IS-02 Machine Learning - Data and Web Science

Final Project

Problem 2 - Regression

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In [1]:
```
#importing necessary libraries
import logging
import pickle
import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
from time import time
from sklearn.decomposition import PCA
from sklearn.ensemble import RandomForestRegressor
from sklearn.feature_selection import SelectKBest
from sklearn.linear_model import LinearRegression, SGDRegressor
from sklearn.model_selection import GridSearchCV
from sklearn.neural_network import MLPRegressor
from sklearn.pipeline import FeatureUnion, Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import SVR
```

For Problem 2 we are trying to predict the fuel cost per 12000 miles when given the specification of a car. We clearly have to deal with a regression problem so first lets take a look into our data and figure out how to process them and what algorithms we are going to use.

In [2]:
```
X = pd.read_csv("fuel_emissions.csv")
X.head()
```

```
/home/hydone/anaconda3/lib/python3.8/site-packages/IPython/core/interactivesh
ell.py:3146: DtypeWarning: Columns (8) have mixed types.Specify dtype option
on import or set low_memory=False.
  has_raised = await self.run_ast_nodes(code_ast.body, cell_name,
```

Out[2]:

	file	year	manufacturer	model	description	euro_standard	tax_band
0	Part_A_Euro_IV_may2005.csv	2005	BMW	1 Series E87	116i	4	NaN
1	Part_A_Euro_IV_may2005.csv	2005	BMW	1 Series E87	118d - from March 2005	4	NaN
2	Part_A_Euro_IV_may2005.csv	2005	BMW	1 Series E87	118d - up to February 2005	4	NaN
3	Part_A_Euro_IV_may2005.csv	2005	BMW	1 Series E87	118i	4	NaN
4	Part_A_Euro_IV_may2005.csv	2005	BMW	1 Series E87	118i	4	NaN

5 rows × 29 columns

Lets take a look at the types because we can see clearly we have a lot of categorical values

In [3]:
```
X.dtypes
```

Out[3]:
```
file                        object
year                         int64
manufacturer                object
model                       object
description                 object
euro_standard                int64
tax_band                    object
transmission                object
transmission_type           object
engine_capacity            float64
fuel_type                   object
urban_metric               float64
extra_urban_metric         float64
combined_metric            float64
urban_imperial             float64
extra_urban_imperial       float64
combined_imperial          float64
noise_level                float64
co2                          int64
thc_emissions              float64
co_emissions               float64
nox_emissions              float64
thc_nox_emissions          float64
particulates_emissions     float64
fuel_cost_12000_miles      float64
standard_12_months         float64
standard_6_months          float64
first_year_12_months       float64
first_year_6_months        float64
dtype: object
```

Ok now lets drop some "useless" columns. First lets remove all imperial columns since we are going to use the metric ones for our algorithms. Next lets drop the file name, the year since we have the euro standard column with which we can tell the range of the manufactured year. Also since we want our models to be generic we can drop the model and the model description columns as well.

In [4]:
```
#Dropping some "useless" columns
X.drop(axis=1,columns=["file","year","model","urban_imperial","extra_urban_im
```

Next lets check if we have any NaN values

In [5]:
```
#check if we have any NaN values
X.isnull().sum()
```

Out[5]:
```
manufacturer                0
euro_standard               0
tax_band                25251
transmission               10
transmission_type         341
engine_capacity             7
fuel_type                   0
urban_metric               13
extra_urban_metric         13
combined_metric             7
noise_level                 0
co2                         0
thc_emissions           16599
co_emissions               24
```

```
nox_emissions                70
thc_nox_emissions         27658
particulates_emissions    19912
fuel_cost_12000_miles        10
standard_12_months        29571
standard_6_months         30162
first_year_12_months      29571
first_year_6_months       31669
dtype: int64
```

We can clearly see that we have some columns with a lot of NaN values. Some columns contain almost exclusively null values. We will drop columns that have more than 25% of their values as NaN and fill the other ones with each column's mean for non categorical columns. For categorical columns we will use the method forward fill and will propagate the last valid observation forward. There are just 10 NaN values in our target column (fuel_cost_12000_miles) so, it is better to remove the rows that contain these values rather than filling them.

In [6]:
```
#Get all column names that have more than 25% NaN values.
alist = [i for i in zip(X.isnull().sum(),X.columns.values)]
columns2drop = [i[1] for i in alist if i[0] > X.shape[0]*.25]
```

In [7]:
```
X.drop(axis=1,columns=columns2drop,inplace=True)
X.dropna(axis=0,subset=["fuel_cost_12000_miles"],inplace=True)
```

In [8]:
```
#New df with dropped columns
X.head()
```

Out[8]:

	manufacturer	euro_standard	transmission	transmission_type	engine_capacity	fuel_type	urba
0	BMW	4	M5	Manual	1596.0	Petrol	
1	BMW	4	M6	Manual	1995.0	Diesel	
2	BMW	4	M6	Manual	1995.0	Diesel	
3	BMW	4	M5	Manual	1995.0	Petrol	
4	BMW	4	A6	Automatic	1995.0	Petrol	

In [9]:
```
#moving target column to y
y = X.fuel_cost_12000_miles
X.drop(axis=1,columns="fuel_cost_12000_miles",inplace=True)
```

In [10]:
```
values = {
          "engine_capacity" : X.engine_capacity.mean(),
          "urban_metric" : X.urban_metric.mean(),
          "extra_urban_metric" : X.extra_urban_metric.mean(),
          "combined_metric" : X.combined_metric.mean(),
          "co_emissions" : X.co_emissions.mean(),
          "nox_emissions" : X.nox_emissions.mean()
          }
X.fillna(value=values,inplace=True)
X.fillna(method="ffill",inplace=True)
```

In [11]:
```
#Check if we have any nan values still left
X.isnull().sum()
```

Out[11]:
```
manufacturer         0
euro_standard        0
transmission         0
transmission_type    0
```

```
engine_capacity       0
fuel_type             0
urban_metric          0
extra_urban_metric    0
combined_metric       0
noise_level           0
co2                   0
co_emissions          0
nox_emissions         0
dtype: int64
```

In [12]:
```
X.dtypes
```

Out[12]:
```
manufacturer           object
euro_standard           int64
transmission           object
transmission_type      object
engine_capacity       float64
fuel_type              object
urban_metric          float64
extra_urban_metric    float64
combined_metric       float64
noise_level           float64
co2                     int64
co_emissions          float64
nox_emissions         float64
dtype: object
```

We will use one-hot encoding for all categorical values left in our data, creating new columns for each unique value inside them.

In [13]:
```
X = pd.get_dummies(X,columns=["manufacturer","transmission","transmission_typ
```

In [14]:
```
#getting dataframe's shape
X.shape
```

Out[14]:
```
(33078, 158)
```

We have 158 columns (features) in our DataFrame. It is suggested to run PCA in order to reduce the dimensionality of our problem and run our algorithms faster like we stated in Problem 1. 40 features are being selected, in this case, and the best 10 from the rest are also added with a Feature Union. So in total 50 features/columns. In all our models we decided to scale our data with Standard Scaler since regression algorithms appear to run better when the data is scaled/normalized. The algorithms we decided to use for the regression problem were:

- LinearRegression
- RandomForestRegressor
- SGDRegressor
- MLPRegressor
- SVR

We used, in total, 19 different variations of the above algorithms.

The metrics we decided to use to rank each model were:

- Mean Squared Error
- Mean Squared Root Error
- Mean Absolute Error
- R2

10-Fold Cross Validated Grid Search was performed on the data and the mean scores of each variation were extracted into a pandas DataFrame. In total we had 190 runs of our pipeline.

> Pipeline([('scale', StandardScaler()),("features", combined_features), ("estimator", RegressionAlgorithm())])

In [15]:
```
try:
   df = pickle.load( open( "models_gscv.p", "rb" ) )
except FileNotFoundError:

    logging.basicConfig(level=logging.INFO,
                        format='%(asctime)s %(levelname)s %(message)s')

    # This dataset is too high-dimensional. Let's do PCA:
    pca = PCA(n_components=40)

    # Maybe some original features where good, too?
    selection = SelectKBest(k=10)

    # Build estimator from PCA and Univariate selection:
    combined_features = FeatureUnion([("pca", pca), ("univ_select", selection

    # Use combined features to transform dataset:
    X_features = combined_features.fit(X, y).transform(X)
    print("Combined space has", X_features.shape[1], "features")


    pipe = Pipeline([('scale', StandardScaler()),("features", combined_featur

    #Our models
    parameters = [
        {
        'estimator': [LinearRegression()],
    },
        {
        'estimator': [RandomForestRegressor()],
        'estimator__n_estimators': [20,50,100],
        'estimator__criterion': ["mse"],
        'estimator__max_depth': [None,10],
    },
        {
        'estimator': [SGDRegressor()],
        'estimator__loss': ["huber"],
        'estimator__penalty': ["l2","elasticnet"],
        'estimator__learning_rate': ["adaptive","invscaling"],
        'estimator__max_iter': [1000 ],
    },
        {
        'estimator': [MLPRegressor()],
        'estimator__activation': ["tanh","relu","logistic"],
        'estimator__solver': ["adam"],
        'estimator__learning_rate_init': [10**-3],
        'estimator__shuffle': [True,False],
    },
        {
        'estimator': [SVR()],
        'estimator__kernel': ["sigmoid","rbf"],
        'estimator__max_iter': [10**5],
    },
    ]
    scoring = ["neg_mean_absolute_error","neg_mean_squared_error","neg_root_m
    if __name__ == "__main__":
```

```
        grid_search = GridSearchCV(pipe, parameters,scoring=scoring, n_jobs=-

        print("Performing grid search...")
        print("pipeline:", [name for name, _ in pipe.steps])
        t0 = time()
        grid_search.fit(X, y)
        print("done in %0.3fs" % (time() - t0))
        print()
        # values = [i[0] for i in grid_search.cv_results_.values()]
        # dflist.append(values)
        print("Best score: %0.3f" % grid_search.best_score_)

        # df = pd.DataFrame(dflist,columns=list(grid_search.cv_results_.keys(
        df = pd.DataFrame(grid_search.cv_results_)
        pickle.dump(df, open( "models_gscv.p", "wb" ) )
```

In [16]:

```
df.head()
```

Out[16]:

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_estimator	param_
0	2.307495	0.048379	0.030996	0.008465	LinearRegression()	
1	18.914201	0.603615	0.023709	0.002768	RandomForestRegressor()	
2	43.256071	0.968224	0.036076	0.002150	RandomForestRegressor()	
3	84.985354	1.880756	0.063278	0.007895	RandomForestRegressor()	
4	12.034566	0.229606	0.015868	0.000935	RandomForestRegressor()	

5 rows × 70 columns

In [17]:

```
fdf = df[['params','param_estimator','mean_test_neg_mean_absolute_error','mea
```

In [18]:

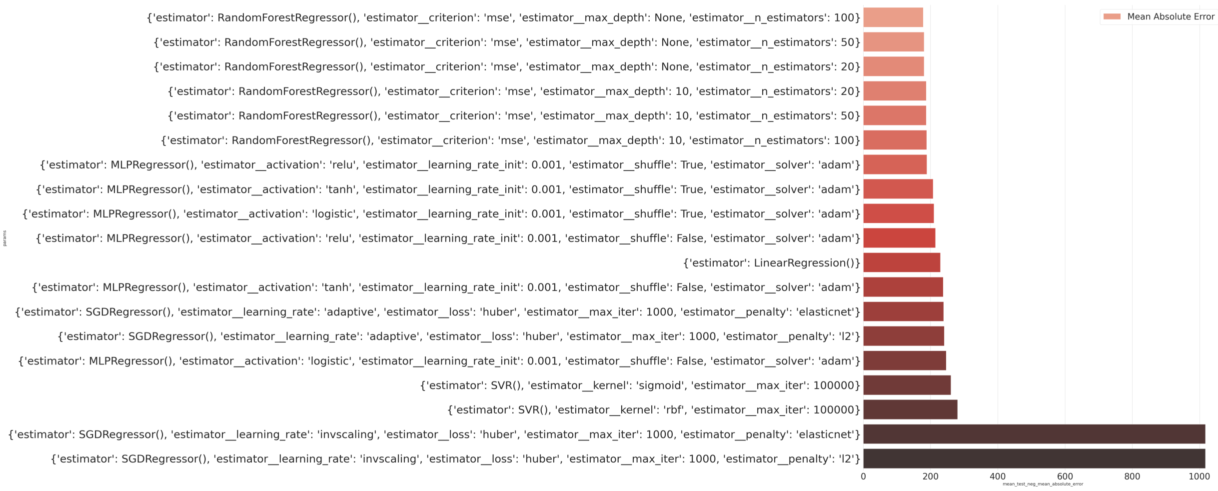
```
fdf["params"] = fdf["params"].astype(str)
```

In [19]:

```
sns.set_theme(style="whitegrid")
f, ax = plt.subplots(figsize=(30, 40))
fdf.sort_values(by="mean_test_r2",ascending=False,inplace=True)
sns.set_color_codes("muted")
sns.barplot(x=[1 for _ in range(19)], y=df["params"].astype(str), data=fdf,
            label="R2 = 1", color="b")
sns.set_color_codes("pastel")
sns.barplot(x="mean_test_r2", y="params", data=fdf,
            label="Mean R2", color="b")
ax.legend(ncol=2, loc="upper left", frameon=True,fontsize=40)
ax.yaxis.label.set_size(20)
for xtick in ax.xaxis.get_major_ticks():
    xtick.label.set_fontsize(40)
for ytick in ax.yaxis.get_major_ticks():
    ytick.label.set_fontsize(50)
ax.xaxis.label.set_size(20)
sns.despine(left=True, bottom=True)
```

For the Coefficient of determination or R2, we can see in the above plot that the best algorithm is the RandomForestRegressor while four of our models scored a negative mean R2 score in the ten folds we tested. All six variations of the RandomForestRegressor algorithm scored a better score than the rest models by a decent margin.

In [20]:
```
sns.set_theme(style="whitegrid")
f, ax = plt.subplots(figsize=(30, 40))
fdf.sort_values(by="mean_test_neg_mean_absolute_error",ascending=False,inplac
sns.set_color_codes("pastel")
sns.barplot(x=fdf["mean_test_neg_mean_absolute_error"].abs(), y="params", dat
            label="Mean Absolute Error", palette="Reds_d")
ax.legend(ncol=1, loc="upper right", frameon=True,fontsize=40)
ax.yaxis.label.set_size(20)
for xtick in ax.xaxis.get_major_ticks():
    xtick.label.set_fontsize(40)
for ytick in ax.yaxis.get_major_ticks():
    ytick.label.set_fontsize(50)
ax.xaxis.label.set_size(20)
sns.despine(left=True, bottom=True)
```



In [21]:
```
sns.set_theme(style="whitegrid")
f, ax = plt.subplots(figsize=(30, 40))
fdf.sort_values(by="mean_test_neg_root_mean_squared_error",ascending=False,in
sns.set_color_codes("pastel")
sns.barplot(x=fdf["mean_test_neg_root_mean_squared_error"].abs(), y="params",
            label="Mean R2", palette="Greens_d")
ax.legend(ncol=1, loc="upper right", frameon=True,fontsize=40)
ax.yaxis.label.set_size(20)
for xtick in ax.xaxis.get_major_ticks():
    xtick.label.set_fontsize(40)
for ytick in ax.yaxis.get_major_ticks():
```

```
    ytick.label.set_fontsize(50)
ax.xaxis.label.set_size(20)
sns.despine(left=True, bottom=True)
```

In [22]:

```
sns.set_theme(style="whitegrid")
f, ax = plt.subplots(figsize=(30, 40))
fdf.sort_values(by="mean_test_neg_mean_squared_error",ascending=False,inplace
sns.set_color_codes("pastel")
sns.barplot(x=fdf["mean_test_neg_mean_squared_error"].abs(), y="params", data
            label="Mean Squared Error / 10^6", palette="Blues_d")
ax.legend(ncol=1, loc="upper right", frameon=True,fontsize=40)
ax.yaxis.label.set_size(20)
for xtick in ax.xaxis.get_major_ticks():
    xtick.label.set_fontsize(40)
for ytick in ax.yaxis.get_major_ticks():
    ytick.label.set_fontsize(50)
ax.xaxis.label.set_size(20)
sns.despine(left=True, bottom=True)
```

For the rest of the metrics (Mean Squared Error, Mean Squared Root Error, Mean Absolute Error) we still observe that the best model is a RandomForestRegressor model. In all our experiments it is clear that the best algorithm, according to our results in this specific problem, is the RandomForestRegressor. The worst algorithm in all our cases is the SGDRegressor with the estimator_learning_rate parameter set to invscaling. Although the results seem to be pretty clear, the difference is marginal and in most cases, running different amounts of folds or different parameters can improve the performance of each algorithm. Like in the case of Multi-Layer Perceptrons we notice that by tuning some of their parameters can drastically change their performance.