Import modules

In [2]:
```python
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn import preprocessing, svm
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
import xgboost as xg
from sklearn.metrics import mean_squared_error as MSE
from sklearn.metrics import make_scorer
from sklearn.neural_network import MLPRegressor
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score
from sklearn.pipeline import Pipeline
from sklearn.pipeline import FeatureUnion
from sklearn.decomposition import PCA
from sklearn.feature_selection import SelectKBest
from tabulate import tabulate
import warnings
```

```
/Users/kobr0v/opt/anaconda3/lib/python3.9/site-packages/xgboost/compat.py:36: FutureWarning: pandas.Int64Index is de
precated and will be removed from pandas in a future version. Use pandas.Index with the appropriate dtype instead.
  from pandas import MultiIndex, Int64Index
```

In [3]:
```python
warnings.filterwarnings('ignore')
def rmse(predict, actual):
    score = np.sqrt(MSE(predict, actual))
    return score

RMSE = make_scorer(rmse)
```

Read the file and prepare the dataset

In [229…
```python
file="large_database.xlsx"
database = pd.read_excel(file, usecols=[1,2,3,4,5,11, 9, 12])
X = pd.read_excel(file, usecols=[1,2,3,4,5])
y = pd.read_excel(file, usecols=[9,11,12])
y1= pd.read_excel(file, usecols=[9])
y2= pd.read_excel(file, usecols=[12])
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, shuffle=True, random_state=20)
y1_train=y_train.iloc[:,0]
y2_train=y_train.iloc[:,2]
y1_test=y_test.iloc[:,0]
y2_test=y_test.iloc[:,2]
```

Descriptive statistics

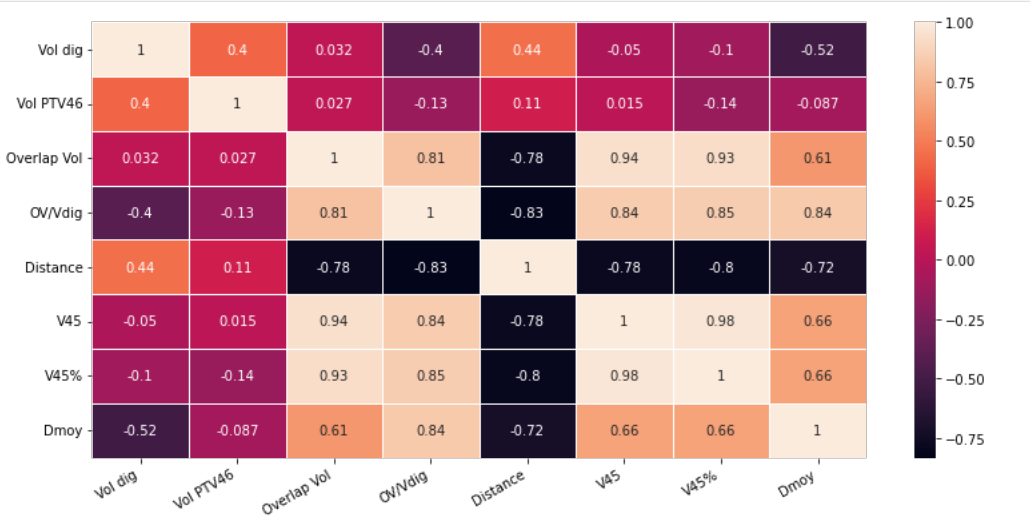
In [230…
```python
database.describe()
```

Out[230]:

	Vol dig	Vol PTV46	Overlap Vol	OV/Vdig	Distance	V45	V45%	Dmoy
count	48.000000	48.000000	48.000000	48.000000	48.000000	48.000000	48.000000	48.000000
mean	1373.485571	971.240832	44.469771	0.038613	8.298153	40.348828	0.042395	16.659639
std	612.312042	177.198329	34.831949	0.035407	1.983831	34.406977	0.035242	5.506392
min	293.393004	665.105557	2.672223	0.001253	2.191926	0.215625	0.000143	7.771517
25%	912.240196	850.297525	19.104834	0.010301	7.220885	18.377344	0.018851	12.799274
50%	1254.637830	944.967107	32.599803	0.028017	8.151168	28.523437	0.029917	15.544078
75%	1747.808000	1076.448962	62.377415	0.057959	9.749421	55.094531	0.057217	20.164501
max	2911.111661	1503.124779	139.933084	0.182168	12.185881	172.640625	0.158789	32.765113

Correlation matrix

In [231…
```python
cormat = database.corr()
plt.figure(figsize=(13, 6))
sns.heatmap(corrmat, vmax=1, annot=True, linewidths=.5)
plt.xticks(rotation=30, horizontalalignment="right")
plt.show()
```



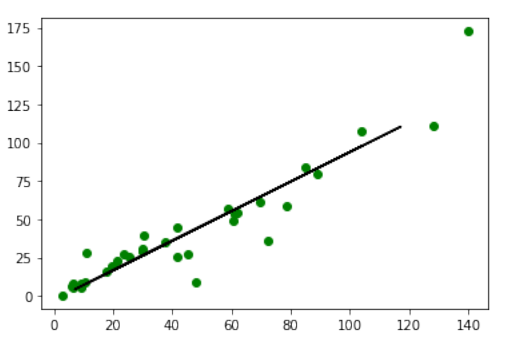
Replication of CFJ models

Linear Regression V45 = F(Overlap Vol)

In [232…
```python
regressor = LinearRegression()
regressor.fit(X_train["Overlap Vol"].array.reshape(-1,1), y1_train.array)
y1_pred = regressor.predict(X_test["Overlap Vol"].array.reshape(-1,1))
r_squared_train = regressor.score(X_train["Overlap Vol"].array.reshape(-1,1),y1_train)
r_squared_test = regressor.score(X_test["Overlap Vol"].array.reshape(-1,1),y1_test)
print("Training coefficient of determination R2: ",r_squared_train)
print("Testing coefficient of determination R2: ",r_squared_test)
plt.scatter(X_train["Overlap Vol"].array.reshape(-1,1), y1_train,color='g')
plt.plot(X_test["Overlap Vol"].array.reshape(-1,1), y1_pred,color='k')
```

```
Training coefficient of determination R2:  0.8754562517157654
Testing coefficient of determination R2:  0.9501134180471098
```

Out[232]:
```
[<matplotlib.lines.Line2D at 0x7f9842aea370>]
```

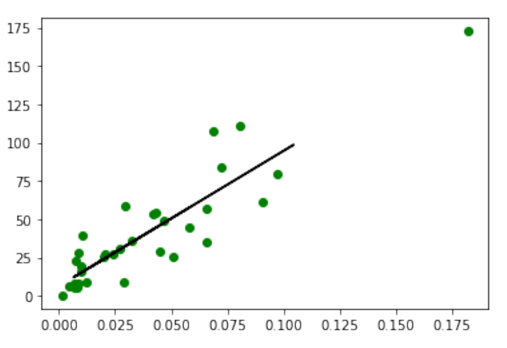


Linear Regression V45 = F(OV/Vol)

In [233…
```python
regressor = LinearRegression()
regressor.fit(X_train["OV/Vdig"].array.reshape(-1,1), y1_train.array)
y1_pred = regressor.predict(X_test["OV/Vdig"].array.reshape(-1,1))
r_squared_test = regressor.score(X_test["OV/Vdig"].array.reshape(-1,1),y1_test)
r_squared_train = regressor.score(X_train["OV/Vdig"].array.reshape(-1,1),y1_train)
print("Training coefficient of determination R2: ",r_squared_train)
print("Testing coefficient of determination R2: ",r_squared_test)
plt.scatter(X_train["OV/Vdig"].array.reshape(-1,1), y1_train,color='g')
plt.plot(X_test["OV/Vdig"].array.reshape(-1,1), y1_pred,color='k')
```

```
Training coefficient of determination R2:  0.8086483932469174
Testing coefficient of determination R2:  0.3459264875385393
```

Out[233]:
```
[<matplotlib.lines.Line2D at 0x7f98122b7dc0>]
```

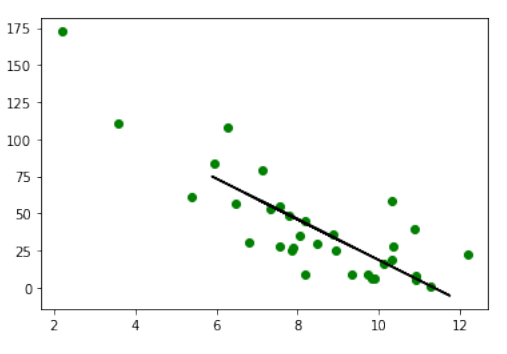


Linear Regression V45 = F(Distance)

In [234…
```python
regressor = LinearRegression()
regressor.fit(X_train["Distance"].array.reshape(-1,1), y1_train.array)
y1_pred = regressor.predict(X_test["Distance"].array.reshape(-1,1))
r_squared_test = regressor.score(X_test["Distance"].array.reshape(-1,1),y1_test)
r_squared_train = regressor.score(X_train["Distance"].array.reshape(-1,1),y1_train)
print("Training coefficient of determination R2: ",r_squared_train)
print("Testing coefficient of determination R2: ",r_squared_test)
plt.scatter(X_train["Distance"].array.reshape(-1,1), y1_train,color='g')
plt.plot(X_test["Distance"].array.reshape(-1,1), y1_pred,color='k')
```

```
Training coefficient of determination R2:  0.6743918380270656
Testing coefficient of determination R2:  0.3795024601681817
```

Out[234]:
```
[<matplotlib.lines.Line2D at 0x7f97f808bdf0>]
```



Multiple Linear Regression V45 = F(Overlap Vol, Distance)

In [235…
```python
regressor = LinearRegression()
regressor.fit(X_train[["Overlap Vol","Distance"]], y1_train.array)
y1_pred = regressor.predict(X_test[["Overlap Vol","Distance"]])
r_squared_test = regressor.score(X_test[["Overlap Vol","Distance"]],y1_test)
r_squared_test = regressor.score(X_train[["Overlap Vol","Distance"]],y1_train)
print("Training coefficient of determination R2: ",r_squared_train)
print("Testing coefficient of determination R2: ",r_squared_test)
```

```
Training coefficient of determination R2:  0.6743918380270656
Testing coefficient of determination R2:  0.883601176377753
```

Creating Principal Component Regression model

In [236…
```python
# create feature union
features = []
features.append(('pca', PCA(n_components=3)))
features.append(('select_best', SelectKBest(k=3)))
feature_union = FeatureUnion(features)
# create pipeline
estimators = []
estimators.append(('standardize', StandardScaler()))
estimators.append(('feature_union', feature_union))
estimators.append(('linear_regression', LinearRegression()))
PCR = Pipeline(estimators)
kfold = KFold(n_splits=3)
PCR_results1 = cross_val_score(PCR, X, y1, cv=kfold, scoring=RMSE)
PCR_results2 = cross_val_score(PCR, X, y2, cv=kfold, scoring=RMSE)
```

In [237…
```python
PCR.fit(X,y1)
out1 = PCR.predict(X)
PCR.fit(X,y2)
out2 = PCR.predict(X)
print("RMSE Y1: ", rmse(out1,y1))
print("RMSE Y2: ", rmse(out2,y2))

pd.DataFrame(out2).to_clipboard()
```

```
RMSE Y1:  9.97613459288511
RMSE Y2:  2.673158223016091
```

Select ML models to be cross validated

In [ ]:

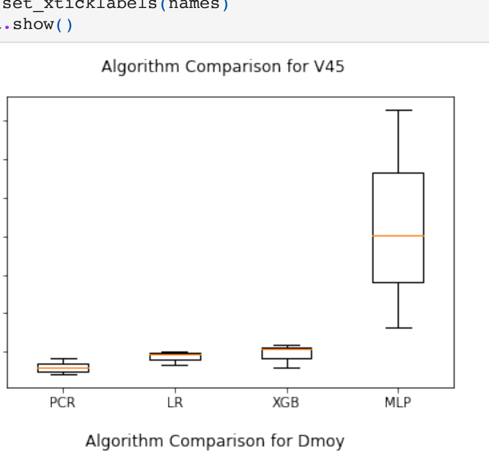
In [238…
```python
# prepare models
models = []
models.append(('LR', LinearRegression()))
models.append(('XGB', xg.XGBRegressor()))
models.append(('MLP', MLPRegressor()))
```

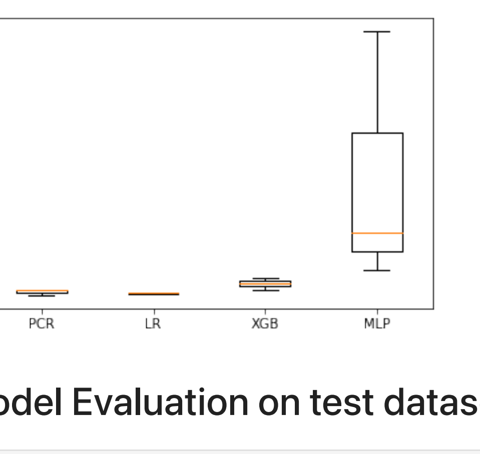
Model evaluation on train dataset

In [239…
```python
# evaluate each model in turn
results1 = [PCR_results1]
results2 = [PCR_results2]
names = ['PCR']
for name, model in models:
    kfold = KFold(n_splits=3)
    cv_results1 = cross_val_score(model, X_train, y1_train, cv=kfold, scoring=RMSE)
    cv_results2 = cross_val_score(model, X_train, y2_train, cv=kfold, scoring=RMSE)
    results1.append(cv_results1)
    results2.append(cv_results2)
    names.append(name)

# boxplot algorithm comparison
fig1 = plt.figure()
fig1.suptitle('Algorithm Comparison for V45')
ax = fig1.add_subplot(111)
plt.boxplot(results1)
ax.set_xticklabels(names)

fig2 = plt.figure()
fig2.suptitle('Algorithm Comparison for Dmoy')
ax = fig2.add_subplot(111)
plt.boxplot(results2)
ax.set_xticklabels(names)
plt.show()
```





Model Evaluation on test dataset

In [240…
```python
PCR1 = PCR.fit(X_train,y1_train)
PCR2 = PCR.fit(X_train,y2_train)

PCR1_pred = PCR1.predict(X_test)
PCR2_pred = PCR2.predict(X_test)
```

In [241…
```python
rmse1 = rmse(PCR1_pred,y1_test)
rmse2 = rmse(PCR2_pred,y2_test)
TestRes1 = [rmse1]
TestRes2 = [rmse2]
ML_names = ['PCR']
```

In [242…
```python
for name, model in models:
    m1 = model.fit(X_train, y1_train)
    m2 = model.fit(X_train, y2_train)
    test_result1 = m1.predict(X_test)
    test_result2 = m2.predict(X_test)
    TestRes1.append(rmse(test_result1,y1_test))
    TestRes2.append(rmse(test_result2,y2_test))
    ML_names.append(name)
```

Summary

In [243…
```python
print("Model comparison for the V45 output")


print(tabulate({"ML model": ML_names, "RMSE": TestRes1}, headers="keys"))

print("-----------------------------------------")

print("Model comparison for the Dmoy output")

print(tabulate({"ML model": ML_names, "RMSE": TestRes2}, headers="keys"))
```

```
Model comparison for the V45 output
ML model       RMSE
----------  -------
PCR         35.5624
LR          35.5624
XGB         35.1013
MLP         48.2692
-----------------------------------------
Model comparison for the Dmoy output
ML model        RMSE
----------  --------
PCR          3.18283
LR           3.18283
XGB          3.05679
MLP         62.5418
```

In [ ]:

In [ ]: