document

Required packages

```
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
```

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

```
-- Attaching packages ------------------------------------ tidymodels 1.2.0 --

v broom        1.0.6      v recipes      1.0.10
v dials        1.2.1      v rsample      1.2.1
v ggplot2      3.5.1      v tibble       3.2.1
v infer        1.0.7      v tune         1.2.1
v modeldata    1.3.0      v workflows    1.1.4
v parsnip      1.2.1      v workflowsets 1.1.0
v purrr        1.0.2      v yardstick    1.3.1
```

```
-- 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()
* Search for functions across packages at https://www.tidymodels.org/find/
```

```
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
```

```
library(vip)
```

```

Adjuntando el paquete: 'vip'

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

    vi
```

```
library(ranger)
```

Load dataset

```
database <- read_rds("../data/database.rds")

colnames(database)
```

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

```
nrow(database)
```

```
[1] 1105
```

```
summary(database)
```

```
   Estación         Temperatura (°C)  Humedad (%)     Presión (hPa)
 Length:1105        Min.   : 0.00    Min.   : 3.00   Min.   :902.0
 Class :character   1st Qu.:11.40    1st Qu.:32.00   1st Qu.:923.2
 Mode  :character   Median :18.00    Median :46.00   Median :927.3
                    Mean   :17.32    Mean   :48.04   Mean   :926.9
                    3rd Qu.:23.50    3rd Qu.:62.00   3rd Qu.:930.5
                    Max.   :36.60    Max.   :95.00   Max.   :940.0

 Velocidad de viento (m/s)   CO (mg/m3)      NO (ug/m3)      NO2 (ug/m3)
 Min.   : 0.000            Min.   :0.000   Min.   :  0.02   Min.   :  1.28
 1st Qu.: 0.310            1st Qu.:0.740   1st Qu.:  3.53   1st Qu.: 30.71
 Median : 1.110            Median :1.120   Median : 26.00   Median : 45.56
 Mean   : 1.484            Mean   :1.172   Mean   : 35.36   Mean   : 44.17
 3rd Qu.: 1.940            3rd Qu.:1.580   3rd Qu.: 55.15   3rd Qu.: 54.11
 Max.   :18.060            Max.   :3.460   Max.   :363.27   Max.   :131.05

  NOX (ug/m3)       O3 (ug/m3)      PM10 (ug/m3)
 Min.   :  4.15   Min.   :  0.00   Min.   :  0.00
 1st Qu.: 40.11   1st Qu.: 13.05   1st Qu.: 15.00
 Median : 93.49   Median : 30.55   Median : 29.00
 Mean   : 98.40   Mean   : 51.02   Mean   : 36.75
 3rd Qu.:137.60   3rd Qu.: 43.86   3rd Qu.: 49.00
 Max.   :559.91   Max.   :487.52   Max.   :318.00
                                   NA's   :11
      time
 Min.   :2022-02-11 17:00:00.00
 1st Qu.:2022-05-02 10:00:00.00
 Median :2023-01-13 02:00:00.00
```

```
 Mean   :2022-11-29 21:23:43.71
 3rd Qu.:2023-03-27 15:00:00.00
 Max.   :2023-10-17 07:00:00.00
```

Cleaning

- Tener en cuenta Temperatura, Humedad relativa, Presión atmosférica, Velocidad de viento, CO, NO, NO2, O3 como variables predictoras de PM10.
- Quitar la variable NOX
- Remuevo NA

```
data <- database %>% select(-one_of(c("Estación","time","NOX (ug/m3)")))
data <- data[complete.cases(data),]
```

- El dataset a entrenar tiene 1094 muestras o filas.
- Cuenta con 9 variables o columnas.
- Las variables se llaman: Temperatura (°C), Humedad (%), Presión (hPa), Velocidad de viento (m/s), CO (mg/m3), NO (ug/m3), NO2 (ug/m3), O3 (ug/m3), PM10 (ug/m3).

```
colnames(data)
```

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

- Procedo a quitar las unidades al nombre de cada variable. Esto hará más legible los gráficos. Por supuesto que en paper debe explicarse cada variable y sus unidades.

```
library(stringr)
```

```
Adjuntando el paquete: 'stringr'

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

    fixed
```

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

- Se lista un resumen de los datos.

```
summary(data)
```

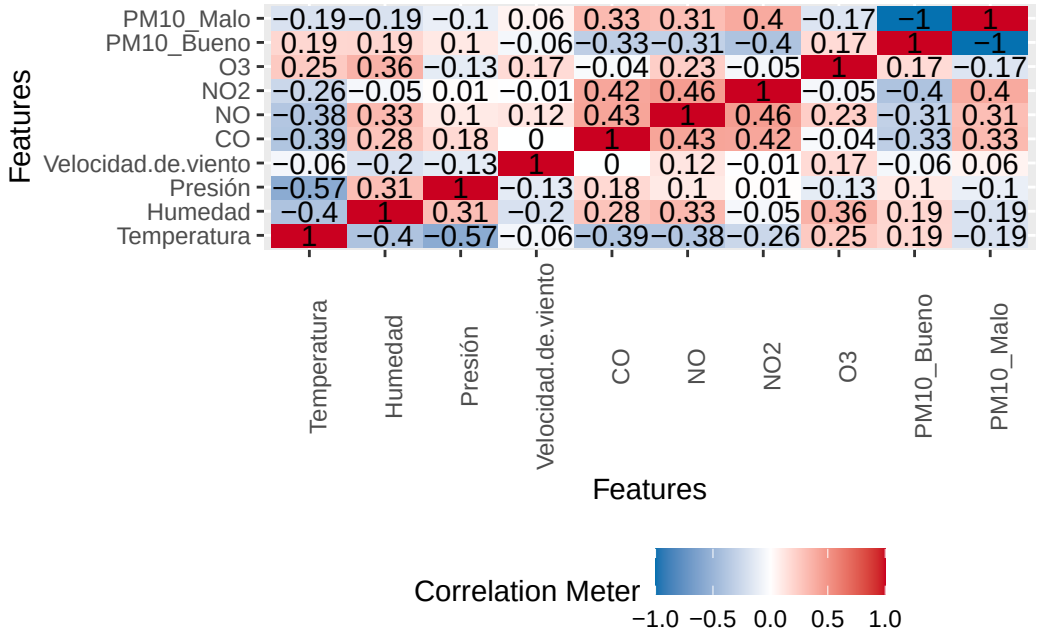
```
  Temperatura       Humedad         Presión      Velocidad de viento
 Min.   : 0.00   Min.   : 5.0   Min.   :902.0   Min.   : 0.000
 1st Qu.:11.31   1st Qu.:32.0   1st Qu.:923.3   1st Qu.: 0.310
 Median :17.90   Median :46.0   Median :927.3   Median : 1.110
 Mean   :17.25   Mean   :48.2   Mean   :927.0   Mean   : 1.483
 3rd Qu.:23.45   3rd Qu.:62.0   3rd Qu.:930.5   3rd Qu.: 1.940
 Max.   :36.60   Max.   :95.0   Max.   :940.0   Max.   :18.060
       CO               NO               NO2               O3
 Min.   :0.000   Min.   :  0.020   Min.   :  1.28   Min.   :  0.00
 1st Qu.:0.740   1st Qu.:  3.542   1st Qu.: 30.94   1st Qu.: 13.05
 Median :1.120   Median : 26.045   Median : 45.73   Median : 30.61
 Mean   :1.174   Mean   : 35.203   Mean   : 44.38   Mean   : 51.27
 3rd Qu.:1.577   3rd Qu.: 55.203   3rd Qu.: 54.13   3rd Qu.: 43.81
 Max.   :3.460   Max.   :196.860   Max.   :131.05   Max.   :487.52
      PM10
 Min.   :  0.00
 1st Qu.: 15.00
 Median : 29.00
 Mean   : 36.75
 3rd Qu.: 49.00
 Max.   :318.00
```

- Discretizar la variable Material Particulado (PM10) tomando como umbral el valor de 45 µg/m3, por debajo del cual se categorizará como “Bueno”. Por encima de 45 µg/m3, se asignará el valor “Malo”.

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

Pearson correlation

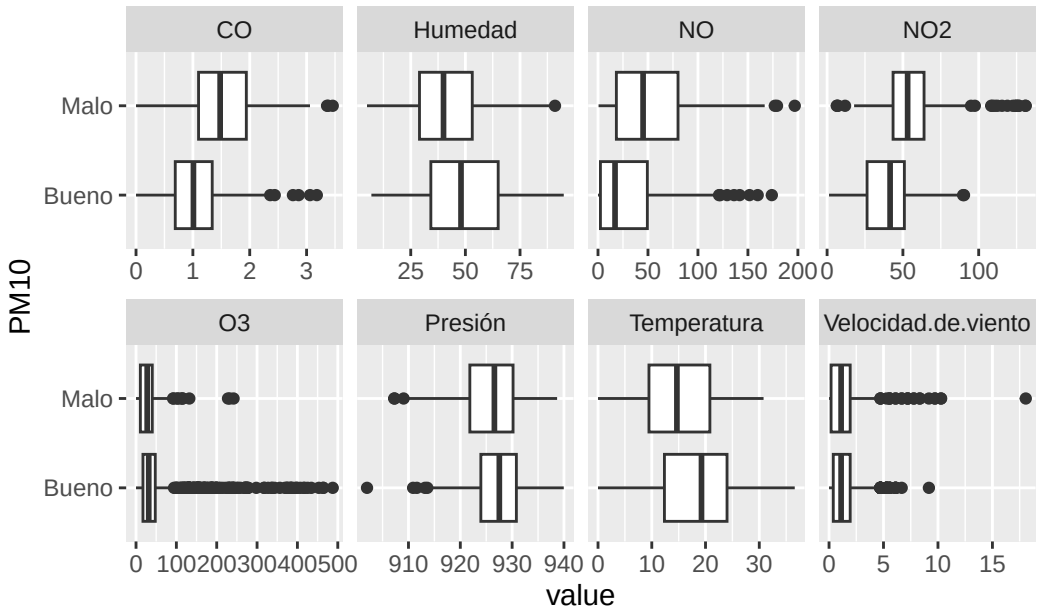
```
plot_correlation(data)
```




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

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

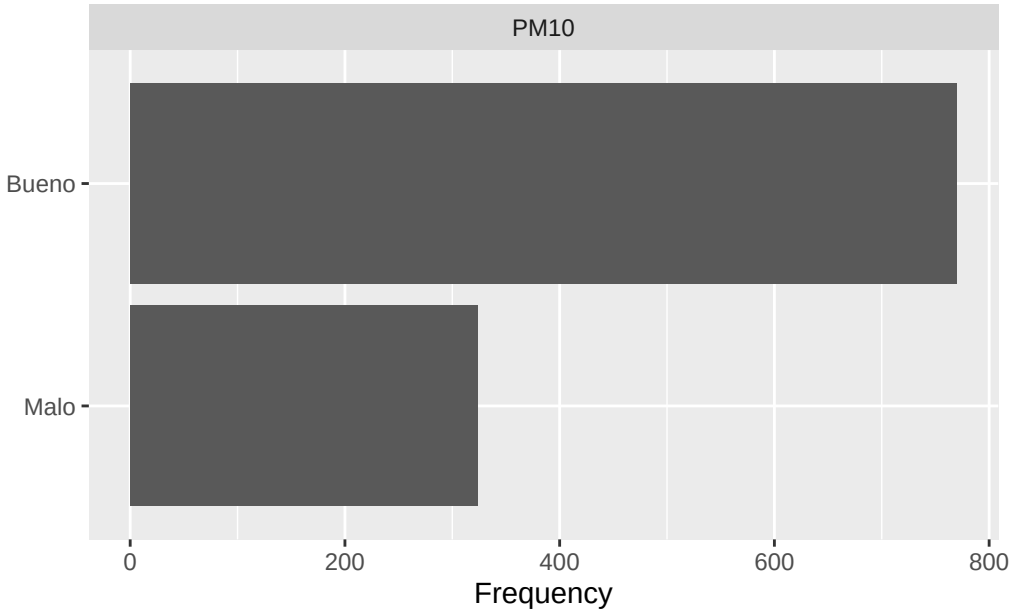
```
plot_boxplot(data, by = "PM10")
```




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

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

```
plot_bar(data)
```



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

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

Modelos

Separación de sets de datos

Los datos del dataset data, se usa un 75 % o 3/4 partes para entrenamiento y un 25% para testeo.

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

data_train <- training(splits) # 75 % entrenamiento
data_test  <- testing(splits)  # 25 % en testeo
```

Clasificación binaria

Para desarrollar el clasificador binario entrenamos dos modelos: regresión logistica (logistic regression) y random forest.

Usaremos la librería tidymodels.

Regresion logistica

- El modelo de regresión logística a usar está implementado en la librería glmnet.
- penalty: representa cuánta de esa regularización utilizaremos. Este es un hiperparámetro que ajustaremos durante el entrenamiento para encontrar el mejor valor para hacer predicciones con nuestros datos.
- mixture = 1 significa que se usará una regularización L1 (L1 regularization, pure lasso model), mixture en un valor de uno significa que el modelo glmnet eliminará potencialmente los predictores irrelevantes y elegirá un modelo más simple.

```
lr_mod <-
  logistic_reg(penalty = tune(), mixture = 1) %>%
  set_engine("glmnet")
```

Receta.

- usamos los datos de entrenamiento (data_train) para predecir la 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())
```

Creamos el flujo de trabajo de tidymodels: el paso a paso de lo que queremos que ejecute.

```
lr_workflow <-
  workflow() %>%
  add_model(lr_mod) %>%
  add_recipe(lr_recipe)
```

Grid tunning

Dado que solo tenemos un hiperparámetro para ajustar aquí, podemos configurar la cuadrícula manualmente usando un tibble de una columna con 30 valores candidatos:

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

Estos son los valores que se probarán en el entrenamiento: difererentes valores para el hiperparámetro penalty.

```
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
```

Con el argumento strata, el muestreo aleatorio (random sampling) se realiza dentro de la variable PM10 (the stratification variable). Esto puede ayudar a garantizar que las nuevas muestras tengan proporciones equivalentes a las del conjunto de datos original. En el caso de una variable categórica como PM10, el muestreo se realiza por separado dentro de cada clase.

Para el tuneo del hiperparámetro penalty se utiliza un set de datos de validación. Dentro del dataset de entrenamiento, un 80 % se mantiene para entrenar, y se usa el 20 % para validar.

Dentro del conjunto de datos de entrenamiento, usamos una porción del mismo como conjunto de validación para entrenar con los distintos valores de penalty (el grid tunning que realizaremos).

```
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.
```

En el siguiente bloque de código se ejecuta todo: la receta o indicaciones que quedaron guardadas en lr_workflow más el tuneo de hiperparámetros tune_grid.

Como métrica de evaluación del clasificador se utiliza ROC_AUC.

```
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
```

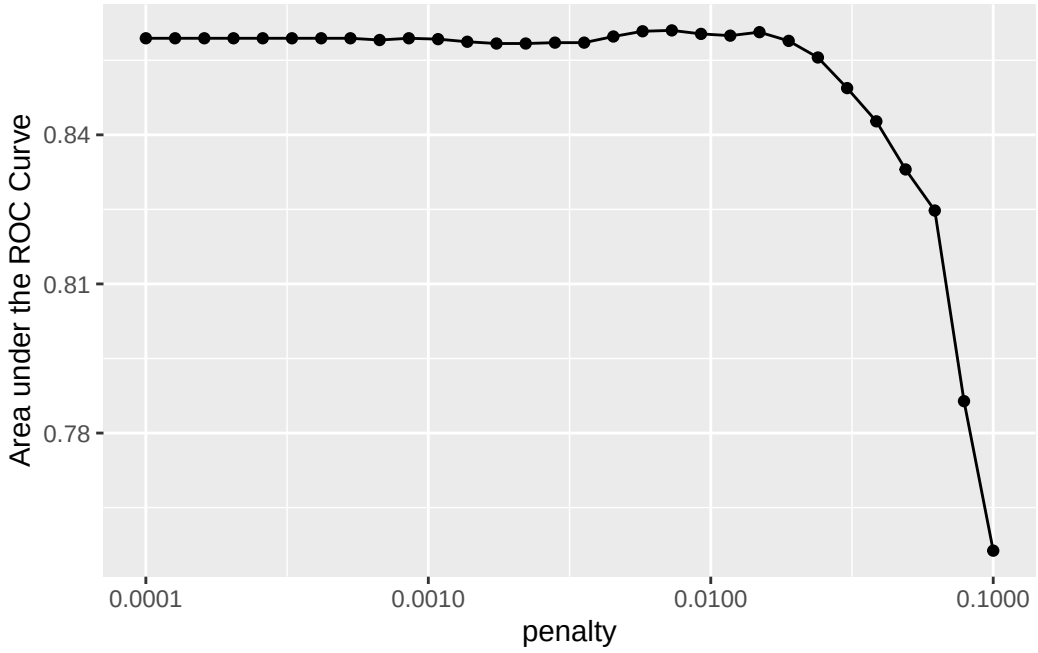
```
# Tuning results
# Validation Set Split (0.8/0.2)  using stratification
# A tibble: 1 x 5
  splits            id         .metrics          .notes           .predictions
  <list>            <chr>      <list>            <list>           <list>
1 <split [655/165]> validation <tibble [30 x 5]> <tibble [0 x 3]> <tibble>
```

Resultados del tuneo de hiperparámetro

Graficamos la variación de los valores de ROC ante diferentes valores de penalty. Mientras más alto es el valor de ROC, mejores son dichos modelos.

```
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
```

Este gráfico nos muestra que el rendimiento del modelo es generalmente mejor con los valores de penalización más bajos. Esto sugiere que la mayoría de los predictores son importantes para el modelo. También vemos una caída pronunciada en el área bajo la curva ROC hacia los valores de penalización más altos. Esto sucede porque una penalización lo suficientemente grande eliminará todos los predictores del modelo y, como era de esperar, la precisión predictiva se desploma usando menos predictores en el modelo.

Mejores modelos de Logistic Regression

Mostramos los mejores 15 modelos según la métrica ROC usando show_best. Mientras más alto es el valor de ROC, mejores son dichos modelos.

Los datos se muestran ordenados de menor a mayor según el valor de penalty.

```
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     0.859     1      NA Preprocessor1_Model01
 2 0.000127 roc_auc binary     0.859     1      NA Preprocessor1_Model02
 3 0.000161 roc_auc binary     0.859     1      NA Preprocessor1_Model03
 4 0.000204 roc_auc binary     0.859     1      NA Preprocessor1_Model04
 5 0.000259 roc_auc binary     0.859     1      NA Preprocessor1_Model05
 6 0.000329 roc_auc binary     0.859     1      NA Preprocessor1_Model06
 7 0.000418 roc_auc binary     0.859     1      NA Preprocessor1_Model07
 8 0.000530 roc_auc binary     0.859     1      NA Preprocessor1_Model08
 9 0.000853 roc_auc binary     0.859     1      NA Preprocessor1_Model10
10 0.00452  roc_auc binary     0.860     1      NA Preprocessor1_Model17
11 0.00574  roc_auc binary     0.861     1      NA Preprocessor1_Model18
12 0.00728  roc_auc binary     0.861     1      NA Preprocessor1_Model19
13 0.00924  roc_auc binary     0.860     1      NA Preprocessor1_Model20
14 0.0117   roc_auc binary     0.860     1      NA Preprocessor1_Model21
15 0.0149   roc_auc binary     0.861     1      NA Preprocessor1_Model22
```

Muestro la misma información anterior pero ordenada esta vez de forma decreciente por el valor ROC auc

Los datos se muestran ordenados de menor a mayor según el valor de penalty.

```
lr_res %>%
  show_best(metric = "roc_auc", n = 15) %>%
  arrange(desc(mean))
```

```
# A tibble: 15 x 7
    penalty .metric .estimator  mean     n std_err .config
      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
 1 0.00728  roc_auc binary     0.861     1      NA Preprocessor1_Model19
 2 0.00574  roc_auc binary     0.861     1      NA Preprocessor1_Model18
 3 0.0149   roc_auc binary     0.861     1      NA Preprocessor1_Model22
 4 0.00924  roc_auc binary     0.860     1      NA Preprocessor1_Model20
 5 0.0117   roc_auc binary     0.860     1      NA Preprocessor1_Model21
 6 0.00452  roc_auc binary     0.860     1      NA Preprocessor1_Model17
 7 0.0001   roc_auc binary     0.859     1      NA Preprocessor1_Model01
 8 0.000127 roc_auc binary     0.859     1      NA Preprocessor1_Model02
 9 0.000161 roc_auc binary     0.859     1      NA Preprocessor1_Model03
10 0.000204 roc_auc binary     0.859     1      NA Preprocessor1_Model04
11 0.000259 roc_auc binary     0.859     1      NA Preprocessor1_Model05
12 0.000329 roc_auc binary     0.859     1      NA Preprocessor1_Model06
13 0.000418 roc_auc binary     0.859     1      NA Preprocessor1_Model07
14 0.000530 roc_auc binary     0.859     1      NA Preprocessor1_Model08
15 0.000853 roc_auc binary     0.859     1      NA Preprocessor1_Model10
```

Observamos que el valor de penalty de 0.0072789538 aparece en el PUESTO 1.

Otra forma de observar esto es usando la función select_best() que encuentra la mejor combinación de hiperparámetros basándose en una medida de performance. En nuestro caso es un sólo hiperparámetro, penalty para el modelo de regresión logística, y la medida con la que evaluamos los modelos es ROC_AUC.

```
  lr_res %>%
  select_best(metric = "roc_auc")
```

```
# A tibble: 1 x 2
  penalty .config
    <dbl> <chr>
1 0.00728 Preprocessor1_Model19
```

Nos indica que el modelo nro 19 es el mejorcito y el valor de penalty 0.007278954. Aunque si observamos con respecto a los otros valores de penalty menores, es muy poca la variación de ROC.

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

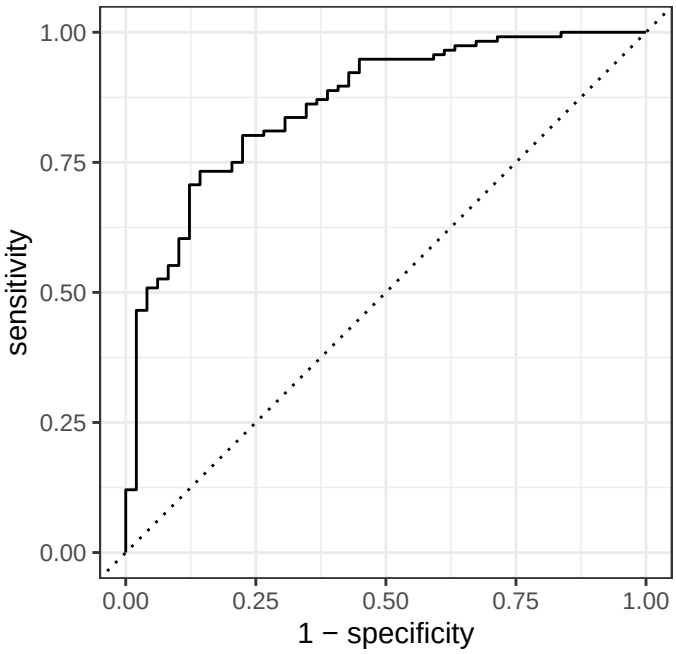
```
# A tibble: 1 x 7
  penalty .metric .estimator  mean     n std_err .config
    <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
1 0.00728 roc_auc binary     0.861     1      NA Preprocessor1_Model19
```

Ahora tenemos nuestro modelo candidato: una logistic regresion con el valor de penalty mostrado arriba.

Graficamos la curva ROC para ese modelo con su performance en el conjunto de entrenamiento.

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

autoplot(lr_auc)
```




```
ggsave(filename = "./figs-to-paper/05-log-reg-ROC-best-on-training.tiff",units = "px", dpi=30
```

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

RESULTADOS en conjunto de datos de testeo

Primero extraigo el mejor modelo, como ya explicamos antes.

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

best_model
```

```
# A tibble: 1 x 2
  penalty .config
    <dbl> <chr>
1 0.00728 Preprocessor1_Model19
```

Actualizamos nuestro workflow de trabajo.

```
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 = 0.00727895384398315
  mixture = 1

Computational engine: glmnet
```

Podemos utilizar la función last_fit() con nuestro modelo finalizado; esta función ajusta el modelo finalizado en el conjunto de datos de entrenamiento completo y evalúa el modelo finalizado en los datos de prueba.

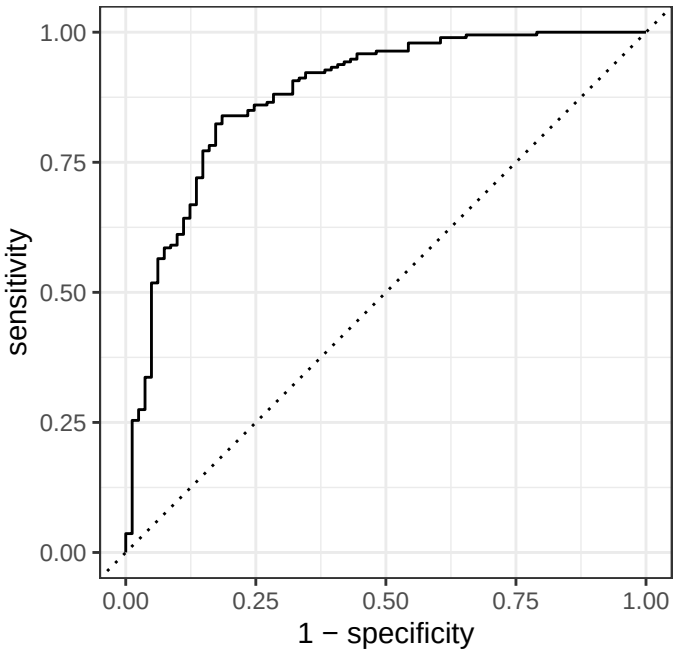
```
final_fit <-
  final_wf %>%
  last_fit(splits)
```

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

```
# A tibble: 3 x 4
  .metric     .estimator .estimate .config
  <chr>       <chr>          <dbl> <chr>
1 accuracy    binary         0.839 Preprocessor1_Model1
2 roc_auc     binary         0.881 Preprocessor1_Model1
3 brier_class binary         0.120 Preprocessor1_Model1
```

ROC CURVE SOBRE EL CONJUNTO DE TESTEO

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




```
ggsave(filename = "./figs-to-paper/06-log-reg-ROC-best-on-testing.tiff",units = "px", dpi=300
```

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

Predecimos en el conjunto de datos de testeo, ese 25 % de datos que dejamos reservado para este momento.

```
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)
```

Matriz de confusión

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

```
          Truth
Prediction Bueno Malo
     Bueno   177   28
     Malo     16   53
```

```
# check
nrow(data_test) == 177 + 16 +28 + 53
```

```
[1] TRUE
```

Métricas de accuracy, sensitivity, specificity

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

```
# A tibble: 13 x 3
   .metric              .estimator .estimate
   <chr>                <chr>          <dbl>
 1 accuracy             binary         0.839
 2 kap                  binary         0.597
 3 sens                 binary         0.917
 4 spec                 binary         0.654
 5 ppv                  binary         0.863
```

```
 6 npv                   binary         0.768
 7 mcc                   binary         0.601
 8 j_index               binary         0.571
 9 bal_accuracy          binary         0.786
10 detection_prevalence  binary         0.748
11 precision             binary         0.863
12 recall                binary         0.917
13 f_meas                binary         0.889
```

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         0.889
```

Random Forest

Vamos a entrenar un modelo de random forest para clasificación binaria.

Para ello usaremos la implementación de random forest de la librería ranger.

Durante el entrenamiento tunearemos dos hiperparámetros: mtry y min_n.

Dejamos trees en 100.

```
# nro de cores en el procesador de la COMPU donde esto se corre.
cores <- parallel::detectCores()

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

Receta: vamos a usar PM10 como variable a predecir que contiene los valores que queremos clasificar.

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

Armado del workflow tidymodels con el modelo y receta.

```
rf_workflow <-
  workflow() %>%
  add_model(rf_mod) %>%
  add_recipe(rf_recipe)
```

Se tunea usando el conjunto de datos de entrenamiento, dentro del mismo establecemos una porción para validación, lo mismo que realizamos en el apartado anterior.

Se establece que la grilla sea de tamaño 25.

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

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

Podemos observar todas los resultados para cada valor de mtry y min_n ejecutando lo siguiente:

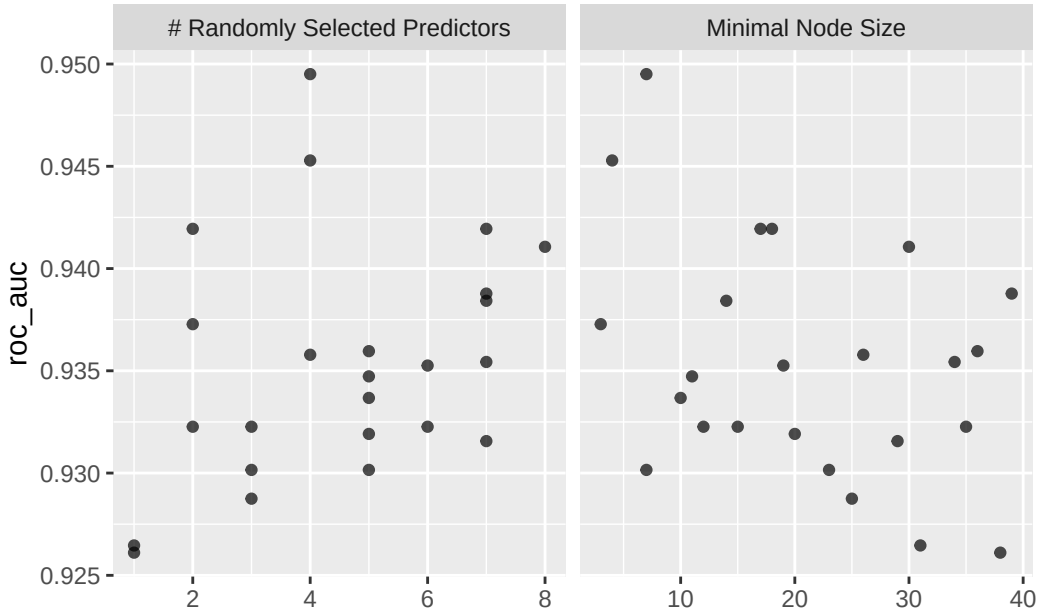
```
rf_res %>% collect_metrics()
```

```
# A tibble: 24 x 8
    mtry min_n .metric .estimator  mean     n std_err .config
   <int> <int> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
 1     4     7 roc_auc binary     0.950     1      NA Preprocessor1_Model01
 2     8    30 roc_auc binary     0.941     1      NA Preprocessor1_Model02
 3     3    25 roc_auc binary     0.929     1      NA Preprocessor1_Model03
 4     7    34 roc_auc binary     0.935     1      NA Preprocessor1_Model04
 5     4     4 roc_auc binary     0.945     1      NA Preprocessor1_Model05
 6     5    10 roc_auc binary     0.934     1      NA Preprocessor1_Model06
 7     1    38 roc_auc binary     0.926     1      NA Preprocessor1_Model07
```

```
 8     5    11 roc_auc binary     0.935     1      NA Preprocessor1_Model08
 9     6    19 roc_auc binary     0.935     1      NA Preprocessor1_Model09
10     7    29 roc_auc binary     0.932     1      NA Preprocessor1_Model10
# i 14 more rows
```

Graficamos resultados del tuneo de hiperparámetros.

```
autoplot(rf_res)
```




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

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

Observamos los mejores modelos.

```
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     4     7 roc_auc binary     0.950     1      NA Preprocessor1_Model01
```

```
2     4     4 roc_auc binary     0.945     1      NA Preprocessor1_Model05
3     7    17 roc_auc binary     0.942     1      NA Preprocessor1_Model21
4     2    18 roc_auc binary     0.942     1      NA Preprocessor1_Model23
5     8    30 roc_auc binary     0.941     1      NA Preprocessor1_Model02
```

Nos quedamos con el mejor modelo.

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

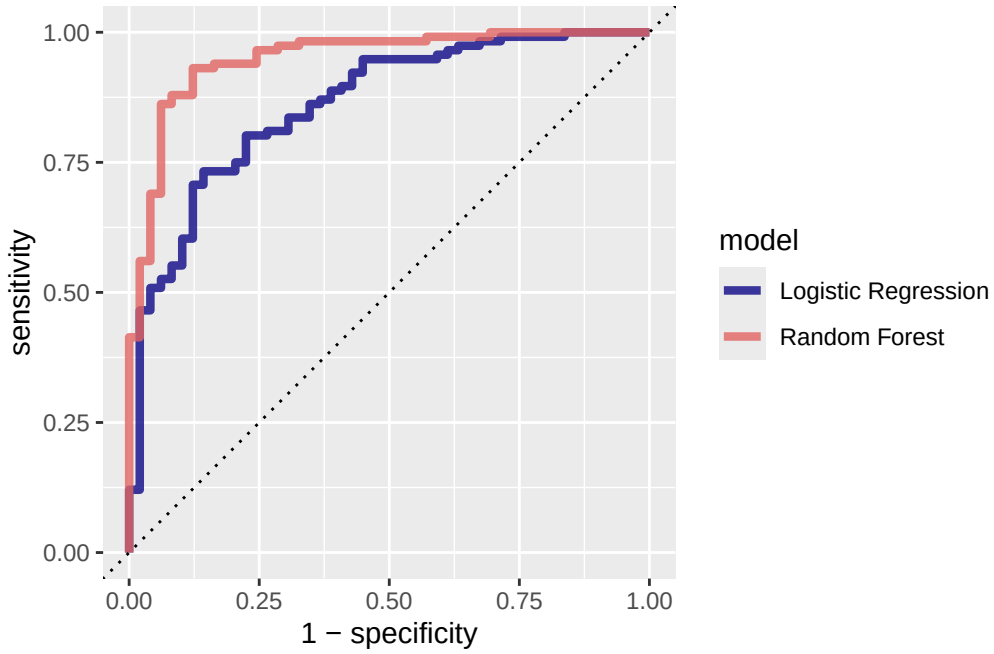
```
# A tibble: 1 x 3
   mtry min_n .config
  <int> <int> <chr>
1     4     7 Preprocessor1_Model01
```

Para filtrar las predicciones solo para nuestro mejor modelo, podemos usar el argumento de parámetros y pasarle nuestro tibble con los mejores valores de hiperparámetros del ajuste, al que llamamos rf_best:

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

ROC curve comparación de ambos modelos en el entrenamiento.

```
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=30
```

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

Observamos que el modelo de random forest es mejor en todo el umbral de probabilidad de eventos.

RESULTADOS FINALES

Armamos un modelo con los parámetros seleccionados, lo entrenamos, y luego queremos que prediga usando el conjunto de testeo.

```
# the last model
last_rf_mod <-
  rand_forest(mtry = 4, min_n = 7, 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)
```

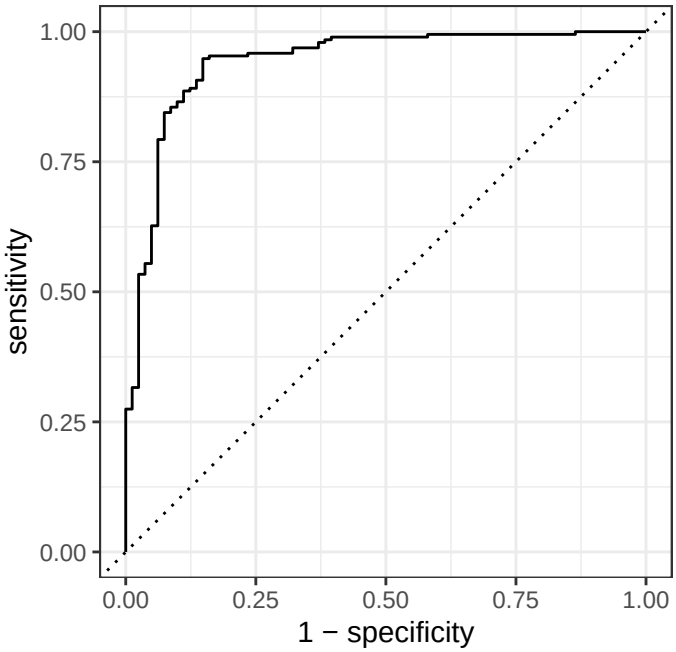
```r
# the last fit
set.seed(345)
last_rf_fit <-
  last_rf_workflow %>%
  last_fit(splits)

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 [820/274]> train/test split <tibble> <tibble> <tibble>     <workflow>
```

ROC curve plot

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



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

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

MATRIZ DE CONFUSION

```
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)
```

Matriz de confusión

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

```
          Truth
Prediction Bueno Malo
     Bueno   183   13
     Malo     10   68
```

MÉTRICAS VARIAS

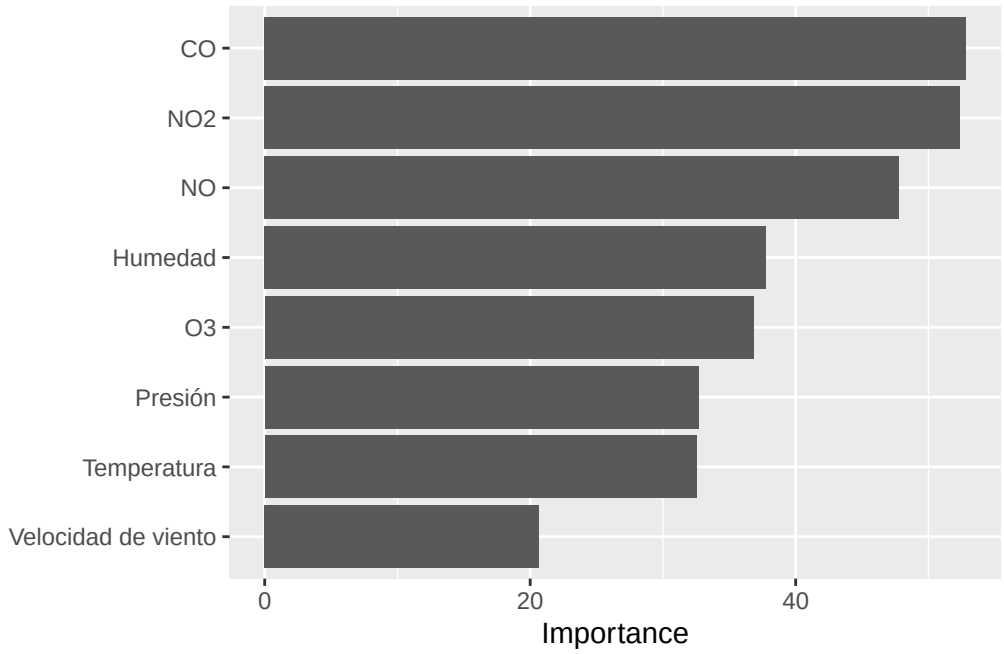
```r
summary(conf_mat(RF_results, truth = PM10,
         estimate = .pred_class))
```

```
# A tibble: 13 x 3
   .metric              .estimator .estimate
   <chr>                <chr>          <dbl>
 1 accuracy             binary         0.916
 2 kap                  binary         0.796
 3 sens                 binary         0.948
 4 spec                 binary         0.840
 5 ppv                  binary         0.934
 6 npv                  binary         0.872
 7 mcc                  binary         0.797
 8 j_index              binary         0.788
 9 bal_accuracy         binary         0.894
10 detection_prevalence binary         0.715
11 precision            binary         0.934
12 recall               binary         0.948
13 f_meas               binary         0.941
```

Vip Variable importance

Listamos de mayor a menor importancia las variables. Significa las variables que más colaboran en la predicción del modelo RF.

```r
last_rf_fit %>%
  extract_fit_parsnip() %>%
  vip(num_features = 10)
```




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

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

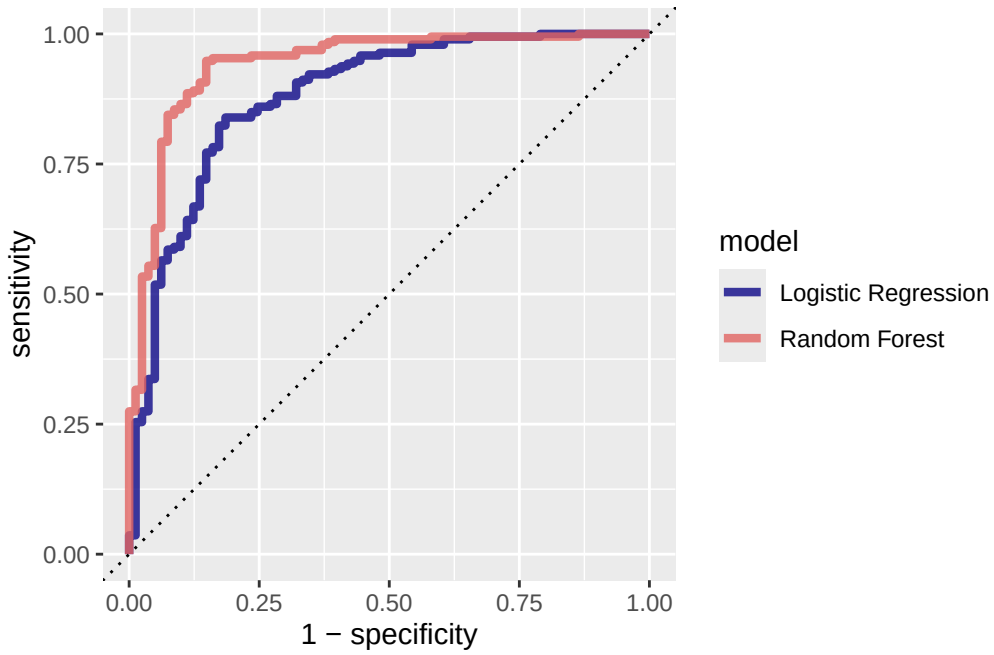
COMPARACION

ROC CURVE

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

```
rf_auc_f <- last_rf_fit %>%
            collect_predictions() %>%
            roc_curve(PM10, .pred_Bueno) %>%
            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
```

METRICAS

Agrego una fila con el resultado ROC_AUC

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

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.881
```

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

```r
m_lr
```

```
# A tibble: 14 x 4
   .metric              .estimator .estimate model
   <chr>                <chr>          <dbl> <chr>
 1 accuracy             binary         0.839 Logistic Regression
 2 kap                  binary         0.597 Logistic Regression
 3 sens                 binary         0.917 Logistic Regression
 4 spec                 binary         0.654 Logistic Regression
 5 ppv                  binary         0.863 Logistic Regression
 6 npv                  binary         0.768 Logistic Regression
 7 mcc                  binary         0.601 Logistic Regression
 8 j_index              binary         0.571 Logistic Regression
 9 bal_accuracy         binary         0.786 Logistic Regression
10 detection_prevalence binary         0.748 Logistic Regression
11 precision            binary         0.863 Logistic Regression
12 recall               binary         0.917 Logistic Regression
13 f_meas               binary         0.889 Logistic Regression
14 roc_auc              binary         0.881 Logistic Regression
```

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

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc binary         0.942
```

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

```r
m_rf
```

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

```
   .metric              .estimator .estimate model
   <chr>                <chr>          <dbl> <chr>
 1 accuracy             binary         0.916 Random Forest
 2 kap                  binary         0.796 Random Forest
 3 sens                 binary         0.948 Random Forest
 4 spec                 binary         0.840 Random Forest
 5 ppv                  binary         0.934 Random Forest
 6 npv                  binary         0.872 Random Forest
 7 mcc                  binary         0.797 Random Forest
 8 j_index              binary         0.788 Random Forest
 9 bal_accuracy         binary         0.894 Random Forest
10 detection_prevalence binary         0.715 Random Forest
11 precision            binary         0.934 Random Forest
12 recall               binary         0.948 Random Forest
13 f_meas               binary         0.941 Random Forest
14 roc_auc              binary         0.942 Random Forest
```

TABLA COMPARATIVA METRICAS POR CADA MODELO

```
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                       0.916                 0.839
 2 kap                            0.796                 0.597
 3 sens                           0.948                 0.917
 4 spec                           0.840                 0.654
 5 ppv                            0.934                 0.863
 6 npv                            0.872                 0.768
 7 mcc                            0.797                 0.601
 8 j_index                        0.788                 0.571
 9 bal_accuracy                   0.894                 0.786
10 detection_prevalence           0.715                 0.748
11 precision                      0.934                 0.863
12 recall                         0.948                 0.917
13 f_meas                         0.941                 0.889
14 roc_auc                        0.942                 0.881
```

Guardo los resultados en un archivo csv

```r
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

```r
sessionInfo()
```

```
R version 4.4.1 (2024-06-14)
Platform: x86_64-pc-linux-gnu
Running under: Ubuntu 22.04.4 LTS

Matrix products: default
BLAS:   /usr/lib/x86_64-linux-gnu/atlas/libblas.so.3.10.3
LAPACK: /usr/lib/x86_64-linux-gnu/atlas/liblapack.so.3.10.3;  LAPACK version 3.10.0

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/Buenos_Aires
tzcode source: system (glibc)

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

other attached packages:
 [1] stringr_1.5.1      ranger_0.16.0      vip_0.4.1          glmnet_4.1-8
 [5] Matrix_1.6-5       yardstick_1.3.1    workflowsets_1.1.0 workflows_1.1.4
 [9] tune_1.2.1         tibble_3.2.1       rsample_1.2.1      recipes_1.0.10
[13] purrr_1.0.2        parsnip_1.2.1      modeldata_1.3.0    infer_1.0.7
[17] ggplot2_3.5.1      dials_1.2.1        scales_1.3.0       broom_1.0.6
[21] tidymodels_1.2.0   DataExplorer_0.8.3 tidyr_1.3.1        dplyr_1.1.4
[25] readr_2.1.5
```

```
loaded via a namespace (and not attached):
 [1] gridExtra_2.3       rlang_1.1.3         magrittr_2.0.3
 [4] furrr_0.3.1         compiler_4.4.1      vctrs_0.6.5
 [7] reshape2_1.4.4      lhs_1.1.6           crayon_1.5.2
[10] pkgconfig_2.0.3     shape_1.4.6.1       fastmap_1.2.0
[13] backports_1.5.0     ellipsis_0.3.2      labeling_0.4.3
[16] utf8_1.2.4          rmarkdown_2.27      prodlim_2023.08.28
[19] tzdb_0.4.0          bit_4.0.5           tinytex_0.51
[22] xfun_0.44           jsonlite_1.8.8      parallel_4.4.1
[25] R6_2.5.1            stringi_1.8.4       parallelly_1.37.1
[28] rpart_4.1.23        lubridate_1.9.3     Rcpp_1.0.12
[31] iterators_1.0.14    knitr_1.46          future.apply_1.11.2
[34] splines_4.4.1       nnet_7.3-19         igraph_2.0.3
[37] timechange_0.3.0    tidyselect_1.2.1    rstudioapi_0.16.0
[40] yaml_2.3.8          timeDate_4032.109   codetools_0.2-19
[43] listenv_0.9.1       lattice_0.22-5      plyr_1.8.9
[46] withr_3.0.0         evaluate_0.23       future_1.33.2
[49] survival_3.7-0      pillar_1.9.0        foreach_1.5.2
[52] generics_0.1.3      vroom_1.6.5         hms_1.1.3
[55] munsell_0.5.1       globals_0.16.3      class_7.3-22
[58] glue_1.7.0          tools_4.4.1         data.table_1.15.4
[61] gower_1.0.1         grid_4.4.1          ipred_0.9-14
[64] colorspace_2.1-0    networkD3_0.4       cli_3.6.2
[67] DiceDesign_1.10     fansi_1.0.6         viridisLite_0.4.2
[70] lava_1.8.0          gtable_0.3.5        GPfit_1.0-8
[73] digest_0.6.35       htmlwidgets_1.6.4   farver_2.1.2
[76] htmltools_0.5.8.1   lifecycle_1.0.4     hardhat_1.3.1
[79] bit64_4.0.5         MASS_7.3-60
```