

Evaluation Metrics For Regression Models

To be able to measure the performance of a regression model and compare several models, different metrics could use: R2 Score, MSE, RMSE, MAE, MAPE

1. Loading the dataset and fitting the model

We will use the Diabetes data used in the "Least Angle Regression" paper: N=442 patients, p=10 predictors. One row per patient, and the last column is the response variable.

dataset(raw): <https://www4.stat.ncsu.edu/~boos/var.select/diabetes.tab.txt>

In [26]: `pip install -U scikit-learn`

Requirement already satisfied: scikit-learn in c:\users\kiran\anaconda3\lib\site-packages (1.2.2) Note: you may need to restart the kernel to use updated packages.

Requirement already satisfied: numpy>=1.17.3 in c:\users\kiran\anaconda3\lib\site-packages (from scikit-learn) (1.21.5)

Requirement already satisfied: threadpoolctl>=2.0.0 in c:\users\kiran\anaconda3\lib\site-packages (from scikit-learn) (2.2.0)

Requirement already satisfied: scipy>=1.3.2 in c:\users\kiran\anaconda3\lib\site-packages (from scikit-learn) (1.9.1)

Requirement already satisfied: joblib>=1.1.1 in c:\users\kiran\anaconda3\lib\site-packages (from scikit-learn) (1.2.0)

In [110]...

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import normalize
from sklearn.preprocessing import MinMaxScaler
import time
from pandas.io.json import json_normalize
from sklearn.datasets import make_classification
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
from sklearn.pipeline import make_pipeline
from sklearn.linear_model import LinearRegression, Lasso
from sklearn.metrics import r2_score
from sklearn.metrics import explained_variance_score, mean_squared_error, mean_absolute_error
```

In [35]: `df=pd.read_csv('https://www4.stat.ncsu.edu/~boos/var.select/diabetes.tab.txt', sep='\t')`
`print(df.shape)`
`df.head()`

(442, 11)

Out[35]:

	AGE	SEX	BMI	BP	S1	S2	S3	S4	S5	S6	Y
0	59	2	32.1	101.0	157	93.2	38.0	4.0	4.8598	87	151
1	48	1	21.6	87.0	183	103.2	70.0	3.0	3.8918	69	75
2	72	2	30.5	93.0	156	93.6	41.0	4.0	4.6728	85	141
3	24	1	25.3	84.0	198	131.4	40.0	5.0	4.8903	89	206
4	50	1	23.0	101.0	192	125.4	52.0	4.0	4.2905	80	135

We will also normalize data, to have the same order of magnitude among the independent variables:

```
In [43]: # Scaled data : X-mean: # Start by subtracting the mean with StandardScaler, without c
df_sc=StandardScaler(with_std=False).fit_transform(df)
df_sc=pd.DataFrame(data=df_sc,columns=df.columns)

### Normalize data: divide each feature by its L2 norm
# If axis=0 no need to transpose, this available in normalize method but not in normal

df_norm=normalize(df_sc.iloc[:, :-1], norm='l2')

#or transpose the dataframe: (as axis=1 is the default value)
#df_norm=normalize(df_sc.iloc[:, :-1], T, norm='l2')
#(not to forget to transpose the results too, to go back to the initial shape)

df_norm=pd.DataFrame(data=df_norm, columns=df.columns[:-1])
df_norm['Y']=df_sc['Y']
print('Normalized data:Scaled data/L2 norm')
df_norm.head()
```

Normalized data:Scaled data/L2 norm

Out[43]:

	AGE	SEX	BMI	BP	S1	S2	S3	S4	S5	
0	0.242521	0.012301	0.132441	0.146990	-0.743632	-0.514549	-0.272751	-0.001625	0.005053	-0
1	-0.015115	-0.013662	-0.139324	-0.223086	-0.179130	-0.357052	0.589631	-0.031222	-0.021868	-0
2	0.493611	0.011176	0.086695	-0.034622	-0.696639	-0.459079	-0.184742	-0.001477	0.000660	-0
3	-0.722696	-0.013804	-0.031710	-0.313832	0.261150	0.470463	-0.288525	0.027405	0.007336	-0
4	0.086518	-0.027342	-0.197088	0.370906	0.166959	0.581543	0.129116	-0.004101	-0.020487	-0

1.2 Model to Fit

To illustrate the computation of the the different metrics, step by step, let's take the predicted values given

by the OLS model 'y_predict_ols'. In this example we will not be splitting the dataset to train and test sets.

It's no the objective of this notebook

```

In [57]: features=df.columns[:-1]
X=df_norm[features]
y=df_norm['Y']

### OLS:Ordinary Least Square
reg_ols=LinearRegression(fit_intercept=False)
reg_ols.fit(X,y)
#Predict Values
y_predict_ols=reg_ols.predict(X)
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols

df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
df_errors['(y_yhat)**2']=df_errors['y_yhat']**2
mean_y=df_errors['y_true'].mean()
df_errors['(y_ymean)**2']=(df_errors['y_true']-mean_y)**2

r2_recomp=1-(np.sum(df_errors['(y_yhat)**2'])/np.sum(df_errors['(y_ymean)**2']))
r2_recomp

```

Out[57]: 0.48233609146755896

SKLEARN

```

In [61]: r2_sk_learn=r2_score(y,y_predict_ols)
r2_sk_learn

```

Out[61]: 0.48233609146755885

Both

```

In [62]: print('r2 recomputed:',r2_recomp,'r2_sk_learn',r2_sk_learn)

r2 recomputed: 0.48233609146755896 r2_sk_learn 0.48233609146755885

```

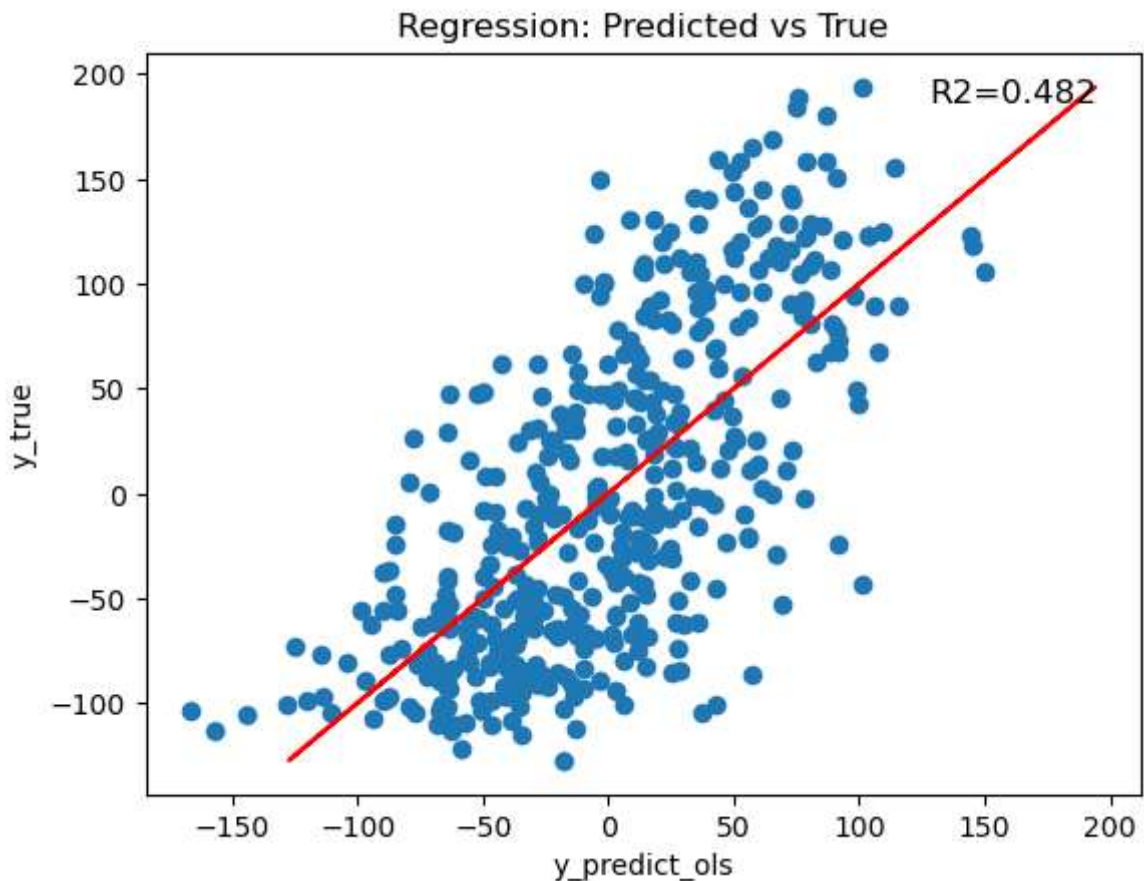
Let's Visualize

```

In [63]: plt.scatter(y_predict_ols,y)
plt.plot(y,y,'-r')
plt.annotate(r"R2={0}".format(round(r2_recomp,3)),xy=(200,200),xytext=(-65,-10),
            textcoords='offset points',fontsize=12)
plt.xlabel('y_predict_ols')
plt.ylabel('y_true')
plt.title('Regression: Predicted vs True')

```

Out[63]: Text(0.5, 1.0, 'Regression: Predicted vs True')



Explained Variable Score

In [66]: `N=y.shape[0]`

```
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols

mean_y=df_errors['y_true'].mean()
df_errors['(y_ymean)**2']=(df_errors['y_true']-mean_y)**2
var_y=np.sum(df_errors['(y_ymean)**2'])/N
df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
mean_yyhat=df_errors['y_yhat'].mean()
df_errors['(y_yhat_yyhatmean)**2']=(df_errors['y_yhat']-mean_yyhat)**2
var_yyhat=np.sum(df_errors['(y_yhat_yyhatmean)**2'])/N

explained_variance_recomp=1-var_yyhat/var_y
explained_variance_recomp
```

Out[66]: 0.4824491425011799

SKLearn

In [70]: `explained_variance_sklearn=explained_variance_score(y,y_predict_ols)`
`explained_variance_sklearn`

Out[70]: 0.4824491425011799

Both

```
In [72]: print('Explained variance recomputed:',explained_variance_recomp,'Explained variance from sklearn:',explained_variance_sklearn)
```

Explained variance recomputed: 0.4824491425011799 Explained variance from sklearn 0.4824491425011799

One can see that the explained variance and the R2 score are equal. That's because the mean of the residual is ~0

```
In [73]: mean_yyhat=df_errors['y_yhat'].mean()
mean_yyhat
```

Out[73]: 0.8187671322471713

MSE : Mean Squared Error

```
In [74]: N=y.shape[0]
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols
df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
df_errors['(y_yhat)**2']=df_errors['y_yhat']**2
mse_recomp=np.sum(df_errors['(y_yhat)**2'])/N
mse_recomp
```

Out[74]: 3069.6873928821205

SKLearn

```
In [78]: mse_sklearn=mean_squared_error(y,y_predict_ols)
mse_sklearn
```

Out[78]: 3069.6873928821205

Both

```
In [80]: print('MSE Recomputed:',mse_recomp,'MSE from sklearn',mse_sklearn)
```

MSE Recomputed: 3069.6873928821205 MSE from sklearn 3069.6873928821205

RMSE: Root Mean Squared Error

```
In [82]: rmse_recomp=np.sqrt(mse_recomp)
rmse_recomp
```

Out[82]: 55.40475965909536

SK Learn

```
In [83]: rmse_sklearn=mean_squared_error(y,y_predict_ols,squared=False)
rmse_sklearn
```

Out[83]: 55.40475965909536

Both

```
In [84]: print('RMSE Recomputed:',rmse_recomp,'RMSE from sklearn:',rmse_sklearn)
```

RMSE Recomputed: 55.40475965909536 RMSE from sklearn: 55.40475965909536

MAE : Mean Absolute Error

```
In [93]: N=y.shape[0]
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols
df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
df_errors['abs(y_yhat)']=df_errors['y_yhat'].abs()
mae_recomp=np.sum(df_errors['abs(y_yhat)'])/N
mae_recomp
```

Out[93]: 45.885213649138834

SK Learn

```
In [94]: mae_sklearn=mean_absolute_error(y,y_predict_ols)
mae_sklearn
```

Out[94]: 45.885213649138834

Both

```
In [92]: print('MAE recomputed:',mae_recomp,'MAE from sklearn:',mae_sklearn)
```

MAE recomputed: 45.885213649138834 MAE from sklearn: 45.885213649138834

MAPE: Mean Absolute Percentage Error

```
In [96]: N=y.shape[0]
epsilon=0.0001
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols
df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
df_errors['abs(y_yhat)']=df_errors['y_yhat'].abs()
df_errors['abs(y_true)']=df_errors['y_true'].apply(lambda x:max(epsilon,np.abs(x)))
df_errors['|(y_yhat)/y|']=df_errors['abs(y_yhat)']/df_errors['abs(y_true)']
mape_recomp=np.sum(df_errors['|(y_yhat)/y|'])/N
mape_recomp
```

Out[96]: 3.03466206442493

SK Learn

```
In [98]: mape_sklearn=mean_absolute_percentage_error(y,y_predict_ols)
mape_sklearn
```

Out[98]: 3.03466206442493

Both

```
In [99]: print('MAPE recomputed:', mape_recomp, 'MAPE from sklearn:', mape_sklearn)
```

```
MAPE recomputed: 3.03466206442493 MAPE from sklearn: 3.03466206442493
```

```
In [101]: N=y.shape[0]
epsilon=0.0001
df_errors=pd.DataFrame()
df_errors['y_true']=y
df_errors['yhat']=y_predict_ols
df_errors['y_yhat']=df_errors['y_true']-df_errors['yhat']
df_errors['abs(y_yhat)']=df_errors['y_yhat'].abs()

medae_recomp=np.median(df_errors['abs(y_yhat)'])
medae_recomp
```

```
Out[101]: 42.166118060703866
```

SK Learn

```
In [104]: medae_sklearn=median_absolute_error(y,y_predict_ols)
medae_sklearn
```

```
Out[104]: 42.166118060703866
```

Both

```
In [105]: print('MEDAE Recomputed:', medae_recomp, 'MEDAE from sklearn', medae_sklearn)
```

```
MEDAE Recomputed: 42.166118060703866 MEDAE from sklearn 42.166118060703866
```

Evaluation Metrics to compare among models

We will use 2 regression models, to fit the data and evaluate their performance. As explained at the beginning, we will not be splitting the dataset to train and test sets. Its not the objective of this notebook.

```
In [111]: features=df.columns[:-1]
X=df_norm[features]
y=df_norm['Y']

### OLS: Ordinary Least Square

reg_ols=LinearRegression(fit_intercept=False)
reg_ols.fit(X,y)

## Predict Values
y_predict_ols=reg_ols.predict(X)

## LASSO
reg_lasso=Lasso(alpha=1,fit_intercept=False) # Without cross-validation to find the be
reg_lasso.fit(X,y)
#Predict values
y_predict_lasso=reg_lasso.predict(X)
```

Now what we fit the models, let`s compute the different metrics for each of them:


```

In [114... predicted_values=[y_predict_ols,y_predict_lasso]
models=['OLS','LASSO']

measures_list=[]

i=0

for y_predict in predicted_values:
    r2=r2_score(y,y_predict)
    explained_variance=explained_variance_score(y,y_predict)
    mse=mean_squared_error(y,y_predict)
    rmse=mean_squared_error(y,y_predict,squared=False)
    mae=mean_absolute_error(y,y_predict)
    mape=mean_absolute_percentage_error(y,y_predict)
    medae=median_absolute_error(y,y_predict)
    measures_list.append([models[i],r2,explained_variance,mse,rmse,mae,mape,medae])
    i+=1

df_results=pd.DataFrame(data=measures_list,
                        columns=['model','r2','explained_var','mse','rmse','mae','mape','medae'])

```

```
In [115... df_results
```

```
Out[115]:
```

	model	r2	explained_var	mse	rmse	mae	mape	medae
0	OLS	0.482336	0.482449	3069.687393	55.40476	45.885214	3.034662	42.166118
1	LASSO	0.428986	0.429100	3386.045847	58.18974	48.293216	3.093502	44.530827

As shown in the results, the R2 is higher for the OLS(0.48) than the Lasso model(0.12) (even if the value in absolute terms is not that high)

At this stage, we can assume that the OLS is a better model than the Lasso for our dataset

Furthermore, the MSE and RMSE are lower for the OLS than Lasso. Once again, OLS is a good fit for our dataset

MAE and MedAE are also showing better results for OLS than Lasso

However, MAPE is lower for the Lasso than the OLS, showing that there are some values of the true y that could be high, making the relative value of the residual lower. It could be interesting to study the outliers in the dataset, and remove them if any.

Globally, the OLS model is showing better metrics than the Lasso model. Thus between these 2 models, OLS will be a good fit for our Dataset.

I hope you enjoyed it.

```
In [ ]:
```