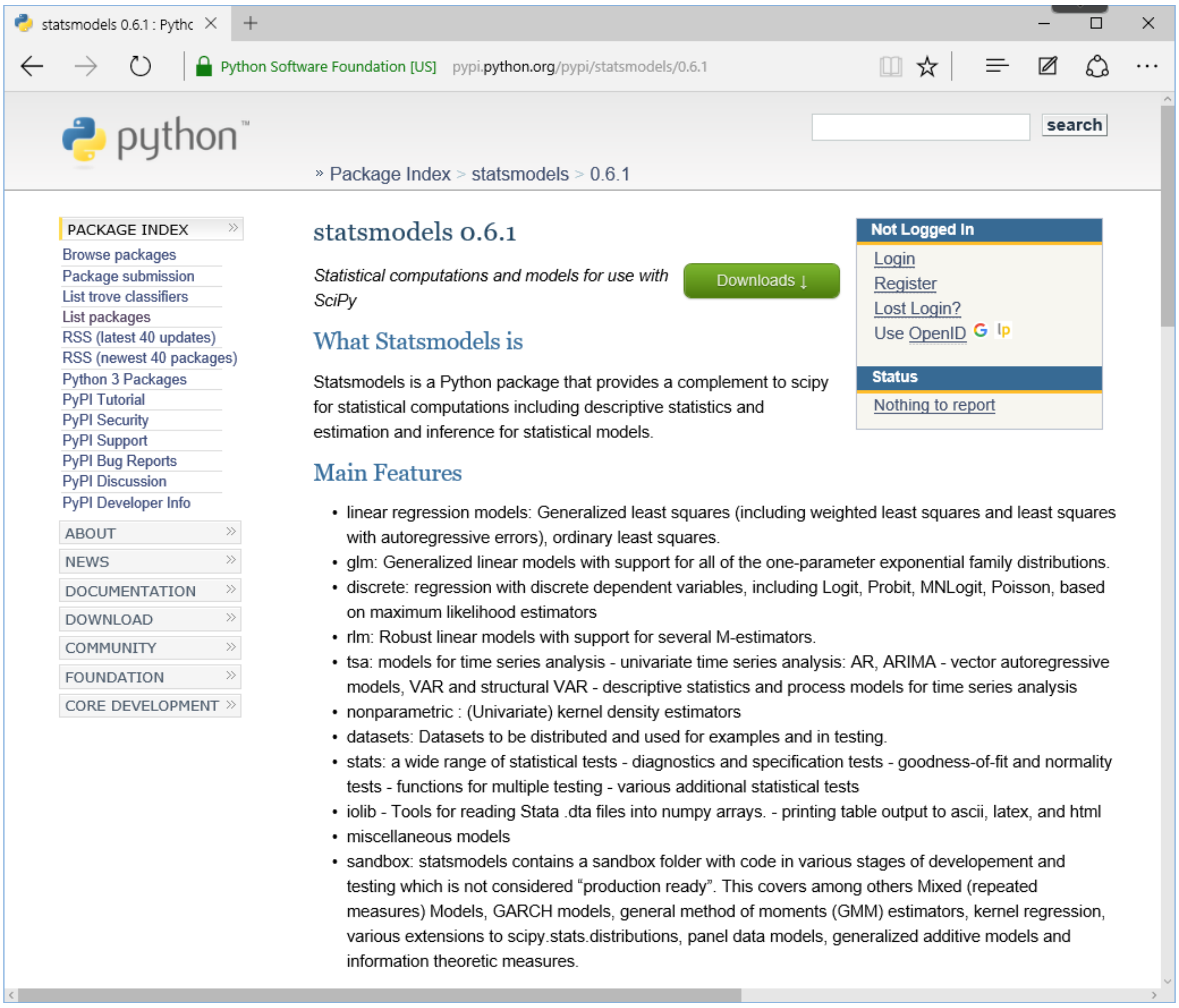
1 Introduction

Regression analysis with the StatsModels package for Python.

Statsmodels is a Python module that provides classes and functions for the estimation of many different statistical models, as well as for conducting statistical tests, and statistical data exploration. The description of the library is available on the PyPI page, the repository that lists the tools and packages devoted to Python[1].



statsmodels 0.6.1

Statistical computations and models for use with SciPy

What Statsmodels is

Statsmodels is a Python package that provides a complement to scipy for statistical computations including descriptive statistics and estimation and inference for statistical models.

Main Features

- linear regression models: Generalized least squares (including weighted least squares and least squares with autoregressive errors), ordinary least squares.
- glm: Generalized linear models with support for all of the one-parameter exponential family distributions.
- discrete: regression with discrete dependent variables, including Logit, Probit, MNLogit, Poisson, based on maximum likelihood estimators
- rlm: Robust linear models with support for several M-estimators.
- tsa: models for time series analysis - univariate time series analysis: AR, ARIMA - vector autoregressive models, VAR and structural VAR - descriptive statistics and process models for time series analysis
- nonparametric : (Univariate) kernel density estimators
- datasets: Datasets to be distributed and used for examples and in testing.
- stats: a wide range of statistical tests - diagnostics and specification tests - goodness-of-fit and normality tests - functions for multiple testing - various additional statistical tests
- iolib - Tools for reading Stata .dta files into numpy arrays. - printing table output to ascii, latex, and html
- miscellaneous models
- sandbox: statsmodels contains a sandbox folder with code in various stages of developement and testing which is not considered "production ready". This covers among others Mixed (repeated measures) Models, GARCH models, general method of moments (GMM) estimators, kernel regression, various extensions to scipy.stats.distributions, panel data models, generalized additive models and information theoretic measures.

In this tutorial, we will try to identify the potentialities of StatsModels by conducting a case study in multiple linear regression. We will discuss about: the estimation of model parameters using the ordinary least squares method, the implementation of some statistical tests, the checking of the model assumptions by analyzing the residuals, the detection of

[1] The French version of this tutorial was written in September 2015. We were using the **version 0.6.1**.

outliers and influential points, the analysis of multicollinearity, the calculation of the prediction interval for a new instance.

About the regression analysis, an excellent reference is the online course available on the PennState Eberly College of Science website: "STAT 501 - Regression Methods".

2 Dataset

We use the "vehicules_1.txt" data file for the construction of the model. It describes n = 26 vehicles from their characteristics: engine size (cylindrée), horsepower (puissance), weight (poids) and consumption (conso, liter per 100 km).

modele	cylindree	puissance	poids	conso
Maserati Ghibli GT	2789	209	1485	14.5
Daihatsu Cuore	846	32	650	5.7
Toyota Corolla	1331	55	1010	7.1
Fort Escort 1.4i PT	1390	54	1110	8.6
Mazda Hachtback V	2497	122	1330	10.8
Volvo 960 Kombi aut	2473	125	1570	12.7
Toyota Previa salon	2438	97	1800	12.8
Renault Safrane 2.2. V	2165	101	1500	11.7
Honda Civic Joker 1.4	1396	66	1140	7.7
VW Golt 2.0 GTI	1984	85	1155	9.5
Suzuki Swift 1.0 GLS	993	39	790	5.8
Lancia K 3.0 LS	2958	150	1550	11.9
Mercedes S 600	5987	300	2250	18.7
Volvo 850 2.5	2435	106	1370	10.8
VW Polo 1.4 60	1390	44	955	6.5
Hyundai Sonata 3000	2972	107	1400	11.7
Opel Corsa 1.2i Eco	1195	33	895	6.8
Opel Astra 1.6i 16V	1597	74	1080	7.4
Peugeot 306 XS 108	1761	74	1100	9
Mitsubishi Galant	1998	66	1300	7.6
Citroen ZX Volcane	1998	89	1140	8.8
Peugeot 806 2.0	1998	89	1560	10.8
Fiat Panda Mambo L	899	29	730	6.1
Seat Alhambra 2.0	1984	85	1635	11.6
Ford Fiesta 1.2 Zetec	1242	55	940	6.6

We want to explain / predict the consumption of the cars (y : CONSO) from **p = 3** input (explanatory, predictor) variables (X_1 : cylindrée, X_2 : puissance, X_3 : poids).

The regression equation is written as

$$y_i = a_0 + a_1 x_{i1} + a_2 x_{i2} + a_3 x_{i3} + \varepsilon_i, \; i = 1, \ldots, n$$

The aim of the regression analysis is to estimate the values of the coefficients (a_0, a_1, a_2, a_3) using the available dataset.

3 Data importation

We use the Pandas package for importing the data file into a data frame structure.

```
#modifying the default directory
import os
os.chdir("… directory containing the data file …")

#importing the Pandas library
#reading the data file with read.table()
import pandas
cars = pandas.read_table("vehicules_1.txt",sep="\t",header=0,index_col=0)
```

In the **read_table()** command, we specify: the first row represents the name of the variables (**header = 0**), the first column (n°0) represents the labels of the instances (**index_col = 0**). We display the dimensions of the dataset. We retrieve the values of **n** (number of instances) and **p** (number of input variables for the regression).

```
#dimensions
print(cars.shape)

#number of instances
n = cars.shape[0]

#number of input variables for the regression
p = cars.shape[1] - 1
```

We have **n = 26** rows and 4 columns, of which **p = 3** explanatory variables.

We display the type of the variables:

```
#list of variables and their types
print(cars.dtypes)
```

All the variables are numeric (integer or float). The first column (n°0) which represents the labels of the instances is not accounted for here.

```
cylindree      int64
puissance      int64
poids          int64
conso        float64
dtype: object
```

We access to the labels with the **index** property.

```
#list of the cars
```

```
print(cars.index)
```

We obtain:

```
Index(['Maserati Ghibli GT', 'Daihatsu Cuore', 'Toyota Corolla',
       'Fort Escort 1.4i PT', 'Mazda Hachtback V', 'Volvo 960 Kombi aut',
       'Toyota Previa salon', 'Renault Safrane 2.2. V',
       'Honda Civic Joker 1.4', 'VW Golt 2.0 GTI', 'Suzuki Swift 1.0 GLS',
       'Lancia K 3.0 LS', 'Mercedes S 600', 'Volvo 850 2.5', 'VW Polo 1.4 60',
       'Hyundai Sonata 3000', 'Opel Corsa 1.2i Eco', 'Opel Astra 1.6i 16V',
       'Peugeot 306 XS 108', 'Mitsubishi Galant', 'Citroen ZX Volcane',
       'Peugeot 806 2.0', 'Fiat Panda Mambo L', 'Seat Alhambra 2.0',
       'Ford Fiesta 1.2 Zetec'],
      dtype='object', name='modele')
```

4 Regression analysis

4.1 Launching the analysis

We can perform the modelling step by importing the Statsmodels package. We have two options. (1) The first consists of dividing the data into two parts: a vector containing the values of the target variable CONSO, a matrix with the explanatory variables CYLINDREE, POWER, CONSO. Then, we pass them to the OLS tool. This implies some manipulation of data, and especially we must convert the data frame structure into numpy vector and matrix. (2) The second is based on a specific tool (ols) which directly recognizes formulas similar to the ones used under R [e. g. lm() function for R]. The Pandas data frame structure can be used directly in this case. We prefer this second solution.

```
#regression with formula
import statsmodels.formula.api as smf

#instantiation
reg = smf.ols('conso ~ cylindree + puissance + poids', data = cars)

#members of reg object
print(dir(reg))
```

reg is an instance of the class **ols**. We can list their members with the **dir()** command i.e. properties and methods.

```
['__class__', '__delattr__', '__dict__', '__dir__', '__doc__', '__eq__',
'__format__', '__ge__', '__getattribute__', '__gt__', '__hash__', '__init__',
'__le__', '__lt__', '__module__', '__ne__', '__new__', '__reduce__',
'__reduce_ex__', '__repr__', '__setattr__', '__sizeof__', '__str__',
'__subclasshook__', '__weakref__', '_data_attr', '_df_model', '_df_resid',
'_get_init_kwds', '_handle_data', '_init_keys', 'data', 'df_model', 'df_resid',
'endog', 'endog_names', 'exog', 'exog_names', 'fit', 'fit_regularized', 'formula',
'from_formula', 'hessian', 'information', 'initialize', 'k_constant', 'loglike',
'nobs', 'predict', 'rank', 'score', 'weights', 'wendog', 'wexog', 'whiten']
```

We use the **fit()** command to launch the modelling process on the dataset.

```
#launching the modelling process
res = reg.fit()

#members of the object provided by the modelling
print(dir(res))
```

The **res** object has also various properties and methods.

```
['HC0_se', 'HC1_se', 'HC2_se', 'HC3_se', '_HCCM', '__class__', '__delattr__',
'__dict__', '__dir__', '__doc__', '__eq__', '__format__', '__ge__',
'__getattribute__', '__gt__', '__hash__', '__init__', '__le__', '__lt__',
'__module__', '__ne__', '__new__', '__reduce__', '__reduce_ex__', '__repr__',
'__setattr__', '__sizeof__', '__str__', '__subclasshook__', '__weakref__',
'_cache', '_data_attr', '_get_robustcov_results', '_is_nested',
'_wexog_singular_values', 'aic', 'bic', 'bse', 'centered_tss', 'compare_f_test',
'compare_lm_test', 'compare_lr_test', 'condition_number', 'conf_int',
'conf_int_el', 'cov_HC0', 'cov_HC1', 'cov_HC2', 'cov_HC3', 'cov_kwds',
'cov_params', 'cov_type', 'df_model', 'df_resid', 'eigenvals', 'el_test', 'ess',
'f_pvalue', 'f_test', 'fittedvalues', 'fvalue', 'get_influence',
'get_robustcov_results', 'initialize', 'k_constant', 'llf', 'load', 'model',
'mse_model', 'mse_resid', 'mse_total', 'nobs', 'normalized_cov_params',
'outlier_test', 'params', 'predict', 'pvalues', 'remove_data', 'resid',
'resid_pearson', 'rsquared', 'rsquared_adj', 'save', 'scale', 'ssr', 'summary',
'summary2', 't_test', 'tvalues', 'uncentered_tss', 'use_t', 'wald_test', 'wresid']
```

summary() displays the details of the result.

```
#detailed results
print(res.summary())
```

The presentation is conventional, as seen in most of statistical tools.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  conso   R-squared:                       0.957
Model:                            OLS   Adj. R-squared:                  0.951
Method:                 Least Squares   F-statistic:                     154.7
Date:                Sun, 27 Sep 2015   Prob (F-statistic):           1.79e-14
Time:                        09:35:48   Log-Likelihood:                -24.400
No. Observations:                  25   AIC:                             56.80
Df Residuals:                      21   BIC:                             61.68
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
Intercept      1.2998      0.614      2.117      0.046         0.023     2.577
cylindree     -0.0005      0.000     -0.953      0.351        -0.002     0.001
puissance      0.0303      0.007      4.052      0.001         0.015     0.046
poids          0.0052      0.001      6.447      0.000         0.004     0.007
==============================================================================
Omnibus:                        0.799   Durbin-Watson:                   2.419
Prob(Omnibus):                  0.671   Jarque-Bera (JB):                0.772
Skew:                          -0.369   Prob(JB):                        0.680
Kurtosis:                       2.558   Cond. No.                     1.14e+04
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.14e+04. This might indicate that there are
strong multicollinearity or other numerical problems.
```

The coefficient of determination is equal to $R^2 = 0.975$. The regression is globally significant at the 5% level [F-statistic = 154.7, with Prob(F-statistic) = 1.79e-14]. All the coefficients seem also significant at the 5% level (see t and P>|t| into the coefficients table).

Everything seems to be going well. But a warning message alerts us nevertheless. A collinearity problem between explanatory variables is suspected. We will check it later.

4.2 Intermediate computations

The object **res** enables to perform intermediate calculations. Some are relatively simple. Below, we display some important results (estimated coefficients, R2). We try to calculate manually the F-Statistic. We have the same as the value provided by the **res** object of course.

```
#estimated coefficients
print(res.params)

#R2
print(res.rsquared)

#calculating the F-statistic
F = res.mse_model / res.mse_resid
print(F)

#F provided by the res object
print(res.fvalue)
```

Other calculations are possible, giving us access to sophisticated procedures such as tests that a subset of the slopes is null.

We try to test that all the slopes are 0. This is a special case of the testing that a subset is null. The null hypothesis may be written in a matrix format.

$$H_0 : Ra = 0$$

Where

- a = (a_0,a_1,a_2,a_3) is the vector of the coefficients;
- R is the matrix of constraints:

$$R = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

We can write the test in a more explicit form:

$$H_0 : \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\Leftrightarrow H_0 : \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

In Python, we describe the R matrix, then we call the **f_test()** procedure:

```
#test for a linear combination of coefficients
#all the slopes are zero
import numpy as np

#matrix R
R = np.array([[0,1,0,0],[0,0,1,0],[0,0,0,1]])

#F-statistic
print(res.f_test(R))
```

We obtain the F-statistic for the global significance (model significance).

```
<F test: F=array([[ 154.67525358]]), p=1.7868899968536844e-14, df_denom=21, df_num=3>
```

5 Regression diagnostic

5.1 Model assumptions – Test for error normality

One of the main assumption for the inferential part of the regression (OLS - ordinary least squares) is the assumption that the errors follow a normal distribution. A first important verification is to check the compatibility of the residuals (the errors observed on the sample) with this assumption.

Jarque-Bera Test. We use the **stattools** module in order to perform the Jarque-Bera test. This test checks if the observed skewness and kurtosis matching a normal distribution.

```
#Jarque-Bera normality test
import statsmodels.api as sm
JB, JBpv,skw,kurt = sm.stats.stattools.jarque_bera(res.resid)
print(JB,JBpv,skw,kurt)
```

We have respectively: the statistic JB, the p-value of the test JBpv, the skewness skw and the kurtosis kurt.

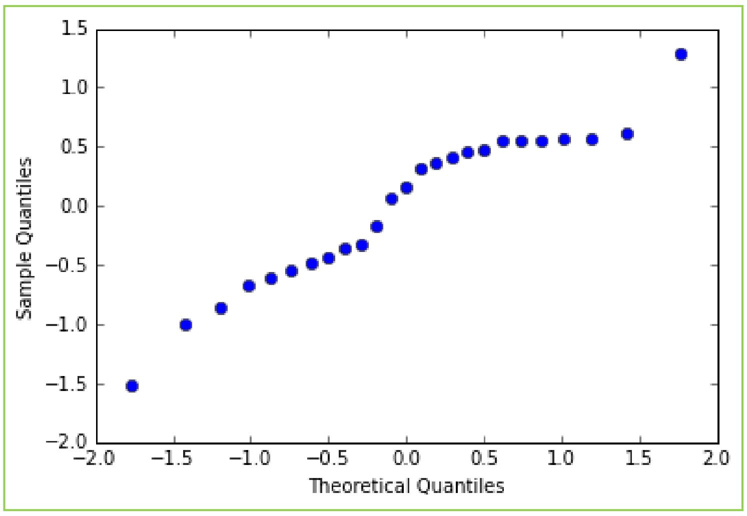
```
0.7721503004927122 0.679719442677 -0.3693040742424057 2.5575948785729956
```

We observe that the values obtained (JB, JBpv) are consistent with those provided by the summary() command above (page 5). Here, we can assume that the errors are a normal distribution at the 5% level.

Normal probability plot. The normal probability plot is a graphical technique to identify substantive departures from normality. It is based on the comparison between the observed distribution and the theoretical distribution under the normal assumption. The null hypothesis (normal distribution) is rejected if the points are not aligned on a straight line. We use the **qqplot()** procedure.

```
#qqpolot vs. normal distribution
sm.qqplot(res.resid)
```

We have a graphical representation.



The graph confirms the Jarque-Bera test. The points are approximately aligned. But there seems to be some problems with the high values of the residuals. This suggests the existence of atypical points in our data.

5.2 Detection of outliers and influential points

We use a specific object provided by the regression result to analyze the influential points.

```
#object for the analysis of influential points
infl = res.get_influence()

#members
print(dir(infl))
```

We have some properties and methods.

```
['__class__', '__delattr__', '__dict__', '__dir__', '__doc__', '__eq__',
'__format__', '__ge__', '__getattribute__', '__gt__', '__hash__', '__init__',
'__le__', '__lt__', '__module__', '__ne__', '__new__', '__reduce__',
'__reduce_ex__', '__repr__', '__setattr__', '__sizeof__', '__str__',
'__subclasshook__', '__weakref__', '_get_drop_vari', '_ols_xnoti', '_res_looo',
'aux_regression_endog', 'aux_regression_exog', 'cooks_distance', 'cov_ratio',
'det_cov_params_not_obsi', 'dfbetas', 'dffits', 'dffits_internal', 'endog',
'ess_press', 'exog', 'get_resid_studentized_external', 'hat_diag_factor',
'hat_matrix_diag', 'influence', 'k_vars', 'model_class', 'nobs', 'params_not_obsi',
'resid_press', 'resid_std', 'resid_studentized_external',
'resid_studentized_internal', 'resid_var', 'results', 'sigma2_not_obsi',
'sigma_est', 'summary_frame', 'summary_table']
```

Leverage and internally studentized residuals (standardized residuals). We display for instance the leverage and the internally studentized residuals.

```
#leverage
print(infl.hat_matrix_diag)
```

```
#internally studentized residuals
print(infl.resid_studentized_internal)
```

We have, respectively: leverage,

```
[ 0.72183931  0.17493953  0.06052439  0.05984303  0.05833457  0.09834565
  0.3069384   0.09434881  0.07277269  0.05243782  0.11234304  0.08071319
  0.72325833  0.05315383  0.08893405  0.25018637  0.10112179  0.0540076
  0.05121573  0.10772156  0.05567033  0.16884879  0.13204031  0.24442832
  0.07603257]
```

and internally studentized residuals.

```
[ 1.27808674  0.70998577 -0.71688165  0.81147383  0.10804304  0.93643923
  0.61326258  0.85119912 -1.28230456  0.82173104 -0.4825047  -0.89285915
 -1.47915409  0.46985347 -0.65771702  2.12388261  0.62133156 -1.46735362
  0.84071707 -2.28450314 -0.25846374 -0.56426915  0.84517318  0.26915841
 -0.98733251]
```

Knowing how to code allows us to verify by calculation the results proposed by the different procedures. For instance, we can obtain the internally studentized residuals (*t*$_i$) from the residuals $\hat{\varepsilon}_i = y_i - \hat{y}_i$, the leverage h_i and the regression standard error $\hat{\sigma}_\varepsilon$ obtained from the **scale** property of the object resulting from the regression (**res.scale**):

$$t_i = \frac{\hat{\varepsilon}_i}{\hat{\sigma}_\varepsilon \sqrt{1-h_i}}$$

We use the following commands:

```
#checking the values of the internally studentized residuals
import numpy as np
residus = res.resid.as_matrix() #residuals
leviers = infl.hat_matrix_diag #leverage
sigma_err = np.sqrt(res.scale) #regression standard error
res_stds = residus/(sigma_err*np.sqrt(1.0-leviers))
print(res_stds)
```

The values are consistent to those provided directly with the property "resid_studenized_internal". Fortunately, we would have been quite disturbed otherwise.

Externally studentized residuals. We repeat the approach for the externally studentized residuals, using the following formula:

$$t_i^* = t_i \sqrt{\frac{n-p-2}{n-p-1-t_i^2}}$$

We compare the values provided by the property resid_studentized_external and the values obtained by the formula above.

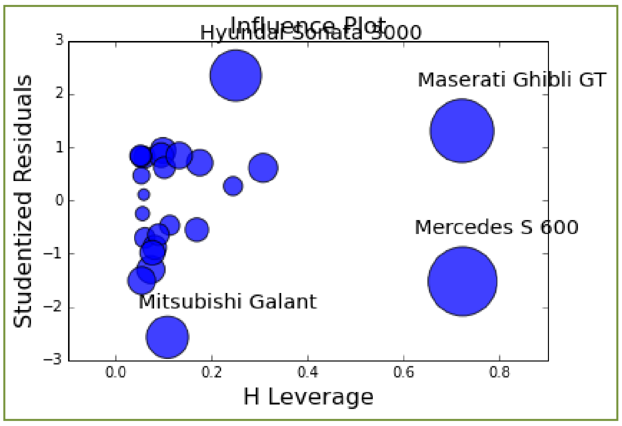
```
#values provided by the property of the object
print(infl.resid_studentized_external)
#checking with the formula
res_studs = res_stds*np.sqrt((n-p-2)/(n-p-1-res_stds**2))
print(res_studs)
```

Here also, the results are consistent.

```
[ 1.29882255  0.70134375 -0.70832574  0.80463315  0.10546853  0.933571
  0.60391521  0.8453972  -1.30347228  0.81513961 -0.4735084  -0.88836644
 -1.52514011  0.46095935 -0.64858111  2.33908893  0.61200904 -1.51157649
  0.83462166 -2.57180996 -0.25263694 -0.55489299  0.83920081  0.26312597
 -0.98671171]
```

Graphical representation. StatsModels provides a graphical tool to identify the suspicious observations.

```
#graphical representation of the influences()
sm.graphics.influence_plot(res)
```



The problem concern Mitsubishi Galant, Hyundai Sonata, Mercedes S 600 and Maserati Ghibli GT.

Automatic detection – Comparison to a threshold value. Visually inspecting the data is a good thing. But being able to detect outliers and/or influential points automatically is preferable, especially when the number of observations is high. To do this, we need to define threshold values from which a point becomes suspect.

Leverage. For the leverage, the threshold value may be:

$$s_h = 2 \times \frac{p+1}{n}$$

An observation is suspicious if $h_i > s_h$

```
#threshold leverage
seuil_levier = 2*(p+1)/n
print(seuil_levier)

#identification
atyp_levier = leviers > seuil_levier
print(atyp_levier)
```

Python displays a vector of Boolean values. True represents instances with a leverage higher than the threshold value.

```
[ True False False False False False False False False False False False
  True False False False False False False False False False False False False]
```

The reading is not easy. It is more convenient to display the index of the vehicles.

```
#which vehicles?
print(cars.index[atyp_levier],leviers[atyp_levier])
```

We have both the car model and the values of the leverage.

```
Index(['Maserati Ghibli GT', 'Mercedes S 600'], dtype='object', name='modele') [
0.72183931  0.72325833]
```

Externally studentized residuals. The probability distribution of the externally studentized residuals is a Student distribution with (n-p-2) degrees of freedom. Thus, at the 5% level, the threshold value is

$$s_t = t_{1-0.05/2}(n-p-2)$$

Where $\mathbf{t_{1-0.05/2}}$ is the quantile of the t distribution for a probability 0.975.

An observation is suspicious if

$$\left|t_i^*\right| > s_t$$

```
#threshold externally studentized residuals
import scipy
seuil_stud = scipy.stats.t.ppf(0.975,df=n-p-2)
print(seuil_stud)

#detection - absolute value > threshold
atyp_stud = np.abs(res_studs) > seuil_stud

#which ones?
print(cars.index[atyp_stud],res_studs[atyp_stud])
```

These are,

```
Index(['Hyundai Sonata 3000', 'Mitsubishi Galant'], dtype='object', name='modele')
[ 2.33908893 -2.57180996]
```

Combination of leverage and externally studentized residuals. By combining the two approaches with the logical operator OR,

```
#suspicious observations with one of the two criteria
pbm_infl = np.logical_or(atyp_levier,atyp_stud)
print(cars.index[pbm_infl])
```

We identify 4 vehicles which are highlighted into the graphical representation above.

```
Index(['Maserati Ghibli GT', 'Mercedes S 600', 'Hyundai Sonata 3000',
       'Mitsubishi Galant'], dtype='object', name='modele')
```

Other criteria. The tool provides other criteria such as DFFITS, Cook's distance, etc. We can present them in a tabular form.

```
#Other criteria for detecting influential points
print(infl.summary_frame().filter(["hat_diag","student_resid","dffits","cooks_d"]))
```

Values should be compared with their respective thresholds:

- $|DFFITS_i| > 2\sqrt{\frac{p+1}{n}}$ for DFFITS ;
- $D_i > \frac{4}{n-p-1}$ for Cook's distance.

```
                     hat_diag  student_resid    dffits   cooks_d
modele
Maserati Ghibli GT   0.721839       1.298823  2.092292  1.059755
Daihatsu Cuore       0.174940       0.701344  0.322948  0.026720
Toyota Corolla       0.060524      -0.708326 -0.179786  0.008277
Fort Escort 1.4i PT  0.059843       0.804633  0.203004  0.010479
Mazda Hachtback V    0.058335       0.105469  0.026251  0.000181
Volvo 960 Kombi aut  0.098346       0.933571  0.308322  0.023912
Toyota Previa salon  0.306938       0.603915  0.401898  0.041640
Renault Safrane 2.2. V  0.094349    0.845397  0.272865  0.018870
Honda Civic Joker 1.4  0.072773    -1.303472 -0.365168  0.032263
VW Golt 2.0 GTI      0.052438       0.815140  0.191757  0.009342
Suzuki Swift 1.0 GLS  0.112343     -0.473508 -0.168453  0.007366
Lancia K 3.0 LS      0.080713      -0.888366 -0.263232  0.017498
Mercedes S 600       0.723258      -1.525140 -2.465581  1.429505
Volvo 850 2.5        0.053154       0.460959  0.109217  0.003098
VW Polo 1.4 60       0.088934      -0.648581 -0.202639  0.010557
Hyundai Sonata 3000  0.250186       2.339089  1.351145  0.376280
```

```
Opel Corsa 1.2i Eco     0.101122       0.612009  0.205272  0.010858
Opel Astra 1.6i 16V     0.054008      -1.511576 -0.361172  0.030731
Peugeot 306 XS 108      0.051216       0.834622  0.193913  0.009538
Mitsubishi Galant       0.107722      -2.571810 -0.893593  0.157516
Citroen ZX Volcane      0.055670      -0.252637 -0.061340  0.000985
Peugeot 806 2.0         0.168849      -0.554893 -0.250103  0.016171
Fiat Panda Mambo L      0.132040       0.839201  0.327318  0.027167
Seat Alhambra 2.0       0.244428       0.263126  0.149659  0.005859
Ford Fiesta 1.2 Zetec   0.076033      -0.986712 -0.283049  0.020054
```

Note: Detecting outliers or influential points is one thing, dealing them is another. Indeed, we cannot remove them systematically. It is necessary to identify why an observation is problematic and thus to determine the most appropriate solution, which may be deletion, but not systematically. For instance, let us take a simple situation. A point can be atypical because it takes an unusual value on a variable. If the variable selection process leads to its exclusion from the model, what should be done then? Re-enter the point? Leave as is? There is no pre-determined solution. The modelling process is exploratory in nature.

6 Multicollinearity problem

The multicollinearity problem disturbs the statistical inference, in part because it inflates the estimated standard error of coefficients. There are different ways of identifying the multicollinearity. We study a few detection techniques based on the analysis of the correlation matrix in this section.

Correlation matrix. A rule of thumb is to compare the absolute value of the correlation between each pair of variables with the threshold value 0.8. In Python, we copy the explanatory variables in a matrix. Then, we use **corrcoef()** procedure form the scipy library.

```
#correlation matrix
import scipy
mc = scipy.corrcoef(cars_exog,rowvar=0)
print(mc)
```

There are clearly problems with our data.

```
[[ 1.          0.94703153  0.87481759]
 [ 0.94703153  1.          0.82796562]
 [ 0.87481759  0.82796562  1.        ]]
```

All pairs of predictors are highly correlated.

Klein's rule of thumb. It consists in comparing the square of the correlation between the pairs of predictors with the overall R2 ($R^2 = 0.957$) of the regression. It is interesting because it takes into account the characteristics of the regression.

```
#Klein's rule of thumb
mc2 = mc**2
print(mc2)
```

None of the values exceed the R^2, but there are uncomfortable similarities nonetheless.

```
[[ 1.          0.89686872  0.76530582]
 [ 0.89686872  1.          0.68552706]
 [ 0.76530582  0.68552706  1.        ]]
```

Variance Inflation Factor (VIF). This criterion makes it possible to evaluate the relationship of one predictor with all other explanatory variables. We can read its value on the diagonal of the inverse of the correlation matrix.

```
#VIF criterion
vif = np.linalg.inv(mc)
print(vif)
```

A possible rule for multicollinearity detection is (VIF > 4). Here also, we note that the multicollinearity problem affects our regression.

```
[[ 12.992577    -9.20146328  -3.7476397 ]
 [ -9.20146328   9.6964853    0.02124552]
 [ -3.7476397    0.02124552   4.26091058]]
```

Possible solutions. Regularized least squares or variable selection approaches are possible solution for the multicollinearity problem. It seems that they are not available in the Statsmodels package. But it is not matter , Python is a powerful programming language, it would be easy for us to program additional calculations from the objects provided by Statsmodels.

7 Prediction and prediction interval

Applying the model on unseen instances (instances for which only the values of the explanatory variables are available) to obtain the expected values of the target variable is one of the objectives of the regression. The prediction is all the more credible if we can provide a prediction interval with a certain probability (confidence level) of containing the true value of the target variable.

In our case, this is above all an exercise. We apply the model on a set of observations not used during the modelling process. We therefore have the values of both predictors and target variable. This would allow us to verify the reliability of our model by comparing predicted and observed values. It is a kind of holdout validation scheme. This approach is widely use in classification problems.

7.1 Data importation

Here is the “vehicules_2.txt” data file:

modele	cylindree	puissance	poids	conso
Nissan Primera 2.0	1997	92	1240	9.2
Fiat Tempra 1.6 Liberty	1580	65	1080	9.3
Opel Omega 2.5i V6	2496	125	1670	11.3
Subaru Vivio 4WD	658	32	740	6.8
Seat Ibiza 2.0 GTI	1983	85	1075	9.5
Ferrari 456 GT	5474	325	1690	21.3

For these n*=6 vehicles, we calculate the prediction and we compare them to the observed values of the target attribute.

We load the data file in a new data frame **cars2**.

```
#loading the second data file
cars2 = pandas.read_table("vehicules_2.txt",sep="\t",header=0,index_col=0)

#number of instances
n_pred = cars2.shape[0]

#description of the new cars
print(cars2)
```

The structure of the data file (index, columns) is identical to the first dataset.

```
                         cylindree  puissance  poids  conso
modele
Nissan Primera 2.0            1997         92   1240    9.2
Fiat Tempra 1.6 Liberty       1580         65   1080    9.3
Opel Omega 2.5i V6            2496        125   1670   11.3
Subaru Vivio 4WD               658         32    740    6.8
Seat Ibiza 2.0 GTI            1983         85   1075    9.5
Ferrari 456 GT                5474        325   1690   21.3
```

7.2 Punctual prediction

The predicted value of the response is obtained by applying the model on the predictor values. Using the matrix form is better when the number of instances to process is high:

$$y_* = X_* \times \hat{a}$$

Where â is the vector of estimated coefficients, including the intercept. So that the calculation is consistent, we must add to the X∗ matrix a column of 1. The dimension of the matrix X∗ is (n*, p+1).

In Python, we create the matrix with the new column, we use the **add_constant()** procedure.

```
#predictor columns
cars2_exog = cars2[['cylindree','puissance','poids']]
#add a column of 1
cars2_exog = sm.add_constant(cars2_exog)
print(cars2_exog)
```

The constant value 1 is in the first column. The target variable CONSO is not included in the X∗ matrix of course.

```
                          const  cylindree  puissance  poids
modele
Nissan Primera 2.0            1       1997         92   1240
Fiat Tempra 1.6 Liberty       1       1580         65   1080
Opel Omega 2.5i V6            1       2496        125   1670
Subaru Vivio 4WD              1        658         32    740
Seat Ibiza 2.0 GTI            1       1983         85   1075
Ferrari 456 GT                1       5474        325   1690
```

Then, we apply the coefficients of the regression with the **predict**() command…

```
#punctual prediction by applying the regression coefficients
pred_conso = reg.predict(res.params,cars2_exog)
print(pred_conso)
```

… to obtain the predicted values.

```
[  9.58736855   8.1355859   12.58619059   5.80536066   8.52394228  17.33247145]
```

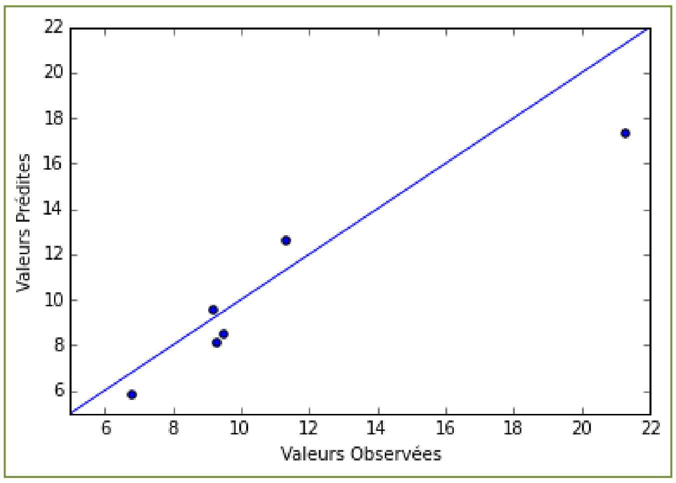
7.3 Comparison of predicted values and observed values

A scatterplot enables to check the quality of prediction. We set in the x axis the observed values of the response variable, in the y axis the predicted values. If the prediction is perfect, the plotted points are aligned in the diagonal. We use the **matplotlib** package for Python.

```
#comparison obs. Vs. pred.
import matplotlib.pyplot as plt
```

```
plt.scatter(cars2['conso'],pred_conso)
plt.plot(np.arange(5,23),np.arange(5,23))
plt.xlabel('Valeurs Observées')
plt.ylabel('Valeurs Prédites')
plt.xlim(5,22)
plt.ylim(5,22)
plt.show()
```

The prediction is acceptable for 5 points. For the 6th, the Ferrari, the regression model strongly underestimates the consumption (17.33 vs. 21.3).



7.4 Prediction interval

A punctual prediction is a first step. A prediction interval is always more interesting because we can associate a probability of error to the result provided.

Standard error of the prediction. The calculation is quite complex. We need to calculate the standard error of the prediction for each individual, we use the following formula (squared value of the standard error of the prediction) for a new instance i*

$$\hat{\sigma}^2_{\hat{\varepsilon}_{i*}} = \hat{\sigma}^2_{\varepsilon}\left[1 + X_{i*}(X'X)^{-1}X'_{i*}\right]$$

Some information is provided by the Python objects **reg** and **res** (sections 4.1 and **Erreur ! Source du renvoi introuvable.**) : $\hat{\sigma}^2_{\varepsilon}$ is the square of the residual standard error, $(X'X)^{-1}$ is obtained from the matrix of explanatory variables. Other information is related to the new individual: X_{i*} is the values of the input attributes, including the constant 1. For instance, for (Nissan Primera 2.0), we have the vector (1 ; 1997 ; 92 ; 1240).

Let us see how to organize this in a Python program.

```
#retrieving the matrix (X'X)-1
inv_xtx = reg.normalized_cov_params
print(inv_xtx)

#description of the new instances: transformation in matrix
X_pred = cars2_exog.as_matrix()

#### squared value of the standard error of the prediction ###
#initialization
var_err = np.zeros((n_pred,))
#for each individual to process
for i in range(n_pred):
    #description of the individual
    tmp = X_pred[i,:]
    #matrix product
    pm = np.dot(np.dot(tmp,inv_xtx),np.transpose(tmp))
    #squared values
    var_err[i] = res.scale * (1 + pm)
#
print(var_err)
```

We obtain:

```
[ 0.51089413  0.51560511  0.56515759  0.56494062  0.53000431  1.11282003]
```

Confidence interval. Now we calculate the lower and upper bounds for a 95% confidence level, using the quantile of the Student distribution and the punctual prediction.

```
#quantile of the Student distribution (0.975)
qt = scipy.stats.t.ppf(0.975,df=n-p-1)

#lower bound
yb = pred_conso - qt * np.sqrt(var_err)
print(yb)

#upper bound
yh = pred_conso + qt * np.sqrt(var_err)
print(yh)
```

For the 6 cars of the second data file, we obtain:

```
[  8.1009259    6.6423057   11.02280004   4.24227024   7.00995439  15.13868086]
[ 11.07381119   9.62886611  14.14958114   7.36845108  10.03793016  19.52626203]
```

Checking of the prediction interval. The evaluation takes on a concrete dimension here since we check, for a given confidence level, if the confidence interval contains the true (observed) value of the response variable. We organize the presentation in such a way that the observed values are surrounded by the lower and upper bounds of the intervals.

```
#matrix with the various values (lower bound, observed, upper bound)
a = np.resize(yb,new_shape=(n_pred,1))
y_obs = cars2['conso']
a = np.append(a,np.resize(y_obs,new_shape=(n_pred,1)),axis=1)
a = np.append(a,np.resize(yh,new_shape=(n_pred,1)),axis=1)

#transforming in a data frame object to obtain better displaying
df = pandas.DataFrame(a)
df.index = cars2.index
df.columns = ['B.Basse','Y.Obs','B.Haute']
print(df)
```

It is confirmed, the Ferrari is crossing the limits (if I may say so).

```
                          B.Basse  Y.Obs    B.Haute
modele
Nissan Primera 2.0       8.100926    9.2  11.073811
Fiat Tempra 1.6 Liberty  6.642306    9.3   9.628866
Opel Omega 2.5i V6      11.022800   11.3  14.149581
Subaru Vivio 4WD         4.242270    6.8   7.368451
Seat Ibiza 2.0 GTI       7.009954    9.5  10.037930
Ferrari 456 GT          15.138681   21.3  19.526262
```

8 Conclusion

The StatsModels package provides interesting features for statistical modeling. Coupled with the Python language and other packages (numpy, scipy, pandas, etc.), the possibilities become immense. The skills that we have been able to develop under R are very easy to transpose here.