Air quality project : Time Series Analysis

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12 janvier, 2020

Contents

Preliminary

Our project consists of time series analysis using R programming language. Our data set contains the responses of a gas mutisensor device deployed on the field in an Italian city, in a significantly polluted area, at road level. The data set contains 9358 instances of hourly averaged responses from an array of 5 metal oxide chemical sensors embedded in an Air Quality Chemical Multisensor Device. Data were recorded from March 2004 to February 2005.

```r
dim(data)
```

```
## [1] 9471   17
```

```r
str(data)
```

```
## 'data.frame':    9471 obs. of  17 variables:
##  $ Date         : chr  "10/03/2004" "10/03/2004" "10/03/2004" "10/03/2004" ...
##  $ Time         : chr  "18.00.00" "19.00.00" "20.00.00" "21.00.00" ...
##  $ CO.GT.       : chr  "2,6" "2" "2,2" "2,2" ...
##  $ PT08.S1.CO.  : int  1360 1292 1402 1376 1272 1197 1185 1136 1094 1010 ...
##  $ NMHC.GT.     : int  150 112 88 80 51 38 31 31 24 19 ...
##  $ C6H6.GT.     : chr  "11,9" "9,4" "9,0" "9,2" ...
##  $ PT08.S2.NMHC.: int  1046 955 939 948 836 750 690 672 609 561 ...
##  $ NOx.GT.      : int  166 103 131 172 131 89 62 62 45 -200 ...
##  $ PT08.S3.NOx. : int  1056 1174 1140 1092 1205 1337 1462 1453 1579 1705 ...
##  $ NO2.GT.      : int  113 92 114 122 116 96 77 76 60 -200 ...
##  $ PT08.S4.NO2. : int  1692 1559 1555 1584 1490 1393 1333 1333 1276 1235 ...
##  $ PT08.S5.O3.  : int  1268 972 1074 1203 1110 949 733 730 620 501 ...
##  $ T            : chr  "13,6" "13,3" "11,9" "11,0" ...
##  $ RH           : chr  "48,9" "47,7" "54,0" "60,0" ...
##  $ AH           : chr  "0,7578" "0,7255" "0,7502" "0,7867" ...
##  $ X            : logi  NA NA NA NA NA NA ...
##  $ X.1          : logi  NA NA NA NA NA NA ...
```

Attribute	Description
Date	Date (DD/MM/YYYY)
Time	Time (HH.MM.SS)
CO(GT)	True hourly averaged concentration CO in mg/m^3 (reference analyzer)
PT08.S1(CO)	PT08.S1 (tin oxide) hourly averaged sensor response (nominally CO targeted)
NMHC(GT)	True hourly averaged overall Non Metanic Hydro Carbons concentration in microg/m^3(reference analyzer
C6H6(GT)	True hourly averaged Benzene concentration in microg/m^3 (reference analyzer)
PT08.S2(NMHC)	PT08.S2 (titania) hourly averaged sensor response (nominally NMHC targeted)
NOx(GT)	True hourly averaged NOx concentration in ppb (reference analyzer)
PT08.S3(NOx)	PT08.S3 (tungsten oxide) hourly averaged sensor response (nominally NOx targeted)
NO2(GT)	True hourly averaged NO2 concentration in microg/m^3 (reference analyzer)
PT08.S4(NO2)	PT08.S4 (tungsten oxide) hourly averaged sensor response (nominally NO2 targeted)
PT08.S5(O3)	PT08.S5 (indium oxide) hourly averaged sensor response (nominally O3 targeted)
T	Temperature in °C
RH	Relative Humidity (%)
AH	AH Absolute Humidity

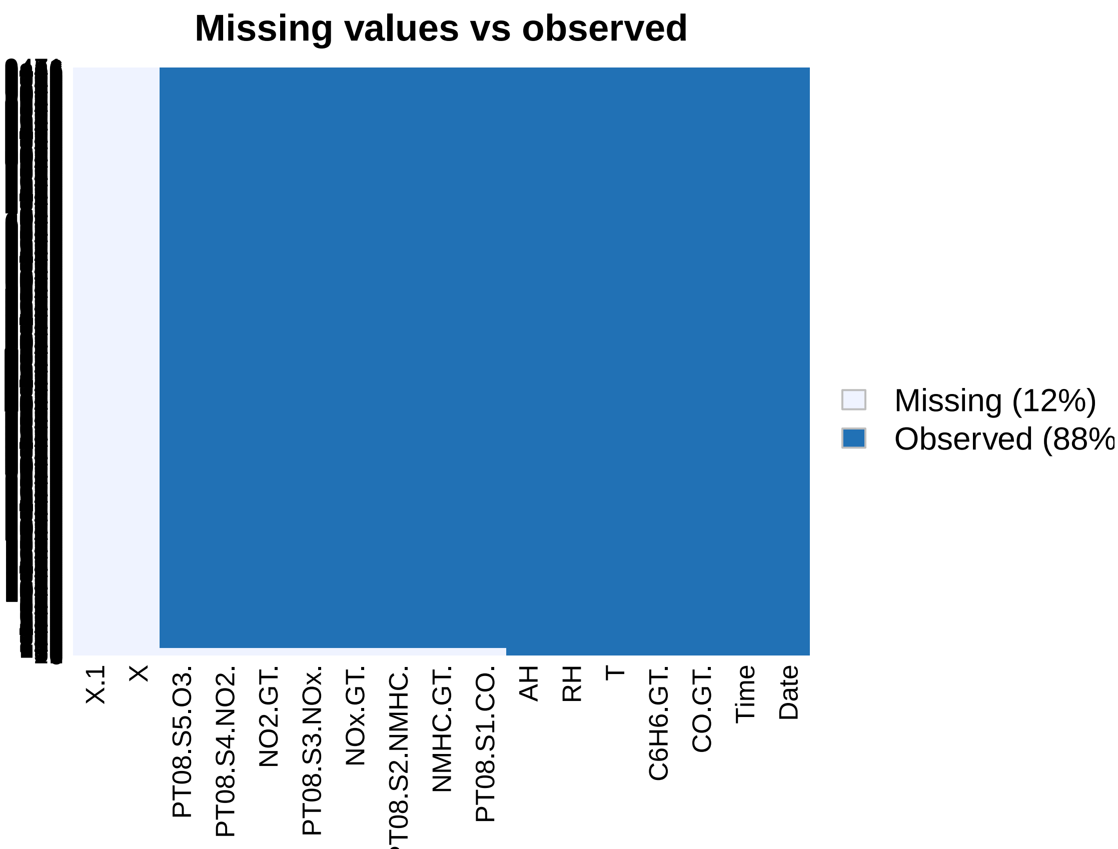
I)-Cleaning and preprocessing

1) Data cleaning

As we can see in the str(dim) output, our data contains missing values, some are directly reported as NA and others have been assigned to -200. It also contains a certain number of numeric variables that are characters which makes it not directly exploitable and some numbers have commas within them. For all these reasons, we had to clean our data set first so that we can exploit it afterwards.

```
## Loading required package: Rcpp
```

```
## ##
## ## Amelia II: Multiple Imputation
## ## (Version 1.7.6, built: 2019-11-24)
## ## Copyright (C) 2005-2020 James Honaker, Gary King and Matthew Blackwell
## ## Refer to http://gking.harvard.edu/amelia/ for more information
## ##
```



We remove X1 and X beacause they have no data within them, also we compute the necessary changes so that our data is exploitable afterwards.

We noticed that NHMC contains a lot of -200 values, so we prefered to delet it along with all the lines that contain -200.

```
summary(data$NMHC.GT.)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  -200.0  -200.0  -200.0  -159.1  -200.0  1189.0
```

```r
str(data)
```

```
## 'data.frame':    6941 obs. of  14 variables:
##  $ Date         : Date, format: "2004-03-10" "2004-03-10" ...
##  $ Time         : chr  "18.00.00" "19.00.00" "20.00.00" "21.00.00" ...
##  $ CO.GT.       : num  2.6 2 2.2 2.2 1.6 1.2 1.2 1 0.9 0.7 ...
##  $ PT08.S1.CO.  : int  1360 1292 1402 1376 1272 1197 1185 1136 1094 1066 ...
##  $ C6H6.GT.     : num  11.9 9.4 9 9.2 6.5 4.7 3.6 3.3 2.3 1.1 ...
##  $ PT08.S2.NMHC.: int  1046 955 939 948 836 750 690 672 609 512 ...
##  $ NOx.GT.      : int  166 103 131 172 131 89 62 62 45 16 ...
##  $ PT08.S3.NOx. : int  1056 1174 1140 1092 1205 1337 1462 1453 1579 1918 ...
##  $ NO2.GT.      : int  113 92 114 122 116 96 77 76 60 28 ...
##  $ PT08.S4.NO2. : int  1692 1559 1555 1584 1490 1393 1333 1333 1276 1182 ...
##  $ PT08.S5.O3.  : int  1268 972 1074 1203 1110 949 733 730 620 422 ...
##  $ T            : num  13.6 13.3 11.9 11 11.2 11.2 11.3 10.7 10.7 11 ...
##  $ RH           : num  48.9 47.7 54 60 59.6 59.2 56.8 60 59.7 56.2 ...
##  $ AH           : num  0.758 0.726 0.75 0.787 0.789 ...
```

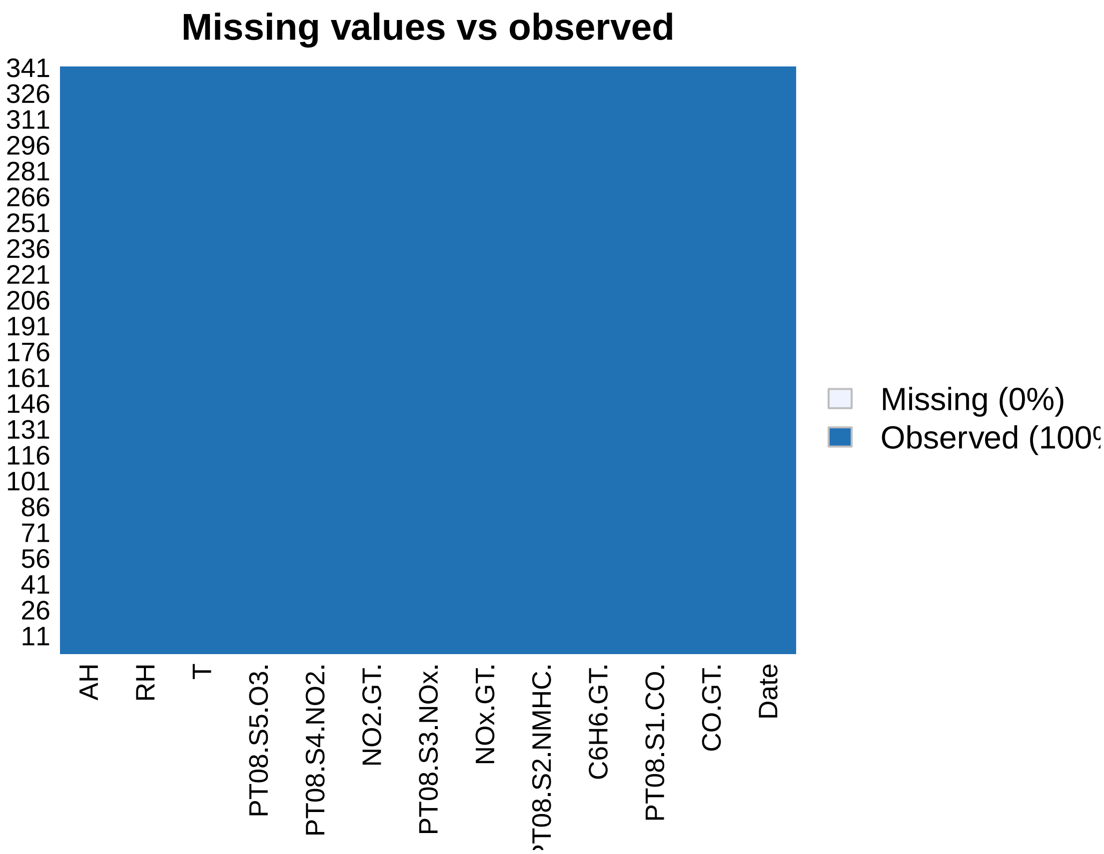
Now that our data is nearly clean, we chose to consider the daily concentration of the different gases our main focus of study by taking the average of the concentrations observed daily.

We obtain 341 observations of 13 variables.

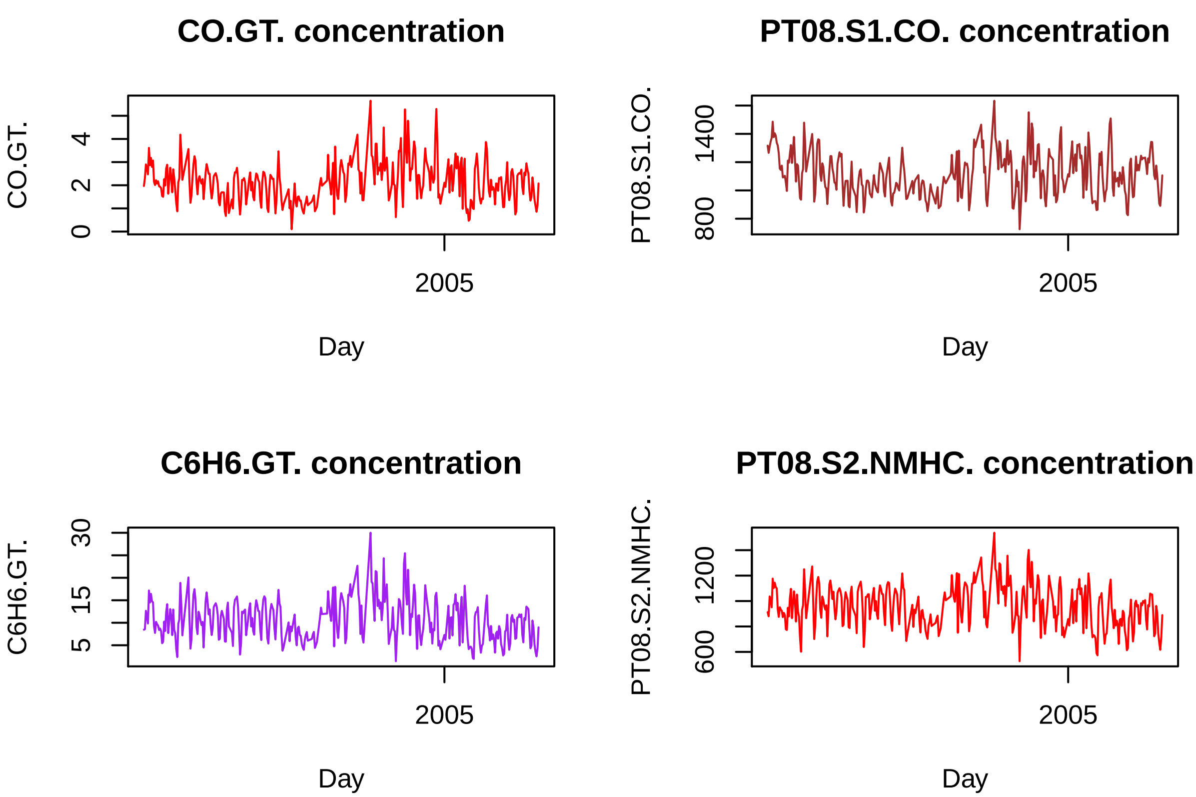
```r
str(daily_data)
```

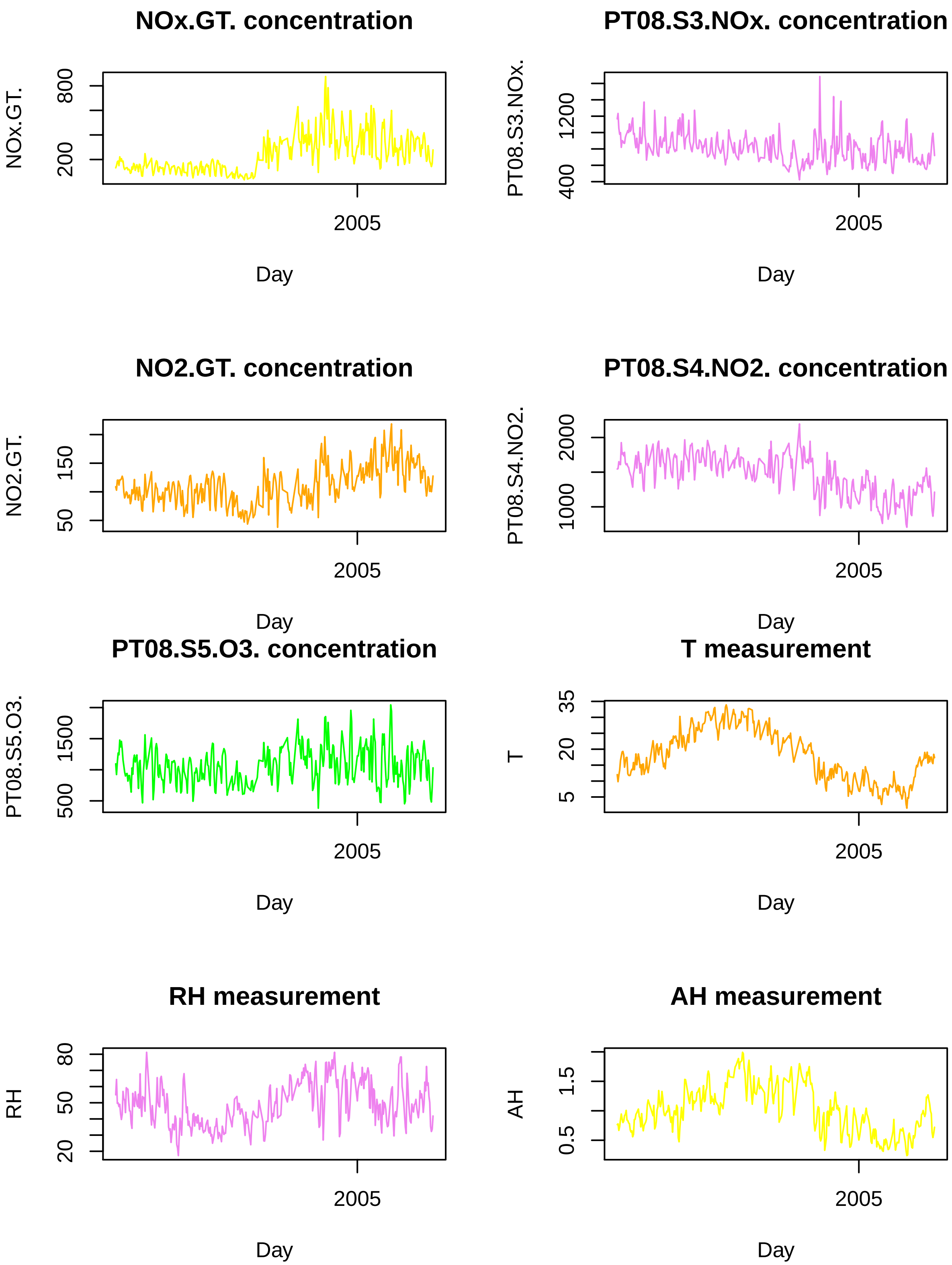
```
## 'data.frame':    341 obs. of  13 variables:
##  $ Date         : Date, format: "2004-03-10" "2004-03-11" ...
##  $ CO.GT.       : num  1.97 2.31 2.9 2.74 2.47 ...
##  $ PT08.S1.CO.  : num  1316 1265 1309 1346 1372 ...
##  $ C6H6.GT.     : num  8.45 8.57 12.67 11.38 9.84 ...
##  $ PT08.S2.NMHC.: num  912 880 1036 1010 951 ...
##  $ NOx.GT.      : num  132 150 181 188 150 ...
##  $ PT08.S3.NOx. : num  1167 1233 1053 978 999 ...
##  $ NO2.GT.      : num  109 103 120 120 112 ...
##  $ PT08.S4.NO2. : num  1546 1551 1651 1614 1608 ...
##  $ PT08.S5.O3.  : num  1096 923 1121 1269 1241 ...
##  $ T            : num  12 9.8 11.8 13.4 16.4 ...
##  $ RH           : num  54.9 64.4 49.6 49.9 47.6 ...
##  $ AH           : num  0.766 0.778 0.667 0.734 0.848 ...
```

```r
missmap(daily_data, main = "Missing values vs observed")
```



Since our data is all observed now, we can start plotting it to visualize what our data set looks like.





The variables starting with PT are the responses of the sensors measuring the concentration of the gas concerned. When investigating our data and by doing some research on air pollution, we found that the main air pollutants belong to the nitrogen oxides family (NOx). Thus, we wanted to see the relation between this gas concentration and the other ones. A linear regression was run between the NOx concentration and the other gases.

```r
summary(reg)
```

```
##
## Call:
## lm(formula = daily_data$PT08.S3.NOx. ~ +daily_data$PT08.S1.CO. +
##     daily_data$PT08.S2.NMHC. + daily_data$PT08.S4.NO2. + daily_data$PT08.S5.O3. +
##     daily_data$T + daily_data$RH + daily_data$AH)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -182.43  -60.67  -12.99   32.68  736.42
##
## Coefficients:
##                           Estimate Std. Error t value Pr(>|t|)
## (Intercept)             1499.58349   73.78298  20.324  < 2e-16 ***
## daily_data$PT08.S1.CO.     -0.30643    0.09141  -3.352 0.000894 ***
## daily_data$PT08.S2.NMHC.   -0.46111    0.10894  -4.233 2.99e-05 ***
## daily_data$PT08.S4.NO2.     0.51459    0.05633   9.135  < 2e-16 ***
## daily_data$PT08.S5.O3.     -0.26128    0.06138  -4.256 2.70e-05 ***
## daily_data$T               -4.07044    3.05090  -1.334 0.183057
## daily_data$RH              -0.70990    1.08830  -0.652 0.514660
## daily_data$AH            -263.09360   48.56193  -5.418 1.16e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 95.89 on 333 degrees of freedom
## Multiple R-squared:  0.714,  Adjusted R-squared:  0.708
## F-statistic: 118.8 on 7 and 333 DF,  p-value: < 2.2e-16
```

We will build the NOx concentration as a time series beacause it comes from sensor measurements, thus noise will be modeled accordingly. Since it is linearly related to the other gases (except for the temperature, relative humidity and absolute humidity that we will exclude from our study). We will focus on the NOx model.

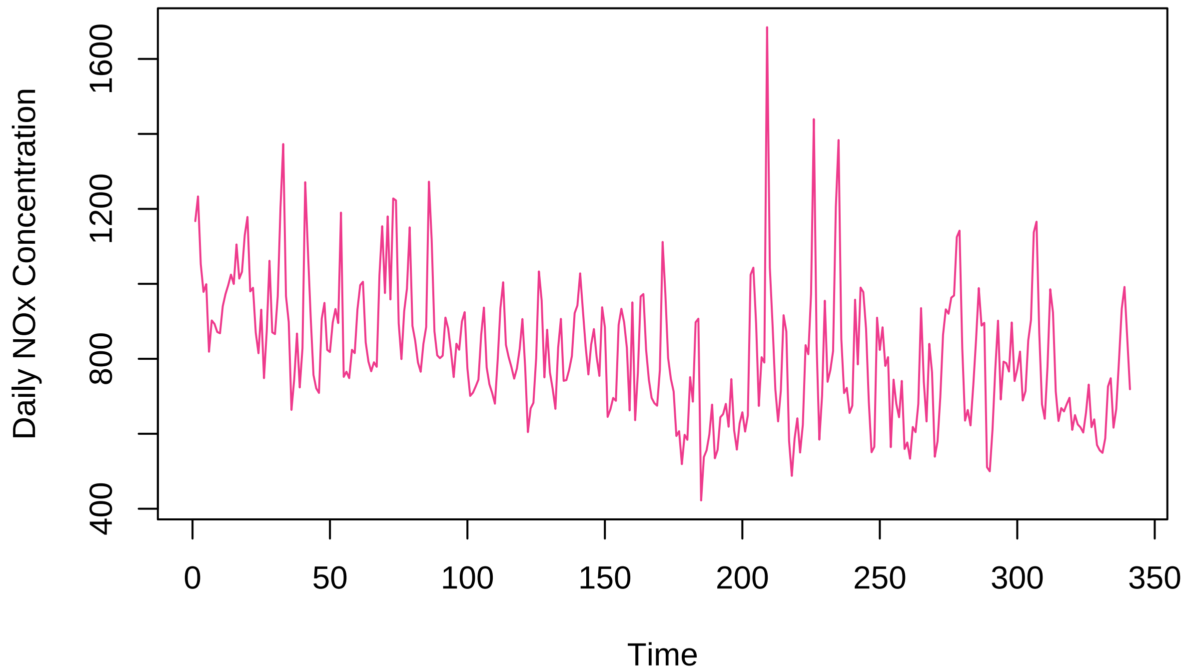
2) Data preprocessing

We count one PT08.S3.NOX observation per day for 341 days. We suppose that our time series follows an additive model :

$$D_t = S_t + T_t + X_t$$

Where $(S_t)_t$ is the seasonality, $(T_t)_t$ the trend and $(X_t)_t$ is assumed to be stationary.

We obtain this representation :

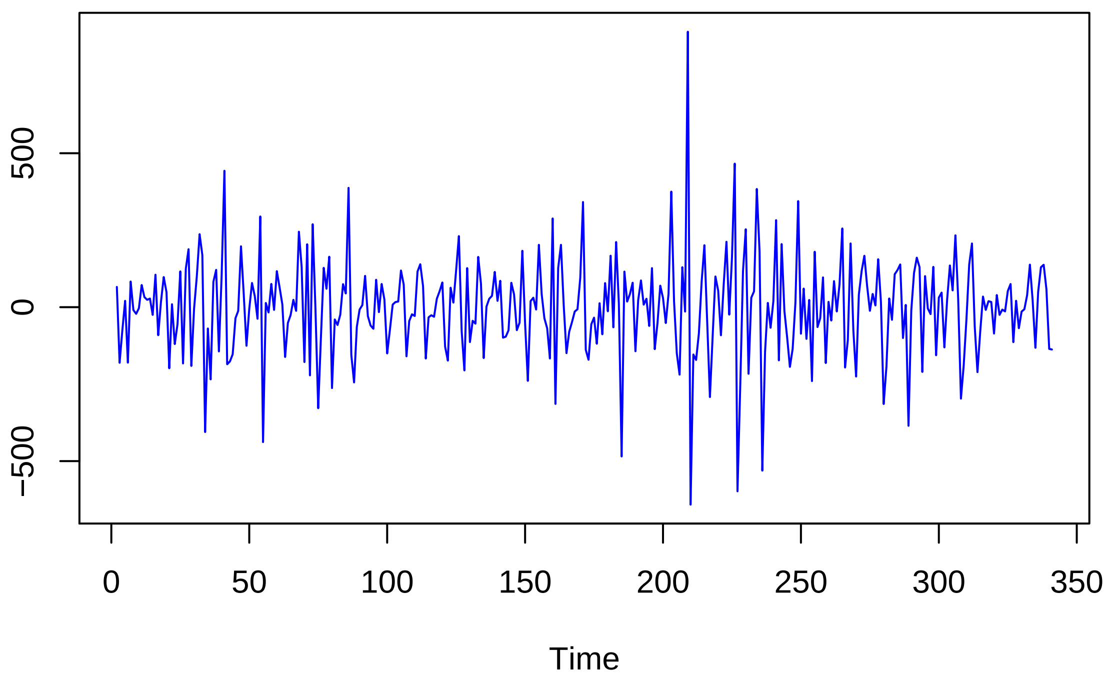


Before building any model, we have to stationarise it first by removing the seasonal and trend components.

$$X_t = D_t - T_t - S_t$$

So we use differencing :

$$D_t - D_{t-1}$$



We want to make sure of the stationarity of our series, so we use the Augmented Dickey-Fuller Test that tests the null hypothesis that a unit root is present in a time series sample.

We obtain these results :

```
## Warning in adf.test(ts_stat_PT08.S3.NOx.): p-value smaller than printed p-value
```

```
##
##  Augmented Dickey-Fuller Test
##
## data:  ts_stat_PT08.S3.NOx.
## Dickey-Fuller = -11.962, Lag order = 6, p-value = 0.01
## alternative hypothesis: stationary
```

Since our p-value is smalled than 0.01, we reject the null hypothesis with level of confidence of 99%

II)-Model fitting on the time series of interest

In order to test different models, we take out the last 10 most recent data that will be used for testing, the other observations will be used for the training.

Let $(X_t)_t$ be a centered second order stationary process. For $h \in Z$, we define :

- The autocovariance function :

$$\gamma_X(h) = Cov(X_t, X_{t+h}) = Cov(X_0, X_h) = E[X_0 X_h]$$

- The autorrelation function (ACF):

$$\rho_X(h) = \rho(X_t, X_{t+h}) = \frac{\gamma_X(h)}{\gamma_X(0)}$$

- The partial autocorrelation function (PACF):

$$\tilde{\rho}_X(h) = \rho_X(X_0 - \pi_{h-1}(X_0), X_h - \pi_{h-1}(X_h))$$

with the convention $\pi_0(X_1) = 0$ where $\pi_{h-1}(X_0)$ is the projection of X_0 on the linear span of $(X_1, X_2, ..., X_{h-1})$

1) MA model

A MA(q) process, with $q \in N$, is a solution to the equation :

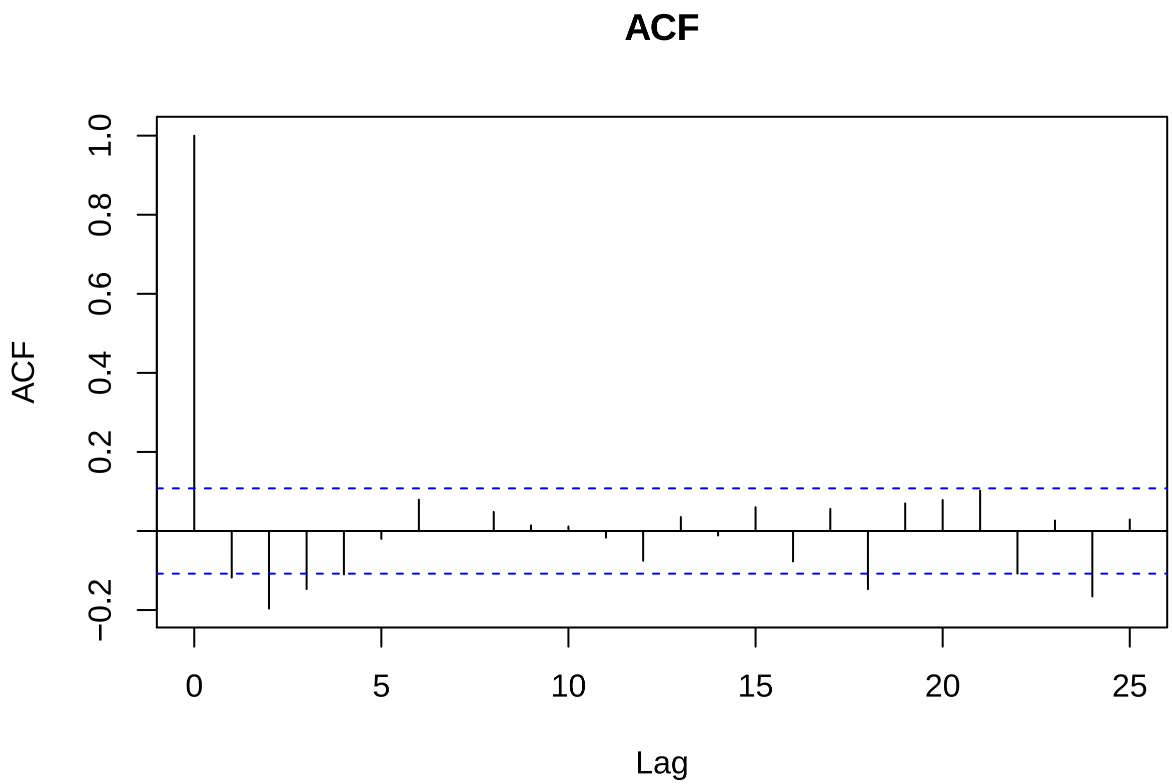
$$X_t = Z_t + \gamma_1 Z_{t-1} + ... + \gamma_q Z_{t-q}$$

with $t \in Z$ and $(Z_t)_t$ a white noise.

In order to find q, we use this MA(q) property :

$$\gamma_X(h) = 0 \ \forall h \geq p$$

We choose the q parameter accordingly to the last lag in the acf that is significantly non-null, outside the blue confident band.



We notice that we can not fit our data into a MA model, which is quite unexpected, because the data comes from sensor measurements so we have expected a strong noise presence. Thus, we will try other models.

2) AR model

A second model is the AR(p).

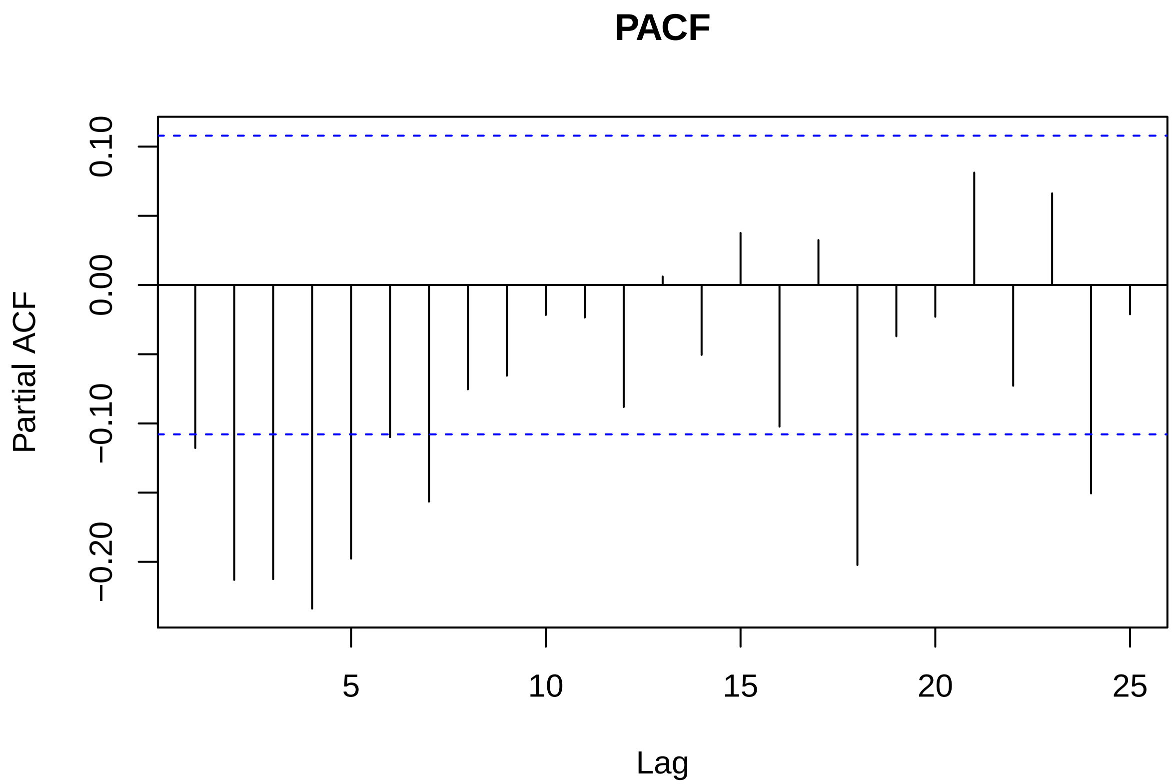
An AR(p) process, with $p \in N$, is a solution of the equation :

$$X_t = \phi_1 X_{t-1} + \phi_2 X_{t-2} + ... + \phi_p X_{t-p} + Z_t$$

We will use a pacf AR(p) proprety, equivalent to the acf MA(q) property :

$$\tilde{\rho}_X(h) = 0 \ \forall h > p$$

We obtain this pacf plot :



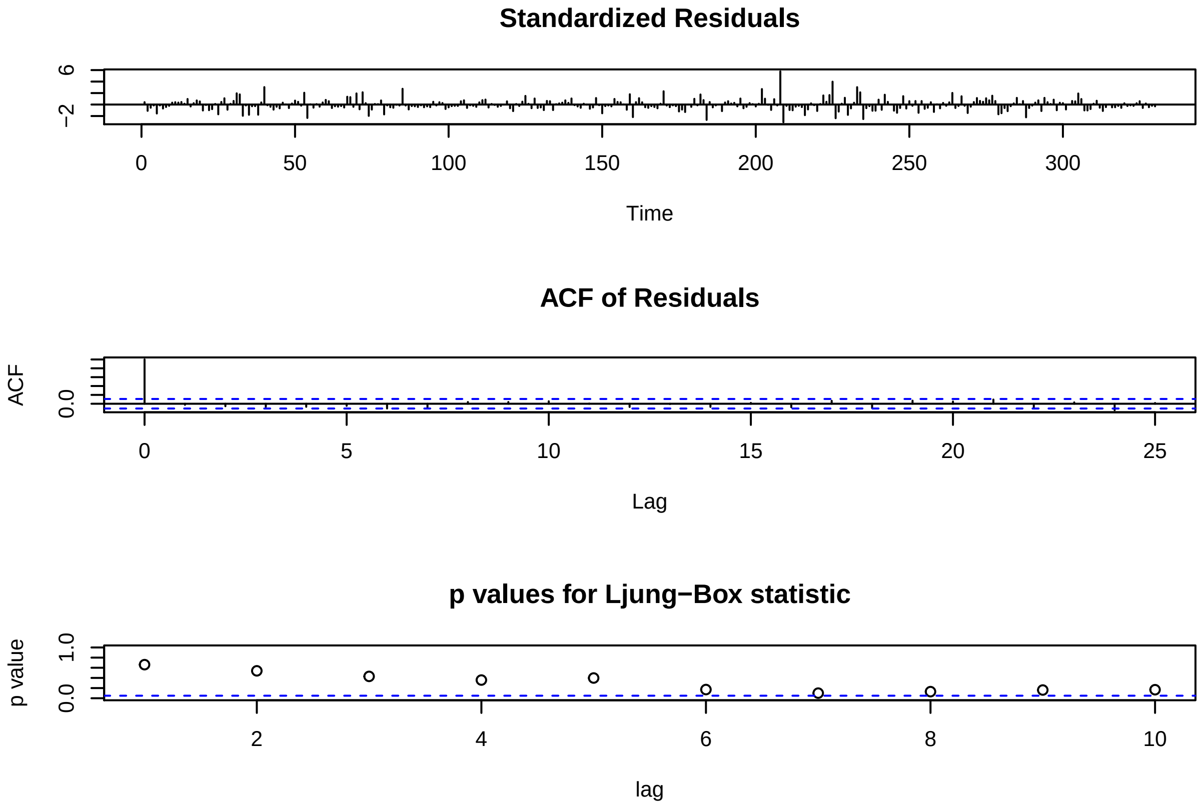
The PACF plot indicates a significant value at lag 5. Thus, we choose an AR(5) model.

```
##
## Call:
## arima(x = ts_stat_PT08.S3.NOx._train_set, order = c(5, 0, 0), include.mean = FALSE)
##
## Coefficients:
##           ar1      ar2      ar3      ar4      ar5
##       -0.2842  -0.3523  -0.3167  -0.2801  -0.1998
## s.e.   0.0539   0.0541   0.0546   0.0538   0.0539
##
## sigma^2 estimated as 20679:  log likelihood = -2108.17,  aic = 4228.34
```

So we have :

$$X_t = -0.2842X_{t-1} - 0.3523X_{t-2} - 0.3167X_{t-3} - 0.2801X_{t-4} - 0.1998X_{t-5}$$

Now we check that the residuals are likely white noise.



The ACF plot of residuals show no significant lags, so the AR(5) is likely a good representation of the series. Also, the p-values for Ljung-Box statistic are all greater than 0.05, so we cannot reject the hypothesis that the autocorrelation is different from 0. Therefore, the AR(5) model is an appropriate one.

3) ARMA model

4) Residuals

5) GARCH model

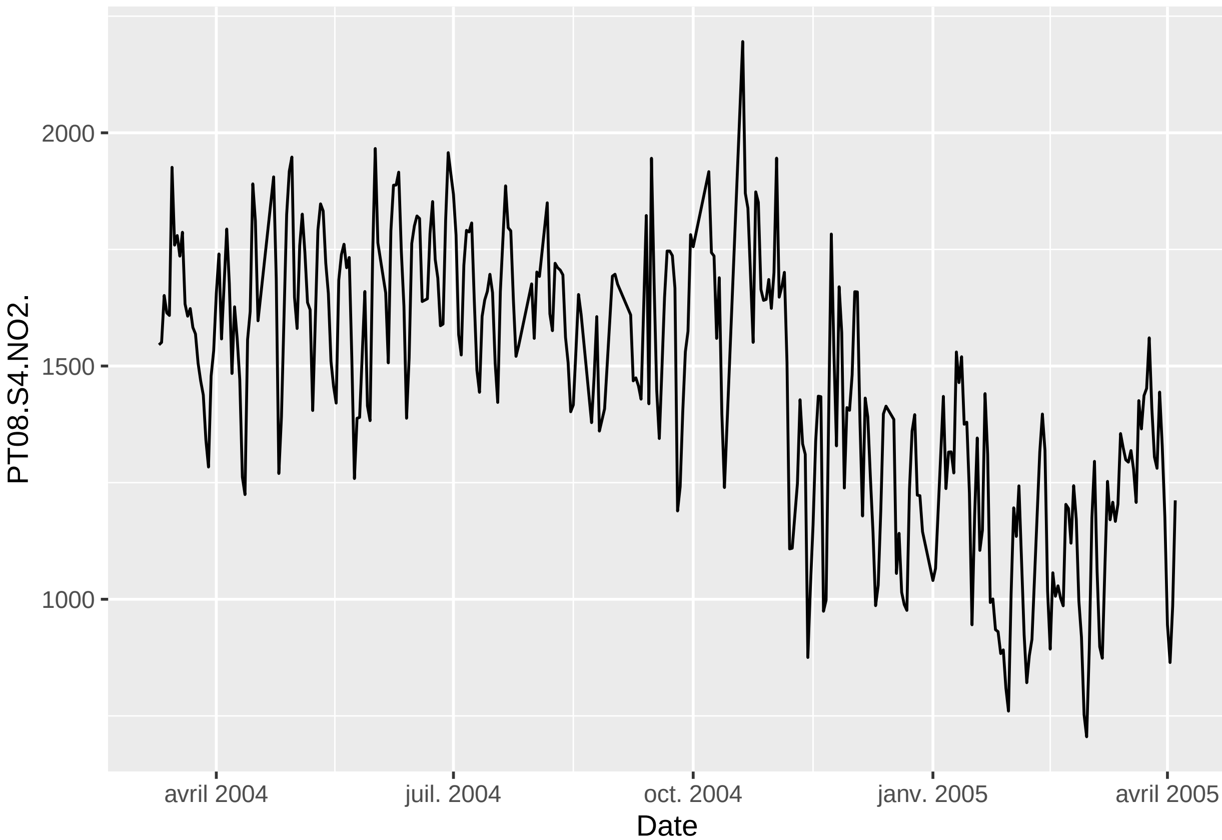
6) Prediction intervals for the 10 most recent data

III)-Training on the times series of interest using explanatory times series

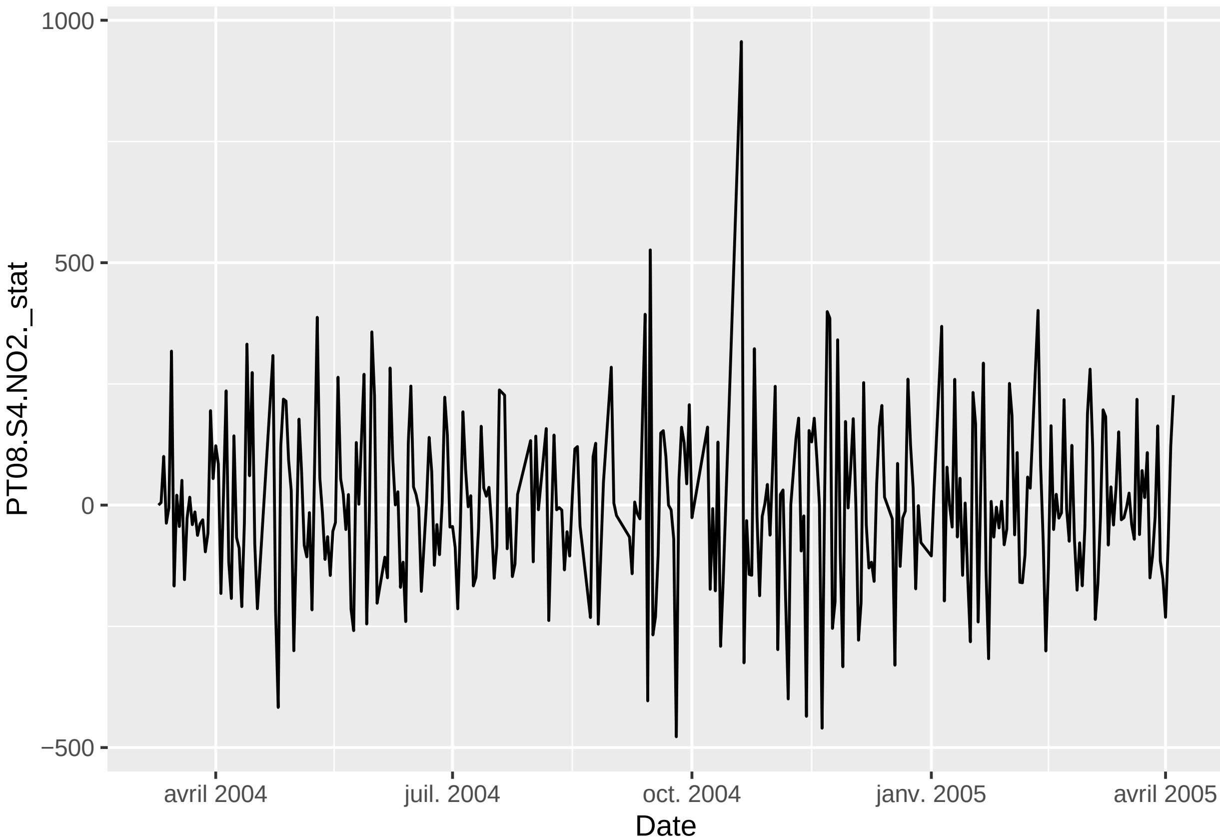
Yet, we will introduce other components, that we didn'tuse in the models previously. We do it in order to find better predictions and better confidence intervals.

1) Preprocessing

First, we have to stationarise our data with the same method as before. This means that we remove seasonal and trend components by using differencing.



We see indeed that this data need to be stationarised



As before, we apply the Augmented Dickey-Fuller Test

```
library(tseries)
test_stationnarity = adf.test(ts_stat_PT08.S4.NO2.)
```

```
## Warning in adf.test(ts_stat_PT08.S4.NO2.): p-value smaller than printed p-value
```

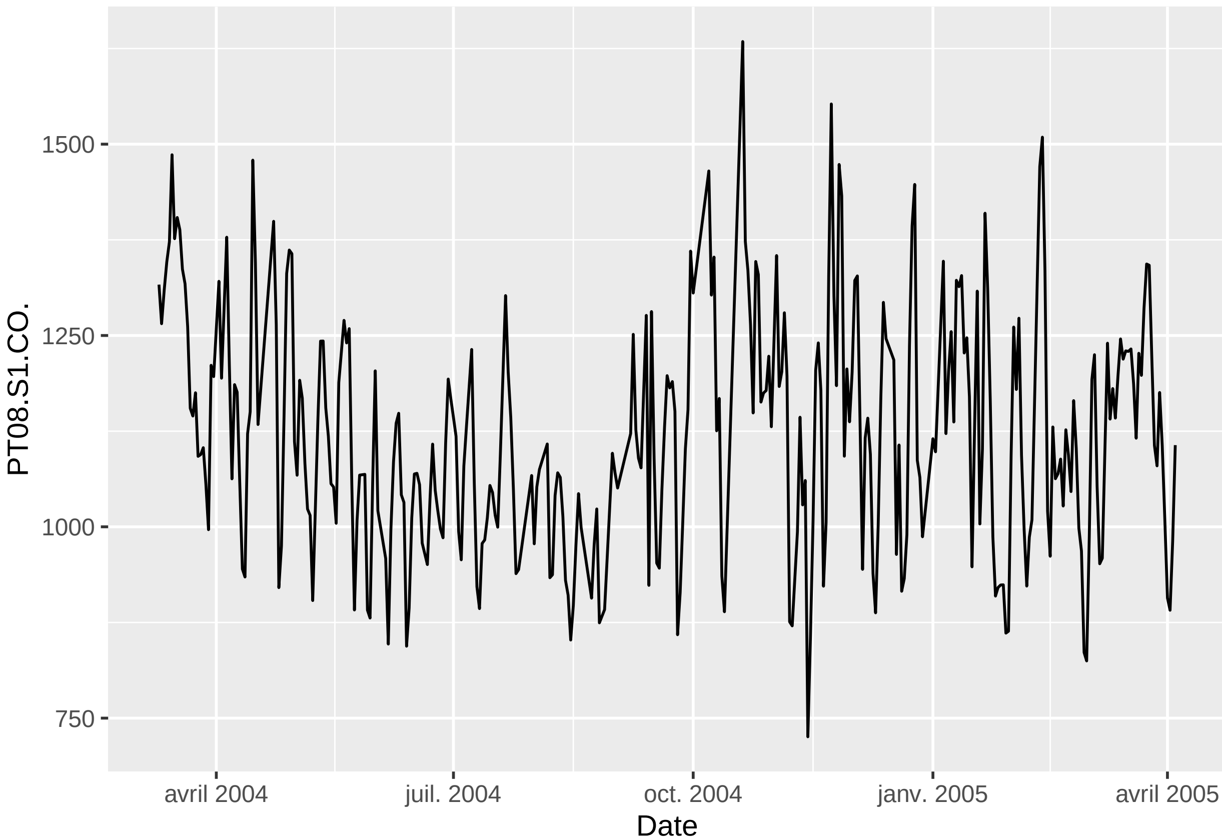
```
print(test_stationnarity)
```

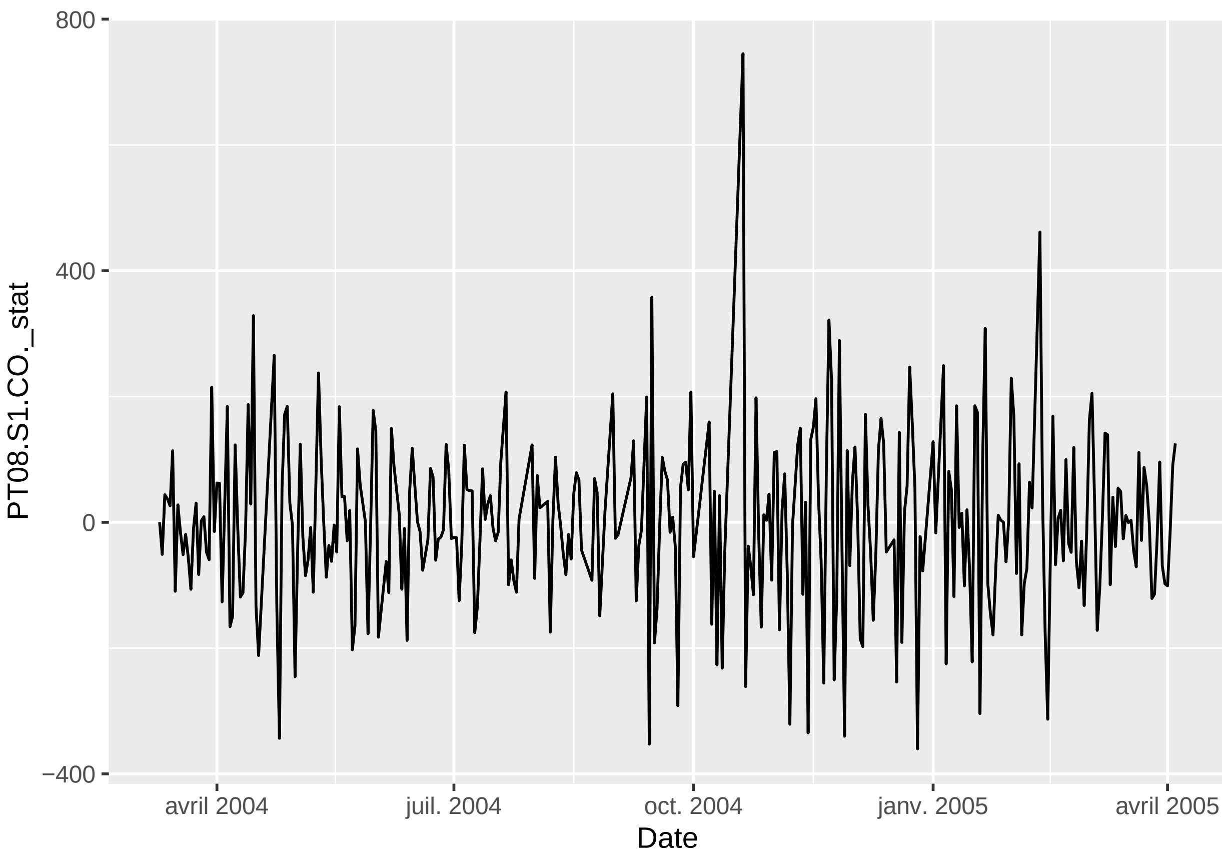
```
##
##  Augmented Dickey-Fuller Test
##
## data:  ts_stat_PT08.S4.NO2.
## Dickey-Fuller = -11.191, Lag order = 6, p-value = 0.01
## alternative hypothesis: stationary
```

We do it for each component with a name starting with PT.

To be sure that everything is fine, we use the Augmented Dickey-Fuller Test.

Here are the results for each component.


PT08.S1.CO.
1500
1250
1000
750
avril 2004
juil. 2004
oct. 2004
janv. 2005
avril 2005
Date

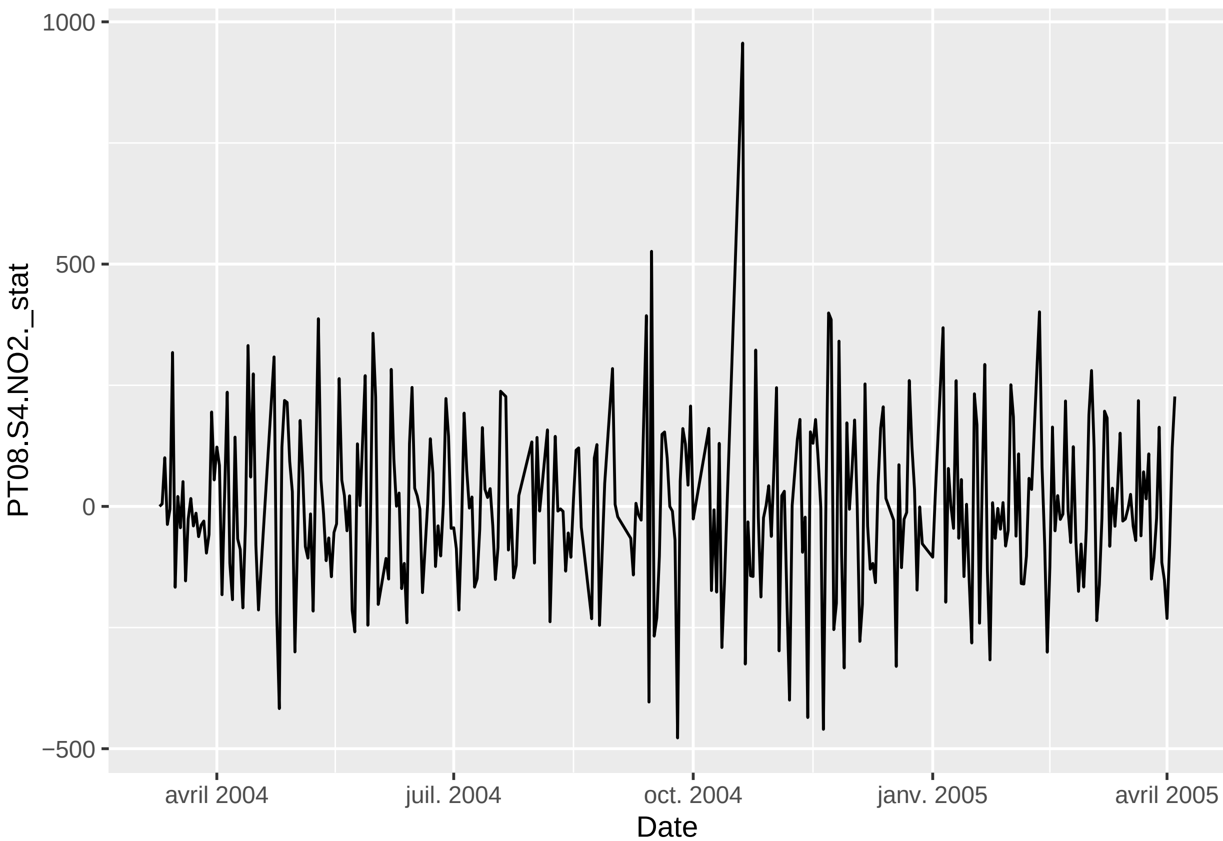

PT08.S1.CO._stat
800
400
0
−400
avril 2004
juil. 2004
oct. 2004
janv. 2005
avril 2005
Date

```r
library(tseries)
test_stationnarity = adf.test(ts_stat_PT08.S1.CO.)
```

```
## Warning in adf.test(ts_stat_PT08.S1.CO.): p-value smaller than printed p-value
```

```r
print(test_stationnarity)
```

```
##
##  Augmented Dickey-Fuller Test
##
## data:  ts_stat_PT08.S1.CO.
## Dickey-Fuller = -11.123, Lag order = 6, p-value = 0.01
## alternative hypothesis: stationary
```

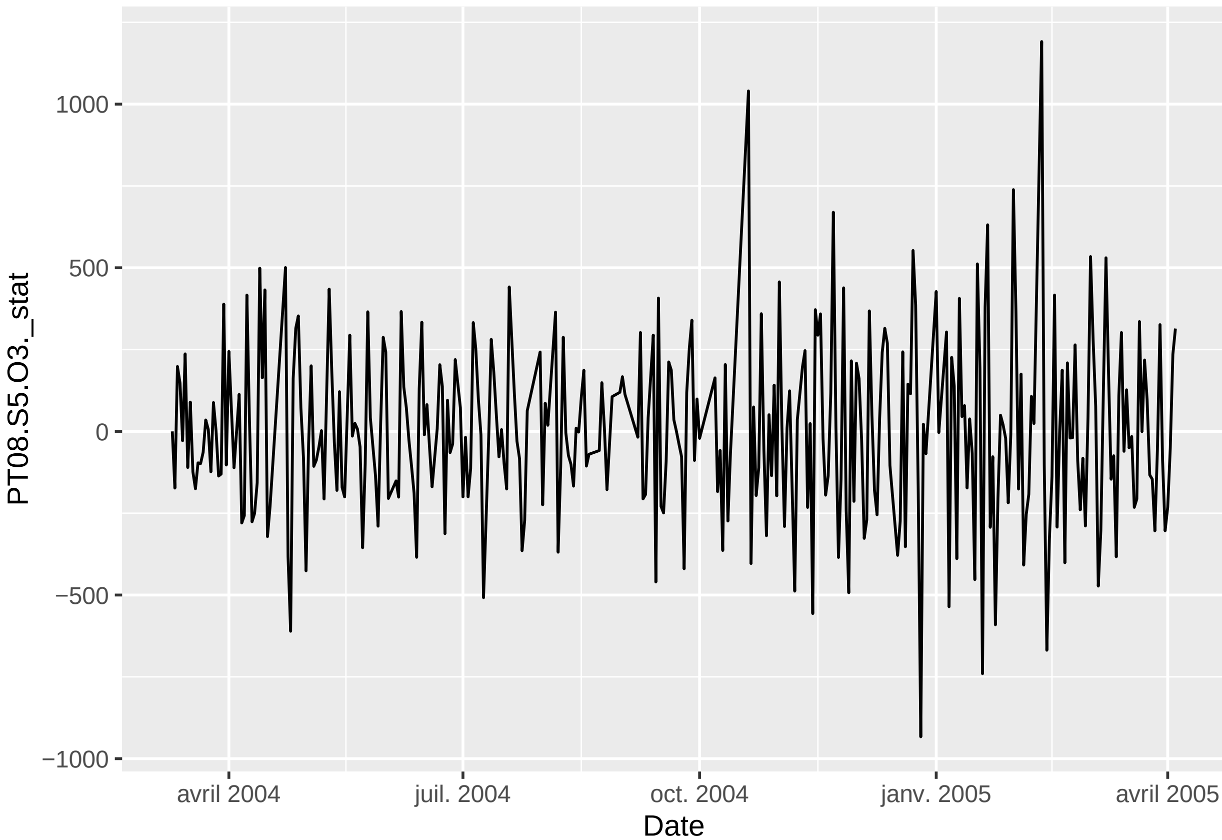



```r
#
library(tseries)
test_stationnarity = adf.test(ts_stat_PT08.S2.NMHC.)
```

```
## Warning in adf.test(ts_stat_PT08.S2.NMHC.): p-value smaller than printed p-value
```

```r
print(test_stationnarity)
```

```
##
##  Augmented Dickey-Fuller Test
##
## data:  ts_stat_PT08.S2.NMHC.
## Dickey-Fuller = -11.266, Lag order = 6, p-value = 0.01
## alternative hypothesis: stationary
```




```r
#
library(tseries)
test_stationnarity = adf.test(ts_stat_PT08.S5.O3.)
```

```
## Warning in adf.test(ts_stat_PT08.S5.O3.): p-value smaller than printed p-value
```

```r
print(test_stationnarity)
```

```
##
##  Augmented Dickey-Fuller Test
##
## data:  ts_stat_PT08.S5.O3.
## Dickey-Fuller = -11.178, Lag order = 6, p-value = 0.01
## alternative hypothesis: stationary
```

2) Time varying coefficients

Now we want to build a dynamical model thanks to the explanatory time series. We know that the order of the AR model was 5, so we will use 5 past values of the time series of interest for predicting the present value of the time series of interest too.

```
##          ytraining lag(ytraining, 1) lag(ytraining, 2) lag(ytraining, 3)
## [334,]  -14.251812         -6.708333          38.74275         138.21558
## [335,]   -6.708333         38.742754         138.21558          22.08333
## [336,]   38.742754        138.215580          22.08333        -131.90761
## [337,]  138.215580         22.083333        -131.90761                NA
## [338,]   22.083333       -131.907609                NA                NA
## [339,] -131.907609                NA                NA                NA
```

```
##        lag(ytraining, 4) lag(ytraining, 5) lag(ytraining, 6) lag(ytraining, 7)
## [334,]          22.08333         -131.9076                NA                NA
## [335,]        -131.90761                NA                NA                NA
## [336,]                NA                NA                NA                NA
## [337,]                NA                NA                NA                NA
## [338,]                NA                NA                NA                NA
## [339,]                NA                NA                NA                NA
##        lag(ytraining, 8) lag(ytraining, 9) lag(ytraining, 10)
## [334,]                NA                NA                 NA
## [335,]                NA                NA                 NA
## [336,]                NA                NA                 NA
## [337,]                NA                NA                 NA
## [338,]                NA                NA                 NA
## [339,]                NA                NA                 NA
```

We use the SSModel function. Our target variable is ts_PTO8.S3.NOx. and our covariates are the other components starting with PT.

3) QLIK

We have our model so we can use it with a QFAS in order to tune the hyperparameter.

4) Prediction

We have everything yet in order to do the prediction. The intervals of prediction can indeed be produced thanks to the use of the Kalman's recursion on the tuned dynamical model.

Let's explain why we use this : by contrast with the AR models, it is much more difficult to find the best possible (linear) prediction of an ARMA mode. Indeed, as soon as the MA part is non degenerate, the filter can have infinitely many non null coefficients.

One way to solve the problem is to consider ARMA model as a more general linear model called state space models. Those models have been introduced in signal processing and the best linear prediction can be computed recursively by the Kalman's recursion. How does this work ? A state space linear model of dimension r with constant coefficient is given by a system of space euqation and state equations of the form : $X_t = G^T Y_t + Z_T$ $Y_t = FY_{t-1} + V_t$ which are respectively the Space equation and the State equation, where (Z_t) and (V_t) are uncorrelated white noise with variance R and Q, G ∈ Rr, F ∈ M(r,r) and Y ∈ Rr is the random state of the system. The Kalman theorem says : In a state-space model with constant coefficients, if $\widehat{Y_0}$ and Ω_0 are well chosen, one can compute recursively

$$\widehat{X_n} = \pi_{n-1}(X_n)$$
$$R_n^L = E[(X_n - \widehat{X_n})^2]$$
$$\widehat{Y_n} = \pi_{n-1}(Y_n)$$
$$and\ \Omega_n = E[(Y_n - \widehat{Y_n})(Y_n - \widehat{Y_n})^T]$$
$$by\ the\ following\ recursion\ : \widehat{Y_{n+1}} = F\widehat{Y_n} + \frac{F\Omega_n G}{R_n^L} * (X_n - G^T\widehat{Y_n})$$
$$\widehat{X_{n+1}} = (G)^T * \widehat{Y_{n+1}}$$
$$\Omega_{n+1} = F\Omega_n F^T + Q - \frac{F\Omega_n G}{R_n} * G^T\Omega_n F^T$$

$$R_{n+1}^L = G^T \Omega_{n+1} G + R$$

The Kalman's recursion has several advantages : - It is a recursve procedures - Each step requires the inversion of a scalar RL n and not the entire covariance matrix - The recursion can handle missing values nicely

However, there are also some drawbacks : - Tuning hyperparameters requires a non explicit minimization - The recursion can be instable

Our target variable is ts_PTO8.S3.NOx. and our covariates are the other components starting with PT.

IV) Conclusion