499
```

```
## Test RMSE: 5.1527

## Test R-squared: 0.5213

##
## === Variable Importance ===
```



4.5 Conclusion

Model	CV_MSE	CV_RMSE	CV_R2	Test_MSE	Test_RMSE	Test_R2
Basic rpart	54.0182	7.2328	0.2399	39.0057	6.2455	0.2967
Fine-tuned rpart	54.0182	7.2328	0.2399	45.6268	6.7548	0.1773
Basic random forest	32.1680	5.5379	0.5766	26.3880	5.1369	0.5242
Random forest with VSURF	32.1680	5.5379	0.5766	27.4477	5.2391	0.5051

The performance comparison shows that the random forest models outperform the decision tree models. Both versions of the random forest (basic and VSURF-enhanced) have lower cross-validation and test MSE as well as higher R-squared values compared to the rpart models. Notably, the basic random forest achieves the best performance on the test set with a Test MSE of 26.388 and a Test R^2 of 0.5242, indicating that ensemble methods capture the underlying patterns more effectively.

On the other hand, while the fine-tuned rpart model (with only 5 nodes) offers a simpler and more interpretable tree structure, its test performance (Test R^2 of 0.1773) is considerably poorer than that of the more complex basic rpart model (Test R^2 of 0.2967). This suggests that in this case, the additional complexity in the basic rpart tree is beneficial for prediction.

5. Overall Conclusion

```
##                  Model  CV MSE CV RMSE  CV R²  Test MSE Test RMSE Test R²
## 1  Stepwise Selection 34.2779  5.7463 0.5378  27.8327    5.2757  0.4981
## 2               Lasso 34.5082  5.8744 0.5364  27.9424    5.2861  0.4961
## 3 Basic random forest 32.1680  5.5379 0.5766  26.3880    5.1369  0.5242
```

While the enhancements achieved by Stepwise Selection and Lasso over the basic OLS model are minimal, the Basic random forest offers the best performance among the compared models. However, even this improvement is moderate, indicating that while the random forest does yield better predictive accuracy, the gains are not extraordinarily large. It's worth noting that the concept of the reduction of the number of features is not very efficient for this dataset. Even within the random forest models, employing a variable selection method such as VSURF resulted in worse performance compared to the Basic random forest. This reinforces the idea that with a relatively small set of predictors, using all available features can be more effective than reducing the feature set.