5.5: Python Assignment

Quantitative Structure-Property Relationships

Downloadable Files

- **QSPR.ipynb**
- Excel_multiple_linear_regression_assignment.docx
- BP.csv
- 102BP.csv

- Download the ipynb file and run your Jupyter notebook.
  - You can use the notebook you created in section 1.5 or the Jupyter hub at LibreText: https://jupyter.libretexts.org (see your instructor if you do not have access to the hub).
  - This page is an html version of the above .ipynb file.
    - If you have questions on this assignment you should use this web page and the hypothes.is annotation to post a question (or comment) to the 2019OLCCStu class group. Contact your instructor if you do not know how to access the 2019OLCCStu group within the hypothes.is system.
- You will need to have the BP.csv and 102BP.csv files in the same directory as the QSPR.ipynb Jupyter notebook file.
- Your instructor may have you use Excel and multiple linear regression assignment in addition to this notebook.

Required Modules

- RDKit
- mordred (in your conda environment type- conda install -c mordred-descriptor mordred)
- pandas
- statsmodels (in your conda environment type- conda install statsmodels)

Objectives

- Use RDKit to calculate molecular descriptors
- Use molecular descriptors to create a predictive model for boiling points of alkanes.
- Use statsmodels to visualize data

Quantitative Structure-Property Relationships

Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) use statistical models to relate a set of predictor values to a response variable. Molecules are described using a set of *descriptors*, and then mathematical relationships can be developed to explain observed properties. In QSPR and QSAR, physico-chemical properties of theoretical descriptors of chemicals are used to predict either a physical property or a biological outcome.

Molecular Descriptors

A molecular descriptor is “final result of a logical and mathematical procedure, which transforms chemical information encoded within a symbolic repre-sentation of a molecule into a useful number or the result of some standardized experiment” (Todeschini, R.; Consonni, V. *Molecular descriptors for chemoinformatics* **2009** Wiley-VCH, Weinheim). You are already familiar with descriptors such as molecular weight or number of heavy atoms and we have queried PubChem for data such as XLogP. We’ll examine just a few simple descriptors, but thousands have been developed for applications in QSPR.

Using rdkit and mordred to calculate descriptors

Clearly we have been using algorithms for calculating these indices. This is time consuming for an individual, but programs can be used to complete this much easier. We will use the rdkit and mordred python libraries to help us out.

In [1]:

```
from rdkit import Chem                              # imports the Chem module from rdki
from mordred import Calculator, descriptors         # imports mordred descriptor librar
calc = Calculator(descriptors, ignore_3D=True)      # sets up a function reading descri
len(calc.descriptors) # tells us how many different types of descriptors are availabl
```

Out[1]:

```
1613
```

Wiener Index

We already calculated the Wiener index for *n*-pentane and 2-methylpentane. Now let's have mordred do it for us.

In [2]:

```
from mordred import WienerIndex
pentane = Chem.MolFromSmiles('CCCCC')                   # Use rdkit to create a mol fi
methyl_pentane = Chem.MolFromSmiles('CCCC(C)C')         #  and for 2-methylpentane
wiener_index = WienerIndex.WienerIndex()                # create descriptor instance f
result1 = wiener_index(pentane)                         # calculate wiener index for n
result2 = wiener_index(methyl_pentane)                  #  and for 2-methylpentane
print("The Wiener index for n-pentane is: ", result1)  # display result
print("The Wiener index for 2-methylpentane is: ", result2)
```

```
The Wiener index for n-pentane is:  20
The Wiener index for 2-methylpentane is:  32
```

Zagreb Indices

And we can do the same for the different Zagreb indices for *n*-pentane and 2-methylpentane.

In [3]:

```
from mordred import ZagrebIndex

zagreb_index1 = ZagrebIndex.ZagrebIndex(version = 1)            # create descriptor i
zagreb_index2 = ZagrebIndex.ZagrebIndex(version = 2)            # create descriptor i

result_Z1 = zagreb_index1(pentane)                              # calculate Z1 descri
result_Z2 = zagreb_index2(pentane)                              # calculate Z2 descri
print("The Zagreb index 1 for n-pentane is:", result_Z1)
print("The Zagreb index 2 for n-pentane is:", result_Z2)

result_Z1 = zagreb_index1(methyl_pentane)                       # and for 2-methylpen
result_Z2 = zagreb_index2(methyl_pentane)
print("The Zagreb index 1 for 2-methylpentane is:", result_Z1)
print("The Zagreb index 2 for 2-methylpentane is:", result_Z2)
```

```
The Zagreb index 1 for n-pentane is: 14.0
The Zagreb index 2 for n-pentane is: 12.0
```

```
The Zagreb index 1 for 2-methylpentane is: 20.0
The Zagreb index 2 for 2-methylpentane is: 18.0
```

As you can see from the code above, each index will have different code that needs to be followed for programming. Each descriptor and the resulting code syntax can be found here http://mordred-descriptor.github.io/documentation/master/api/modules.html

Looping through a list of molecules

Now that we have an understanding on how rdkit and mordred work to get our descriptors, let's simplify the code using a looping structure:

In [4]:

```
smiles = ["CCC", "CCCC", "CCCCC", "CCCC(C)C","CC(C)C(C)C"]         #store smiles stri

for smile in smiles:
    mol = Chem.MolFromSmiles(smile)                        # convert smiles string to m
    result_Z1 = zagreb_index1(mol)                         # calculate Z1 descriptor va
    result_Z2 = zagreb_index2(mol)                         # calculate Z2 descriptor va
    print("The Zagreb index 1 for", smile, "is:", result_Z1)
    print("The Zagreb index 2 for", smile, "is:", result_Z2)
    print()
```

```
The Zagreb index 1 for CCC is: 6.0
The Zagreb index 2 for CCC is: 4.0

The Zagreb index 1 for CCCC is: 10.0
The Zagreb index 2 for CCCC is: 8.0

The Zagreb index 1 for CCCCC is: 14.0
The Zagreb index 2 for CCCCC is: 12.0

The Zagreb index 1 for CCCC(C)C is: 20.0
The Zagreb index 2 for CCCC(C)C is: 18.0

The Zagreb index 1 for CC(C)C(C)C is: 22.0
The Zagreb index 2 for CC(C)C(C)C is: 21.0
```

Using descriptors to predict molecular properties

For this exercise we will take a series of alkanes and create an equation that will allow us to predict boiling points. We will start with a 30 molecule alkane training set. We will obtain various descriptors and see how they can predict the physical property boiling point.

For this exercise we will be using the pandas (Python Data Analysis) library to help us read, write and manage data. We will also use matplotlib to generate graphs.

Boiling Point data

Let's start by reading and graphing a set of boiling point data. First we read our csv file into a pandas "dataframe". Notice that we can generate a nicely formatted table from our dataframe by just entering the name of the dataframe on the last line.

In [5]:

```
import pandas as pd         # import the Python Data Analysis Library with the shorten
df = pd.read_csv("BP.csv") # read in the file into a pandas dataframe
df                          # print the dataframe
```

Out[5]:

	compound	name	BP_C	BP_K	SMILES	MW
0	1	Methane	-162.2	110.95	C	16.043
1	2	Ethane	-88.6	184.55	CC	30.070
2	3	propane	-42.2	230.95	CCC	44.100
3	4	butane	-0.1	273.05	CCCC	58.120
4	5	2-methylpropane	-11.2	261.95	CC(C)C	58.120
5	6	pentane	36.1	309.25	CCCCC	72.150
6	7	2-methylbutane	27.0	300.15	CC(C)CC	72.150
7	8	2,2-dimethylpropane	9.5	282.65	CC(C)(C)C	72.150
8	9	hexane	68.8	341.95	CCCCCC	86.180
9	10	2-methylpentane	60.9	334.05	CC(C)CCC	86.180
10	11	3-methylpentane	63.3	336.45	CC(CC)CC	86.180
11	12	2,2-dimethylbutane	49.8	322.95	CC(C)(CC)C	86.180
12	13	2,3-dimethylbutane	58.1	331.25	CC(C)C(C)C	86.180
13	14	heptane	98.5	371.65	CCCCCCC	100.200
14	15	3-ethylpentane	93.5	366.65	C(C)C(CC)CC	100.200
15	16	2,2-dimethylpentane	79.2	352.35	CC(C)(CCC)C	100.200
16	17	2,3-dimethylpentane	89.8	362.95	CC(C)C(CC)C	100.200
17	18	2,4-dimethylpentane	80.6	353.75	CC(C)CC(C)C	100.200
18	19	2-methylhexane	90.1	363.25	CC(C)CCCC	100.205
19	20	3-methylhexane	91.8	364.95	CC(CC)CCC	100.200
20	21	octane	125.6	398.75	CCCCCCCC	114.230
21	22	3-methylheptane	118.9	392.05	CC(CC)CCCC	114.232
22	23	2,2,3,3-tetramethylbutane	106.5	379.65	CC(C)(C(C)(C)C)C	114.230

	compound	name	BP_C	BP_K	SMILES	MW
23	24	2,3,3-trimethylpentane	114.7	387.85	CC(C)C(CC)(C)C	114.230
24	25	2,3,4-trimethylpentane	113.7	386.85	CC(C)C(C(C)C)C	114.230
25	26	2,2,4-trimethylpentane	99.3	372.45	CC(C)(CC(C)C)C	114.230
26	27	nonane	150.7	423.85	CCCCCCCCC	128.250
27	28	2-methyloctane	143.0	416.15	CC(C)CCCCCC	128.259
28	29	decane	174.2	447.35	CCCCCCCCCC	142.280
29	30	2-methylnonane	166.9	440.05	CC(C)CCCCCCC	142.280

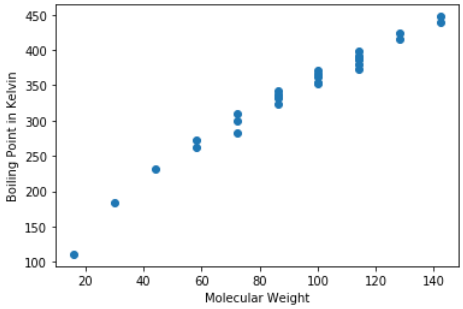
Graphing the data

Now we can graph the data using matplotlib.

In [16]:

```
import matplotlib.pyplot as plt

plt.scatter(df.MW, df.BP_K)     # plot of boiling point (in K) vs molecular weight
plt.xlabel('Molecular Weight')
plt.ylabel('Boiling Point in Kelvin')
plt.show()
```



Clearly from the data we can see that we have multiple molecules with the same molecular weight, but different boiling points. Molecular weight is therefore not the best predictor of boiling point. We can see if there are other descriptors that we can use such as Weiner or Zagreb. Let's add various descriptors to the dataframe.

Adding descriptors to the dataset

We can now calculate the Wiener and Zagreb indices for each of our hydrocarbons and add them to the dataframe.

In [7]:

```
# create new lists to store results we calculate
result_Wiener= []
result_Z1= []
result_Z2= []
```

```
for index, row in df.iterrows():                # iterate through each row of the CSV
    SMILE = row['SMILES']                       # get SMILES string from row
    mol = Chem.MolFromSmiles(SMILE)             # convert smiles string to mol file
    result_Wiener.append(wiener_index(mol))     # calculate Wiener index descripter v
    result_Z1.append(zagreb_index1(mol))        # calculate zagreb (Z1) descriptor va
    result_Z2.append(zagreb_index2(mol))        # calculate zagreb (Z2) descriptor va

df['Wiener'] = result_Wiener            # add the results for WienerIndex to dataframe
df['Z1'] = result_Z1                    # add the results for Zagreb 1 to dataframe
df['Z2'] = result_Z2                    # add the results for Zagreb 2 to dataframe
df                                      # print the updated dataframe
```

Out[7]:

	compound	name	BP_C	BP_K	SMILES	MW	Wiener	Z1	Z2
0	1	Methane	-162.2	110.95	C	16.043	0	0.0	0.0
1	2	Ethane	-88.6	184.55	CC	30.070	1	2.0	1.0
2	3	propane	-42.2	230.95	CCC	44.100	4	6.0	4.0
3	4	butane	-0.1	273.05	CCCC	58.120	10	10.0	8.0
4	5	2-methylpropane	-11.2	261.95	CC(C)C	58.120	9	12.0	9.0
5	6	pentane	36.1	309.25	CCCCC	72.150	20	14.0	12.0
6	7	2-methylbutane	27.0	300.15	CC(C)CC	72.150	18	16.0	14.0
7	8	2,2-dimethylpropane	9.5	282.65	CC(C)(C)C	72.150	16	20.0	16.0
8	9	hexane	68.8	341.95	CCCCCC	86.180	35	18.0	16.0
9	10	2-methylpentane	60.9	334.05	CC(C)CCC	86.180	32	20.0	18.0
10	11	3-methylpentane	63.3	336.45	CC(CC)CC	86.180	31	20.0	19.0
11	12	2,2-dimethylbutane	49.8	322.95	CC(C)(CC)C	86.180	28	24.0	22.0
12	13	2,3-dimethylbutane	58.1	331.25	CC(C)C(C)C	86.180	29	22.0	21.0

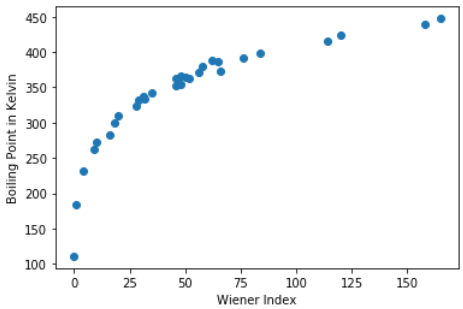
	compound	name	BP_C	BP_K	SMILES	MW	Wiener	Z1	Z2
13	14	heptane	98.5	371.65	CCCCCCC	100.200	56	22.0	20.0
14	15	3-ethylpentane	93.5	366.65	C(C)C(CC)CC	100.200	48	24.0	24.0
15	16	2,2-dimethylpentane	79.2	352.35	CC(C)(CCC)C	100.200	46	28.0	26.0
16	17	2,3-dimethylpentane	89.8	362.95	CC(C)C(CC)C	100.200	46	26.0	26.0
17	18	2,4-dimethylpentane	80.6	353.75	CC(C)CC(C)C	100.200	48	26.0	24.0
18	19	2-methylhexane	90.1	363.25	CC(C)CCCC	100.205	52	24.0	22.0
19	20	3-methylhexane	91.8	364.95	CC(CC)CCC	100.200	50	24.0	23.0
20	21	octane	125.6	398.75	CCCCCCCC	114.230	84	26.0	24.0
21	22	3-methylheptane	118.9	392.05	CC(CC)CCCC	114.232	76	28.0	27.0
22	23	2,2,3,3-tetramethylbutane	106.5	379.65	CC(C)(C(C)(C)C)C	114.230	58	38.0	40.0
23	24	2,3,3-trimethylpentane	114.7	387.85	CC(C)C(CC)(C)C	114.230	62	34.0	36.0
24	25	2,3,4-trimethylpentane	113.7	386.85	CC(C)C(C(C)C)C	114.230	65	32.0	33.0
25	26	2,2,4-trimethylpentane	99.3	372.45	CC(C)(CC(C)C)C	114.230	66	34.0	32.0
26	27	nonane	150.7	423.85	CCCCCCCCC	128.250	120	30.0	28.0
27	28	2-methyloctane	143.0	416.15	CC(C)CCCCCC	128.259	114	32.0	30.0

	compound	name	BP_C	BP_K	SMILES	MW	Wiener	Z1	Z2
28	29	decane	174.2	447.35	CCCCCCCCCC	142.280	165	34.0	32.0
29	30	2-methylnonane	166.9	440.05	CC(C)CCCCCCC	142.280	158	36.0	34.0

Now we can see how each of these descriptors are related to the boiling points of their respective compounds.

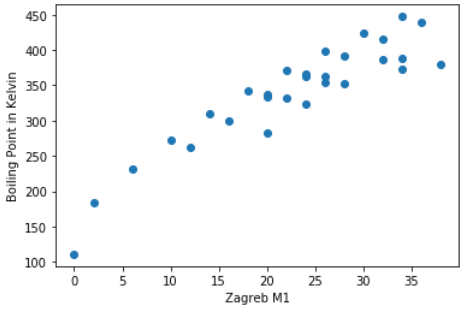
In [8]:

```
plt.scatter(df.Wiener, df.BP_K) # plot of BP versus Wiener index
plt.xlabel('Wiener Index')
plt.ylabel('Boiling Point in Kelvin')
plt.show()
```



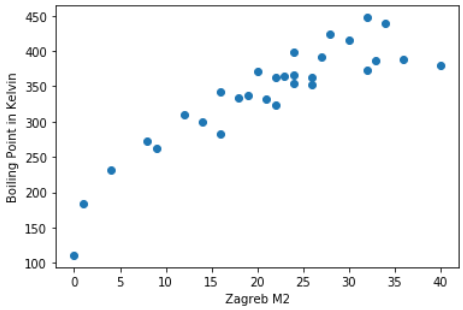
In [9]:

```
plt.scatter(df.Z1, df.BP_K) # plot of BP versus Zagreb M1
plt.xlabel('Zagreb M1')
plt.ylabel('Boiling Point in Kelvin')
plt.show()
```



In [10]:

```
plt.scatter(df.Z2, df.BP_K) # plot of BP versus Zagreb M2
plt.xlabel('Zagreb M2')
plt.ylabel('Boiling Point in Kelvin')
plt.show()
```



Clearly molecular weight was somewhat predictive, but problematic. It looks like using the other indicators we have have some other ways to predict boiling point.

One option is write this data to a new CSV file and work in Microsoft Excel to perform a regression analysis. Exporting the data is straightforward and your instructor may provide instructions on how to analyze the data using Excel.

In [11]:

```
df.to_csv('bp_descriptor_data.csv', encoding='utf-8', index=False)
```

Mulitple regression analysis using statsmodels

The statsmodels package provides numerous tools for performaing statistical analysis using Python. In this case, we want to perform a *multiple linear regression* using all of our descriptors (molecular weight, Wiener index, Zagreb indices) to help predict our boiling point.

In [12]:

```
import statsmodels.api as sm            # import the statsmodels library as sm
X = df[["MW", "Wiener", "Z1", "Z2"]]    # select our independent variables
X = sm.add_constant(X)                  # add an intercept to our model
y = df[["BP_K"]]                        # select BP as our dependent variable
model = sm.OLS(y,X).fit()               # set up our model
predictions = model.predict(X)          # make the predictions
print(model.summary())                  # print out statistical summary
```

```
C:\ProgramData\Miniconda3\envs\OLCC2019\lib\site-packages\numpy\core\fromnumeric.py:2
  return ptp(axis=axis, out=out, **kwargs)
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   BP_K   R-squared:                       0.994
Model:                            OLS   Adj. R-squared:                  0.994
Method:                 Least Squares   F-statistic:                     1124.
Date:                Wed, 16 Oct 2019   Prob (F-statistic):           8.16e-28
Time:                        19:04:48   Log-Likelihood:                -93.019
No. Observations:                  30   AIC:                             196.0
Df Residuals:                      25   BIC:                             203.0
Df Model:                           4
Covariance Type:            nonrobust
==============================================================================
```

```
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         55.5695      6.745      8.238      0.000      41.677      69.462
MW             4.4325      0.203     21.853      0.000       4.015       4.850
Wiener        -0.6411      0.064     -9.960      0.000      -0.774      -0.509
Z1            -4.3920      1.238     -3.549      0.002      -6.941      -1.843
Z2             0.2982      0.943      0.316      0.754      -1.644       2.240
==============================================================================
Omnibus:                        3.756   Durbin-Watson:                   1.285
Prob(Omnibus):                  0.153   Jarque-Bera (JB):                2.259
Skew:                          -0.583   Prob(JB):                        0.323
Kurtosis:                       3.671   Cond. No.                         755.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly spec
```

Note above that we now have coeffiecients for an equation that can be used for prediction of boiling points for molecules not included in our dataset. The equation would be:

```
Predicted BP = 4.4325 * MW - 0.6411 * Weiner - 4.3920 * Z1 + 0.2982 * Z2 + 55.5695
```

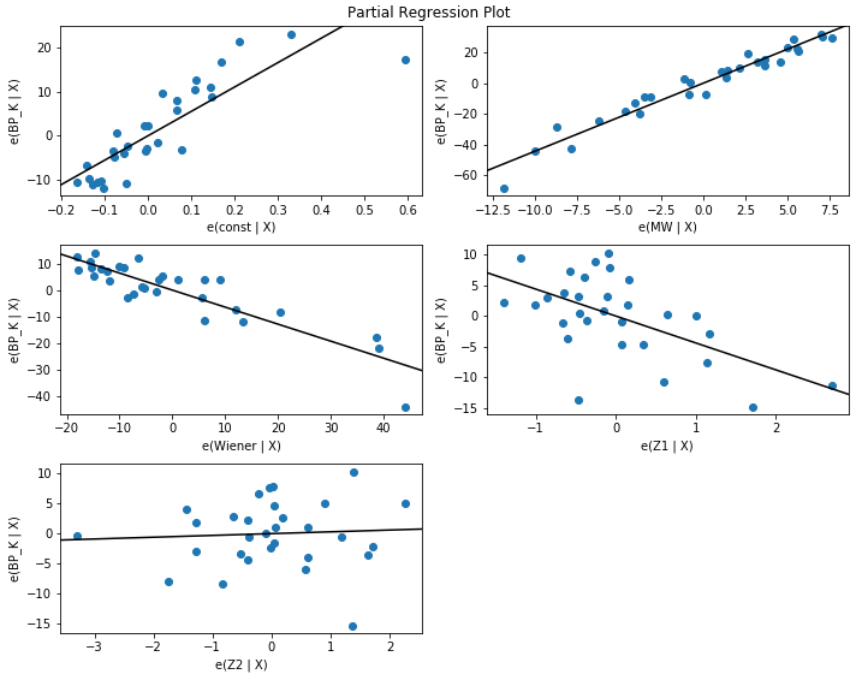
We can use this equation to predict the boiling point of a new molecule. However, before we do, we need to explore the validity of the model.

Model summary and analysis using partial regression plots

A quick look at the results summary shows that the model has an excellent R-squared value. Upon more careful examination, you may notice that one of our descriptors has a very large P value. This would indicate that perhaps the Z2 descriptor is not working well in this case. We can generate a more graphical interpretation that will make this more obvious.

In [13]:

```
fig = plt.figure(figsize=(10,8))
fig = sm.graphics.plot_partregress_grid(model, fig=fig)
```



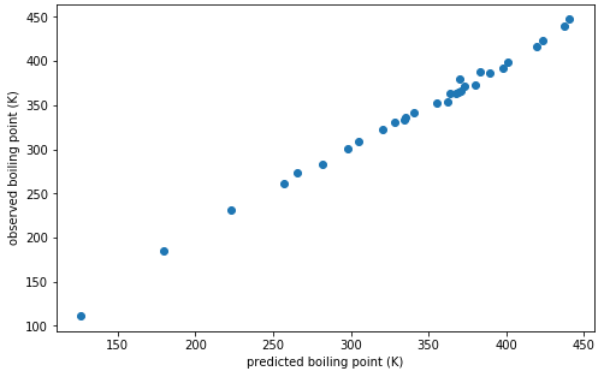
Part of the reason that Z2 may not be predictive in this model is that there is colinearity with the Z1 descriptor. Both descriptors have similar calculations (as outlined in the Libretexts page for this activity). Later on in this exercise we can explore dropping this descriptor.

How good is our model?

If we look at a plot of actual versus predicted boiling points

In [14]:

```
pred_bp = model.fittedvalues.copy()       # use our model to create a set of predicte
fig, ax = plt.subplots(figsize=(8, 5))
lmod = sm.OLS(pred_bp, df.BP_K)           # linear regression of observed vs predicte
res = lmod.fit()                          # run fitting
plt.scatter(pred_bp, df.BP_K)             # plot of of observed vs predicted bp's
plt.ylabel('observed boiling point (K)')
plt.xlabel('predicted boiling point (K)')
plt.show()
print(res.summary())                      # print linear regression stats summary
```



```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared (uncentered):                   1.0
Model:                            OLS   Adj. R-squared (uncentered):              1.0
Method:                 Least Squares   F-statistic:                          1.213e+
Date:                Wed, 16 Oct 2019   Prob (F-statistic):                    4.52e-
Time:                        19:05:22   Log-Likelihood:                         -93.0
No. Observations:                  30   AIC:                                      188
Df Residuals:                      29   BIC:                                      189
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
BP_K           0.9998      0.003    348.263      0.000       0.994       1.006
==============================================================================
Omnibus:                        3.635   Durbin-Watson:                   1.284
Prob(Omnibus):                  0.162   Jarque-Bera (JB):                2.167
Skew:                           0.574   Prob(JB):                        0.338
Kurtosis:                       3.643   Cond. No.                         1.00
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly spec
```

The model appears to have very good predictability (R-squared = 1.000) within the original 30 molecule data set. One way to test this model is to use a new molecule with its descriptors to see how well it is predicted. One molecule in the dataset is 2-methylheptane. It has the following data: MW = 114.232 Wiener Index = 79 Z1 = 28 Z2 = 26 Boiling Point = 390.6 K

Using the equation from above we can determine that the boiling point from the equation Predicted BP = 4.4325 *MW* - *0.6411* Weiner - 4.3920 *Z1* + *0.2982* Z2 + 55.5695 is 396.0 K. The model gives a 1.4% error for prediction of the boiling point outide the training set.

We had mentioned earlier that Z2 may not be very predictive in this model. We can remove the variable an rerun the analysis to see if we can improve the predictability of the model.

In [15]:

```
import statsmodels.api as sm            # import the statsmodels library as sm
X = df[["MW", "Wiener", "Z1"]]          # select our independent variables, this time
X = sm.add_constant(X)                  # add an intercept to our model
y = df[["BP_K"]]                        # select BP as our dependent variable
model = sm.OLS(y,X).fit()               # set up our model
predictions = model.predict(X)          # make the predictions
print(model.summary())                  # print out statistical summary
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    BP_K   R-squared:                       0.994
```

```
Model:                            OLS   Adj. R-squared:                  0.994
Method:                 Least Squares   F-statistic:                     1552.
Date:                Wed, 16 Oct 2019   Prob (F-statistic):           1.99e-29
Time:                        19:05:30   Log-Likelihood:                -93.078
No. Observations:                  30   AIC:                             194.2
Df Residuals:                      26   BIC:                             199.8
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         55.4979      6.624      8.378      0.000      41.882      69.113
MW             4.4114      0.188     23.433      0.000       4.024       4.798
Wiener        -0.6397      0.063    -10.139      0.000      -0.769      -0.510
Z1            -4.0260      0.430     -9.364      0.000      -4.910      -3.142
==============================================================================
Omnibus:                        2.917   Durbin-Watson:                   1.326
Prob(Omnibus):                  0.233   Jarque-Bera (JB):                1.624
Skew:                          -0.507   Prob(JB):                        0.444
Kurtosis:                       3.521   Cond. No.                         741.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly spec
```

IThe model appears to have very good predictability (R-squared = 0.994) within the original 30 molecule data set. Let's reexamine 2-methylheptane: MW = 114.232 Wiener Index = 79 Z1 = 28 Boiling Point = 390.6 K

Using the equation from above we can determine that the boiling point from the equation Predicted BP = 4.4114 *MW* - *0.6397* Weiner - 4.0260 * Z1 + 55.4979 is 396.2 K. The model also gives a 1.4% error for prediction of the boiling point outide the training set.

We can see here that Z2 doesn't really change the result of the calculation, and can probably be best left out to simplify the model.

Keep in mind that we have completed this analysis with only a training set of 30 molecules. If the training set had more molecules, you should be able to develop a better model.

Assignment

You originally ran this analysis on a 30 molecule data set (BP.CSV). You also have available to you a 102 molecule data set (102BP.CSV).

- Complete the above analysis using the expanded data set to determine if a better predictive model can be obtained with a larger training set. Note that 2-methylheptane is in this new dataset so you will need to choose a new test molecule.

When you have completed the analysis, you will create a new analysis:

- Choose four new topological and other calculated descriptors found in Mordred http://mordred-descriptor.github.io/documentation/master/api/modules.html
- Complete simple linear analysis for each of your new descriptors.
- Complete a multiple linear regression to create an equation that best represents the data boiling point data and your descriptors.
- Create a separate sheet that has your regression data.
- Make a plot of Actual vs Predicted BP for your regression.
- Choose a new molecule not in the dataset (not 2-methylheptane, be creative and use chemical intuition).

- Use your multiple linear equation to predict this molecule's BP and look of the literature value.
- Write a short one-two page paper that includes:
  - What your new chosen descriptors mean
  - Which new chosen descriptors correlate
  - What is the overall equation calculated
  - How to choose the molecule to test
  - How close this multiple linear regression predicts your boiling point of your molecule

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