Data analysis & modeling report

```
The following required system packages are not installed:
- libglpk-dev  [required by igraph]
- libx11-dev   [required by clipr]
- pandoc       [required by DataExplorer, knitr, rmarkdown]
The R packages depending on these system packages may fail to install.

An administrator can install these packages with:
- sudo apt install libglpk-dev libx11-dev pandoc

- The library is already synchronized with the lockfile.
```

Required packages

```r
library(readr)
library(dplyr)
```

```
Adjuntando el paquete: 'dplyr'

The following objects are masked from 'package:stats':

    filter, lag

The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

```r
library(tidyr)
library(DataExplorer)
library(tidymodels)
```

```
-- Attaching packages -------------------------------------- tidymodels 1.3.0 --

v broom        1.0.8     v recipes      1.2.1
v dials        1.4.0     v rsample      1.3.0
v ggplot2      3.5.2     v tibble       3.2.1
v infer        1.0.7     v tune         1.3.0
v modeldata    1.4.0     v workflows    1.2.0
v parsnip      1.3.1     v workflowsets 1.1.0
v purrr        1.0.4     v yardstick    1.3.2

-- Conflicts ----------------------------------------- tidymodels_conflicts() --
x purrr::discard()  masks scales::discard()
x dplyr::filter()   masks stats::filter()
x dplyr::lag()      masks stats::lag()
x yardstick::spec() masks readr::spec()
x recipes::step()   masks stats::step()
```

```r
library(glmnet)
```

```
Cargando paquete requerido: Matrix


Adjuntando el paquete: 'Matrix'

The following objects are masked from 'package:tidyr':

    expand, pack, unpack

Loaded glmnet 4.1-8
```

```r
library(vip)
```

```

Adjuntando el paquete: 'vip'
```

```
The following object is masked from 'package:utils':

    vi
```

```r
library(ranger)
library(readxl)
library(kernelshap)
library(shapviz)
```

Load dataset

```r
database <- read_excel("database_2021_2024_con out.xlsx",
    col_types = c("date", "numeric", "text",
        "date", "numeric", "numeric", "numeric",
        "skip", "skip", "numeric", "numeric",
        "numeric", "numeric", "numeric",
        "numeric", "numeric"))

colnames(database)
```

```
 [1] "Dia"                          "Año"
 [3] "Estación"                     "Hora"
 [5] "Temperatura (°C)"             "Humedad (%)"
 [7] "Presión (hPa)"                "Velocidad de viento (m/s)"
 [9] "CO (mg/m3)"                   "NO (ug/m3)"
[11] "NO2 (ug/m3)"                  "NOX (ug/m3)"
[13] "O3 (ug/m3)"                   "PM10 (ug/m3)"
```

```r
nrow(database)
```

```
[1] 1747
```

```r
summary(database)
```

```
      Dia                              Año          Estación
 Min.   :2021-07-27 00:00:00.00   Min.   :2021   Length:1747
 1st Qu.:2022-02-16 00:00:00.00   1st Qu.:2022   Class :character
 Median :2023-01-12 00:00:00.00   Median :2023   Mode  :character
```

```
 Mean   :2022-12-05 06:32:21.16   Mean   :2022  
 3rd Qu.:2023-10-12 00:00:00.00   3rd Qu.:2023  
 Max.   :2024-04-04 00:00:00.00   Max.   :2024  
                                                
      Hora                        Temperatura (°C)  Humedad (%)   
 Min.   :1899-12-31 00:00:00.00   Min.   :-1.70    Min.   : 3.00  
 1st Qu.:1899-12-31 06:00:00.00   1st Qu.:12.18    1st Qu.:33.00  
 Median :1899-12-31 13:00:00.00   Median :19.20    Median :46.00  
 Mean   :1899-12-31 16:00:37.09   Mean   :18.03    Mean   :48.05  
 3rd Qu.:1899-12-31 19:00:00.00   3rd Qu.:24.00    3rd Qu.:62.00  
 Max.   :1900-01-05 08:00:00.00   Max.   :36.60    Max.   :95.00  
                                                                  
 Presión (hPa)   Velocidad de viento (m/s)   CO (mg/m3)      NO (ug/m3)     
 Min.   :902.0   Min.   : 0.000            Min.   :0.000   Min.   :  0.020  
 1st Qu.:923.4   1st Qu.: 0.290            1st Qu.:0.700   1st Qu.:  4.955  
 Median :927.2   Median : 0.950            Median :1.130   Median : 17.390  
 Mean   :927.1   Mean   : 1.438            Mean   :1.188   Mean   : 32.230  
 3rd Qu.:930.5   3rd Qu.: 1.940            3rd Qu.:1.595   3rd Qu.: 47.910  
 Max.   :942.5   Max.   :18.060            Max.   :3.460   Max.   :417.340  
 NA's   :160                                                                
  NO2 (ug/m3)      NOX (ug/m3)       O3 (ug/m3)      PM10 (ug/m3)   
 Min.   :  1.28   Min.   :  4.15   Min.   :  0.00   Min.   :  0.00  
 1st Qu.: 28.23   1st Qu.: 40.81   1st Qu.:  6.61   1st Qu.: 16.00  
 Median : 43.22   Median : 71.98   Median : 30.75   Median : 28.50  
 Mean   : 43.80   Mean   : 90.56   Mean   : 58.83   Mean   : 36.37  
 3rd Qu.: 54.23   3rd Qu.:127.17   3rd Qu.: 64.16   3rd Qu.: 48.50  
 Max.   :131.05   Max.   :559.91   Max.   :509.65   Max.   :318.00  
                                                    NA's   :16      
```

Cleaning

Delete columns

- Keep variables Temperatura, Humedad relativa, Presión atmosférica, Velocidad de viento, CO, NO, NO2, O3.
- Delete column NOX
- Delete NA

```
data <- database %>% select(-one_of(c("Estación","Dia","Año","Hora","NOX (ug/m3)")))
```

Clean the features' names

```r
library(stringr)
```

```
Adjuntando el paquete: 'stringr'

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

    fixed
```

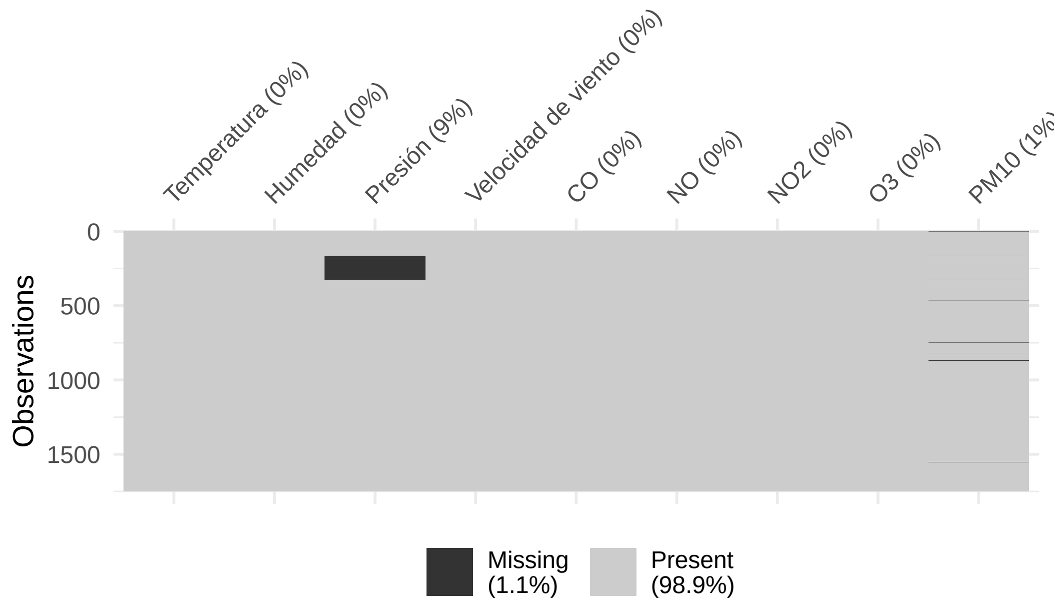
```r
colnames(data) <- str_replace(colnames(data),pattern="\\s+\\(\\S+", "")
```

Missing values

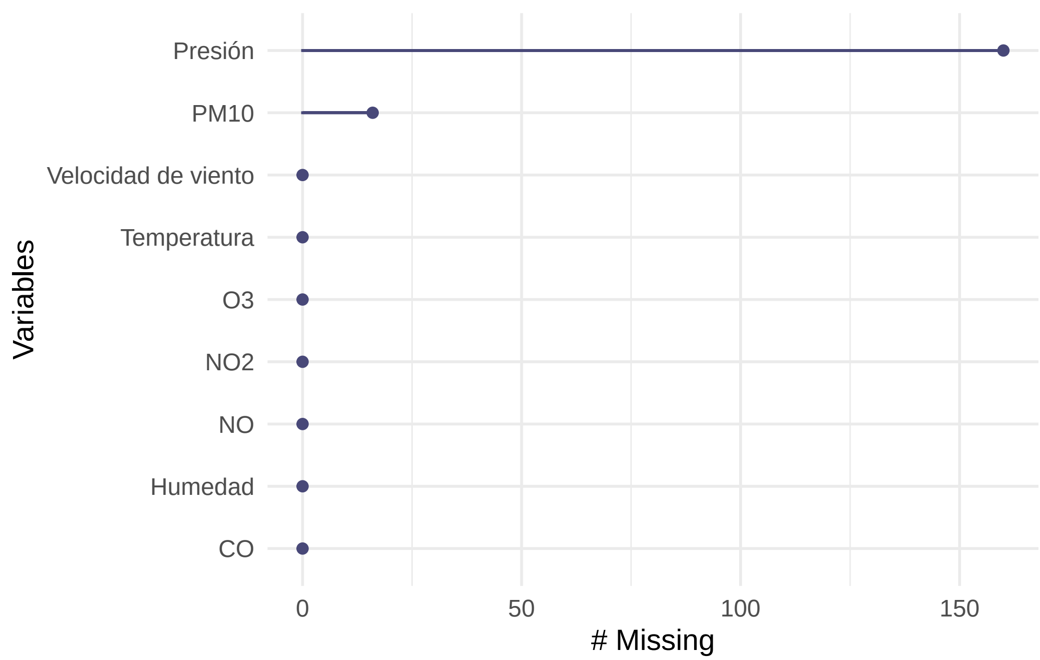
```r
# visualizar los valores perdidos del dataset data. Instalar la libreria naniar si no está i
if(!require(naniar)){
  install.packages("naniar")
  library(naniar)
}
```

```
Cargando paquete requerido: naniar
```

```r
vis_miss(data)
```




```
gg_miss_var(data)
```



```r
data_imputed <- data %>%
  mutate(
    PM10 = ifelse(is.na(PM10), median(PM10, na.rm = TRUE), PM10),
    Presión = ifelse(is.na(Presión), median(Presión, na.rm = TRUE), Presión)
  )
```

- The dataset has 1747 samples (rows) and 9 variables (columns).
- The features (variables) are: Temperatura, Humedad, Presión, Velocidad de viento, CO, NO, NO2, O3, PM10.

Variable name

```r
data <- data_imputed
colnames(data)
```

```
[1] "Temperatura"         "Humedad"             "Presión"
[4] "Velocidad de viento" "CO"                  "NO"
[7] "NO2"                 "O3"                  "PM10"
```

- Translate names to English

```r
colnames(data)[1:4] <- c("Temperature","Humidity","Pressure","Wind speed")
```

```r
colnames(data)
```

```
[1] "Temperature" "Humidity"    "Pressure"    "Wind speed"  "CO"
[6] "NO"          "NO2"         "O3"          "PM10"
```

- Data summary

```r
summary(data)
```

```
  Temperature       Humidity         Pressure        Wind speed
 Min.   :-1.70   Min.   : 3.00   Min.   :902.0   Min.   : 0.000
 1st Qu.:12.18   1st Qu.:33.00   1st Qu.:924.0   1st Qu.: 0.290
 Median :19.20   Median :46.00   Median :927.2   Median : 0.950
 Mean   :18.03   Mean   :48.05   Mean   :927.1   Mean   : 1.438
 3rd Qu.:24.00   3rd Qu.:62.00   3rd Qu.:930.1   3rd Qu.: 1.940
```

```
 Max.   :36.60   Max.   :95.00   Max.   :942.5   Max.   :18.060  
       CO               NO                NO2                O3        
 Min.   :0.000   Min.   :  0.020   Min.   :  1.28   Min.   :  0.00  
 1st Qu.:0.700   1st Qu.:  4.955   1st Qu.: 28.23   1st Qu.:  6.61  
 Median :1.130   Median : 17.390   Median : 43.22   Median : 30.75  
 Mean   :1.188   Mean   : 32.230   Mean   : 43.80   Mean   : 58.83  
 3rd Qu.:1.595   3rd Qu.: 47.910   3rd Qu.: 54.23   3rd Qu.: 64.16  
 Max.   :3.460   Max.   :417.340   Max.   :131.05   Max.   :509.65  
      PM10      
 Min.   :  0.0  
 1st Qu.: 16.0  
 Median : 28.5  
 Mean   : 36.3  
 3rd Qu.: 48.0  
 Max.   :318.0  
```

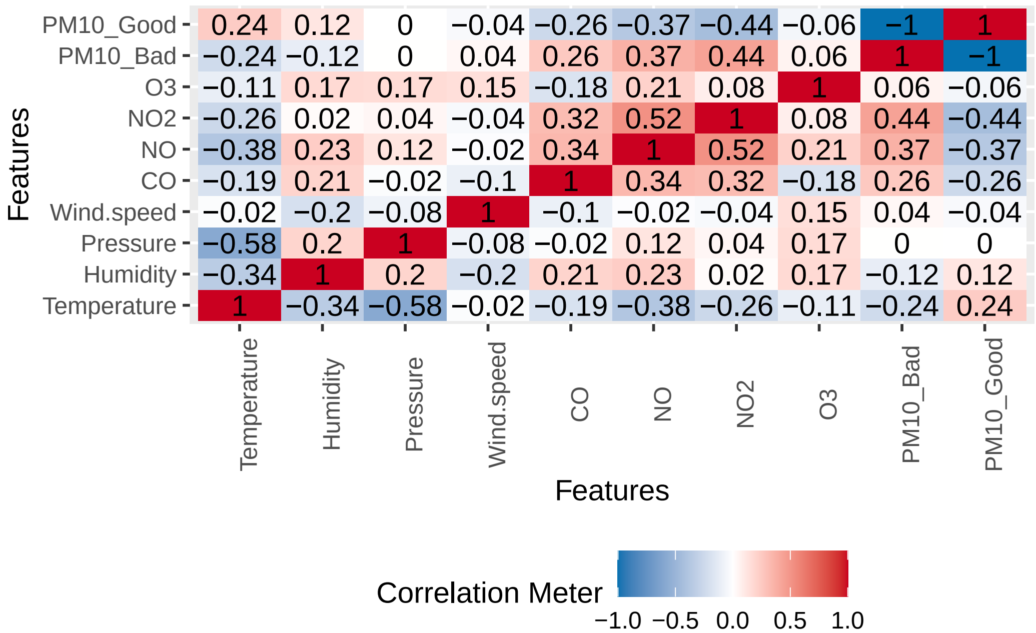
- The variable Particulate Matter (PM10) will be discretized using a threshold value of 45 µg/m3, below which it will be categorized as "Good." Above 45 µg/m3, it will be assigned the value "Bad."

```
y_col_name <- colnames(data)[10]
y_cut <- cut(data$PM10,breaks=c(-10,45,400),labels = c("Good","Bad"))
data$PM10 <- y_cut
```

EDA

Pearson correlation

```
plot_correlation(data)
```

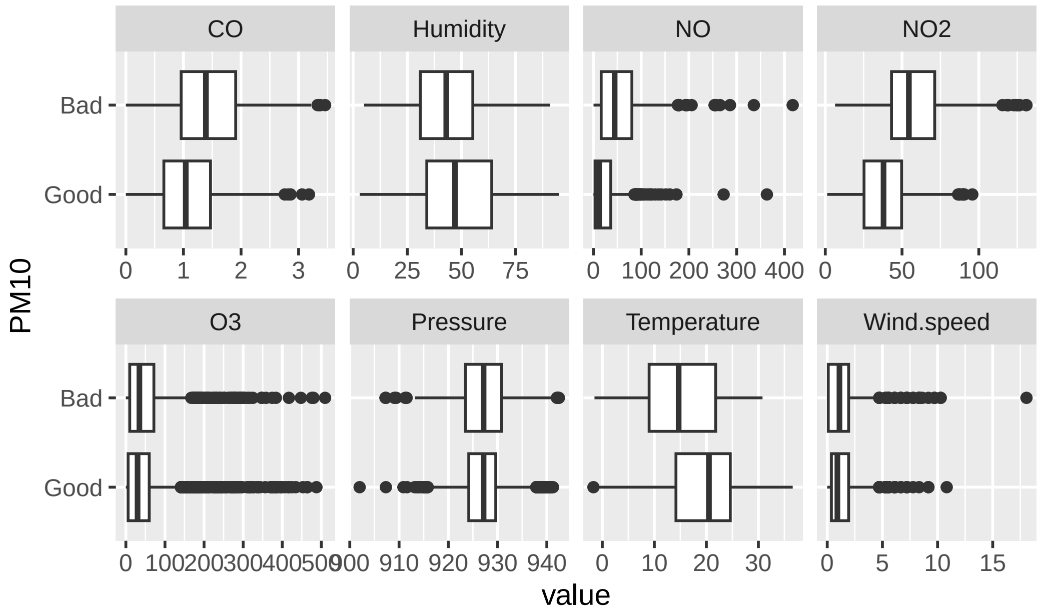



```r
ggsave(filename = "./figs-to-paper/01-pearson-correlation.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

Box plot

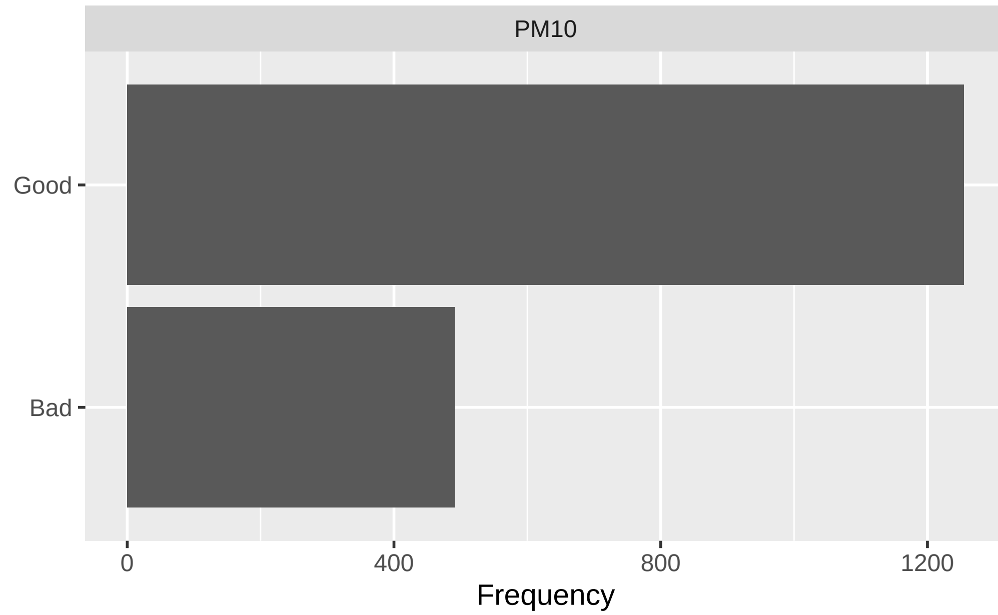
```r
plot_boxplot(data, by = "PM10")
```




```r
ggsave(filename = "./figs-to-paper/02-boxplot.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

```r
plot_bar(data)
```




```
ggsave(filename = "./figs-to-paper/03-dataset-desbalanceado.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

Machine learning models

Slipt train & test set

We split the dataset to use a 75 % for training and a 25 % for testing.

```
set.seed(123)
splits      <- initial_split(data, strata = PM10, prop = 3/4)

data_train <- training(splits) # 75 % train set
data_test  <- testing(splits)  # 25 % testing set
```

Binary clasification with Logistic regression

- We train two models to develop the binary classifier: logistic regression and random forest.

- We will use the tidymodels library.
- The logistic regression model is implemented in the glmnet package.
- mixture = 1 means L1 regularization (a pure Lasso model) will be used. A mixture value of 1 means that the glmnet model will potentially eliminate irrelevant predictors and choose a simpler model.
- penalty: This hyperparameter represents how much of this regularization we will use. We will adjust it during training to find the best value for making predictions with our data.

```
lr_mod <-
  logistic_reg(penalty = tune(), mixture = 1) %>%
  set_engine("glmnet") # we use the package glmnet
```

Tidymodels recipe

- data_train dataset will be used to train the logistic model. We want to predict the variable PM10.

- step_normalize() creates a specification of a recipe step that will normalize numeric data to have a standard deviation of one and a mean of zero.

```
lr_recipe <-
  recipe(PM10 ~ ., data = data_train) %>%
  step_normalize(all_predictors())
```

Tidymodels workflow

```
lr_workflow <-
  workflow() %>%  # create a workflow
  add_model(lr_mod) %>% # add the model
  add_recipe(lr_recipe) # add the recipe
```

Grid tunning

We have a hyperparameter to adjust: the penalty for L1 regularization. We can configure the grid manually using a one-column table with 30 candidate values.

```
lr_reg_grid <- tibble(penalty = 10^seq(-4, -1, length.out = 30))
```

List of the different values for the penalty hyperparameter to try in the training phase.

```
lr_reg_grid
```

```
# A tibble: 30 x 1
    penalty
      <dbl>
 1 0.0001
 2 0.000127
 3 0.000161
 4 0.000204
 5 0.000259
 6 0.000329
 7 0.000418
 8 0.000530
 9 0.000672
10 0.000853
# i 20 more rows
```

Validation set

With the strata argument, random sampling is performed within the variable PM10 (the stratification variable). This can help ensure that the new samples have proportions equivalent to those in the original dataset. In the case of a categorical variable like PM10, sampling is performed separately within each class.

A validation dataset is used to tune the penalty hyperparameter. Within the training dataset, 80% is kept for training and 20% for validation.

Within the training dataset, we use a portion of it as a validation set to train with the different penalty values (the grid tuning we will perform).

```
set.seed(234)
# 20 %
val_set <- validation_split(data_train,
                            strata = PM10,
                            prop = 0.80)
```

```
Warning: `validation_split()` was deprecated in rsample 1.2.0.
i Please use `initial_validation_split()` instead.
```

Training execution

- The following code block executes everything: the recipe or instructions saved in `lr_workflow` plus the hyperparameter tuning (tune_grid).
- ROC_AUC is the classifier evaluation metric.

```
lr_res <-
  lr_workflow %>%
  tune_grid(val_set,
            grid = lr_reg_grid,
            control = control_grid(save_pred = TRUE),
            metrics = metric_set(roc_auc))
```

```
lr_res
```

```
# Tuning results
# Validation Set Split (0.8/0.2)  using stratification
# A tibble: 1 x 5
  splits             id         .metrics          .notes           .predictions
  <list>             <chr>      <list>            <list>           <list>
1 <split [1047/263]> validation <tibble [30 x 5]> <tibble [0 x 3]> <tibble>
```

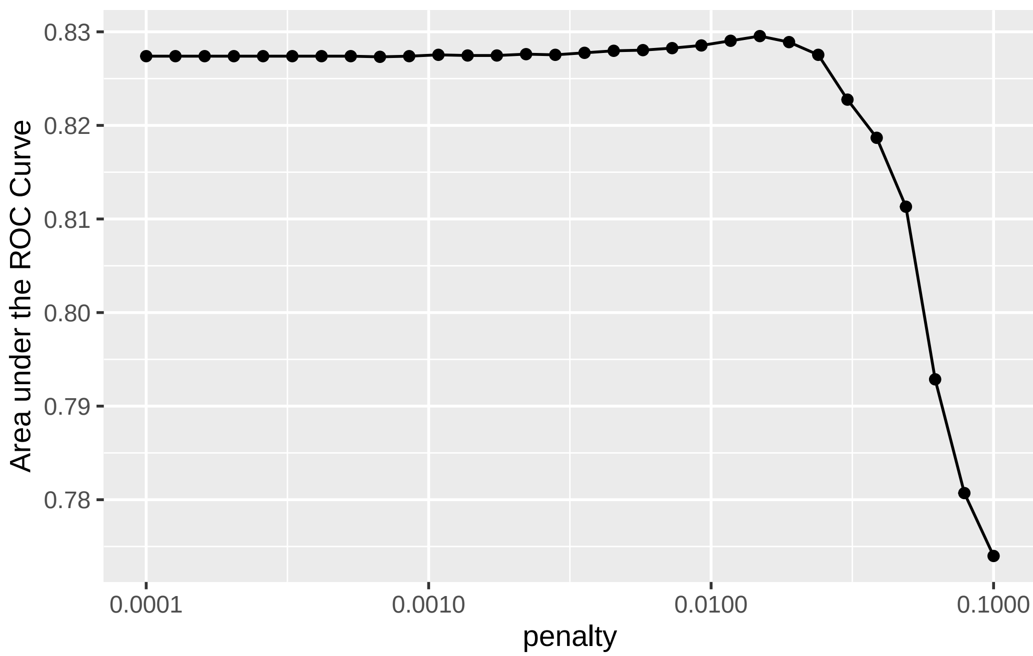
Hyperparameter tuning results

We plot the variation in ROC values for different penalty values.

The higher the ROC value, the better the models.

```
lr_plot <-
  lr_res %>%
  collect_metrics() %>%
  ggplot(aes(x = penalty, y = mean)) +
  geom_point() +
  geom_line() +
  ylab("Area under the ROC Curve") +
  scale_x_log10(labels = scales::label_number())

lr_plot
```




```
ggsave(filename = "./figs-to-paper/04-log-reg-tunning-results.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

The graph above shows that model performance is generally better with lower penalty values, which suggests that most predictors are important to the model.

We also see a steep drop in the area under the ROC curve toward higher penalty values, which happens because a large enough penalty will remove all predictors from the model, and, as expected, predictive accuracy plummets with fewer predictors in the model.

Best Logistic Regression Models

We display the top 15 models based on the ROC metric using show_best. The higher the ROC value, the better the models.

The data is displayed in order from lowest to highest penalty value.

```
top_models <-
  lr_res %>%
  show_best(metric = "roc_auc", n = 15) %>%
  arrange(penalty)
top_models
```

```
# A tibble: 15 x 7
   penalty .metric .estimator  mean     n std_err .config
     <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
 1 0.0001  roc_auc binary     0.827     1      NA Preprocessor1_Model01
 2 0.00108 roc_auc binary     0.828     1      NA Preprocessor1_Model11
 3 0.00137 roc_auc binary     0.827     1      NA Preprocessor1_Model12
 4 0.00174 roc_auc binary     0.827     1      NA Preprocessor1_Model13
 5 0.00221 roc_auc binary     0.828     1      NA Preprocessor1_Model14
 6 0.00281 roc_auc binary     0.828     1      NA Preprocessor1_Model15
 7 0.00356 roc_auc binary     0.828     1      NA Preprocessor1_Model16
 8 0.00452 roc_auc binary     0.828     1      NA Preprocessor1_Model17
 9 0.00574 roc_auc binary     0.828     1      NA Preprocessor1_Model18
10 0.00728 roc_auc binary     0.828     1      NA Preprocessor1_Model19
11 0.00924 roc_auc binary     0.829     1      NA Preprocessor1_Model20
12 0.0117  roc_auc binary     0.829     1      NA Preprocessor1_Model21
13 0.0149  roc_auc binary     0.830     1      NA Preprocessor1_Model22
14 0.0189  roc_auc binary     0.829     1      NA Preprocessor1_Model23
15 0.0240  roc_auc binary     0.828     1      NA Preprocessor1_Model24
```

The same information as above, but this time sorted by descending ROC_AUC value.

The data is displayed sorted from lowest to highest according to the penalty value.

```r
top_models %>%
  arrange(desc(mean))
```

```
# A tibble: 15 x 7
   penalty .metric .estimator  mean     n std_err .config
     <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
 1 0.0149  roc_auc binary     0.830     1      NA Preprocessor1_Model22
 2 0.0117  roc_auc binary     0.829     1      NA Preprocessor1_Model21
 3 0.0189  roc_auc binary     0.829     1      NA Preprocessor1_Model23
 4 0.00924 roc_auc binary     0.829     1      NA Preprocessor1_Model20
 5 0.00728 roc_auc binary     0.828     1      NA Preprocessor1_Model19
 6 0.00574 roc_auc binary     0.828     1      NA Preprocessor1_Model18
 7 0.00452 roc_auc binary     0.828     1      NA Preprocessor1_Model17
 8 0.00356 roc_auc binary     0.828     1      NA Preprocessor1_Model16
 9 0.00221 roc_auc binary     0.828     1      NA Preprocessor1_Model14
10 0.0240  roc_auc binary     0.828     1      NA Preprocessor1_Model24
11 0.00108 roc_auc binary     0.828     1      NA Preprocessor1_Model11
12 0.00281 roc_auc binary     0.828     1      NA Preprocessor1_Model15
13 0.00137 roc_auc binary     0.827     1      NA Preprocessor1_Model12
```

```
14 0.00174 roc_auc binary     0.827     1       NA Preprocessor1_Model13
15 0.0001  roc_auc binary     0.827     1       NA Preprocessor1_Model01
```

```r
penalty_value <-  lr_res %>%
  select_best(metric = "roc_auc") %>% # find the best hyperparameter combination given a per
  select(penalty)
```

The best logistic regression model is the one with penalty = 0.0148735210729351.

We observed minimal ROC variation at the other penalty values.

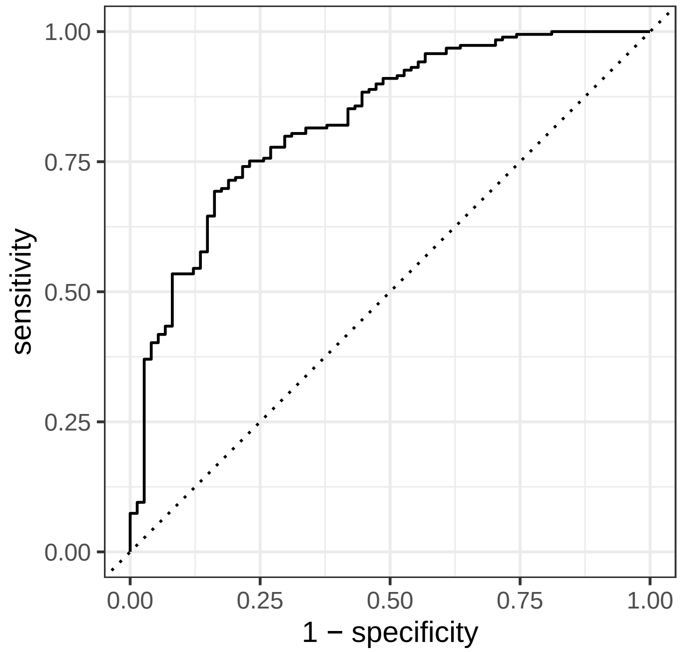
```r
lr_best <- lr_res %>%
        collect_metrics() %>%
        arrange(desc(mean)) %>%
        slice(1)
lr_best
```

```
# A tibble: 1 x 7
  penalty .metric .estimator  mean     n std_err .config
    <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1  0.0149 roc_auc binary     0.830     1      NA Preprocessor1_Model22
```

Roc curve in training set

```r
lr_auc <-
  lr_res %>%
  collect_predictions(parameters = lr_best) %>%
  roc_curve(PM10, .pred_Good) %>%
  mutate(model = "Logistic Regression")

autoplot(lr_auc)
```




```
ggsave(filename = "./figs-to-paper/05-log-reg-ROC-best-on-training.tiff",units = "px", dpi=3
```

```
Saving 1650 x 1050 px image
```

Results (test set)

Get the best model.

```
best_model <- lr_res %>%
  select_best(metric = "roc_auc")

best_model
```

```
# A tibble: 1 x 2
  penalty .config
    <dbl> <chr>
1  0.0149 Preprocessor1_Model22
```

Update the workflow.

```r
final_wf <- lr_workflow %>%
            finalize_workflow(best_model)

final_wf
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: logistic_reg()

-- Preprocessor ----------------------------------------------------------------
1 Recipe Step

* step_normalize()

-- Model -----------------------------------------------------------------------
Logistic Regression Model Specification (classification)

Main Arguments:
  penalty = 0.0148735210729351
  mixture = 1

Computational engine: glmnet
```

We can use the last_fit() function with our finalized model; this function fits the finalized model on the full training dataset and evaluates the finalized model on the test data.

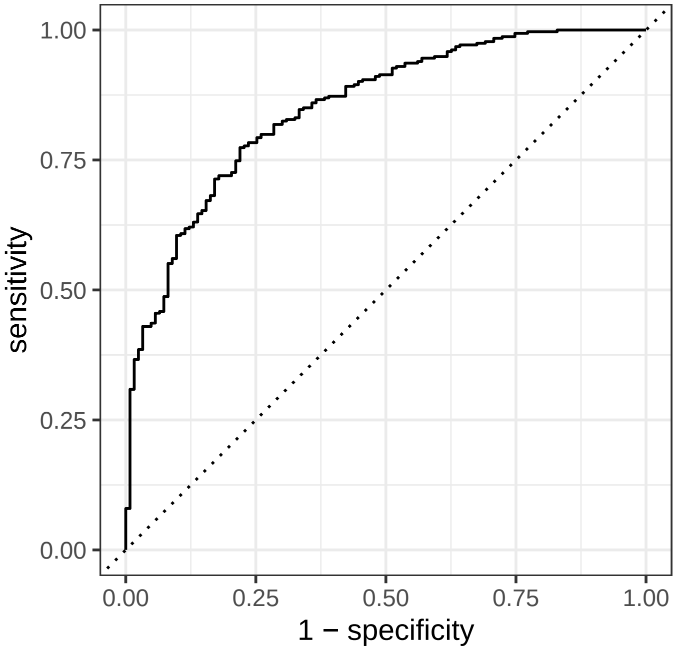
```r
final_fit <-
  final_wf %>%
  last_fit(splits)
```

```r
final_fit %>%
  collect_metrics()
```

```
# A tibble: 3 x 4
  .metric     .estimator .estimate .config
  <chr>       <chr>          <dbl> <chr>
1 accuracy    binary         0.801 Preprocessor1_Model1
2 roc_auc     binary         0.850 Preprocessor1_Model1
3 brier_class binary         0.136 Preprocessor1_Model1
```

ROC CURVE IN TEST SET

```
final_fit %>%
  collect_predictions() %>%
  roc_curve(PM10, .pred_Good) %>%
  mutate(model = "Logistic Regression") %>%
  autoplot()
```




```
ggsave(filename = "./figs-to-paper/06-log-reg-ROC-best-on-testing.tiff",units = "px", dpi=30(
```

```
Saving 1650 x 1050 px image
```

We use the best LR model to predict on the test set.

```
lr_model <- extract_workflow(final_fit)

# Class prediction
pred_class <- predict(lr_model,
                      new_data = data_test,
                      type = "class")
```

```
# Prediction Probabilities
pred_proba <- predict(lr_model,
                      new_data = data_test,
                      type = "prob")
```

```
lr_results <- data_test %>%
              select(PM10) %>%
              bind_cols(pred_class, pred_proba)
```

Confusion matrix (on test set)

```
conf_mat(lr_results, truth = PM10,
         estimate = .pred_class)
```

```
          Truth
Prediction Good Bad
      Good  297  70
      Bad    17  53
```

Accuracy, sensitivity, specificity, etc

```
summary(conf_mat(lr_results, truth = PM10,
         estimate = .pred_class))
```

```
# A tibble: 13 x 3
   .metric              .estimator .estimate
   <chr>                <chr>          <dbl>
 1 accuracy             binary         0.801
 2 kap                  binary         0.434
 3 sens                 binary         0.946
 4 spec                 binary         0.431
 5 ppv                  binary         0.809
 6 npv                  binary         0.757
 7 mcc                  binary         0.462
 8 j_index              binary         0.377
 9 bal_accuracy         binary         0.688
10 detection_prevalence binary         0.840
```

```
11 precision            binary         0.809
12 recall               binary         0.946
13 f_meas               binary         0.872
```

F-measure

```
f_meas(lr_results, truth = PM10,
         estimate = .pred_class)
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 f_meas  binary         0.872
```

Random Forest

We train a random forest model for binary classification.

We use the random forest implementation from the ranger package.

We tune two hyperparameters: mtry and min_n, in training time.

We set the parameter trees to 100.

```
# detect the number of cores from the CPU
cores <- parallel::detectCores()

rf_mod <-
  rand_forest(mtry = tune(), min_n = tune(), trees = 100) %>%
  set_engine("ranger", num.threads = cores) %>% # use the ranger package
  set_mode("classification") # classification task
```

Tidymodels recipe

- data_train dataset will be used to train the RF model.
- We want to predict the variable PM10.

```
rf_recipe <-
  recipe(PM10 ~ ., data = data_train)
```

Tidymodels workflow setup

```
rf_workflow <-
  workflow() %>%
  add_model(rf_mod) %>% ## add model RF
  add_recipe(rf_recipe) ## add recipe
```

RF training

Within the training dataset, we use a portion of it as a validation set to tune the hyperparameters (mtry and min_n).

```
set.seed(345)
rf_res <-
  rf_workflow %>%
  tune_grid(val_set,
            grid = 25, # grid size
            control = control_grid(save_pred = TRUE),
            metrics = metric_set(roc_auc))
```

```
i Creating pre-processing data to finalize unknown parameter: mtry
```

RF hyperparameter tunning results

Results for each value of mtry and min_n:

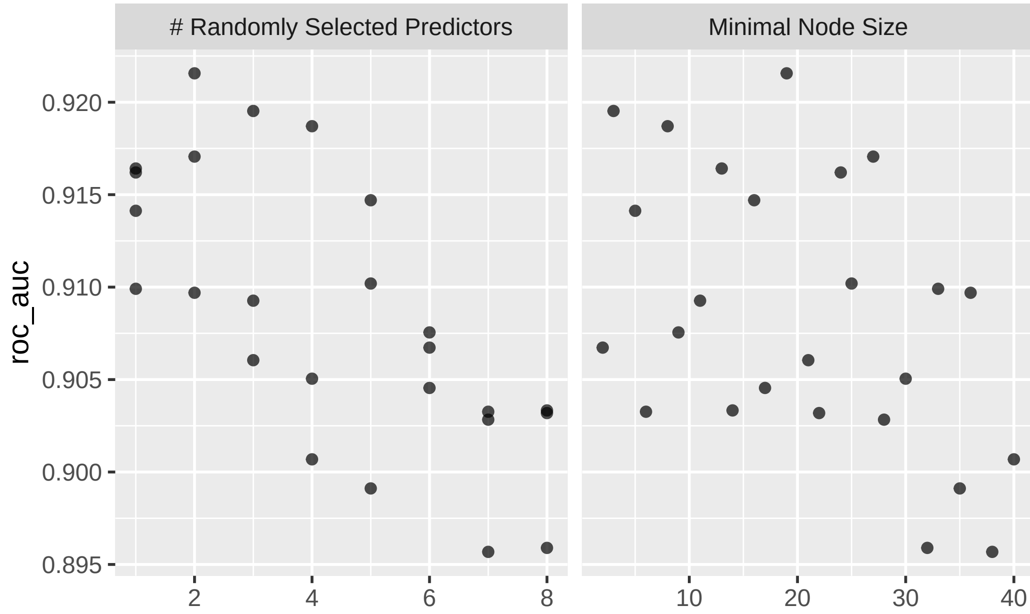
```
rf_res %>% collect_metrics()
```

```
# A tibble: 25 x 8
    mtry min_n .metric .estimator  mean     n std_err .config
   <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
 1     1    24 roc_auc binary     0.916     1      NA Preprocessor1_Model01
 2     1    13 roc_auc binary     0.916     1      NA Preprocessor1_Model02
 3     1    33 roc_auc binary     0.910     1      NA Preprocessor1_Model03
 4     1     5 roc_auc binary     0.914     1      NA Preprocessor1_Model04
 5     2    19 roc_auc binary     0.922     1      NA Preprocessor1_Model05
 6     2    27 roc_auc binary     0.917     1      NA Preprocessor1_Model06
 7     2    36 roc_auc binary     0.910     1      NA Preprocessor1_Model07
 8     3    11 roc_auc binary     0.909     1      NA Preprocessor1_Model08
```

```
 9      3      3 roc_auc binary      0.920      1       NA Preprocessor1_Model09
10      3     21 roc_auc binary      0.906      1       NA Preprocessor1_Model10
# i 15 more rows
```

Plot hyperparameter tunning results.

```
autoplot(rf_res)
```




```
ggsave(filename = "./figs-to-paper/07-RF-tunning.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

RF best models

List the best RF models.

```
rf_res %>%
  show_best(metric = "roc_auc")
```

```
# A tibble: 5 x 8
   mtry min_n .metric .estimator  mean     n std_err .config
  <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1     2    19 roc_auc binary     0.922     1      NA Preprocessor1_Model05
2     3     3 roc_auc binary     0.920     1      NA Preprocessor1_Model09
3     4     8 roc_auc binary     0.919     1      NA Preprocessor1_Model13
4     2    27 roc_auc binary     0.917     1      NA Preprocessor1_Model06
5     1    13 roc_auc binary     0.916     1      NA Preprocessor1_Model02
```

We show the best one.

```
rf_best <-
  rf_res %>%
  select_best(metric = "roc_auc")
rf_best
```

```
# A tibble: 1 x 3
   mtry min_n .config
  <int> <int> <chr>
1     2    19 Preprocessor1_Model05
```

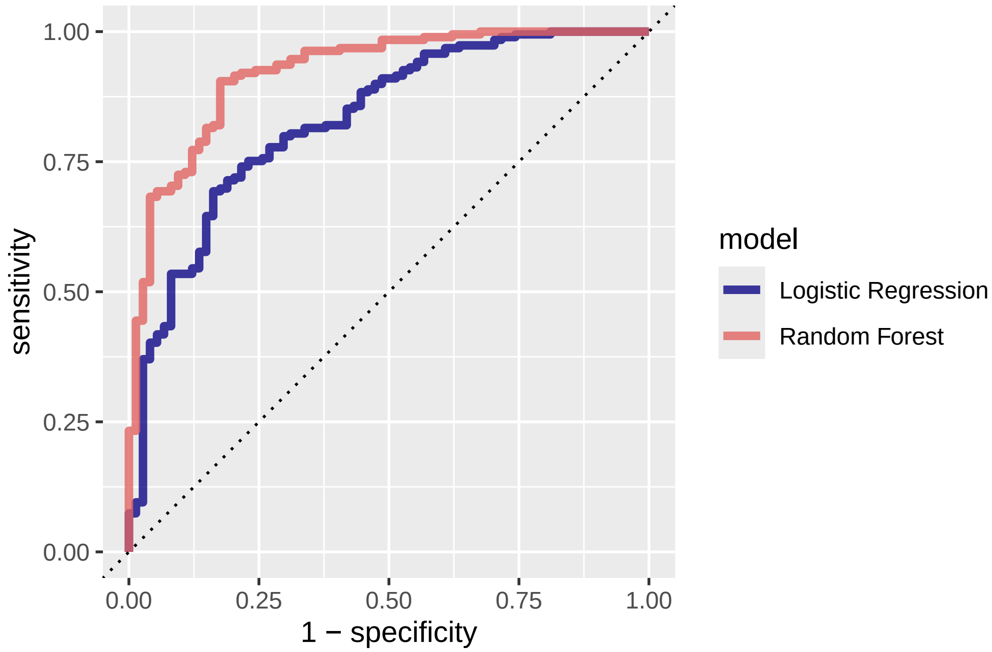
RF ROC curve dataset generation

```
# Para filtrar las predicciones solo para nuestro mejor modelo, podemos usar el argumento de

rf_auc <-
  rf_res %>%
  collect_predictions(parameters = rf_best) %>%
  roc_curve(PM10, .pred_Good) %>%
  mutate(model = "Random Forest")
```

ROC curve to compare Logistic regression model vs Random Forest model .

```
bind_rows(rf_auc, lr_auc) %>%
  ggplot(aes(x = 1 - specificity, y = sensitivity, col = model)) +
  geom_path(lwd = 1.5, alpha = 0.8) +
  geom_abline(lty = 3) +
  coord_equal() +
  scale_color_viridis_d(option = "plasma", end = .6)
```




```
ggsave(filename = "./figs-to-paper/08-ROC-on-training-set-by-model.tiff",units = "px", dpi=3
```

```
Saving 1650 x 1050 px image
```

Conclusion: the RF model was superior across the entire event probability threshold.

Final results

We built a model with the selected parameters, trained it, then predict using the test set.

```
# the last model
last_rf_mod <-
  rand_forest(mtry = rf_best$mtry, min_n = rf_best$min_n, trees = 100) %>%
  set_engine("ranger", num.threads = cores, importance = "impurity") %>%
  set_mode("classification")

# the last workflow
last_rf_workflow <-
  rf_workflow %>%
  update_model(last_rf_mod)
```

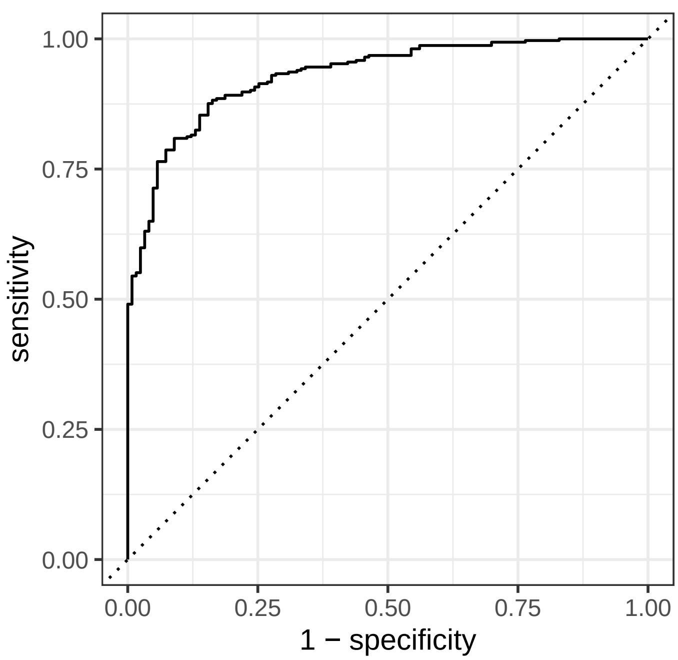
```
# the last fit
set.seed(345)
last_rf_fit <-
  last_rf_workflow %>%
  last_fit(splits)

last_rf_fit
```

```
# Resampling results
# Manual resampling
# A tibble: 1 x 6
  splits             id               .metrics .notes   .predictions .workflow
  <list>             <chr>            <list>   <list>   <list>       <list>
1 <split [1310/437]> train/test split <tibble> <tibble> <tibble>     <workflow>
```

ROC curve plot for Random Forest (test set)

```
last_rf_fit %>%
  collect_predictions() %>%
  roc_curve(PM10, .pred_Good) %>%
  autoplot()
```



```
ggsave(filename = "./figs-to-paper/09-ROC-RF-testset.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

Random Forest confusion matrix (test set)

```
RF_model <- extract_workflow(last_rf_fit)

# Class prediction
pred_class_rf <- predict(RF_model,
                      new_data = data_test,
                      type = "class")

# Prediction Probabilities
pred_proba_rf <- predict(RF_model,
                      new_data = data_test,
                      type = "prob")
```

```
RF_results <- data_test %>%
              select(PM10) %>%
              bind_cols(pred_class_rf, pred_proba_rf)
```

Print the confusion matrix.

```
conf_mat(RF_results, truth = PM10,
         estimate = .pred_class)
```

```
          Truth
Prediction Good Bad
      Good  294  39
      Bad    20  84
```

Summary of metrics

```
summary(conf_mat(RF_results, truth = PM10,
         estimate = .pred_class))
```

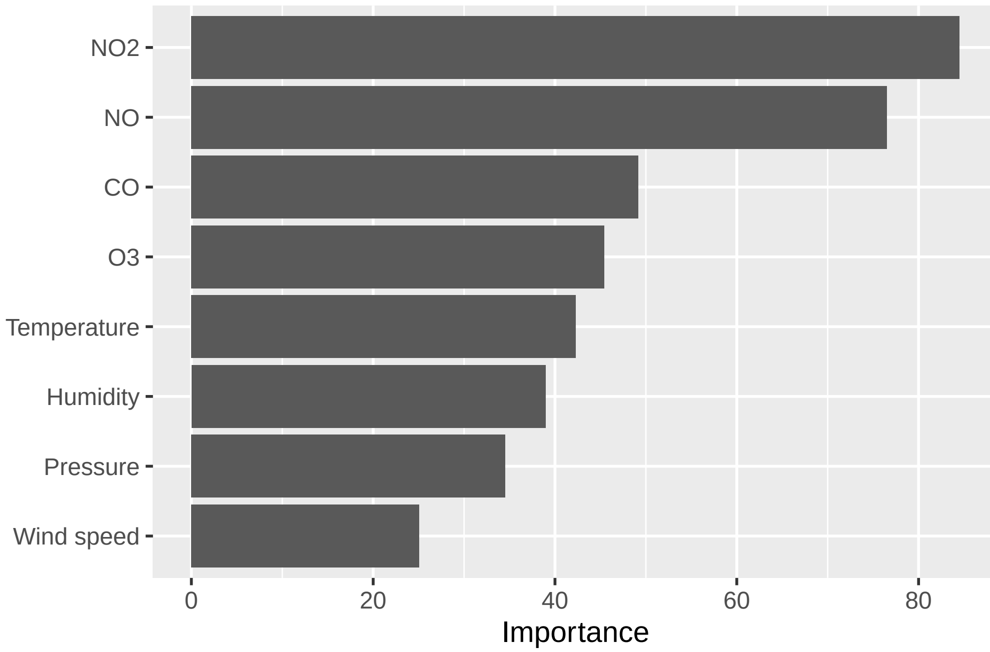
```
# A tibble: 13 x 3
   .metric              .estimator .estimate
   <chr>                <chr>          <dbl>
 1 accuracy             binary         0.865
 2 kap                  binary         0.650
 3 sens                 binary         0.936
 4 spec                 binary         0.683
 5 ppv                  binary         0.883
 6 npv                  binary         0.808
 7 mcc                  binary         0.654
 8 j_index              binary         0.619
 9 bal_accuracy         binary         0.810
10 detection_prevalence binary         0.762
11 precision            binary         0.883
12 recall               binary         0.936
13 f_meas               binary         0.909
```

Variable importance Score

Compute the VIP.

When using the vip function with a random forest model, the default method computes the mean decrease in impurity (or Gini importance) for each variable. This is calculated by accumulating the improvement in the split criterion at each split in each tree, and normalizing by the standard deviation of the differences.

```
last_rf_fit %>%
  extract_fit_parsnip() %>%
  vip(num_features = 10) # check vip package documentation
```




```
ggsave(filename = "./figs-to-paper/10-RF-VIP.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

SHAP values

Recordamos que rf_best no es un objeto del modelo entrenado, sino un conjunto de hiperparámetros seleccionados que representan el mejor modelo. Requiero un objeto de la libreria ranger que represente el mejor modelo randoom forest, para luego ser usado para SHAP

Setup and computing

```
rf_best <- rf_res %>% select_best(metric = "roc_auc")
# hiperparámetros "ganadores"
rf_best
```

```
# A tibble: 1 x 3
   mtry min_n .config
  <int> <int> <chr>
1     2    19 Preprocessor1_Model05
```

```r
# workflow setup: update the hyperparameters
final_rf_workflow <- rf_workflow %>% finalize_workflow(rf_best)

# Train a RF model
rf_final_fit <- final_rf_workflow %>% fit(data = data_train)
```

```r
# Get the final model (a ranger::ranger object)
modelo_final <- extract_fit_parsnip(rf_final_fit)$fit
modelo_final
```

```
Ranger result

Call:
 ranger::ranger(x = maybe_data_frame(x), y = y, mtry = min_cols(~2L,      x), num.trees = ~1(

Type:                             Probability estimation
Number of trees:                  100
Sample size:                      1310
Number of independent variables:  8
Mtry:                             2
Target node size:                 19
Variable importance mode:         none
Splitrule:                        gini
OOB prediction error (Brier s.):  0.1016491
```

`modelo_final` is an object of the class ranger

```r
class(modelo_final)
```

```
[1] "ranger"
```

We create a dataset called X with all the predictors features (without PM10)

```r
library(fastshap)
```

```
Adjuntando el paquete: 'fastshap'
```

```
The following object is masked from 'package:vip':

    gen_friedman


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

    explain
```

```
library(shapviz)

# Creo X (sin PM10, solo predictoras)
X <- data %>% select(-PM10)

head(X)
```

```
# A tibble: 6 x 8
  Temperature Humidity Pressure `Wind speed`    CO    NO   NO2     O3
        <dbl>    <dbl>    <dbl>        <dbl> <dbl> <dbl> <dbl>  <dbl>
1         3         53     938.         0     2.52  99.8  65.6   9.45
2         6.9       42     938.         1.11  1.97  94.2  77.0  13.7
3        10.1       31     938.         1.11  1.91  33.0  48.0  22.0
4        10.4       32     938.         1.11  1.56  15.1  31.4  56.3
5        11.6       30     937.         2.5   1.39  15.6  38.2 146.
6        12.4       30     936.         2.5   1.23  10.2  34.7 290.
```

Prediction function definition for class Good

```
#

pred_fun_good <- function(object, newdata) {
  # get the probabilities matrix
  prob_matrix <- predict(object, data = newdata, response = "prob")
  return(prob_matrix$predictions[,1]) # return predictions for class Good
  # return(prob_matrix$predictions[,2]) # return predictions for class Bad

}
```

```
# pred_fun(modelo_final, X)$predictions
```

Prediction function definition for class Bad

```
pred_fun_bad <- function(object, newdata) {
  # get the probabilities matrix
  prob_matrix <- predict(object, data = newdata, response = "prob")
  return(prob_matrix$predictions[,2]) # return predictions for class Bad

}
```

SHAP values for class Good

Calculate SHAP values with fastshap package

```
# Cálculo de SHAP values con fastshap
shap_values_good <- fastshap::explain(
  object = modelo_final,
  X = X,
  pred_wrapper = pred_fun_good,
  nsim = 100, # Aumentar para mayor precisión
)
```

SHAP values for class Bad

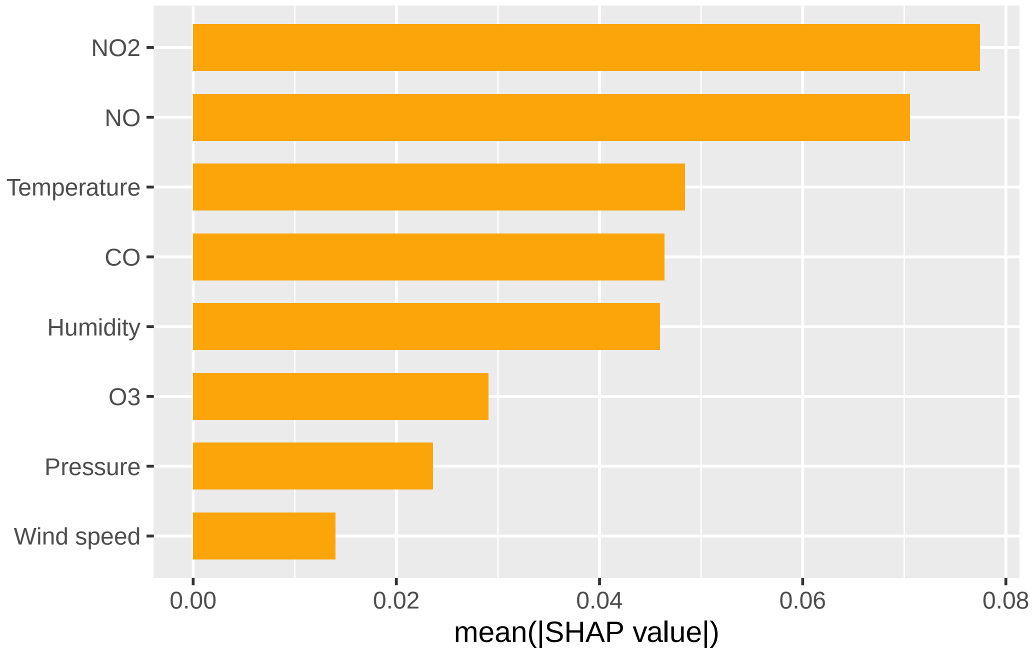
```
# Cálculo de SHAP values con fastshap
shap_values_bad <- fastshap::explain(
  object = modelo_final,
  X = X,
  pred_wrapper = pred_fun_bad,
  nsim = 100, # Aumentar para mayor precisión
)
```

Plots for class Good

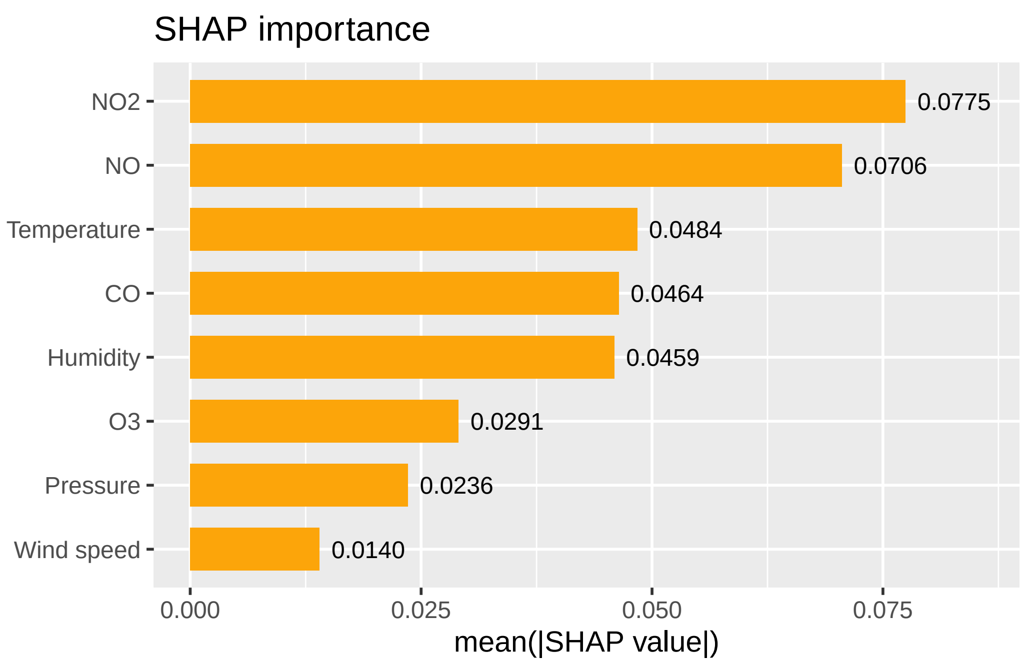
Importance plot.

```
shap <- shapviz(shap_values_good, X = X )

# Gráfico de importancia
sv_importance(shap)
```



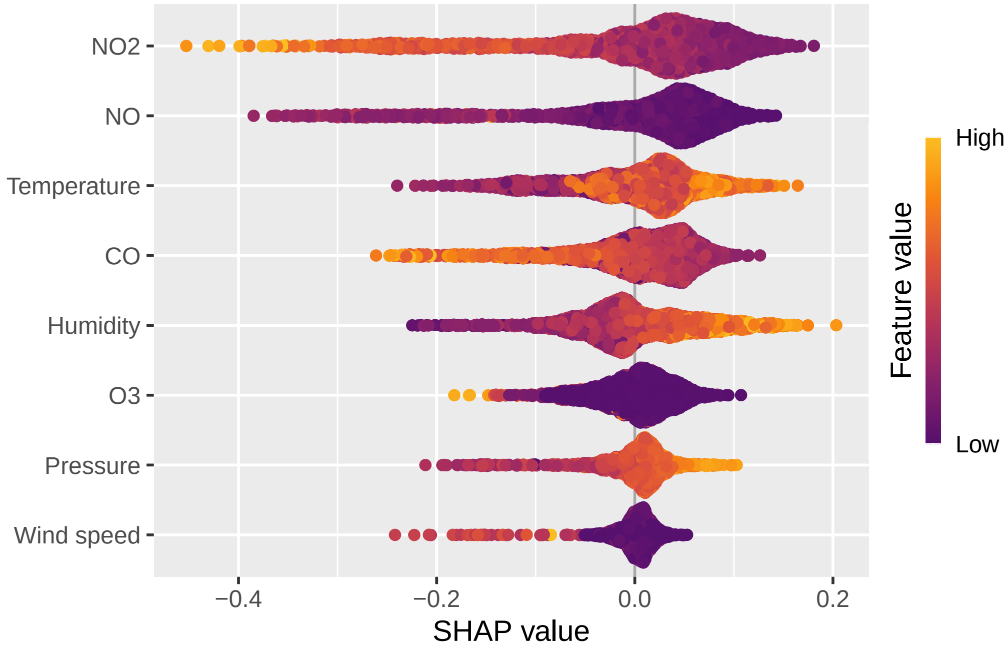

```
sv_importance(shap,show_numbers = TRUE) +
 ggtitle("SHAP importance")
```



```r
ggsave(filename = "./figs-to-paper/12-SHAP_importance_good.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

```r
sv_importance(shap,"bee")
```




```r
ggsave(filename = "./figs-to-paper/13-SHAP_importance_bee_good.tiff",units = "px", dpi=300)
```

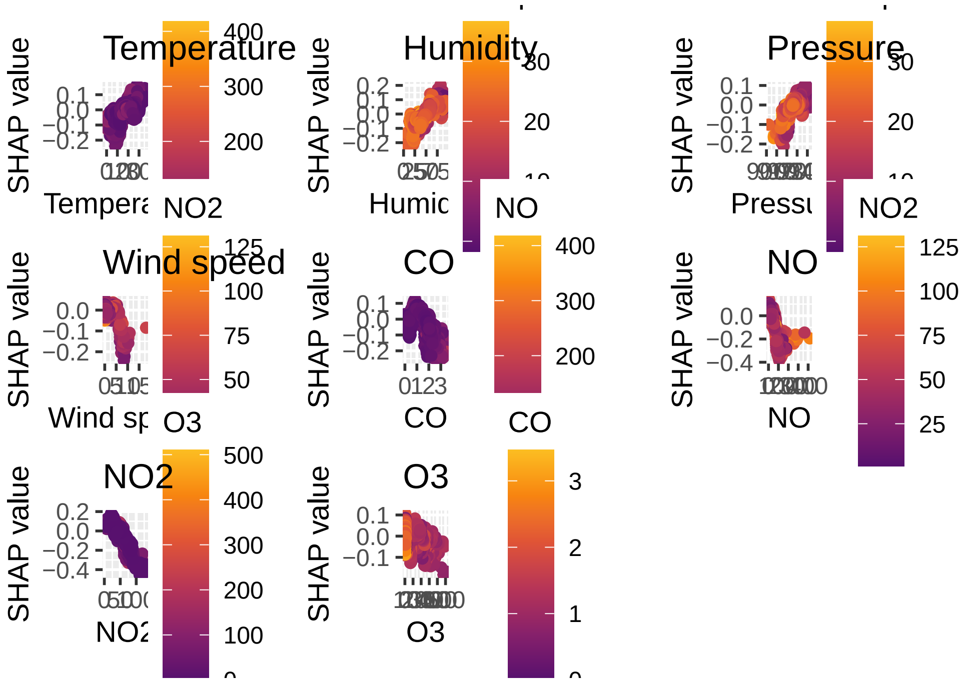
```
Saving 1650 x 1050 px image
```

Plot interaction

```r
colnames(data)[-9]
```

```
[1] "Temperature" "Humidity"    "Pressure"    "Wind speed"  "CO"
[6] "NO"          "NO2"         "O3"
```

```r
sv_dependence(shap, colnames(data)[-9])
```




```
ggsave(filename = "./figs-to-paper/14-SHAP_dependence_good.tiff",units = "px", dpi=300)
```

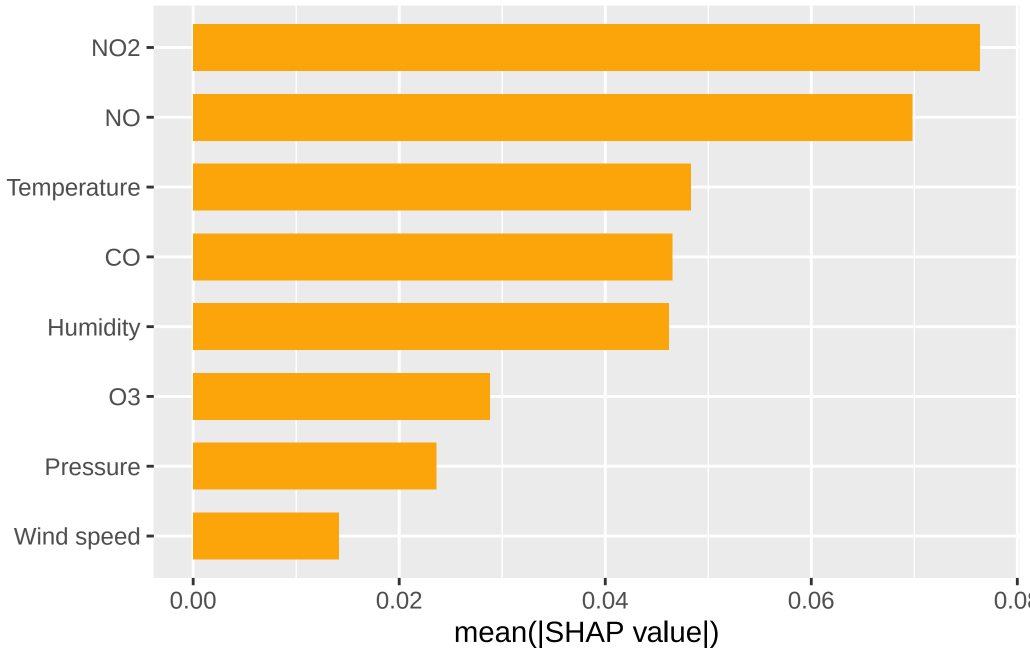
```
Saving 1650 x 1050 px image
```

Plots for class Bad

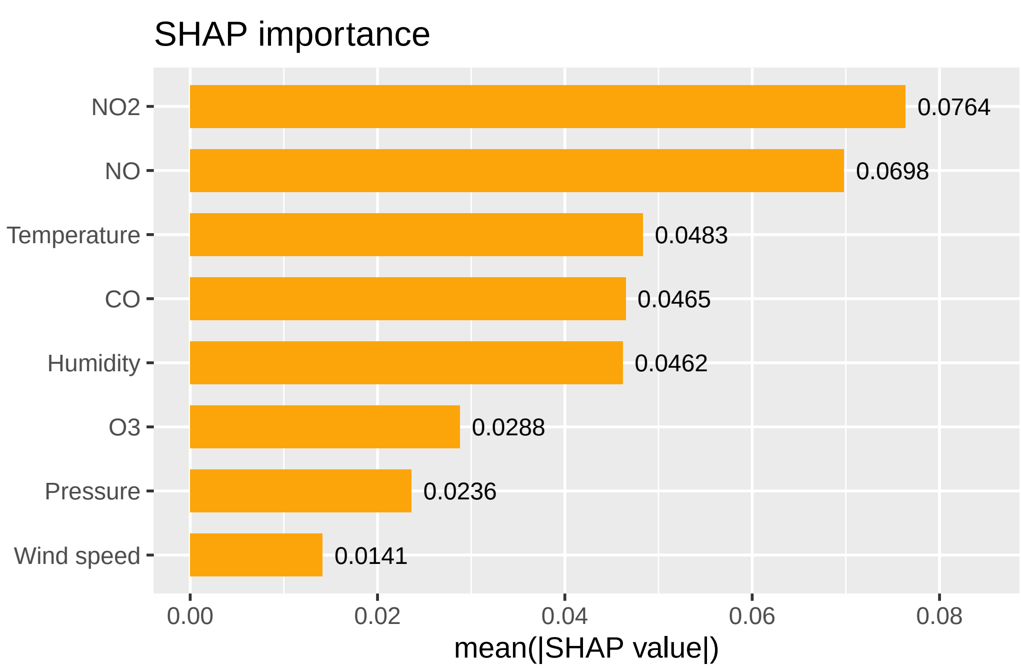
Importance plot.

```
shap <- shapviz(shap_values_bad, X = X )

# Gráfico de importancia
sv_importance(shap)
```



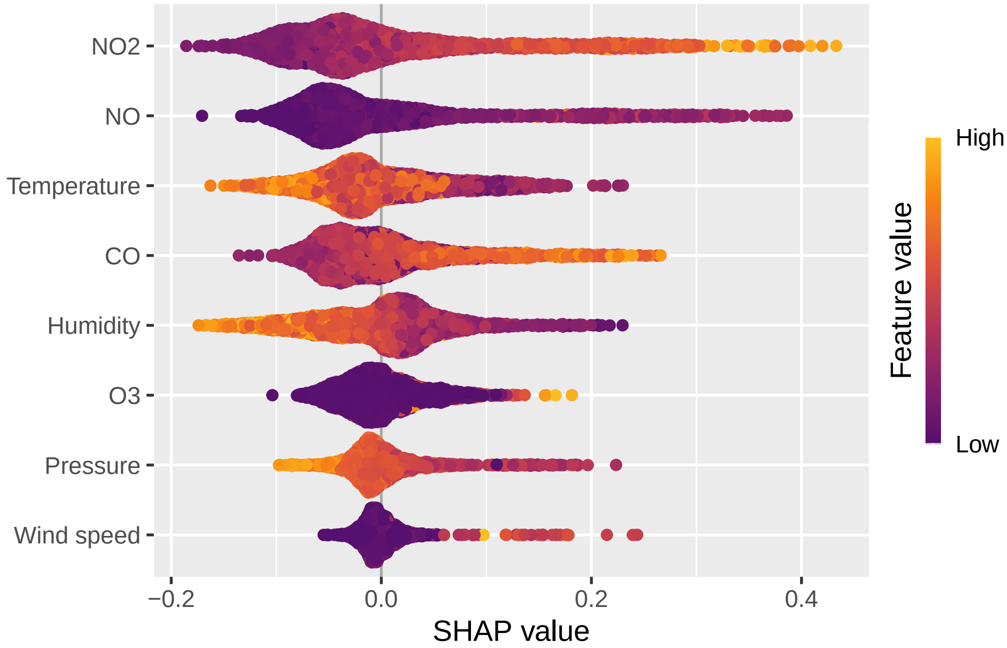

```r
sv_importance(shap,show_numbers = TRUE) +
 ggtitle("SHAP importance")
```



```r
ggsave(filename = "./figs-to-paper/12-SHAP_importance_bad.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

```r
sv_importance(shap,"bee")
```




```r
ggsave(filename = "./figs-to-paper/13-SHAP_importance_bee_bad.tiff",units = "px", dpi=300)
```

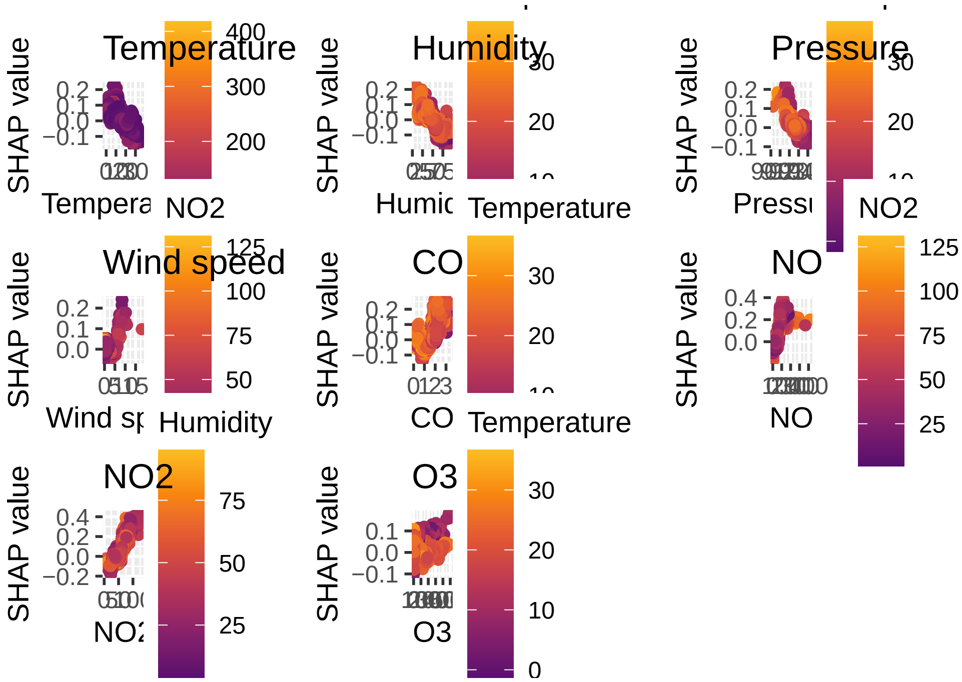
```
Saving 1650 x 1050 px image
```

Plot interaction

```r
colnames(data)[-9]
```

```
[1] "Temperature" "Humidity"    "Pressure"    "Wind speed"  "CO"
[6] "NO"          "NO2"         "O3"
```

```r
sv_dependence(shap, colnames(data)[-9])
```



```
ggsave(filename = "./figs-to-paper/14-SHAP_dependence_bad.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

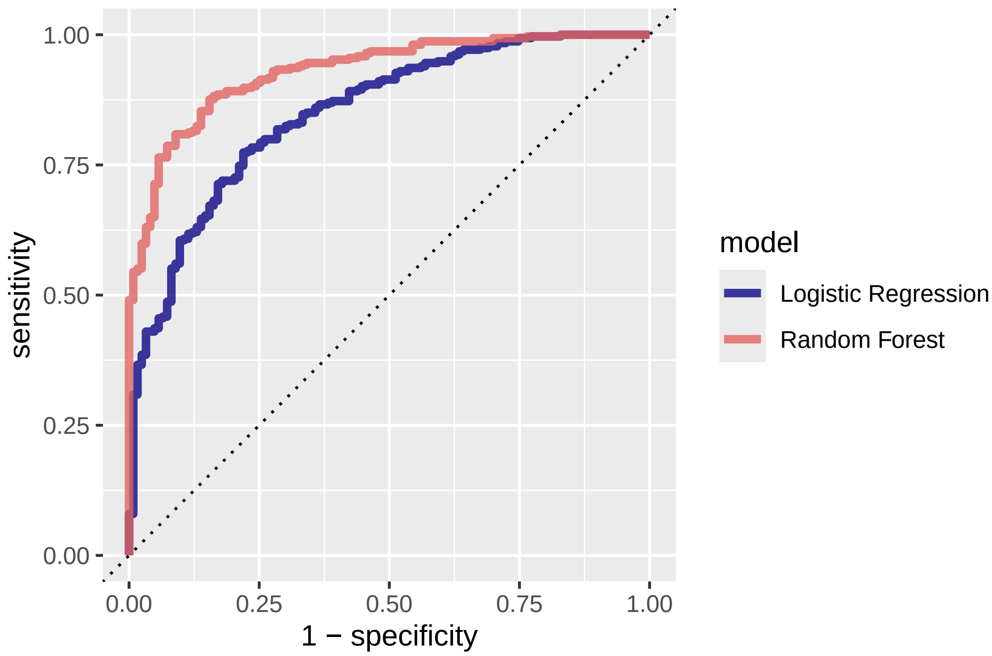
FINAL RESULTS

ROC CURVE

```
lr_auc_f <- final_fit %>%
  collect_predictions() %>%
  roc_curve(PM10, .pred_Good) %>%
  mutate(model = "Logistic Regression")
```

```
rf_auc_f <- last_rf_fit %>%
            collect_predictions() %>%
            roc_curve(PM10, .pred_Good) %>%
            mutate(model = "Random Forest")
```

```r
bind_rows(rf_auc_f, lr_auc_f) %>%
  ggplot(aes(x = 1 - specificity, y = sensitivity, col = model)) +
  geom_path(lwd = 1.5, alpha = 0.8) +
  geom_abline(lty = 3) +
  coord_equal() +
  scale_color_viridis_d(option = "plasma", end = .6)
```




```r
ggsave(filename = "./figs-to-paper/11-ROC-on-test-set.tiff",units = "px", dpi=300)
```

```
Saving 1650 x 1050 px image
```

Metrics

Agrego una fila con el resultado ROC_AUC

```r
roc_auc(lr_results, truth = PM10, .pred_Good)
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.850
```

```r
m_lr <- summary(conf_mat(lr_results, truth = PM10,
         estimate = .pred_class)) %>%
        bind_rows(roc_auc(lr_results, truth = PM10, .pred_Good)) %>%
        mutate(model = "Logistic Regression")
```

```r
m_lr
```

```
# A tibble: 14 x 4
   .metric              .estimator .estimate model
   <chr>                <chr>          <dbl> <chr>
 1 accuracy             binary         0.801 Logistic Regression
 2 kap                  binary         0.434 Logistic Regression
 3 sens                 binary         0.946 Logistic Regression
 4 spec                 binary         0.431 Logistic Regression
 5 ppv                  binary         0.809 Logistic Regression
 6 npv                  binary         0.757 Logistic Regression
 7 mcc                  binary         0.462 Logistic Regression
 8 j_index              binary         0.377 Logistic Regression
 9 bal_accuracy         binary         0.688 Logistic Regression
10 detection_prevalence binary         0.840 Logistic Regression
11 precision            binary         0.809 Logistic Regression
12 recall               binary         0.946 Logistic Regression
13 f_meas               binary         0.872 Logistic Regression
14 roc_auc              binary         0.850 Logistic Regression
```

```r
roc_auc(RF_results, truth = PM10, .pred_Good)
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.930
```

```r
m_rf <- summary(conf_mat(RF_results, truth = PM10,estimate = .pred_class)) %>%
        bind_rows(roc_auc(RF_results, truth = PM10, .pred_Good))  %>%
        mutate(model = "Random Forest")
```

```r
m_rf
```

```
# A tibble: 14 x 4
```

```
   .metric              .estimator .estimate model
   <chr>                <chr>          <dbl> <chr>
 1 accuracy             binary         0.865 Random Forest
 2 kap                  binary         0.650 Random Forest
 3 sens                 binary         0.936 Random Forest
 4 spec                 binary         0.683 Random Forest
 5 ppv                  binary         0.883 Random Forest
 6 npv                  binary         0.808 Random Forest
 7 mcc                  binary         0.654 Random Forest
 8 j_index              binary         0.619 Random Forest
 9 bal_accuracy         binary         0.810 Random Forest
10 detection_prevalence binary         0.762 Random Forest
11 precision            binary         0.883 Random Forest
12 recall               binary         0.936 Random Forest
13 f_meas               binary         0.909 Random Forest
14 roc_auc              binary         0.930 Random Forest
```

Results table to compare each model

```r
bind_rows(m_rf, m_lr) %>%
  select(-one_of(c(".estimator")) ) %>%
  pivot_wider( names_from = "model", values_from = ".estimate")
```

```
# A tibble: 14 x 3
   .metric              `Random Forest` `Logistic Regression`
   <chr>                          <dbl>                 <dbl>
 1 accuracy                       0.865                 0.801
 2 kap                            0.650                 0.434
 3 sens                           0.936                 0.946
 4 spec                           0.683                 0.431
 5 ppv                            0.883                 0.809
 6 npv                            0.808                 0.757
 7 mcc                            0.654                 0.462
 8 j_index                        0.619                 0.377
 9 bal_accuracy                   0.810                 0.688
10 detection_prevalence           0.762                 0.840
11 precision                      0.883                 0.809
12 recall                         0.936                 0.946
13 f_meas                         0.909                 0.872
14 roc_auc                        0.930                 0.850
```

Save the results in a csv file.

```
bind_rows(m_rf, m_lr) %>%
  select(-one_of(c(".estimator")) ) %>%
  pivot_wider( names_from = "model", values_from = ".estimate") %>%
  write_csv(file="./figs-to-paper/final-results.csv")
```

R session info

```
sessionInfo()
```

```
R version 4.4.1 (2024-06-14)
Platform: x86_64-pc-linux-gnu
Running under: Ubuntu 24.10

Matrix products: default
BLAS:   /usr/lib/x86_64-linux-gnu/blas/libblas.so.3.12.0
LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.12.0

locale:
 [1] LC_CTYPE=es_ES.UTF-8       LC_NUMERIC=C
 [3] LC_TIME=es_ES.UTF-8        LC_COLLATE=es_ES.UTF-8
 [5] LC_MONETARY=es_ES.UTF-8    LC_MESSAGES=es_ES.UTF-8
 [7] LC_PAPER=es_ES.UTF-8       LC_NAME=C
 [9] LC_ADDRESS=C               LC_TELEPHONE=C
[11] LC_MEASUREMENT=es_ES.UTF-8 LC_IDENTIFICATION=C

time zone: America/Argentina/Mendoza
tzcode source: system (glibc)

attached base packages:
[1] stats     graphics  grDevices datasets  utils     methods   base

other attached packages:
 [1] fastshap_0.1.1     naniar_1.1.0       stringr_1.5.1      shapviz_0.9.7
 [5] kernelshap_0.7.0   readxl_1.4.5       ranger_0.17.0      vip_0.4.1
 [9] glmnet_4.1-8       Matrix_1.7-0       yardstick_1.3.2    workflowsets_1.1.0
[13] workflows_1.2.0    tune_1.3.0         tibble_3.2.1       rsample_1.3.0
[17] recipes_1.2.1      purrr_1.0.4        parsnip_1.3.1      modeldata_1.4.0
```

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[21] infer_1.0.7        ggplot2_3.5.2      dials_1.4.0        scales_1.3.0
[25] broom_1.0.8        tidymodels_1.3.0   DataExplorer_0.8.3 tidyr_1.3.1
[29] dplyr_1.1.4        readr_2.1.5

loaded via a namespace (and not attached):
 [1] gridExtra_2.3       rlang_1.1.5         magrittr_2.0.3
 [4] furrr_0.3.1         compiler_4.4.1      systemfonts_1.2.2
 [7] reshape2_1.4.4      vctrs_0.6.5         lhs_1.2.0
[10] crayon_1.5.3        pkgconfig_2.0.3     shape_1.4.6.1
[13] fastmap_1.2.0       backports_1.5.0     labeling_0.4.3
[16] utf8_1.2.4          rmarkdown_2.29      prodlim_2024.06.25
[19] tzdb_0.5.0          ragg_1.4.0          visdat_0.6.0
[22] bit_4.6.0           xfun_0.52           jsonlite_2.0.0
[25] parallel_4.4.1      R6_2.6.1            stringi_1.8.7
[28] parallelly_1.43.0   rpart_4.1.23        lubridate_1.9.4
[31] cellranger_1.1.0    xgboost_1.7.9.1     Rcpp_1.0.14
[34] iterators_1.0.14    knitr_1.50          future.apply_1.11.3
[37] splines_4.4.1       nnet_7.3-19         igraph_2.1.4
[40] timechange_0.3.0    tidyselect_1.2.1    rstudioapi_0.17.1
[43] yaml_2.3.10         timeDate_4041.110   codetools_0.2-20
[46] listenv_0.9.1       plyr_1.8.9          lattice_0.22-6
[49] withr_3.0.2         evaluate_1.0.3      future_1.40.0
[52] survival_3.7-0      pillar_1.10.2       renv_1.1.4
[55] foreach_1.5.2       generics_0.1.3      vroom_1.6.5
[58] hms_1.1.3           munsell_0.5.1       globals_0.16.3
[61] class_7.3-22        glue_1.8.0          tools_4.4.1
[64] data.table_1.17.0   gower_1.0.2         grid_4.4.1
[67] ipred_0.9-15        colorspace_2.1-1    patchwork_1.3.0
[70] networkD3_0.4       sfd_0.1.0           cli_3.6.4
[73] DiceDesign_1.10     textshaping_1.0.0   viridisLite_0.4.2
[76] lava_1.8.1          gtable_0.3.6        GPfit_1.0-8
[79] digest_0.6.37       farver_2.1.2        htmlwidgets_1.6.4
[82] htmltools_0.5.8.1   lifecycle_1.0.4     hardhat_1.4.1
[85] bit64_4.6.0-1       sparsevctrs_0.3.2   MASS_7.3-61
```