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00. Introduction

In the R Shiny Dashboard made previously: (https://adrian-

landaverde.shinyapps.io/CrystalCaseStudy/) we made the EDA. In which we could see how the energy from 2005 and 2006 is very different despite the variables are very alike.

So it will be attempted to predict the energy using 2 approaches:

In the fisrt one, it will be implemented one model for each year using the humidity and the temperature

In the second one, it will be used a time series analysis to predict the energy based on the trend and seasonality of the data

01. Libraries and Data

In []:

!pip install statsmodels

Requirement already satisfied: statsmodels in /usr/local/lib/python3.7/dist-pa ckages (0.10.2)

Requirement already satisfied: scipy>=0.18 in /usr/local/lib/python3.7/dist-pa ckages (from statsmodels) (1.4.1)

Requirement already satisfied: patsy>=0.4.0 in /usr/local/lib/python3.7/dist-p ackages (from statsmodels) (0.5.2)

Requirement already satisfied: numpy>=1.11 in /usr/local/lib/python3.7/dist-pa ckages (from statsmodels) (1.21.5)

Requirement already satisfied: pandas>=0.19 in /usr/local/lib/python3.7/dist-p ackages (from statsmodels) (1.3.5)

Requirement already satisfied: pytz>=2017.3 in /usr/local/lib/python3.7/dist-p ackages (from pandas>=0.19->statsmodels) (2018.9)

Requirement already satisfied: python-dateutil>=2.7.3 in /usr/local/lib/python 3.7/dist-packages (from pandas>=0.19->statsmodels) (2.8.2)

Requirement already satisfied: six in /usr/local/lib/python3.7/dist-packages (from patsy>=0.4.0->statsmodels) (1.15.0)

In [2]:

import pandas as pd
import numpy as np

```
import datetime as dt
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.pyplot import figure
import seaborn as sns
from scipy import stats
from sklearn.ensemble import RandomForestRegressor
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model selection import train test split
from sklearn.metrics import r2 score
from sklearn.model selection import GridSearchCV
from sklearn.linear_model import LinearRegression
from sklearn.neural network import MLPRegressor
from sklearn.preprocessing import MinMaxScaler
import statistics
from statsmodels.tsa.stattools import adfuller
from statsmodels.tsa.seasonal import seasonal decompose
from statsmodels.graphics.tsaplots import plot acf, plot pacf
from statsmodels.tsa.statespace.sarimax import SARIMAX
```

/usr/local/lib/python3.7/dist-packages/statsmodels/tools/_testing.py:19: Futur eWarning: pandas.util.testing is deprecated. Use the functions in the public A PI at pandas.testing instead.

import pandas.util.testing as tm

```
import warnings
warnings.filterwarnings("ignore")
```

```
from google.colab import drive
    drive.mount('/content/drive')
```

Mounted at /content/drive

```
In [6]:
    df_energy= pd.read_csv("/content/drive/MyDrive/Universidad/Cuarto Semestre/Cry
    df_energy
```

Out[6]:		Hour	energy_consumpt_2005	energy_consumpt_2006	full_temp_2005	full_humid_200!
	0	1	631.623161	1246.300847	-0.400000	64.000000
	1	2	534.397104	1062.500558	-0.733333	65.333333
	2	3	453.538785	884.586887	-1.066667	66.666667
	3	4	400.699718	786.564121	-1.400000	68.000000
	4	5	378.171092	742.669614	-1.666667	60.333333
	•••					
	8779	8780	950.369306	0.000000	3.333333	64.000000
	8780	8781	880.138770	0.000000	2.666667	68.000000
	8781	8782	792.754026	0.000000	2.000000	72.000000
	8782	8783	740.446668	0.000000	1.333333	76.000000
	8783	8784	706.176769	0.000000	0.666667	80.000000

8784 rows × 7 columns

```
In [ ]:
          df energy["Year"]=2005
          df_energy["Day"]= (((df_energy["Hour"]-1)/24)+1).apply(np.floor)
          df_energy["Week"] = (((df_energy["Day"]-1)/7)+1).apply(np.floor)
           df energy
                Hour energy_consumpt_2005 energy_consumpt_2006 full_temp_2005 full_humid_200!
Out[]:
             0
                    1
                                  631.623161
                                                         1246.300847
                                                                           -0.400000
                                                                                           64.000000
                    2
             1
                                  534.397104
                                                         1062.500558
                                                                           -0.733333
                                                                                           65.333333
             2
                    3
                                  453.538785
                                                          884.586887
                                                                           -1.066667
                                                                                           66.66667
             3
                    4
                                  400.699718
                                                          786.564121
                                                                           -1.400000
                                                                                           68.000000
                    5
                                  378.171092
                                                          742.669614
                                                                           -1.666667
                                                                                           60.333333
             4
                                                            0.000000
                                                                                           64.000000
          8779
                8780
                                  950.369306
                                                                           3.333333
                8781
                                  880.138770
          8780
                                                            0.000000
                                                                           2.666667
                                                                                           68.000000
          8781
                8782
                                  792.754026
                                                            0.000000
                                                                           2.000000
                                                                                           72.000000
          8782
                8783
                                  740.446668
                                                                                           76.000000
                                                            0.000000
                                                                           1.333333
          8783 8784
                                  706.176769
                                                            0.000000
                                                                           0.666667
                                                                                           80.000000
         8784 rows × 10 columns
In [ ]:
          df_energy["Date"]=(np.asarray(df_energy['Year'], dtype='datetime64[Y]')-1970)
           df_energy["Month"]=pd.DatetimeIndex(df_energy['Date']).month
          df energy
Out[]:
                Hour energy_consumpt_2005 energy_consumpt_2006 full_temp_2005 full_humid_200!
             0
                    1
                                  631.623161
                                                         1246.300847
                                                                           -0.400000
                                                                                           64.000000
             1
                    2
                                  534.397104
                                                         1062.500558
                                                                           -0.733333
                                                                                           65.333333
             2
                    3
                                  453.538785
                                                          884.586887
                                                                           -1.066667
                                                                                           66.66667
                                  400.699718
                                                          786.564121
                                                                           -1.400000
                                                                                           68.000000
             3
                    4
                                  378.171092
                                                          742.669614
                                                                           -1.666667
                                                                                           60.333333
          8779
                8780
                                  950.369306
                                                            0.000000
                                                                           3.333333
                                                                                           64.000000
```

0.000000

2.666667

68.000000

880.138770

8780

8781

070	81 8782	792.754026	0.000000	2.000000	72.0000
878	82 8783	740.446668	0.000000	1.333333	76.0000
878	83 8784	706.176769	0.000000	0.666667	80.0000
878	4 rows × 12 columns				
4)
df	energy.isna().sum	()			
ut[]: Hou		0			
ene	ergy_consumpt_2005	34			
	ergy_consumpt_2006	42			
	ll_temp_2005 ll_humid_2005	0 0			
	ll_temp_2006	24			
	ll_humid_2006	24			
Yea		0			
Day	/	0			
Wee	ek	0			
Dat		0			
Mor	nth	0			
dty	/pe: int64				
dty df df df	rpe: int64	nsumpt_2006"].fi] iloc[:-24]			
dty df df df df df df df df	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum	nsumpt_2006"].fi] iloc[:-24] i()			
dty df df df df df df df ene	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ur ergy_consumpt_2005	nsumpt_2006"].fi] iloc[:-24] (() 0 0			
dty df df df df df df ene	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ur ergy_consumpt_2005 ergy_consumpt_2006	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0			
dty df df df df df df df df df d	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ergy_consumpt_2005 ergy_consumpt_2006 Ll_temp_2005	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0			
dty df df df df df df df df df d	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum Ur ergy_consumpt_2005 ergy_consumpt_2006 Ll_temp_2005 Ll_humid_2005	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0			
dty n []: df df df df ut[]: ene ene full full	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ergy_consumpt_2005 ergy_consumpt_2006 Ll_temp_2005	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0 0			
dty df df df df df df df df df d	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ergy_consumpt_2005 ergy_consumpt_2006 ll_temp_2005 ll_humid_2005 ll_temp_2006 ll_temp_2006	nsumpt_2006"].fi] iloc[:-24] (() 0 0 0 0 0 0			
dty df df df df df df df df df d	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ergy_consumpt_2005 ergy_consumpt_2006 ll_temp_2005 ll_humid_2005 ll_temp_2006 ll_temp_2006 ll_temp_2006	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0 0 0 0 0			
dty dfy df df df df df df df df	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum ergy_consumpt_2005 ergy_consumpt_2006 ll_temp_2005 ll_humid_2005 ll_temp_2006 ll_temp_2006 ll_humid_2006 er	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0 0 0 0 0 0 0			
dty dfy df df df df df df df df	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum Ur ergy_consumpt_2005 ergy_consumpt_2006 ll_temp_2005 ll_humid_2005 ll_temp_206 ll_humid_2006 er	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0 0 0 0 0 0 0 0 0			
dty df df df df df df df df df d	E_energy["energy_co E_energy["energy_co E_energy=df_energy. E_energy.isna().sum Ur ergy_consumpt_2005 ergy_consumpt_2006 ll_temp_2005 ll_humid_2005 ll_temp_206 ll_humid_2006 er	nsumpt_2006"].fi] iloc[:-24] i() 0 0 0 0 0 0 0 0 0 0			

02. Machine Learning Regression

Based on the dashboard plots, the energy is more correlated to the mean temperature

per day, and to the humidity per hour

```
meanEnergy2005= df_energy.groupby("Day")['full_temp_2005'].mean()
meanEnergy2006= df_energy.groupby("Day")['full_temp_2006'].mean()
df_energy["temp_per_day_2005"]=(np.repeat(meanEnergy2005,24)).values
df_energy["temp_per_day_2006"]=(np.repeat(meanEnergy2006,24)).values
df_energy["HourOfDay"]=df_energy["Hour"]-((df_energy['Day']-1)*24)
df_energy
```

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:3: SettingWithCop yWarning:

A value is trying to be set on a copy of a slice from a DataFrame. Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy

This is separate from the ipykernel package so we can avoid doing imports un til

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:4: SettingWithCop yWarning:

A value is trying to be set on a copy of a slice from a DataFrame. Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: $https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html\#returning-a-view-versus-a-copy$

after removing the cwd from sys.path.

/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:5: SettingWithCop yWarning:

A value is trying to be set on a copy of a slice from a DataFrame. Try using .loc[row indexer,col indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy

Out[]:	Hour	energy_consumpt_2005	energy_consumpt_2006	full_temp_2005	full_humid_200!
0	1	631.623161	1246.300847	-0.400000	64.000000
1	2	534.397104	1062.500558	-0.733333	65.333333
2	3	453.538785	884.586887	-1.066667	66.666667
3	4	400.699718	786.564121	-1.400000	68.000000
4	5	378.171092	742.669614	-1.666667	60.33333
•••					
8755	8756	927.986980	1933.241699	1.466667	43.33333
8756	8757	909.729665	1763.838385	0.933333	46.666667
8757	8758	848.714914	1569.071986	0.400000	50.000000

```
      8758
      8759
      740.913139
      1468.273109
      -0.066667
      54.000000

      8759
      8760
      613.226705
      1384.624630
      -0.533333
      58.000000
```

8760 rows × 15 columns

```
In []:
    def plotRgresion(y,y_predict,ax,limites,ymin,ymax):
        ax.plot(df_energy["Hour"],y,label="y Real",color="blue")
        ax.plot(df_energy["Hour"],y_predict,label="y Predicted",color="red")
        if(limites):
        ax.set_ylim(ymin,ymax)
        return(ax)

In []:
    X_2005= df_energy[['temp_per_day_2005','HourOfDay','full_humid_2005']]
    y_2005= df_energy['energy_consumpt_2005']
    X_train, X_test, y_train, y_test= train_test_split(X_2005,y_2005,random_statest)
```

02.1 Random Forest

```
In [ ]:
        parameters= {"n estimators":list(range(10,101,10))}
        model = RandomForestRegressor(random state=0)
        grid = GridSearchCV(model, param_grid = parameters,scoring="r2",verbose=3)
        grid.fit(X train,y train)
        print('Grid best parameter (max. R2): ', grid.best params )
        print('Grid best score (R2): ', grid.best_score_)
        print("R2 Score on test:",r2_score(y_test, grid.predict(X_test)))
        fig, ax= plt.subplots(figsize=(20,8))
        ax= plotRgresion(y 2005,grid.predict(X 2005),ax,True,0,1000)
        plt.legend()
        plt.show()
        print("Final R2 Score:",r2_score(y_2005,grid.predict(X_2005)))
        Fitting 5 folds for each of 10 candidates, totalling 50 fits
        [CV 1/5] END .....n_estimators=10;, score=0.662 total time=
                                                                              0.
       1s
        [CV 2/5] END .....n estimators=10;, score=0.235 total time=
        [CV 3/5] END .....n_estimators=10;, score=0.924 total time=
                                                                              0.
        [CV 4/5] END .....n estimators=10;, score=0.377 total time=
                                                                              0.
        [CV 5/5] END .....n_estimators=10;, score=0.118 total time=
                                                                              0.
        [CV 1/5] END .....n estimators=20;, score=0.670 total time=
        [CV 2/5] END .....n estimators=20;, score=0.651 total time=
                                                                              0.
        [CV 3/5] END .....n_estimators=20;, score=0.896 total time=
                                                                              0.
```

[CV 1/5] ENDn_estimators=80;, score=0.673 total time=

[CV 2/5] ENDn_estimators=80;, score=0.723 total time=

[CV 3/5] ENDn_estimators=80;, score=0.931 total time=

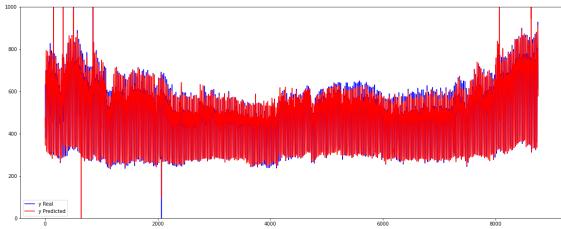
[CV 4/5] FND

0.

0.

0.

```
Crystal_CaseStudy/Energy_Final.ipynb at main · AdrianLandaverde/Crystal_CaseStudy
              ....., SCOLE-0.303 COLET LIME-
9s
[CV 5/5] END .....n_estimators=80;, score=0.259 total time=
[CV 1/5] END .....n_estimators=90;, score=0.673 total time=
                                                                  1.
[CV 2/5] END .....n estimators=90;, score=0.731 total time=
                                                                  1.
[CV 3/5] END .....n_estimators=90;, score=0.932 total time=
                                                                  1.
[CV 4/5] END .....n estimators=90;, score=0.388 total time=
[CV 5/5] END .....n_estimators=90;, score=0.253 total time=
                                                                  1.
[CV 1/5] END .....n estimators=100;, score=0.673 total time=
                                                                  1.
[CV 2/5] END .....n_estimators=100;, score=0.722 total time=
                                                                  1.
[CV 3/5] END .....n_estimators=100;, score=0.933 total time=
[CV 4/5] END .....n estimators=100;, score=0.387 total time=
[CV 5/5] END .....n_estimators=100;, score=0.261 total time=
                                                                  1.
Grid best parameter (max. R2): {'n estimators': 70}
Grid best score (R2): 0.5996080433637754
R2 Score on test: 0.6105817867373805
```



Final R2 Score: 0.8696535631662909

02.2 K-Nearet Neighbours

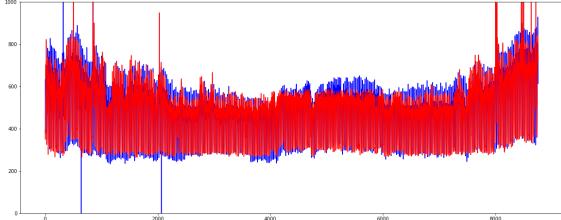
```
In []:
    parametrosKNN= {"n_neighbors":list(range(3,19,2))}
    knn = KNeighborsRegressor()

    grid = GridSearchCV(knn, param_grid = parametrosKNN,scoring="r2",verbose=3)
    grid.fit(X_train,y_train)
    print('Grid best parameter (max. R2): ', grid.best_params_)
    print('Grid best score (R2): ', grid.best_score_)
    print("R2 Score on test:",r2_score(y_test, grid.predict(X_test)))
    fig, ax= plt.subplots(figsize=(20,8))
    ax= plotRgresion(y_2005,grid.predict(X_2005),ax,True,0,1000)
    plt.show()
    print("Final R2 Score:",r2_score(y_2005,grid.predict(X_2005)))
```

Fitting 5 folds for each of 8 candidates, totalling 40 fits

```
[CV 1/5] END .....n_neighbors=3;, score=0.638 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=3;, score=0.515 total time=
                                                             0.
[CV 3/5] END .....n_neighbors=3;, score=0.722 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=3;, score=0.322 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=3;, score=0.382 total time=
                                                             0.
[CV 1/5] END .....n_neighbors=5;, score=0.639 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=5;, score=0.716 total time=
                                                             0.
[CV 3/5] END .....n_neighbors=5;, score=0.821 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=5;, score=0.362 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=5;, score=0.337 total time=
                                                             0.
[CV 1/5] END .....n_neighbors=7;, score=0.632 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=7;, score=0.721 total time=
[CV 3/5] END .....n_neighbors=7;, score=0.802 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=7;, score=0.370 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=7;, score=0.358 total time=
                                                             0.
[CV 1/5] END .....n_neighbors=9;, score=0.616 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=9;, score=0.773 total time=
                                                             0.
[CV 3/5] END .....n_neighbors=9;, score=0.832 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=9;, score=0.371 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=9;, score=0.360 total time=
                                                             0.
[CV 1/5] END .....n_neighbors=11;, score=0.624 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=11;, score=0.779 total time=
                                                             0.
[CV 3/5] END .....n_neighbors=11;, score=0.849 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=11;, score=0.372 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=11;, score=0.339 total time=
                                                             0.
[CV 1/5] END .....n_neighbors=13;, score=0.627 total time=
                                                             0.
[CV 2/5] END .....n_neighbors=13;, score=0.785 total time=
                                                             0.
[CV 3/5] END .....n_neighbors=13;, score=0.844 total time=
                                                             0.
[CV 4/5] END .....n_neighbors=13;, score=0.374 total time=
                                                             0.
[CV 5/5] END .....n_neighbors=13;, score=0.337 total time=
                                                             0.
```

```
Crystal_CaseStudy/Energy_Final.ipynb at main · AdrianLandaverde/Crystal_CaseStudy
[CV 1/5] END .....n_neighbors=15;, score=0.627 total time=
                                                                   0.
[CV 2/5] END ......n neighbors=15;, score=0.790 total time=
                                                                   0.
[CV 3/5] END .....n_neighbors=15;, score=0.850 total time=
                                                                   0.
[CV 4/5] END .....n_neighbors=15;, score=0.374 total time=
                                                                   0.
[CV 5/5] END .....n neighbors=15;, score=0.338 total time=
                                                                   0.
[CV 1/5] END .....n_neighbors=17;, score=0.625 total time=
                                                                   0.
[CV 2/5] END .....n_neighbors=17;, score=0.796 total time=
                                                                   0.
[CV 3/5] END .....n_neighbors=17;, score=0.843 total time=
                                                                   0.
[CV 4/5] END .....n neighbors=17;, score=0.371 total time=
[CV 5/5] END .....n_neighbors=17;, score=0.340 total time=
Grid best parameter (max. R2): {'n_neighbors': 15}
Grid best score (R2): 0.5958735892803727
R2 Score on test: 0.8486469601628195
```

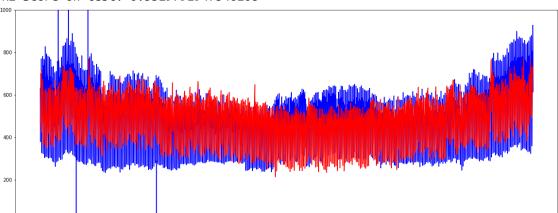


Final R2 Score: 0.6279205764416236

02.3 Linear Regresion

```
In [ ]:
         parametrosLR= {"fit intercept":[True,False],"normalize":[True,False]}
         linear = LinearRegression()
         grid = GridSearchCV(linear, param_grid = parametrosLR,scoring="r2",verbose=3)
         grid.fit(X train,y train)
         print('Grid best parameter (max. R2): ', grid.best_params_)
         print('Grid best score (R2): ', grid.best_score_)
         print("R2 Score on test:",r2_score(y_test, grid.predict(X_test)))
         fig, ax= plt.subplots(figsize=(20,8))
         ax= plotRgresion(y_2005,grid.predict(X_2005),ax,True,0,1000)
         plt.show()
         print("Final R2 Score:",r2_score(y_2005,grid.predict(X_2005)))
        Fitting 5 folds for each of 4 candidates, totalling 20 fits
        [CV 1/5] END fit intercept=True, normalize=True;, score=0.413 total time=
                                                                                     0.
        [CV 2/5] END fit intercept=True, normalize=True;, score=0.540 total time=
```

```
[CV 3/5] END fit intercept=True, normalize=True;, score=0.583 total time=
[CV 4/5] END fit intercept=True, normalize=True;, score=0.224 total time=
0s
[CV 5/5] END fit_intercept=True, normalize=True;, score=0.235 total time=
                                                                            0.
[CV 1/5] END fit intercept=True, normalize=False;, score=0.413 total time=
[CV 2/5] END fit intercept=True, normalize=False;, score=0.540 total time=
0.0s
[CV 3/5] END fit intercept=True, normalize=False;, score=0.583 total time=
0.0s
[CV 4/5] END fit_intercept=True, normalize=False;, score=0.224 total time=
[CV 5/5] END fit intercept=True, normalize=False;, score=0.235 total time=
0.0s
[CV 1/5] END fit intercept=False, normalize=True;, score=-0.037 total time=
0.0s
[CV 2/5] END fit_intercept=False, normalize=True;, score=-0.166 total time=
0.0s
[CV 3/5] END fit intercept=False, normalize=True;, score=-0.137 total time=
[CV 4/5] END fit_intercept=False, normalize=True;, score=-0.135 total time=
0.0s
[CV 5/5] END fit intercept=False, normalize=True;, score=-0.040 total time=
0.05
[CV 1/5] END fit intercept=False, normalize=False;, score=-0.037 total time=
0.0s
[CV 2/5] END fit intercept=False, normalize=False;, score=-0.166 total time=
0.0s
[CV 3/5] END fit intercept=False, normalize=False;, score=-0.137 total time=
0.0s
[CV 4/5] END fit_intercept=False, normalize=False;, score=-0.135 total time=
[CV 5/5] END fit intercept=False, normalize=False;, score=-0.040 total time=
0.0s
Grid best parameter (max. R2): {'fit_intercept': True, 'normalize': True}
Grid best score (R2): 0.3988432306680966
R2 Score on test: 0.5329791947340208
```



Final R2 Score: 0.37299626339069825

02.4 Neural Networks

In []: | layers=[]

```
for i in range(1,11):
 for j in range(1,11):
    layers.append((i,j))
parametrosMLP= {"hidden layer sizes":layers}
mlp = MLPRegressor(max iter=5000)
grid = GridSearchCV(mlp, param grid = parametrosMLP,scoring="r2",verbose=3)
grid.fit(X train,y train)
print('Grid best parameter (max. R2): ', grid.best params )
print('Grid best score (R2): ', grid.best_score_)
print("R2 Score on test:",r2_score(y_test, grid.predict(X_test)))
fig, ax= plt.subplots(figsize=(20,8))
ax= plotRgresion(y_2005,grid.predict(X_2005),ax,True,0,1000)
plt.show()
print("Final R2 Score:",r2 score(y 2005,grid.predict(X 2005)))
```

Fitting 5 folds for each of 100 candidates, totalling 500 fits /usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5 000) reached and the optimization hasn't converged yet. ConvergenceWarning, [CV 1/5] ENDhidden layer sizes=(1, 1);, score=-5.158 total time= 52. [CV 2/5] ENDhidden layer sizes=(1, 1);, score=-0.000 total time= 42. [CV 3/5] ENDhidden_layer_sizes=(1, 1);, score=0.582 total time= 8. 7s [CV 4/5] ENDhidden_layer_sizes=(1, 1);, score=0.221 total time= 12. [CV 5/5] ENDhidden layer sizes=(1, 1);, score=0.234 total time= 22. [CV 1/5] ENDhidden_layer_sizes=(1, 2);, score=0.414 total time= 9. [CV 2/5] ENDhidden layer sizes=(1, 2);, score=0.540 total time= 9. [CV 3/5] ENDhidden_layer_sizes=(1, 2);, score=0.583 total time= 10. [CV 4/5] ENDhidden layer sizes=(1, 2);, score=0.223 total time= 7. [CV 5/5] ENDhidden layer sizes=(1, 2);, score=0.235 total time= 9. [CV 1/5] ENDhidden_layer_sizes=(1, 3);, score=0.410 total time= 6. /usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5 000) reached and the optimization hasn't converged yet. ConvergenceWarning, [CV 2/5] ENDhidden layer sizes=(1, 3);, score=-6.794 total time= 51. 9s [CV 3/5] ENDhidden_layer_sizes=(1, 3);, score=0.583 total time= 7. /usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5 000) reached and the optimization hasn't converged yet. ConvergenceWarning, [CV 4/5] ENDhidden_layer_sizes=(1, 3);, score=-2.699 total time= 58. [CV 5/5] ENDhidden layer sizes=(1, 3);, score=0.235 total time= 5.

```
[CV 1/5] END ......hidden_layer_sizes=(1, 4);, score=0.414 total time=
                                                                        10.
```

```
bS
[CV 2/5] END ......hidden_layer_sizes=(1, 4);, score=0.540 total time=
                                                                          7.
[CV 3/5] END ......hidden_layer_sizes=(1, 4);, score=0.581 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(1, 4);, score=0.221 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(1, 4);, score=0.235 total time=
                                                                          9.
[CV 1/5] END ......hidden layer sizes=(1, 5);, score=-0.000 total time=
                                                                          5.
[CV 2/5] END ......hidden_layer_sizes=(1, 5);, score=0.540 total time=
                                                                         29.
[CV 3/5] END ......hidden_layer_sizes=(1, 5);, score=0.580 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(1, 5);, score=0.221 total time=
                                                                          5.
[CV 5/5] END .....hidden layer sizes=(1, 5);, score=0.235 total time=
                                                                          7.
[CV 1/5] END ......hidden_layer_sizes=(1, 6);, score=0.424 total time=
                                                                         10.
[CV 2/5] END ......hidden_layer_sizes=(1, 6);, score=0.540 total time=
                                                                          9.
[CV 3/5] END .....hidden layer sizes=(1, 6);, score=0.587 total time=
                                                                         10.
[CV 4/5] END .....hidden_layer_sizes=(1, 6);, score=-0.000 total time=
                                                                          4.
[CV 5/5] END ......hidden layer sizes=(1, 6);, score=0.235 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(1, 7);, score=0.421 total time=
                                                                          9.
[CV 2/5] END ......hidden layer sizes=(1, 7);, score=0.546 total time=
                                                                          6.
[CV 3/5] END .....hidden layer sizes=(1, 7);, score=0.582 total time=
                                                                          8.
[CV 4/5] END ......hidden layer sizes=(1, 7);, score=0.223 total time=
                                                                          9.
[CV 5/5] END ......hidden_layer_sizes=(1, 7);, score=0.234 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(1, 8);, score=0.430 total time=
                                                                          9.
[CV 2/5] END ......hidden_layer_sizes=(1, 8);, score=0.540 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(1, 8);, score=0.583 total time=
                                                                          6.
[CV 4/5] END .....hidden layer sizes=(1, 8);, score=-0.000 total time=
                                                                          3.
[CV 5/5] END ......hidden_layer_sizes=(1, 8);, score=0.235 total time=
                                                                          7.
[CV 1/5] END ......hidden_layer_sizes=(1, 9);, score=0.412 total time=
                                                                          6.
[CV 2/5] END ......hidden_layer_sizes=(1, 9);, score=0.540 total time=
                                                                          7.
[CV 3/5] END ......hidden_layer_sizes=(1, 9);, score=0.581 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(1, 9);, score=0.222 total time=
                                                                          7.
[CV 5/5] END .....hidden_layer_sizes=(1, 9);, score=-0.001 total time=
                                                                          4.
[CV 1/5] END .....hidden layer sizes=(1, 10);, score=0.413 total time=
                                                                          7.
```

```
[CV 2/5] END .....hidden_layer_sizes=(1, 10);, score=0.546 total time=
                                                                          10.
[CV 3/5] END ......hidden layer sizes=(1, 10);, score=0.580 total time=
                                                                            6.
5s
[CV 4/5] END ......hidden_layer_sizes=(1, 10);, score=-0.000 total time=
                                                                            4.
[CV 5/5] END ......hidden layer sizes=(1, 10);, score=-0.001 total time=
                                                                            4.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 1/5] END ......hidden layer sizes=(2, 1);, score=-5.159 total time=
                                                                          56.
[CV 2/5] END ......hidden layer sizes=(2, 1);, score=0.539 total time=
                                                                           9.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 3/5] END ......hidden layer sizes=(2, 1);, score=-6.517 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 4/5] END ......hidden layer sizes=(2, 1);, score=-2.723 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 5/5] END ......hidden_layer_sizes=(2, 1);, score=-2.859 total time= 54.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 1/5] END ......hidden layer sizes=(2, 2);, score=-5.149 total time=
                                                                          56.
[CV 2/5] END .....hidden_layer_sizes=(2, 2);, score=-0.000 total time=
                                                                           8.
[CV 3/5] END ......hidden layer sizes=(2, 2);, score=0.581 total time=
                                                                           7.
[CV 4/5] END .....hidden layer sizes=(2, 2);, score=0.223 total time=
                                                                          10.
[CV 5/5] END ......hidden_layer_sizes=(2, 2);, score=0.234 total time=
                                                                            6.
[CV 1/5] END ......hidden layer sizes=(2, 3);, score=0.480 total time=
7s
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 2/5] END ......hidden_layer_sizes=(2, 3);, score=-6.754 total time= 1.1m
[CV 3/5] END ......hidden layer sizes=(2, 3);, score=0.635 total time=
                                                                            6.
[CV 4/5] END ......hidden_layer_sizes=(2, 3);, score=0.223 total time=
                                                                          28.
```

```
[CV 5/5] END ......hidden_layer_sizes=(2, 3);, score=0.237 total time=
                                                                          7.
[CV 1/5] END ......hidden_layer_sizes=(2, 4);, score=0.414 total time=
                                                                          7.
[CV 2/5] END .....hidden layer sizes=(2, 4);, score=0.539 total time=
                                                                         10.
[CV 3/5] END ......hidden_layer_sizes=(2, 4);, score=0.676 total time=
                                                                         10.
[CV 4/5] END ......hidden_layer_sizes=(2, 4);, score=0.230 total time=
                                                                         13.
[CV 5/5] END ......hidden_layer_sizes=(2, 4);, score=0.277 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(2, 5);, score=0.537 total time=
                                                                         13.
[CV 2/5] END .....hidden layer sizes=(2, 5);, score=0.540 total time=
                                                                          7.
[CV 3/5] END ......hidden_layer_sizes=(2, 5);, score=0.583 total time=
                                                                          9.
[CV 4/5] END ......hidden layer sizes=(2, 5);, score=0.232 total time=
                                                                         10.
[CV 5/5] END ......hidden_layer_sizes=(2, 5);, score=0.236 total time=
                                                                          6.
[CV 1/5] END .....hidden layer sizes=(2, 6);, score=0.476 total time=
                                                                          5.
[CV 2/5] END .....hidden layer sizes=(2, 6);, score=0.580 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 3/5] END ......hidden_layer_sizes=(2, 6);, score=-6.489 total time= 1.1m
[CV 4/5] END .....hidden layer sizes=(2, 6);, score=0.220 total time=
[CV 5/5] END ......hidden_layer_sizes=(2, 6);, score=0.237 total time=
                                                                          6.
[CV 1/5] END ......hidden_layer_sizes=(2, 7);, score=0.412 total time=
                                                                          7.
[CV 2/5] END .....hidden layer sizes=(2, 7);, score=0.540 total time=
                                                                          8.
[CV 3/5] END .....hidden_layer_sizes=(2, 7);, score=0.584 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(2, 7);, score=0.222 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(2, 7);, score=0.236 total time=
                                                                          7.
[CV 1/5] END .....hidden layer sizes=(2, 8);, score=0.414 total time=
                                                                          6.
[CV 2/5] END ......hidden_layer_sizes=(2, 8);, score=0.541 total time=
                                                                          7.
[CV 3/5] END ......hidden layer sizes=(2, 8);, score=0.582 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(2, 8);, score=0.255 total time=
                                                                          6.
[CV 5/5] END ......hidden_layer_sizes=(2, 8);, score=0.235 total time=
                                                                          6.
[CV 1/5] END .....hidden layer sizes=(2, 9);, score=0.488 total time=
                                                                          6.
[CV 2/5] END ......hidden_layer_sizes=(2, 9);, score=0.539 total time=
                                                                          9.
```

```
Crystal_CaseStudy/Energy_Final.ipynb at main · AdrianLandaverde/Crystal_CaseStudy
[CV 3/5] END ......nidden_layer_sizes=(2, 9);, score=0.581 total time=
                                                                            /.
[CV 4/5] END ......hidden layer sizes=(2, 9);, score=0.224 total time=
                                                                            7.
[CV 5/5] END ......hidden_layer_sizes=(2, 9);, score=0.272 total time=
                                                                            5.
[CV 1/5] END .....hidden_layer_sizes=(2, 10);, score=0.416 total time=
                                                                            5.
[CV 2/5] END ......hidden layer sizes=(2, 10);, score=0.540 total time=
                                                                            6.
[CV 3/5] END .....hidden_layer_sizes=(2, 10);, score=0.582 total time=
                                                                            6.
[CV 4/5] END .....hidden layer sizes=(2, 10);, score=0.282 total time=
                                                                            9.
[CV 5/5] END .....hidden_layer_sizes=(2, 10);, score=0.237 total time=
                                                                            8.
2s
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 1/5] END .....hidden_layer_sizes=(3, 1);, score=-5.116 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 2/5] END ......hidden layer sizes=(3, 1);, score=-6.727 total time=
                                                                          59.
[CV 3/5] END ......hidden_layer_sizes=(3, 1);, score=0.582 total time=
                                                                            8.
[CV 4/5] END ......hidden_layer_sizes=(3, 1);, score=0.223 total time=
                                                                            9.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 5/5] END .....hidden layer sizes=(3, 1);, score=-2.856 total time= 1.0m
[CV 1/5] END ......hidden_layer_sizes=(3, 2);, score=0.413 total time=
                                                                          12.
[CV 2/5] END .....hidden layer sizes=(3, 2);, score=0.539 total time=
                                                                            8.
[CV 3/5] END .....hidden_layer_sizes=(3, 2);, score=0.578 total time=
                                                                            7.
[CV 4/5] END .....hidden layer sizes=(3, 2);, score=0.244 total time=
                                                                           9.
[CV 5/5] END ......hidden_layer_sizes=(3, 2);, score=0.237 total time=
                                                                            7.
[CV 1/5] END ......hidden_layer_sizes=(3, 3);, score=0.415 total time=
                                                                            5.
[CV 2/5] END .....hidden layer sizes=(3, 3);, score=0.695 total time=
                                                                          12.
[CV 3/5] END ......hidden_layer_sizes=(3, 3);, score=0.722 total time=
                                                                           8.
[CV 4/5] END ......hidden_layer_sizes=(3, 3);, score=0.239 total time=
                                                                            7.
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
```

ConvergenceWarning,

[CV 5/5] FND hidden laver sizes=(3. 3):. score=-2 861 total time= 1 1m

```
in
[CV 1/5] END .....hidden layer sizes=(3, 4);, score=0.414 total time=
                                                                          5.
[CV 2/5] END ......hidden_layer_sizes=(3, 4);, score=0.540 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(3, 4);, score=0.587 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(3, 4);, score=0.308 total time=
                                                                          8.
[CV 5/5] END .....hidden layer sizes=(3, 4);, score=0.236 total time=
                                                                          7.
[CV 1/5] END ......hidden_layer_sizes=(3, 5);, score=0.418 total time=
                                                                          6.
7s
[CV 2/5] END ......hidden_layer_sizes=(3, 5);, score=0.544 total time=
                                                                          6.
[CV 3/5] END ......hidden_layer_sizes=(3, 5);, score=0.588 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(3, 5);, score=0.220 total time=
                                                                          8.
[CV 5/5] END .....hidden layer sizes=(3, 5);, score=0.277 total time=
                                                                          6.
[CV 1/5] END ......hidden_layer_sizes=(3, 6);, score=0.415 total time=
                                                                          5.
[CV 2/5] END ......hidden layer sizes=(3, 6);, score=0.546 total time=
                                                                          6.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 3/5] END .....hidden layer sizes=(3, 6);, score=-6.489 total time= 1.2m
[CV 4/5] END ......hidden_layer_sizes=(3, 6);, score=0.343 total time=
                                                                          7.
[CV 5/5] END ......hidden_layer_sizes=(3, 6);, score=0.236 total time=
                                                                          3.
[CV 1/5] END ......hidden_layer_sizes=(3, 7);, score=0.553 total time=
                                                                         10.
[CV 2/5] END .....hidden layer sizes=(3, 7);, score=0.591 total time=
                                                                          7.
[CV 3/5] END .....hidden_layer_sizes=(3, 7);, score=0.631 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(3, 7);, score=0.261 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(3, 7);, score=0.357 total time=
                                                                         10.
[CV 1/5] END ......hidden_layer_sizes=(3, 8);, score=0.483 total time=
[CV 2/5] END ......hidden_layer_sizes=(3, 8);, score=0.603 total time=
                                                                          8.
[CV 3/5] END ......hidden_layer_sizes=(3, 8);, score=0.770 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(3, 8);, score=0.222 total time=
                                                                          6.
[CV 5/5] END ......hidden_layer_sizes=(3, 8);, score=0.359 total time=
                                                                         12.
[CV 1/5] END ......hidden_layer_sizes=(3, 9);, score=0.415 total time=
                                                                          8.
[CV 2/5] END ......hidden_layer_sizes=(3, 9);, score=0.695 total time=
                                                                         13.
[CV 3/5] END ......hidden_layer_sizes=(3, 9);, score=0.630 total time=
                                                                          7.
```

```
[CV 4/5] END ......hidden_layer_sizes=(3, 9);, score=0.265 total time=
                                                                           9.
[CV 5/5] END ......hidden layer sizes=(3, 9);, score=0.361 total time=
                                                                          13.
[CV 1/5] END ......hidden layer sizes=(3, 10);, score=0.433 total time=
                                                                          14.
[CV 2/5] END .....hidden_layer_sizes=(3, 10);, score=0.548 total time=
                                                                           5.
[CV 3/5] END .....hidden_layer_sizes=(3, 10);, score=0.704 total time=
                                                                           9.
[CV 4/5] END .....hidden_layer_sizes=(3, 10);, score=0.312 total time=
                                                                           7.
[CV 5/5] END ......hidden layer sizes=(3, 10);, score=0.294 total time=
                                                                          19.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 1/5] END .....hidden_layer_sizes=(4, 1);, score=-5.131 total time=
                                                                          54.
[CV 2/5] END ......hidden_layer_sizes=(4, 1);, score=0.601 total time=
                                                                           9.
[CV 3/5] END .....hidden layer sizes=(4, 1);, score=0.632 total time=
                                                                          30.
9s
[CV 4/5] END ......hidden_layer_sizes=(4, 1);, score=0.221 total time=
                                                                          11.
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
[CV 5/5] END ......hidden layer sizes=(4, 1);, score=-2.818 total time=
                                                                          54.
[CV 1/5] END ......hidden_layer_sizes=(4, 2);, score=0.414 total time=
                                                                           6.
[CV 2/5] END ......hidden_layer_sizes=(4, 2);, score=0.543 total time=
                                                                           6.
[CV 3/5] END ......hidden_layer_sizes=(4, 2);, score=0.591 total time=
                                                                           7.
7s
[CV 4/5] END ......hidden_layer_sizes=(4, 2);, score=0.222 total time=
                                                                           8.
[CV 5/5] END ......hidden_layer_sizes=(4, 2);, score=0.335 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 1/5] END ......hidden_layer_sizes=(4, 3);, score=-5.169 total time= 1.0m
[CV 2/5] END ......hidden layer sizes=(4, 3);, score=0.606 total time=
                                                                           7.
7s
[CV 3/5] END .....hidden_layer_sizes=(4, 3);, score=0.642 total time=
                                                                           5.
[CV 4/5] END ......hidden_layer_sizes=(4, 3);, score=0.239 total time=
                                                                           5.
[CV 5/5] END ......hidden_layer_sizes=(4, 3);, score=0.274 total time=
                                                                           4.
[CV 1/5] END ......hidden_layer_sizes=(4, 4);, score=0.414 total time=
                                                                           5.
1s
[CV 2/5] END ......hidden_layer_sizes=(4, 4);, score=0.538 total time=
                                                                           4.
```

```
8s
[CV 3/5] END ......hidden_layer_sizes=(4, 4);, score=0.634 total time=
                                                                          8.
[CV 4/5] END ......hidden_layer_sizes=(4, 4);, score=0.340 total time=
                                                                          6.
[CV 5/5] END ......hidden_layer_sizes=(4, 4);, score=0.237 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(4, 5);, score=0.507 total time=
                                                                         14.
[CV 2/5] END ......hidden_layer_sizes=(4, 5);, score=0.768 total time=
                                                                         12.
[CV 3/5] END .....hidden layer sizes=(4, 5);, score=0.804 total time=
                                                                         22.
[CV 4/5] END ......hidden_layer_sizes=(4, 5);, score=0.232 total time=
                                                                          4.
[CV 5/5] END ......hidden_layer_sizes=(4, 5);, score=0.277 total time=
                                                                          5.
[CV 1/5] END .....hidden layer sizes=(4, 6);, score=0.406 total time=
                                                                          4.
[CV 2/5] END ......hidden_layer_sizes=(4, 6);, score=0.604 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(4, 6);, score=0.810 total time=
                                                                          7.
[CV 4/5] END ......hidden_layer_sizes=(4, 6);, score=0.233 total time=
                                                                          7.
[CV 5/5] END ......hidden layer sizes=(4, 6);, score=0.278 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(4, 7);, score=0.419 total time=
                                                                          7.
[CV 2/5] END ......hidden layer sizes=(4, 7);, score=0.625 total time=
                                                                          9.
[CV 3/5] END ......hidden_layer_sizes=(4, 7);, score=0.589 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(4, 7);, score=0.223 total time=
                                                                          5.
[CV 5/5] END .....hidden layer sizes=(4, 7);, score=0.238 total time=
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[CV 1/5] END ......hidden_layer_sizes=(4, 8);, score=0.442 total time=
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[CV 2/5] END ......hidden_layer_sizes=(4, 8);, score=0.591 total time=
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[CV 3/5] END ......hidden_layer_sizes=(4, 8);, score=0.641 total time=
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[CV 4/5] END ......hidden_layer_sizes=(4, 8);, score=0.358 total time=
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[CV 5/5] END ......hidden layer sizes=(4, 8);, score=0.238 total time=
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[CV 3/5] END ......hidden_layer_sizes=(4, 9);, score=0.587 total time=
                                                                          8.
[CV 4/5] END .....hidden layer sizes=(4, 9);, score=0.243 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(4, 9);, score=0.238 total time=
                                                                          4.
[CV 1/5] END .....hidden layer sizes=(4, 10);, score=0.581 total time=
                                                                          6.
[CV 2/5] END .....hidden_layer_sizes=(4, 10);, score=0.545 total time=
                                                                          6.
```

```
[CV 3/5] END ......hidden_layer_sizes=(4, 10);, score=0.801 total time=
                                                                          6.
[CV 4/5] END .....hidden_layer_sizes=(4, 10);, score=0.235 total time=
                                                                         15.
[CV 5/5] END .....hidden layer sizes=(4, 10);, score=0.277 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(5, 1);, score=0.480 total time=
                                                                          6.
[CV 2/5] END ......hidden layer sizes=(5, 1);, score=0.544 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(5, 1);, score=0.588 total time=
                                                                         18.
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[CV 5/5] END .....hidden layer sizes=(5, 1);, score=0.275 total time=
                                                                          9.
[CV 1/5] END ......hidden_layer_sizes=(5, 2);, score=0.472 total time=
                                                                          6.
[CV 2/5] END ......hidden layer sizes=(5, 2);, score=0.543 total time=
                                                                         21.
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                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(5, 2);, score=0.220 total time=
                                                                          6.
[CV 5/5] END ......hidden_layer_sizes=(5, 2);, score=0.235 total time=
                                                                         22.
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[CV 2/5] END .....hidden layer sizes=(5, 3);, score=0.786 total time=
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[CV 4/5] END ......hidden layer sizes=(5, 3);, score=0.345 total time=
                                                                         17.
[CV 5/5] END ......hidden_layer_sizes=(5, 3);, score=0.236 total time=
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[CV 1/5] END ......hidden layer sizes=(5, 4);, score=0.412 total time=
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[CV 2/5] END ......hidden_layer_sizes=(5, 4);, score=0.768 total time=
                                                                          8.
[CV 3/5] END ......hidden_layer_sizes=(5, 4);, score=0.819 total time=
                                                                          5.
[CV 4/5] END ......hidden_layer_sizes=(5, 4);, score=0.222 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(5, 4);, score=0.355 total time=
                                                                         14.
[CV 1/5] END ......hidden layer sizes=(5, 5);, score=0.565 total time=
                                                                          9.
[CV 2/5] END ......hidden_layer_sizes=(5, 5);, score=0.602 total time=
                                                                          6.
[CV 3/5] END ......hidden_layer_sizes=(5, 5);, score=0.641 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(5, 5);, score=0.212 total time=
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[CV 5/5] END ......hidden_layer_sizes=(5, 5);, score=0.352 total time=
                                                                         13.
[CV 1/5] END .....hidden layer sizes=(5, 6);, score=0.458 total time=
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[CV 2/5] END ......hidden_layer_sizes=(5, 6);, score=0.603 total time=
                                                                          6.
```

```
[CV 3/5] END ......hidden_layer_sizes=(5, 6);, score=0.808 total time=
                                                                         12.
1s
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[CV 1/5] END ......hidden layer sizes=(5, 8);, score=0.590 total time=
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[CV 2/5] END ......hidden_layer_sizes=(5, 8);, score=0.595 total time=
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[CV 3/5] END ......hidden_layer_sizes=(5, 8);, score=0.827 total time=
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[CV 4/5] END ......hidden_layer_sizes=(5, 8);, score=0.331 total time=
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[CV 5/5] END ......hidden_layer_sizes=(5, 8);, score=0.238 total time=
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[CV 4/5] END .....hidden layer sizes=(5, 9);, score=0.249 total time=
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[CV 5/5] END ......hidden_layer_sizes=(5, 9);, score=0.367 total time=
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[CV 3/5] END ......hidden layer sizes=(5, 10);, score=0.582 total time=
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[CV 4/5] END .....hidden_layer_sizes=(5, 10);, score=0.269 total time=
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                                                                         23.
[CV 2/5] END ......hidden_layer_sizes=(6, 1);, score=0.595 total time=
                                                                          7.
[CV 3/5] END ......hidden_layer_sizes=(6, 1);, score=0.586 total time=
                                                                         27.
[CV 4/5] END ......hidden_layer_sizes=(6, 1);, score=0.233 total time=
                                                                         22.
[CV 5/5] END ......hidden_layer_sizes=(6, 1);, score=0.237 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(6, 2);, score=0.478 total time=
                                                                          6.
[CV 2/5] END .....hidden layer sizes=(6, 2);, score=0.778 total time=
```

```
[CV 3/5] END ......hidden_layer_sizes=(6, 2);, score=0.643 total time=
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[CV 5/5] END ......hidden_layer_sizes=(6, 2);, score=0.359 total time=
                                                                         11.
[CV 1/5] END ......hidden_layer_sizes=(6, 3);, score=0.419 total time=
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[CV 2/5] END ......hidden_layer_sizes=(6, 3);, score=0.767 total time=
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[CV 3/5] END .....hidden layer sizes=(6, 3);, score=0.797 total time=
                                                                         28.
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[CV 5/5] END ......hidden_layer_sizes=(6, 3);, score=0.279 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(6, 4);, score=0.597 total time=
                                                                         10.
[CV 2/5] END ......hidden_layer_sizes=(6, 4);, score=0.607 total time=
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[CV 3/5] END .....hidden layer sizes=(6, 4);, score=0.587 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(6, 4);, score=0.359 total time=
                                                                         10.
[CV 5/5] END ......hidden layer sizes=(6, 4);, score=0.277 total time=
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[CV 1/5] END ......hidden_layer_sizes=(6, 5);, score=0.405 total time=
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[CV 2/5] END ......hidden layer sizes=(6, 6);, score=0.597 total time=
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[CV 3/5] END ......hidden_layer_sizes=(6, 6);, score=0.574 total time=
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[CV 4/5] END ......hidden_layer_sizes=(6, 6);, score=0.240 total time=
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[CV 5/5] END ......hidden_layer_sizes=(6, 6);, score=0.237 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(6, 7);, score=0.590 total time=
                                                                          9.
[CV 2/5] END ......hidden_layer_sizes=(6, 7);, score=0.785 total time=
                                                                          8.
[CV 3/5] END ......hidden_layer_sizes=(6, 7);, score=0.571 total time=
                                                                          4.
[CV 4/5] END ......hidden layer sizes=(6, 7);, score=0.346 total time=
                                                                         11.
[CV 5/5] END ......hidden_layer_sizes=(6, 7);, score=0.276 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(6, 8);, score=0.412 total time=
                                                                          4.
[CV 2/5] END ......hidden_layer_sizes=(6, 8);, score=0.869 total time=
                                                                         12.
```

hidden layer circe-/6 0\. cconc-0 700 +o+al +ima-

```
Crystal CaseStudy/Energy Final.ipynb at main AdrianLandaverde/Crystal CaseStudy
[LV 3/3] END ......IILUUEI__tayer__sizes=(0, 0);, Score=0./00 cocat cime=
                                                                           o.
[CV 4/5] END ......hidden_layer_sizes=(6, 8);, score=0.220 total time=
                                                                           6.
[CV 5/5] END .....hidden layer sizes=(6, 8);, score=0.238 total time=
                                                                           4.
[CV 1/5] END .....hidden layer sizes=(6, 9);, score=0.589 total time=
                                                                           8.
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                                                                          11.
[CV 4/5] END ......hidden_layer_sizes=(6, 9);, score=0.222 total time=
                                                                           4.
[CV 5/5] END ......hidden layer sizes=(6, 9);, score=0.238 total time=
                                                                           3.
[CV 1/5] END .....hidden_layer_sizes=(6, 10);, score=0.587 total time=
                                                                           8.
[CV 2/5] END ......hidden_layer_sizes=(6, 10);, score=0.539 total time=
                                                                           3.
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                                                                           6.
[CV 4/5] END .....hidden_layer_sizes=(6, 10);, score=0.225 total time=
                                                                           4.
[CV 5/5] END .....hidden_layer_sizes=(6, 10);, score=0.275 total time=
                                                                           4.
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                                                                          26.
[CV 2/5] END .....hidden layer sizes=(7, 1);, score=0.596 total time=
                                                                           6.
[CV 3/5] END ......hidden_layer_sizes=(7, 1);, score=0.588 total time=
                                                                          24.
9s
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 4/5] END .....hidden layer sizes=(7, 1);, score=-2.734 total time=
                                                                          59.
[CV 5/5] END ......hidden_layer_sizes=(7, 1);, score=0.276 total time=
                                                                           5.
[CV 1/5] END ......hidden_layer_sizes=(7, 2);, score=0.476 total time=
                                                                           6.
[CV 2/5] END .....hidden layer sizes=(7, 2);, score=0.598 total time=
                                                                           5.
[CV 3/5] END ......hidden_layer_sizes=(7, 2);, score=0.804 total time=
                                                                          10.
[CV 4/5] END ......hidden_layer_sizes=(7, 2);, score=0.242 total time=
                                                                           5.
[CV 5/5] END ......hidden_layer_sizes=(7, 2);, score=0.236 total time=
                                                                           5.
[CV 1/5] END ......hidden_layer_sizes=(7, 3);, score=0.479 total time=
                                                                          16.
[CV 2/5] END ......hidden_layer_sizes=(7, 3);, score=0.603 total time=
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[CV 3/5] END ......hidden_layer_sizes=(7, 3);, score=0.640 total time=
                                                                           8.
[CV 4/5] END .....hidden layer sizes=(7, 3);, score=0.349 total time=
                                                                          12.
[CV 5/5] END .....hidden_layer_sizes=(7, 3);, score=0.275 total time=
                                                                           5.
[CV 1/5] END .....hidden laver sizes=(7, 4);, score=0.471 total time=
                                                                           6.
```

```
25
[CV 2/5] END ......hidden_layer_sizes=(7, 4);, score=0.544 total time=
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[CV 4/5] END ......hidden_layer_sizes=(7, 4);, score=0.240 total time=
                                                                          6.
[CV 5/5] END .....hidden layer sizes=(7, 4);, score=0.279 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(7, 5);, score=0.479 total time=
                                                                          4.
[CV 2/5] END ......hidden layer sizes=(7, 5);, score=0.599 total time=
                                                                          4.
[CV 3/5] END ......hidden_layer_sizes=(7, 5);, score=0.637 total time=
                                                                          4.
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[CV 5/5] END .....hidden layer sizes=(7, 5);, score=0.359 total time=
                                                                         10.
[CV 1/5] END ......hidden_layer_sizes=(7, 6);, score=0.485 total time=
                                                                          6.
[CV 2/5] END ......hidden_layer_sizes=(7, 6);, score=0.605 total time=
                                                                          6.
[CV 3/5] END ......hidden_layer_sizes=(7, 6);, score=0.576 total time=
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[CV 5/5] END ......hidden_layer_sizes=(7, 6);, score=0.279 total time=
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[CV 1/5] END ......hidden_layer_sizes=(7, 7);, score=0.408 total time=
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[CV 2/5] END ......hidden_layer_sizes=(7, 7);, score=0.607 total time=
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[CV 4/5] END ......hidden layer sizes=(7, 7);, score=0.262 total time=
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[CV 5/5] END ......hidden_layer_sizes=(7, 7);, score=0.236 total time=
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[CV 1/5] END ......hidden layer sizes=(7, 8);, score=0.485 total time=
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                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(7, 8);, score=0.224 total time=
                                                                          4.
[CV 5/5] END ......hidden_layer_sizes=(7, 8);, score=0.274 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(7, 9);, score=0.480 total time=
                                                                          4.
[CV 2/5] END ......hidden_layer_sizes=(7, 9);, score=0.775 total time=
                                                                          8.
[CV 3/5] END .....hidden layer sizes=(7, 9);, score=0.758 total time=
                                                                          8.
[CV 4/5] END ......hidden_layer_sizes=(7, 9);, score=0.331 total time=
                                                                          7.
[CV 5/5] END ......hidden_layer_sizes=(7, 9);, score=0.357 total time=
                                                                          8.
[CV 1/5] END ......hidden_layer_sizes=(7, 10);, score=0.474 total time=
                                                                          4.
```

```
7s
[CV 2/5] END .....hidden layer sizes=(7, 10);, score=0.761 total time=
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[CV 3/5] END .....hidden_layer_sizes=(7, 10);, score=0.769 total time=
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[CV 4/5] END .....hidden layer sizes=(7, 10);, score=0.344 total time=
                                                                          9.
[CV 5/5] END .....hidden_layer_sizes=(7, 10);, score=0.302 total time=
                                                                          5.
[CV 1/5] END ......hidden_layer_sizes=(8, 1);, score=0.414 total time=
                                                                         12.
[CV 2/5] END .....hidden layer sizes=(8, 1);, score=0.602 total time=
                                                                          6.
0s
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 3/5] END .....hidden_layer_sizes=(8, 1);, score=-6.472 total time=
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[CV 1/5] END ......hidden_layer_sizes=(8, 2);, score=0.503 total time=
                                                                          9.
[CV 2/5] END ......hidden_layer_sizes=(8, 2);, score=0.586 total time=
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[CV 3/5] END ......hidden_layer_sizes=(8, 2);, score=0.629 total time=
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                                                                         11.
[CV 5/5] END ......hidden_layer_sizes=(8, 2);, score=0.276 total time=
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[CV 1/5] END ......hidden_layer_sizes=(8, 3);, score=0.482 total time=
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[CV 3/5] END .....hidden layer sizes=(8, 3);, score=0.802 total time=
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[CV 4/5] END ......hidden_layer_sizes=(8, 3);, score=0.237 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(8, 3);, score=0.352 total time=
                                                                         13.
[CV 1/5] END ......hidden_layer_sizes=(8, 4);, score=0.591 total time=
                                                                          8.
[CV 2/5] END ......hidden_layer_sizes=(8, 4);, score=0.734 total time=
                                                                          9.
[CV 3/5] END .....hidden layer sizes=(8, 4);, score=0.812 total time=
                                                                          9.
[CV 4/5] END ......hidden_layer_sizes=(8, 4);, score=0.239 total time=
                                                                          5.
[CV 5/5] END .....hidden layer sizes=(8, 4);, score=0.360 total time=
                                                                         10.
[CV 1/5] END ......hidden_layer_sizes=(8, 5);, score=0.479 total time=
                                                                          5.
[CV 2/5] END ......hidden_layer_sizes=(8, 5);, score=0.783 total time=
                                                                          9.
[CV 3/5] END .....hidden_layer_sizes=(8, 5);, score=0.785 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(8, 5);, score=0.243 total time=
                                                                          5.
```

```
ΙS
[CV 5/5] END ......hidden_layer_sizes=(8, 5);, score=0.353 total time=
[CV 1/5] END ......hidden_layer_sizes=(8, 6);, score=0.414 total time=
                                                                          5.
[CV 2/5] END ......hidden_layer_sizes=(8, 6);, score=0.769 total time=
                                                                         11.
[CV 3/5] END ......hidden_layer_sizes=(8, 6);, score=0.814 total time=
                                                                         12.
[CV 4/5] END .....hidden layer sizes=(8, 6);, score=0.239 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(8, 6);, score=0.237 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(8, 7);, score=0.591 total time=
                                                                          6.
[CV 2/5] END ......hidden_layer_sizes=(8, 7);, score=0.543 total time=
[CV 3/5] END .....hidden layer sizes=(8, 7);, score=0.589 total time=
[CV 4/5] END ......hidden_layer_sizes=(8, 7);, score=0.344 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(8, 7);, score=0.269 total time=
                                                                          6.
[CV 1/5] END .....hidden layer sizes=(8, 8);, score=0.412 total time=
                                                                          4.
[CV 2/5] END ......hidden_layer_sizes=(8, 8);, score=0.803 total time=
                                                                          8.
[CV 3/5] END ......hidden_layer_sizes=(8, 8);, score=0.584 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(8, 8);, score=0.224 total time=
                                                                          4.
[CV 5/5] END .....hidden layer sizes=(8, 8);, score=0.360 total time=
                                                                          7.
[CV 1/5] END .....hidden layer sizes=(8, 9);, score=0.442 total time=
                                                                          4.
[CV 2/5] END ......hidden_layer_sizes=(8, 9);, score=0.600 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(8, 9);, score=0.637 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(8, 9);, score=0.332 total time=
                                                                          8.
[CV 5/5] END ......hidden_layer_sizes=(8, 9);, score=0.236 total time=
                                                                          4.
[CV 1/5] END .....hidden_layer_sizes=(8, 10);, score=0.403 total time=
                                                                          3.
[CV 2/5] END .....hidden_layer_sizes=(8, 10);, score=0.538 total time=
                                                                          4.
[CV 3/5] END .....hidden_layer_sizes=(8, 10);, score=0.795 total time=
                                                                          7.
                                                                          7.
[CV 4/5] END .....hidden_layer_sizes=(8, 10);, score=0.318 total time=
[CV 5/5] END ......hidden layer sizes=(8, 10);, score=0.357 total time=
                                                                         10.
[CV 1/5] END ......hidden_layer_sizes=(9, 1);, score=0.415 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 2/5] END ......hidden_layer_sizes=(9, 1);, score=-6.754 total time= 1.1m
```

```
[CV 3/5] END ......hidden_layer_sizes=(9, 1);, score=0.587 total time=
                                                                         13.
[CV 4/5] END .....hidden layer sizes=(9, 1);, score=0.222 total time=
7s
[CV 5/5] END ......hidden_layer_sizes=(9, 1);, score=0.276 total time=
                                                                          6.
[CV 1/5] END ......hidden layer sizes=(9, 2);, score=0.588 total time=
                                                                         11.
[CV 2/5] END ......hidden_layer_sizes=(9, 2);, score=0.544 total time=
                                                                         33.
[CV 3/5] END .....hidden layer sizes=(9, 2);, score=0.627 total time=
                                                                          6.
[CV 4/5] END ......hidden_layer_sizes=(9, 2);, score=0.225 total time=
                                                                          5.
[CV 5/5] END ......hidden_layer_sizes=(9, 2);, score=0.277 total time=
                                                                          6.
[CV 1/5] END ......hidden_layer_sizes=(9, 3);, score=0.416 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 2/5] END ......hidden_layer_sizes=(9, 3);, score=-6.757 total time= 1.3m
[CV 3/5] END ......hidden_layer_sizes=(9, 3);, score=0.646 total time=
[CV 4/5] END ......hidden_layer_sizes=(9, 3);, score=0.223 total time=
                                                                         37.
[CV 5/5] END ......hidden_layer_sizes=(9, 3);, score=0.266 total time=
[CV 1/5] END ......hidden_layer_sizes=(9, 4);, score=0.411 total time=
                                                                          5.
[CV 2/5] END ......hidden_layer_sizes=(9, 4);, score=0.601 total time=
                                                                         25.
[CV 3/5] END .....hidden layer sizes=(9, 4);, score=0.792 total time=
                                                                          9.
[CV 4/5] END ......hidden_layer_sizes=(9, 4);, score=0.333 total time=
                                                                         14.
[CV 5/5] END ......hidden_layer_sizes=(9, 4);, score=0.277 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(9, 5);, score=0.621 total time=
                                                                         11.
[CV 2/5] END .....hidden layer sizes=(9, 5);, score=0.545 total time=
                                                                          5.
[CV 3/5] END ......hidden_layer_sizes=(9, 5);, score=0.639 total time=
                                                                          4.
[CV 4/5] END ......hidden_layer_sizes=(9, 5);, score=0.307 total time=
                                                                          9.
[CV 5/5] END ......hidden_layer_sizes=(9, 5);, score=0.366 total time=
                                                                          8.
[CV 1/5] END ......hidden_layer_sizes=(9, 6);, score=0.412 total time=
                                                                          5.
[CV 2/5] END .....hidden layer sizes=(9, 6);, score=0.597 total time=
                                                                          4.
[CV 3/5] END ......hidden_layer_sizes=(9, 6);, score=0.812 total time=
                                                                          9.
[CV 4/5] END ......hidden_layer_sizes=(9, 6);, score=0.224 total time=
                                                                          4.
[CV 5/5] END ......hidden_layer_sizes=(9, 6);, score=0.277 total time=
                                                                          3.
```

```
[CV 1/5] END ......hidden_layer_sizes=(9, 7);, score=0.559 total time=
                                                                           7.
[CV 2/5] END ......hidden_layer_sizes=(9, 7);, score=0.602 total time=
                                                                           5.
[CV 3/5] END .....hidden layer sizes=(9, 7);, score=0.639 total time=
                                                                           4.
[CV 4/5] END ......hidden_layer_sizes=(9, 7);, score=0.222 total time=
                                                                           4.
[CV 5/5] END ......hidden_layer_sizes=(9, 7);, score=0.363 total time=
                                                                           7.
[CV 1/5] END ......hidden_layer_sizes=(9, 8);, score=0.593 total time=
                                                                           5.
[CV 2/5] END ......hidden_layer_sizes=(9, 8);, score=0.774 total time=
                                                                          10.
[CV 3/5] END .....hidden layer sizes=(9, 8);, score=0.854 total time=
                                                                          11.
[CV 4/5] END ......hidden_layer_sizes=(9, 8);, score=0.337 total time=
                                                                           9.
[CV 5/5] END .....hidden layer sizes=(9, 8);, score=0.237 total time=
                                                                           3.
[CV 1/5] END ......hidden_layer_sizes=(9, 9);, score=0.582 total time=
                                                                           6.
[CV 2/5] END .....hidden layer sizes=(9, 9);, score=0.783 total time=
                                                                           7.
[CV 3/5] END .....hidden layer sizes=(9, 9);, score=0.814 total time=
                                                                           6.
[CV 4/5] END ......hidden_layer_sizes=(9, 9);, score=0.342 total time=
                                                                           8.
[CV 5/5] END ......hidden_layer_sizes=(9, 9);, score=0.363 total time=
                                                                           9.
[CV 1/5] END .....hidden_layer_sizes=(9, 10);, score=0.470 total time=
[CV 2/5] END ......hidden layer sizes=(9, 10);, score=0.542 total time=
[CV 3/5] END .....hidden_layer_sizes=(9, 10);, score=0.582 total time=
                                                                           6.
[CV 4/5] END .....hidden_layer_sizes=(9, 10);, score=0.324 total time=
                                                                           5.
[CV 5/5] END ......hidden layer sizes=(9, 10);, score=0.336 total time=
                                                                           9.
[CV 1/5] END .....hidden_layer_sizes=(10, 1);, score=0.463 total time=
[CV 2/5] END .....hidden_layer_sizes=(10, 1);, score=0.599 total time=
/usr/local/lib/python3.7/dist-packages/sklearn/neural_network/_multilayer_perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 3/5] END .....hidden_layer_sizes=(10, 1);, score=-6.533 total time= 1.2m
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
  ConvergenceWarning,
[CV 4/5] END ......hidden_layer_sizes=(10, 1);, score=-2.708 total time= 1.1m
/usr/local/lib/python3.7/dist-packages/sklearn/neural network/ multilayer perc
eptron.py:696: ConvergenceWarning: Stochastic Optimizer: Maximum iterations (5
000) reached and the optimization hasn't converged yet.
 ConvergenceWarning,
```

```
[CV 1/5] END ......hidden_layer_sizes=(10, 3);, score=0.600 total time=
[CV 2/5] END .....hidden_layer_sizes=(10, 3);, score=0.600 total time=
                                                                          4.
[CV 3/5] END ......hidden layer sizes=(10, 3);, score=0.812 total time=
                                                                         11.
[CV 4/5] END .....hidden_layer_sizes=(10, 3);, score=0.246 total time=
[CV 5/5] END .....hidden_layer_sizes=(10, 3);, score=0.238 total time=
                                                                         36.
[CV 1/5] END ......hidden_layer_sizes=(10, 4);, score=0.585 total time=
                                                                         11.
[CV 2/5] END .....hidden_layer_sizes=(10, 4);, score=0.749 total time=
                                                                          6.
[CV 3/5] END ......hidden layer sizes=(10, 4);, score=0.635 total time=
                                                                          6.
[CV 4/5] END .....hidden_layer_sizes=(10, 4);, score=0.238 total time=
                                                                          4.
[CV 5/5] END .....hidden layer sizes=(10, 4);, score=0.360 total time=
                                                                         10.
[CV 1/5] END .....hidden_layer_sizes=(10, 5);, score=0.584 total time=
                                                                          6.
[CV 2/5] END .....hidden_layer_sizes=(10, 5);, score=0.754 total time=
                                                                          7.
[CV 3/5] END .....hidden_layer_sizes=(10, 5);, score=0.585 total time=
                                                                          4.
[CV 4/5] END .....hidden_layer_sizes=(10, 5);, score=0.298 total time=
                                                                          9.
[CV 5/5] END ......hidden layer sizes=(10, 5);, score=0.278 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(10, 6);, score=0.573 total time=
                                                                          8.
[CV 2/5] END ......hidden layer sizes=(10, 6);, score=0.794 total time=
[CV 3/5] END .....hidden_layer_sizes=(10, 6);, score=0.799 total time=
                                                                          8.
[CV 4/5] END .....hidden_layer_sizes=(10, 6);, score=0.330 total time=
                                                                          5.
[CV 5/5] END ......hidden layer sizes=(10, 6);, score=0.279 total time=
                                                                          4.
[CV 1/5] END ......hidden_layer_sizes=(10, 7);, score=0.558 total time=
                                                                          9.
[CV 2/5] END .....hidden_layer_sizes=(10, 7);, score=0.783 total time=
                                                                          6.
[CV 3/5] END .....hidden_layer_sizes=(10, 7);, score=0.821 total time=
                                                                          9.
[CV 4/5] END ......hidden layer sizes=(10, 7);, score=0.319 total time=
                                                                          5.
```

hidden laver sizes=(10. 7):. score=0 272 total time=

[CV 5/5] FND

3

5.

5.

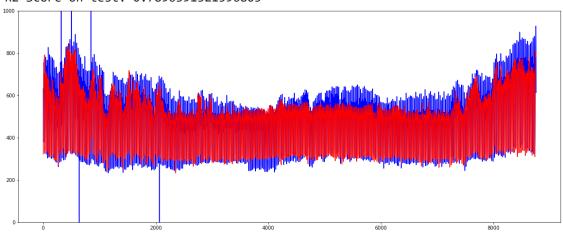
6.

6.

12.

9.

```
6s
[CV 1/5] END ......hidden layer sizes=(10, 8);, score=0.566 total time=
                                                                           7.
[CV 2/5] END .....hidden_layer_sizes=(10, 8);, score=0.538 total time=
                                                                           5.
[CV 3/5] END .....hidden_layer_sizes=(10, 8);, score=0.851 total time=
                                                                           9.
[CV 4/5] END .....hidden_layer_sizes=(10, 8);, score=0.292 total time=
                                                                           4.
[CV 5/5] END .....hidden layer sizes=(10, 8);, score=0.279 total time=
                                                                           3.
[CV 1/5] END .....hidden_layer_sizes=(10, 9);, score=0.590 total time=
                                                                          12.
5s
[CV 2/5] END .....hidden_layer_sizes=(10, 9);, score=0.779 total time=
                                                                           7.
[CV 3/5] END .....hidden_layer_sizes=(10, 9);, score=0.631 total time=
                                                                           4.
[CV 4/5] END .....hidden_layer_sizes=(10, 9);, score=0.316 total time=
                                                                           7.
[CV 5/5] END ......hidden layer sizes=(10, 9);, score=0.350 total time=
                                                                           5.
[CV 1/5] END ......hidden_layer_sizes=(10, 10);, score=0.416 total time=
                                                                           3.
[CV 2/5] END ......hidden layer sizes=(10, 10);, score=0.575 total time=
                                                                           5.
[CV 3/5] END ......hidden_layer_sizes=(10, 10);, score=0.571 total time=
                                                                           4.
[CV 4/5] END ......hidden_layer_sizes=(10, 10);, score=0.247 total time=
                                                                           4.
[CV 5/5] END .....hidden layer sizes=(10, 10);, score=0.365 total time=
                                                                           7.
5s
Grid best parameter (max. R2): {'hidden_layer_sizes': (9, 9)}
Grid best score (R2): 0.5767142177992696
R2 Score on test: 0.7896391321596805
```



Final R2 Score: 0.5542847245302072

Based on the models above, we obtained that the best method to predict the energy was a Random Forest with 70 Trees using the following variables:

'temp_per_day_2005','HourOfDay','full_humid_2005'

- Mean energy per Day
- Hour of the Day
- Humidity of the Hour

Hence, we obtained 2 different models to predict energy, each one for a different year

02.5 Final Model for 2005

```
In [ ]:
         X_2005= df_energy[['temp_per_day_2005','HourOfDay','full_humid_2005']]
         y_2005= df_energy['energy_consumpt_2005']
         X train, X test, y train, y test= train test split(X 2005,y 2005,random state
In [ ]:
         parameters= {"n_estimators":list(range(10,101,10))}
          rf = RandomForestRegressor(random_state=0, n_estimators=70)
          rf.fit(X train,y train)
          print("R2 Score on test:",r2_score(y_test, rf.predict(X_test)))
         fig, axs= plt.subplots(2,1,figsize=(20,8))
          axs[0] = plotRgresion(y 2005, rf.predict(X 2005), axs[0], False, 0, 1000)
          axs[1] = plotRgresion(y 2005, rf.predict(X 2005), axs[1], True, 0, 1000)
          plt.legend()
          plt.show()
          print("Final R2 Score:",r2_score(y_2005,rf.predict(X_2005)))
        R2 Score on test: 0.6105817867373805
        5000
        4000
        3000
        1000
```

0 2000 4000 6000 8000

1000 y Real y Predicted 2000 4000 6000 8000

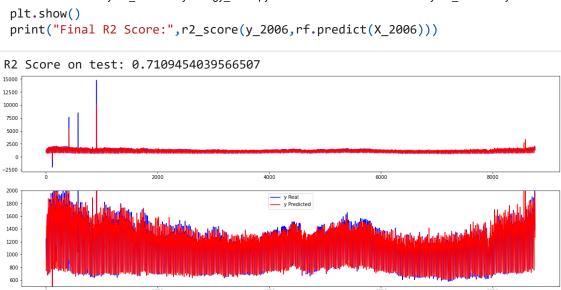
Final R2 Score: 0.8696535631662909

02.6 Final Model for 2006

```
In [ ]:
    X_2006= df_energy[['temp_per_day_2006','HourOfDay','full_humid_2006']]
    y_2006= df_energy['energy_consumpt_2006']
    X_train, X_test, y_train, y_test= train_test_split(X_2006,y_2006,random_state)

In [ ]:
    parameters= {"n_estimators":list(range(10,101,10))}
    rf = RandomForestRegressor(random_state=0, n_estimators=70)
    rf.fit(X_train,y_train)

    print("R2 Score on test:",r2_score(y_test, rf.predict(X_test)))
    fig, axs= plt.subplots(2,1,figsize=(20,8))
    axs[0]= plotRgresion(y_2006,rf.predict(X_2006),axs[0],False,0,1000)
    axs[1]= plotRgresion(y_2006,rf.predict(X_2006),axs[1],True,500,2000)
    plt.legend()
```



Final R2 Score: 0.8857925371269807

03. Time Series Forecast

The previous models can predcit the energy of the hour based on some variables, however, we can see that both years have a similar pattern in the energy, but it has a different scale.

Hence, if we apply a tiem series forecast we might get a better model to predict the energy based on time

```
In [7]: df_energy= pd.read_csv("/content/energy__data-2 (1).csv")
    df_energy
```

Out[7]:		Hour	energy_consumpt_2005	energy_consumpt_2006	full_temp_2005	full_humid_200!
	0	1	631.623161	1246.300847	-0.400000	64.000000
	1	2	534.397104	1062.500558	-0.733333	65.333333
	2	3	453.538785	884.586887	-1.066667	66.666667
	3	4	400.699718	786.564121	-1.400000	68.000000
	4	5	378.171092	742.669614	-1.666667	60.333333
	•••					
	8779	8780	950.369306	0.000000	3.333333	64.000000
	8780	8781	880.138770	0.000000	2.666667	68.000000
	8781	8782	792.754026	0.000000	2.000000	72.000000
	8782	8783	740.446668	0.000000	1.333333	76.000000
	8783	8784	706.176769	0.000000	0.666667	80.000000

8784 rows × 7 columns

03.1 Na & Outliers

We will deal with Na and outliers so that we can get a better representation of the time series

In [8]:

#We will check for Na and interpolate it to get a close prediction of what the df_energy.isna().sum()