APPENDIX

1 Load and Analyze Data

[1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import missingno as msno
from scipy import stats
import sklearn
import statsmodels
import statsmodels.api as sm
import statsmodels.formula.api as smf
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsRegressor
from sklearn.decomposition import PCA
import random
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import make_scorer
from sklearn.pipeline import Pipeline
from numpy import mean
from numpy import std
from sklearn.linear_model import SGDRegressor
from sklearn.linear_model import Ridge
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import Lasso
from sklearn.linear_model import ElasticNet
from sklearn.ensemble import RandomForestRegressor
import umap
import tensorflow as tf
from tensorflow.keras import Model
from tensorflow.keras import Sequential
```

```python
from tensorflow.keras.optimizers import Adam
from sklearn.preprocessing import StandardScaler
from tensorflow.keras.layers import Dense, Dropout
from sklearn.model_selection import train_test_split
from tensorflow.keras.losses import MeanSquaredLogarithmicError
from sklearn.metrics import mean_squared_error
from keras.callbacks import ModelCheckpoint
from statsmodels.stats.outliers_influence import variance_inflation_factor
from sklearn.manifold import TSNE
from statsmodels.tools.tools import maybe_unwrap_results
from statsmodels.graphics.gofplots import ProbPlot
from statsmodels.stats.outliers_influence import variance_inflation_factor
from typing import Type
style_talk = 'seaborn-talk'    #refer to plt.style.available
random.seed(101)
np.random.seed(101)
%matplotlib inline
```

[2]:

```python
class Linear_Reg_Diagnostic():
    """
    Diagnostic plots to identify potential problems in a linear regression fit.
    Mainly,
        a. non-linearity of data
        b. Correlation of error terms
        c. non-constant variance
        d. outliers
        e. high-leverage points
        f. collinearity

"""


    def __init__(self,
                 results: Type[statsmodels.regression.linear_model.
 ↪RegressionResultsWrapper]) -> None:
        """
        For a linear regression model, generates following diagnostic plots:

        a. residual
        b. qq
        c. scale location and
        d. leverage

        and a table

        e. vif

        Args:
```

```
            results (Type[statsmodels.regression.linear_model.
↪RegressionResultsWrapper]):
                must be instance of statsmodels.regression.linear_model object

        Raises:
            TypeError: if instance does not belong to above object

        Example:
        >>> import numpy as np
        >>> import pandas as pd
        >>> import statsmodels.formula.api as smf
        >>> x = np.linspace(-np.pi, np.pi, 100)
        >>> y = 3*x + 8 + np.random.normal(0,1, 100)
        >>> df = pd.DataFrame({'x':x, 'y':y})
        >>> res = smf.ols(formula= "y ~ x", data=df).fit()
        >>> cls = Linear_Reg_Diagnostic(res)
        >>> cls(plot_context="seaborn-paper")

        In case you do not need all plots you can also independently make an␣
↪individual plot/table
        in following ways

        >>> cls = Linear_Reg_Diagnostic(res)
        >>> cls.residual_plot()
        >>> cls.qq_plot()
        >>> cls.scale_location_plot()
        >>> cls.leverage_plot()
        >>> cls.vif_table()
        """

        if isinstance(results, statsmodels.regression.linear_model.
↪RegressionResultsWrapper) is False:
            raise TypeError("result must be instance of statsmodels.regression.
↪linear_model.RegressionResultsWrapper object")

        self.results = maybe_unwrap_results(results)

        self.y_true = self.results.model.endog
        self.y_predict = self.results.fittedvalues
        self.xvar = self.results.model.exog
        self.xvar_names = self.results.model.exog_names

        self.residual = np.array(self.results.resid)
        influence = self.results.get_influence()
        self.residual_norm = influence.resid_studentized_internal
        self.leverage = influence.hat_matrix_diag
        self.cooks_distance = influence.cooks_distance[0]
```

```
        self.nparams = len(self.results.params)

    def __call__(self, plot_context='seaborn-paper'):
        # print(plt.style.available)
        with plt.style.context(plot_context):
            fig, ax = plt.subplots(nrows=2, ncols=2, figsize=(10,10))
            self.residual_plot(ax=ax[0,0])
            self.qq_plot(ax=ax[0,1])
            self.scale_location_plot(ax=ax[1,0])
            self.leverage_plot(ax=ax[1,1])
            plt.show()

        self.vif_table()
        return fig, ax


    def residual_plot(self, ax=None):
        """
        Residual vs Fitted Plot

        Graphical tool to identify non-linearity.
        (Roughly) Horizontal red line is an indicator that the residual has a␣
↪linear pattern
        """
        if ax is None:
            fig, ax = plt.subplots()

        sns.residplot(
            x=self.y_predict,
            y=self.residual,
            lowess=True,
            scatter_kws={'alpha': 0.5},
            line_kws={'color': 'red', 'lw': 1, 'alpha': 0.8},
            ax=ax)

        # annotations
        residual_abs = np.abs(self.residual)
        abs_resid = np.flip(np.sort(residual_abs))
        abs_resid_top_3 = abs_resid[:3]
        for i, _ in enumerate(abs_resid_top_3):
            ax.annotate(
                i,
                xy=(self.y_predict[i], self.residual[i]),
                color='C3')

        ax.set_title('Residuals vs Fitted', fontweight="bold")
        ax.set_xlabel('Fitted values')
```

```
        ax.set_ylabel('Residuals')
        return ax

    def qq_plot(self, ax=None):
        """
        Standarized Residual vs Theoretical Quantile plot

        Used to visually check if residuals are normally distributed.
        Points spread along the diagonal line will suggest so.
        """
        if ax is None:
            fig, ax = plt.subplots()

        QQ = ProbPlot(self.residual_norm)
        QQ.qqplot(line='45', alpha=0.5, lw=1, ax=ax)

        # annotations
        abs_norm_resid = np.flip(np.argsort(np.abs(self.residual_norm)), 0)
        abs_norm_resid_top_3 = abs_norm_resid[:3]
        for r, i in enumerate(abs_norm_resid_top_3):
            ax.annotate(
                i,
                xy=(np.flip(QQ.theoretical_quantiles, 0)[r], self.
↪residual_norm[i]),
                ha='right', color='C3')

        ax.set_title('Normal Q-Q', fontweight="bold")
        ax.set_xlabel('Theoretical Quantiles')
        ax.set_ylabel('Standardized Residuals')
        return ax

    def scale_location_plot(self, ax=None):
        """
        Sqrt(Standarized Residual) vs Fitted values plot

        Used to check homoscedasticity of the residuals.
        Horizontal line will suggest so.
        """
        if ax is None:
            fig, ax = plt.subplots()

        residual_norm_abs_sqrt = np.sqrt(np.abs(self.residual_norm))

        ax.scatter(self.y_predict, residual_norm_abs_sqrt, alpha=0.5);
        sns.regplot(
            x=self.y_predict,
            y=residual_norm_abs_sqrt,
```

```
            scatter=False, ci=False,
            lowess=True,
            line_kws={'color': 'red', 'lw': 1, 'alpha': 0.8},
            ax=ax)

        # annotations
        abs_sq_norm_resid = np.flip(np.argsort(residual_norm_abs_sqrt), 0)
        abs_sq_norm_resid_top_3 = abs_sq_norm_resid[:3]
        for i in abs_sq_norm_resid_top_3:
            ax.annotate(
                i,
                xy=(self.y_predict[i], residual_norm_abs_sqrt[i]),
                color='C3')
        ax.set_title('Scale-Location', fontweight="bold")
        ax.set_xlabel('Fitted values')
        ax.set_ylabel(r'$\sqrt{|\mathrm{Standardized\ Residuals}|}$');
        return ax

    def leverage_plot(self, ax=None):
        """
        Residual vs Leverage plot

        Points falling outside Cook's distance curves are considered␣
↪observation that can sway the fit
        aka are influential.
        Good to have none outside the curves.
        """
        if ax is None:
            fig, ax = plt.subplots()

        ax.scatter(
            self.leverage,
            self.residual_norm,
            alpha=0.5);

        sns.regplot(
            x=self.leverage,
            y=self.residual_norm,
            scatter=False,
            ci=False,
            lowess=True,
            line_kws={'color': 'red', 'lw': 1, 'alpha': 0.8},
            ax=ax)

        # annotations
        leverage_top_3 = np.flip(np.argsort(self.cooks_distance), 0)[:3]
        for i in leverage_top_3:
```

```python
            ax.annotate(
                i,
                xy=(self.leverage[i], self.residual_norm[i]),
                color = 'C3')

        xtemp, ytemp = self.__cooks_dist_line(0.5) # 0.5 line
        ax.plot(xtemp, ytemp, label="Cook's distance", lw=1, ls='--',␣
↪color='red')
        xtemp, ytemp = self.__cooks_dist_line(1) # 1 line
        ax.plot(xtemp, ytemp, lw=1, ls='--', color='red')

        ax.set_xlim(0, max(self.leverage)+0.01)
        ax.set_title('Residuals vs Leverage', fontweight="bold")
        ax.set_xlabel('Leverage')
        ax.set_ylabel('Standardized Residuals')
        ax.legend(loc='upper right')
        return ax

    def vif_table(self):
        """
        VIF table

        VIF, the variance inflation factor, is a measure of multicollinearity.
        VIF > 5 for a variable indicates that it is highly collinear with the
        other input variables.
        """
        vif_df = pd.DataFrame()
        vif_df["Features"] = self.xvar_names
        vif_df["VIF Factor"] = [variance_inflation_factor(self.xvar, i) for i␣
↪in range(self.xvar.shape[1])]

        print(vif_df
                .sort_values("VIF Factor")
                .round(2))


    def __cooks_dist_line(self, factor):
        """
        Helper function for plotting Cook's distance curves
        """
        p = self.nparams
        formula = lambda x: np.sqrt((factor * p * (1 - x)) / x)
        x = np.linspace(0.001, max(self.leverage), 50)
        y = formula(x)
        return x, y
```

[3]:
```
df = pd.read_csv("qsar_fish_toxicity.csv", delimiter = ";", names = ["CIC0",
↪"SM1_Dz", "GATS1i", "NdsCH", "NdssC", "MLOGP", "LC50"])
df.shape
```

[3]: (908, 7)

[4]:
```
df.head()
```

[4]:

	CIC0	SM1_Dz	GATS1i	NdsCH	NdssC	MLOGP	LC50
0	3.260	0.829	1.676	0	1	1.453	3.770
1	2.189	0.580	0.863	0	0	1.348	3.115
2	2.125	0.638	0.831	0	0	1.348	3.531
3	3.027	0.331	1.472	1	0	1.807	3.510
4	2.094	0.827	0.860	0	0	1.886	5.390

[5]:
```
df.tail()
```

[5]:

	CIC0	SM1_Dz	GATS1i	NdsCH	NdssC	MLOGP	LC50
903	2.801	0.728	2.226	0	2	0.736	3.109
904	3.652	0.872	0.867	2	3	3.983	4.040
905	3.763	0.916	0.878	0	6	2.918	4.818
906	2.831	1.393	1.077	0	1	0.906	5.317
907	4.057	1.032	1.183	1	3	4.754	8.201

[6]:
```
df.describe()
```

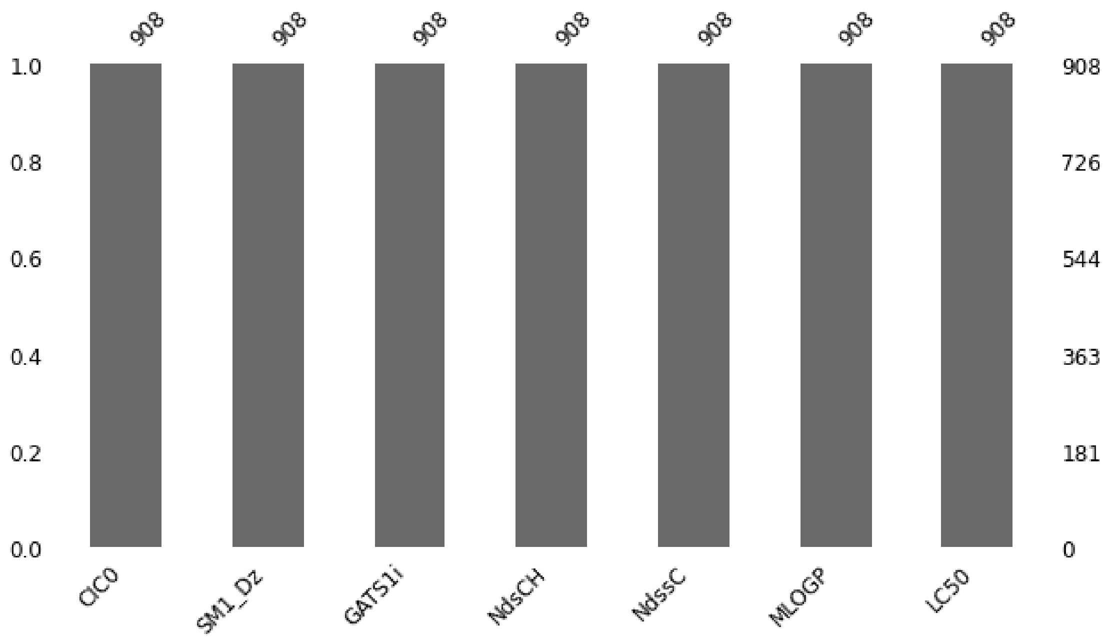
[6]:

	CIC0	SM1_Dz	GATS1i	NdsCH	NdssC	MLOGP	\
count	908.000000	908.000000	908.000000	908.000000	908.000000	908.000000	
mean	2.898129	0.628468	1.293591	0.229075	0.485683	2.109285	
std	0.756088	0.428459	0.394303	0.605335	0.861279	1.433181	
min	0.667000	0.000000	0.396000	0.000000	0.000000	-2.884000	
25%	2.347000	0.223000	0.950750	0.000000	0.000000	1.209000	
50%	2.934000	0.570000	1.240500	0.000000	0.000000	2.127000	
75%	3.407000	0.892750	1.562250	0.000000	1.000000	3.105000	
max	5.926000	2.171000	2.920000	4.000000	6.000000	6.515000	

	LC50
count	908.000000
mean	4.064431
std	1.455698
min	0.053000
25%	3.151750
50%	3.987500
75%	4.907500
max	9.612000

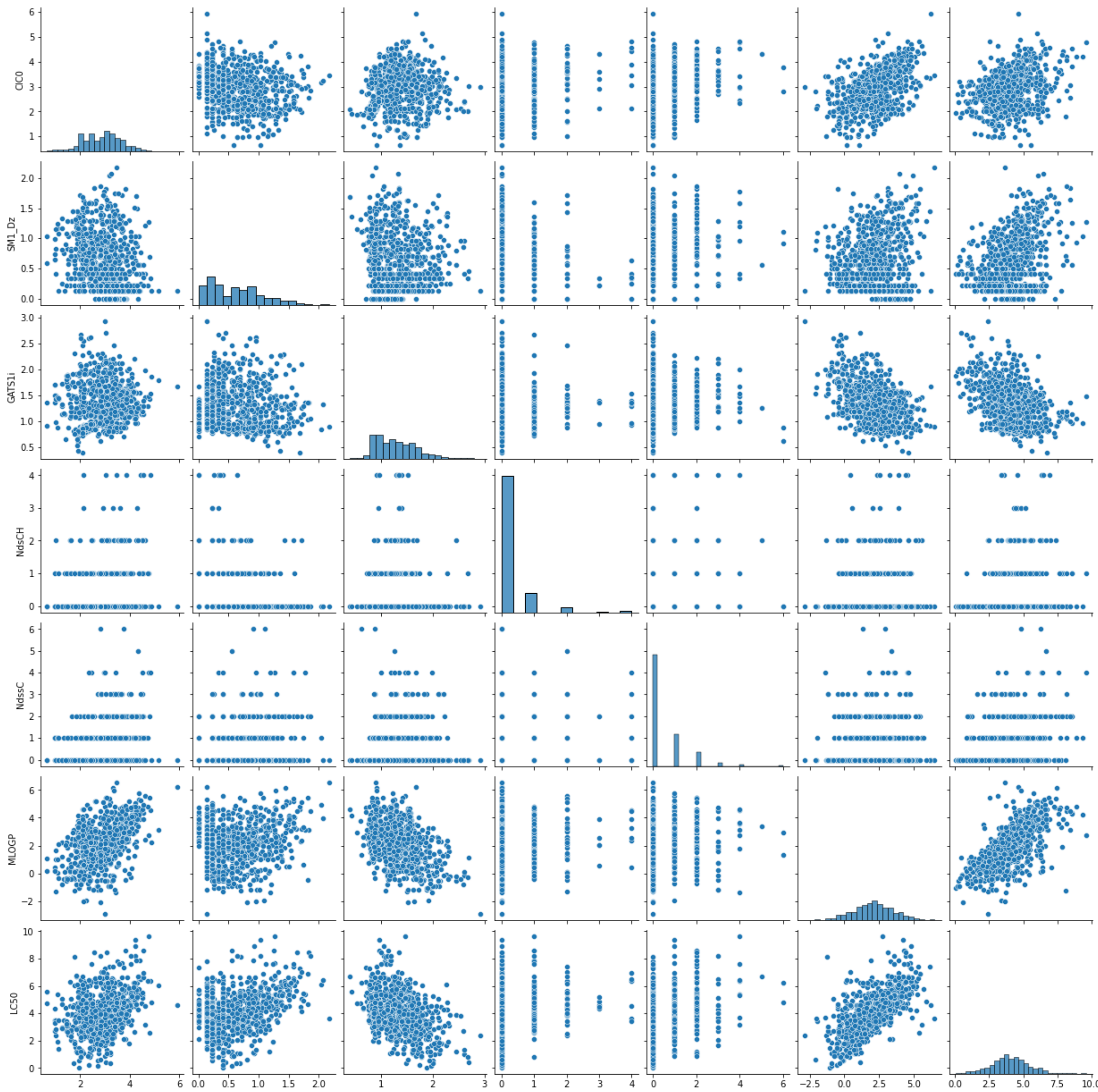
[7]:
```
msno.bar(df, figsize=(10,5), fontsize=12)
```

[7] : <AxesSubplot:>

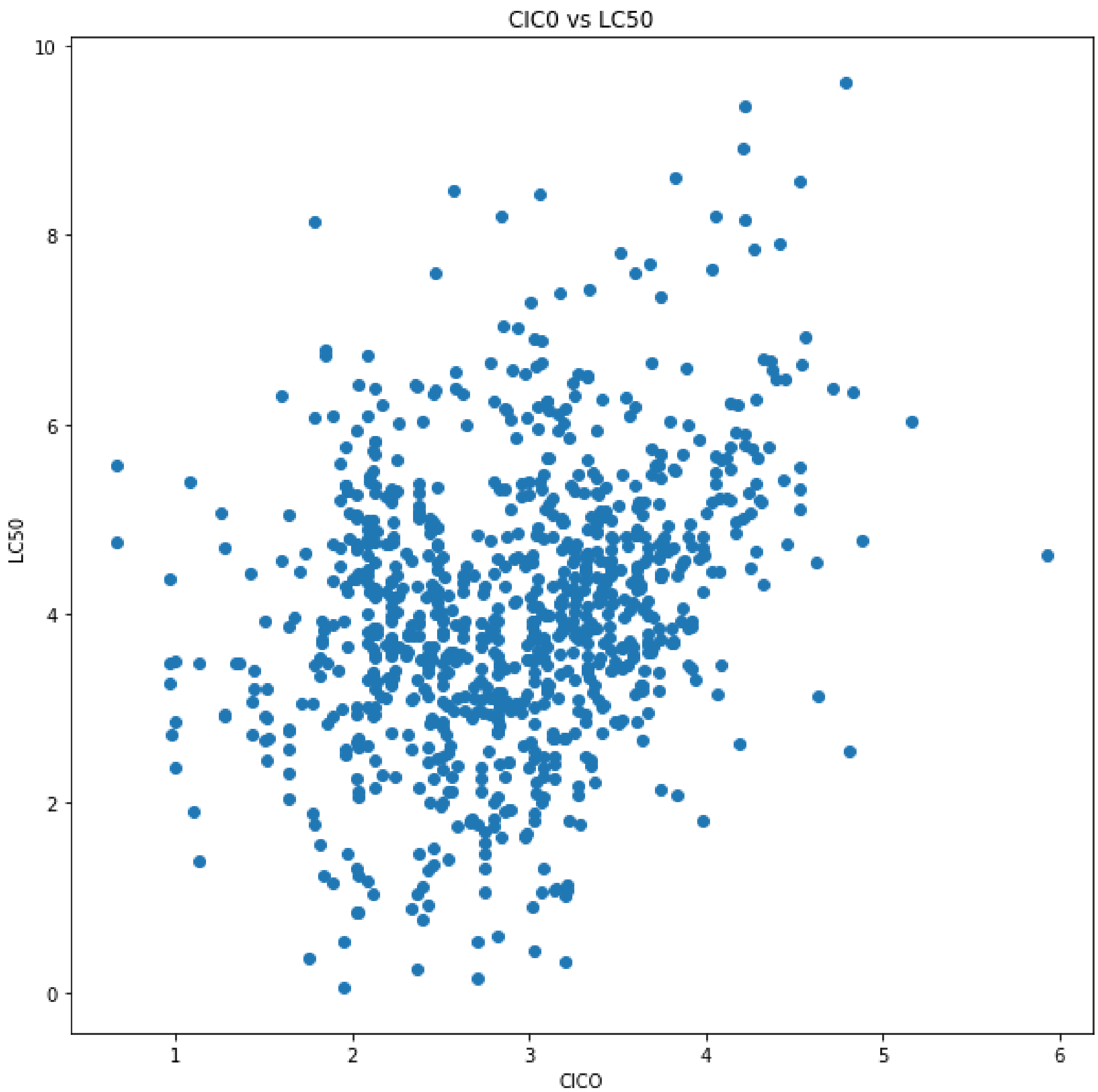


[8]:
```
sns.pairplot(df)
```

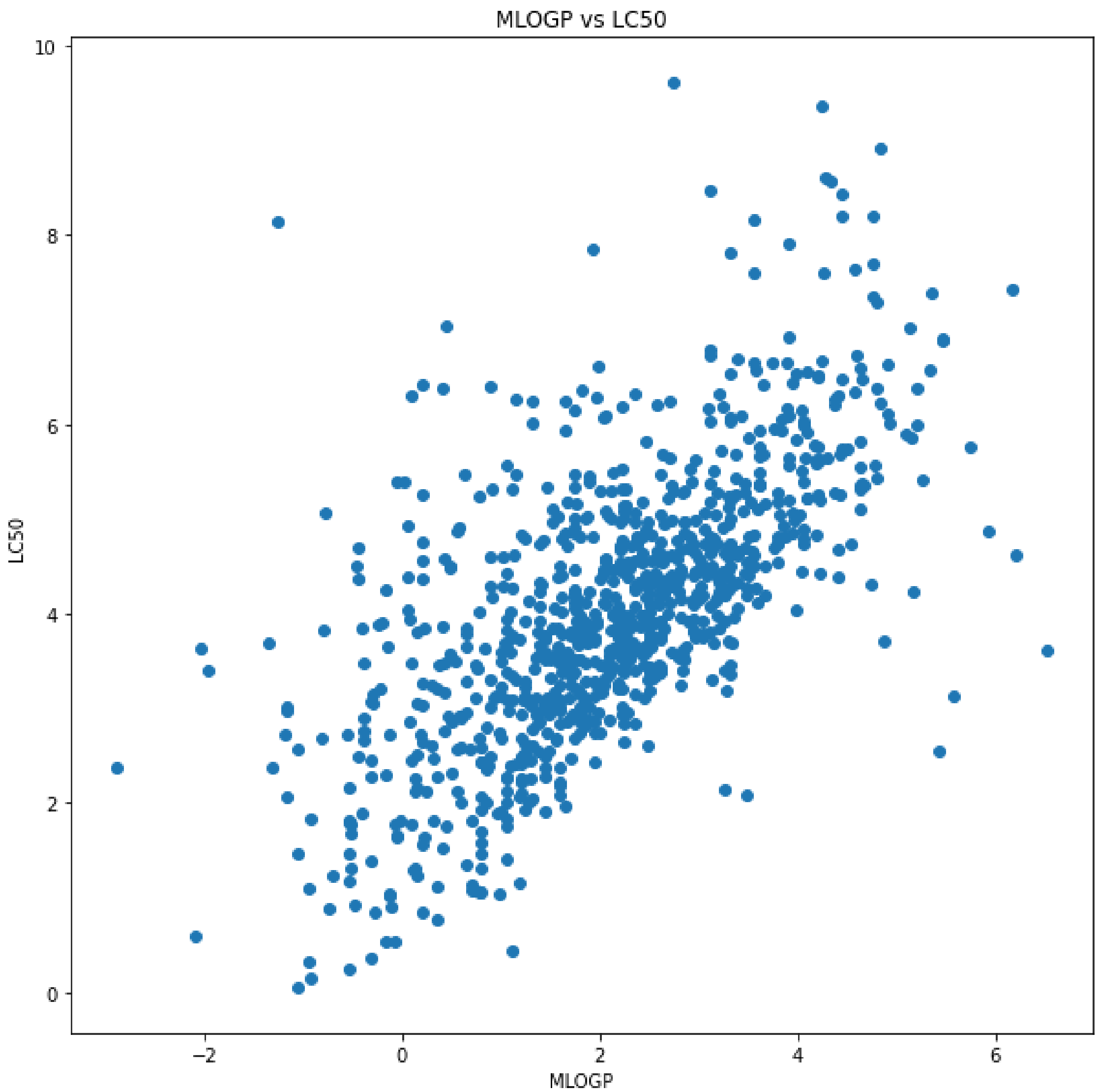
[8] : <seaborn.axisgrid.PairGrid at 0x29ef9575550>



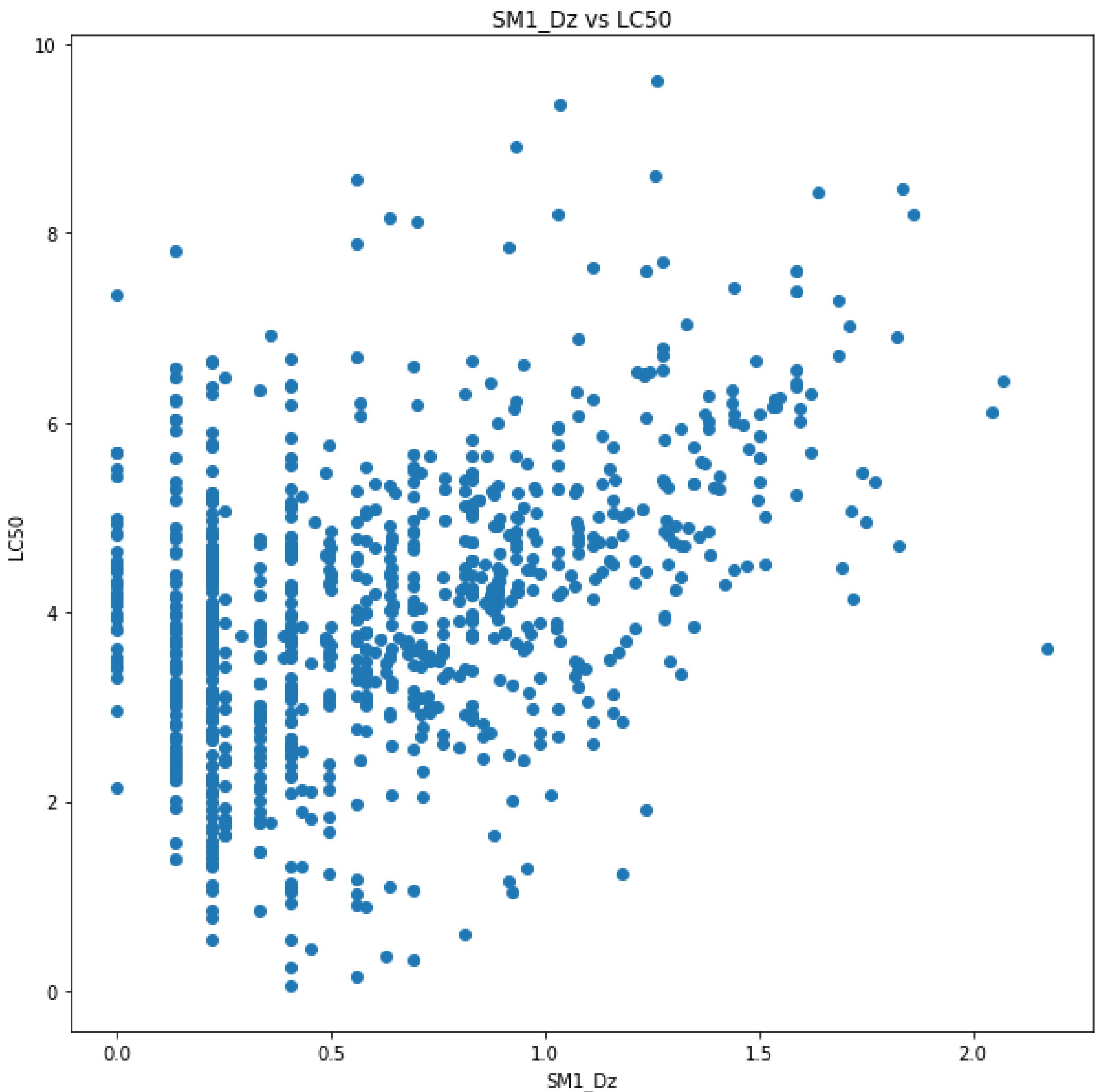
[9]:
```
plt.figure(figsize = (10,10))
plot = plt.scatter(df["CIC0"], df["LC50"])
plt.xlabel("CICO")
plt.ylabel("LC50")
plt.title("CIC0 vs LC50")
plt.show()
```



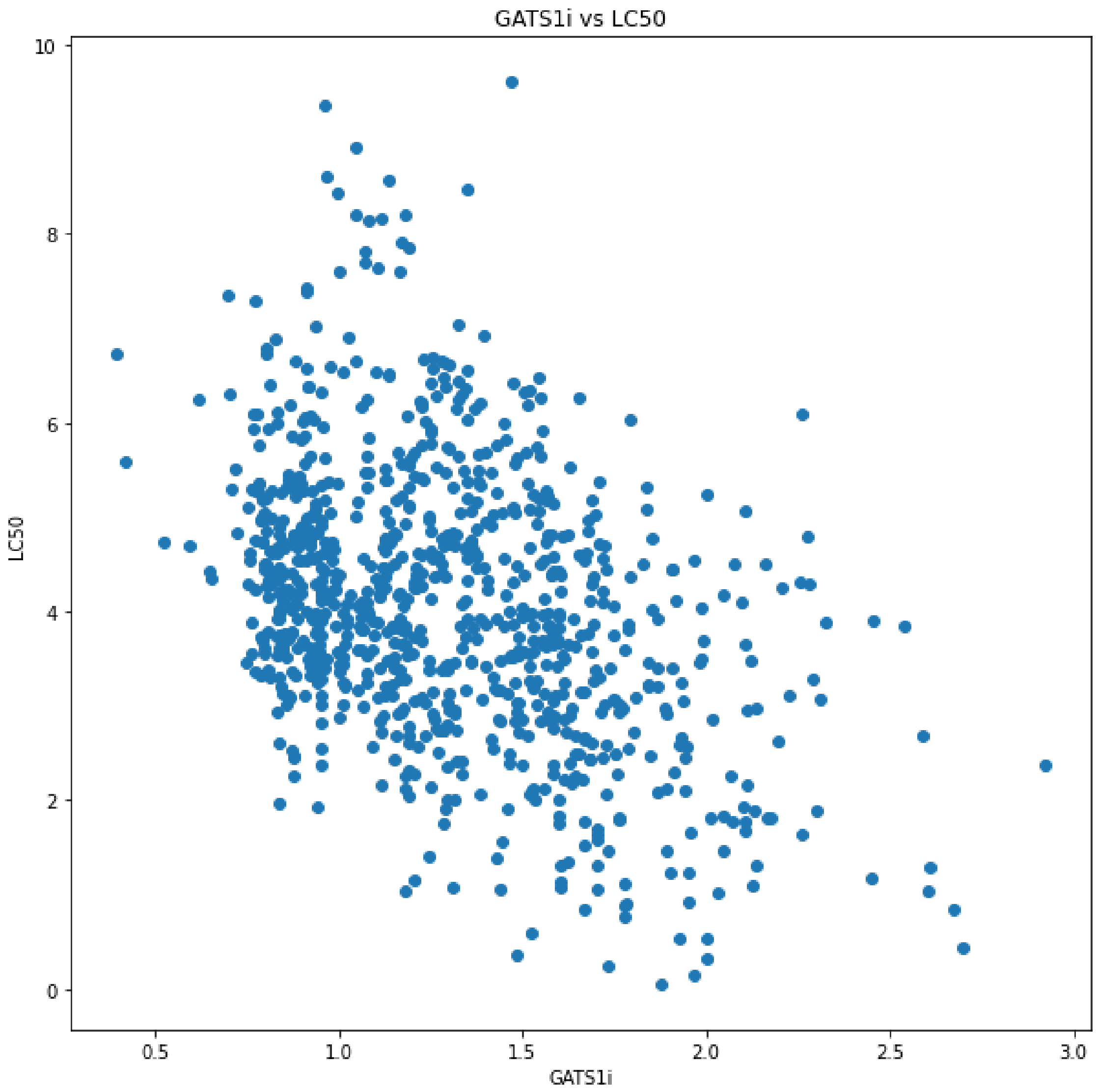
[10]:
```
plt.figure(figsize = (10,10))
plot = plt.scatter(df["MLOGP"], df["LC50"])
plt.xlabel("MLOGP")
plt.ylabel("LC50")
plt.title("MLOGP vs LC50")
plt.show()
```



[11]:
```
plt.figure(figsize = (10,10))
plot = plt.scatter(df["SM1_Dz"], df["LC50"])
plt.xlabel("SM1_Dz")
plt.ylabel("LC50")
plt.title("SM1_Dz vs LC50")
plt.show()
```



[12]:
```
plt.figure(figsize = (10,10))
plot = plt.scatter(df["GATS1i"], df["LC50"])
plt.xlabel("GATS1i")
plt.ylabel("LC50")
plt.title("GATS1i vs LC50")
plt.show()
```



[13]:
```
sns.pairplot(df, hue = "NdsCH")
```

[13]: <seaborn.axisgrid.PairGrid at 0x29efc718b50>

[14]:
```
sns.pairplot(df, hue = "NdssC")
```

[14]: <seaborn.axisgrid.PairGrid at 0x29efcaa7400>

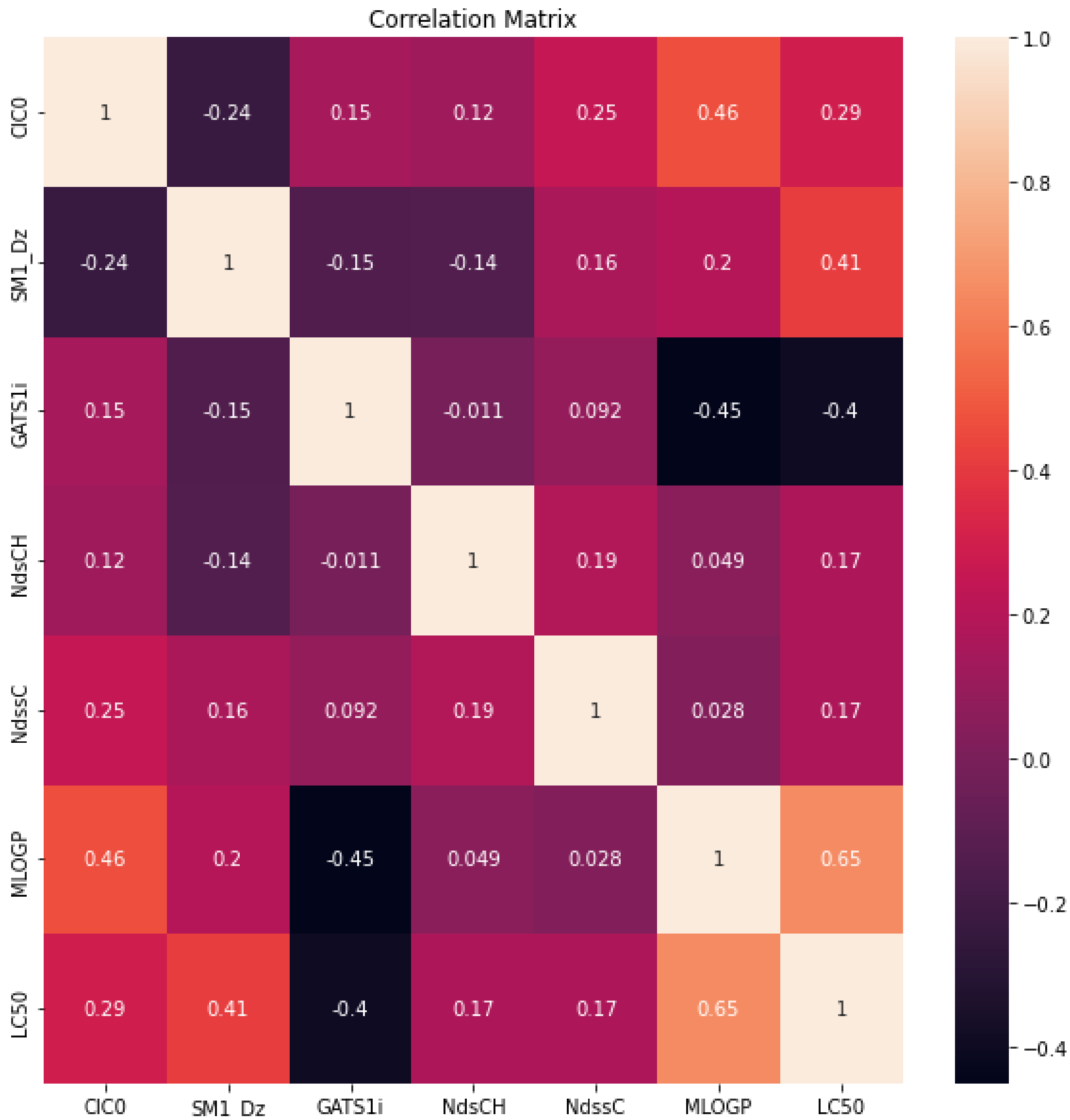
[15]:

```
sns.pairplot(df, hue = "LC50")
```

[15]: <seaborn.axisgrid.PairGrid at 0x29efeb51280>


```
[16]: corr = df.corr()
      plt.figure(figsize = (10,10))
      sns.heatmap(corr, annot = True).set(title = "Correlation Matrix")
```

```
[16]: [Text(0.5, 1.0, 'Correlation Matrix')]
```

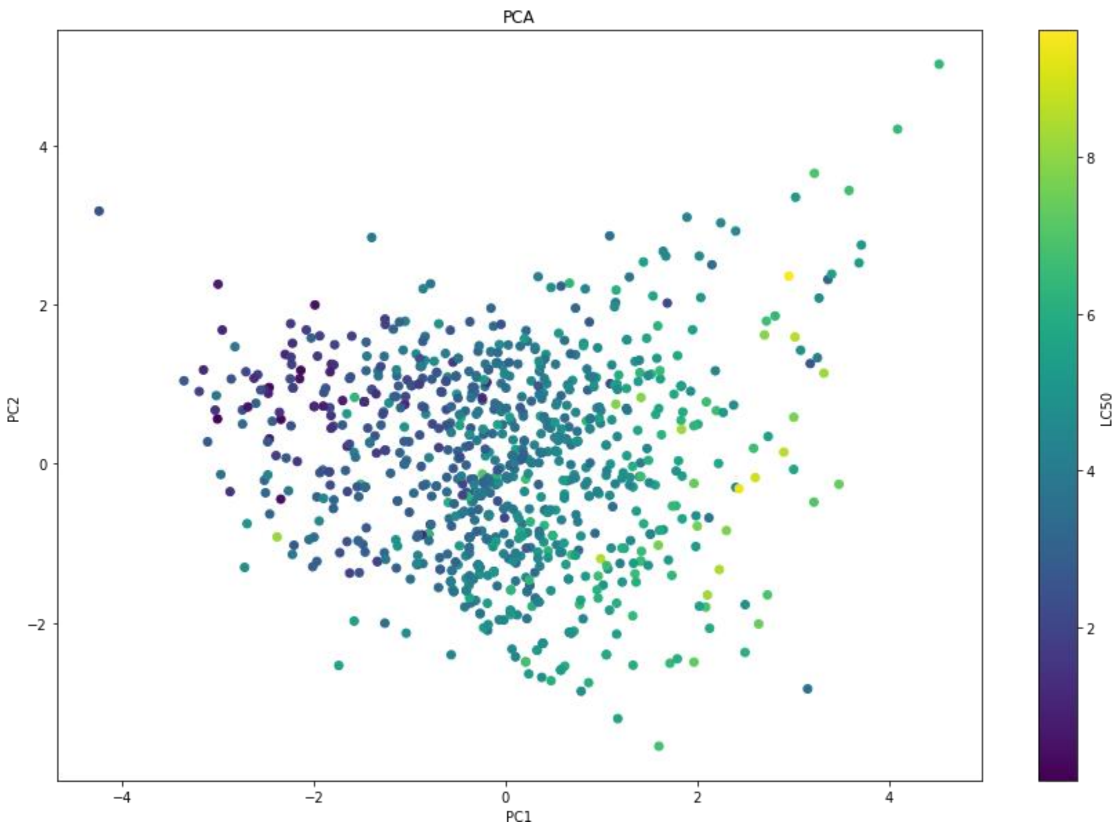


2 Normalize, Split the Data, and Perform Dimensionality Reduction

[17]:
```
X = df.iloc[:, 0:6]
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)
df_scaled = df
df_scaled.iloc[:, 0:6] = X_scaled
Train, Test = train_test_split(df_scaled, test_size=0.2, random_state=101)
X_test = Test.iloc[:, 0:6]
```

```
y_test = Test.iloc[:, 6:]
X_train = Train.iloc[:, 0:6]
y_train = Train.iloc[:, 6:]
```

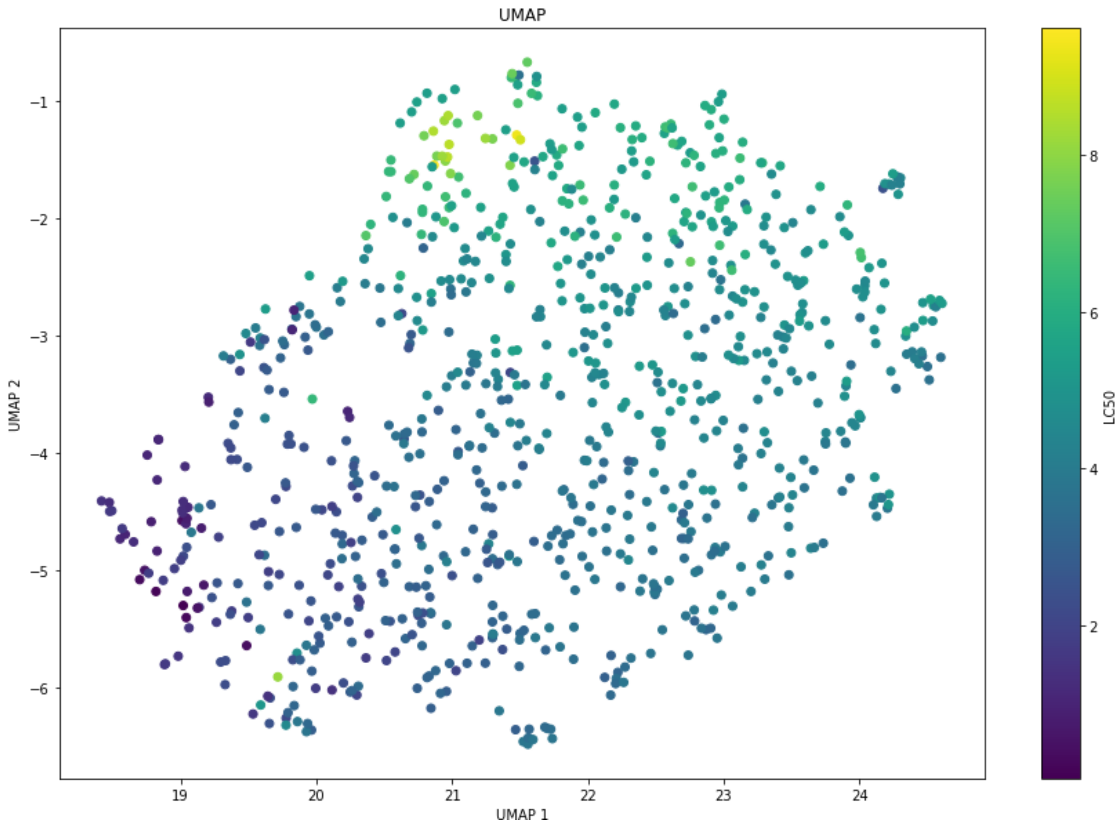
[81]:
```
plt.figure(figsize = (15,10))
pca = PCA(n_components=2)
pc = pca.fit_transform(X_scaled)
plot = plt.scatter(pc[:,0], pc[:,1], c=df.iloc[:, 6:].values)
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.title("PCA")
plt.colorbar(plot, label = "LC50")
plt.show()
```



[74]:
```
reducer = umap.UMAP(target_metric='l1', random_state=101)
embedding = reducer.fit_transform(X_scaled, y = df.iloc[:, 6:].values)
```

[75]:
```
plt.figure(figsize = (15,10))
plot = plt.scatter(embedding[:,0], embedding[:,1], c=df.iloc[:, 6:].values)
plt.title("UMAP")
plt.xlabel("UMAP 1")
```

```
plt.ylabel("UMAP 2")
plt.colorbar(plot, label = "LC50")
plt.show()
```



3 Univariate Model Exploration

3.1 CIC0 vs LC50

[15]:
```
mod = smf.ols(formula = "LC50~CIC0", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
```

```
Dep. Variable:                   LC50   R-squared:                       0.099
Model:                            OLS   Adj. R-squared:                  0.098
Method:                 Least Squares   F-statistic:                     79.97
Date:                Wed, 27 Jul 2022   Prob (F-statistic):           3.14e-18
Time:                        13:00:21   Log-Likelihood:                -1257.0
No. Observations:                 726   AIC:                             2518.
Df Residuals:                     724   BIC:                             2527.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0056      0.051     78.850      0.000       3.906       4.105
CIC0           0.4496      0.050      8.943      0.000       0.351       0.548
==============================================================================
Omnibus:                       16.273   Durbin-Watson:                   1.946
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               19.812
Skew:                           0.269   Prob(JB):                     4.99e-05
Kurtosis:                       3.605   Cond. No.                         1.01
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
             df       sum_sq     mean_sq          F        PR(>F)
CIC0        1.0   149.824163  149.824163  79.968749  3.137657e-18
Residual  724.0  1356.438551    1.873534        NaN           NaN
MAE: 1.1518681199451974
MSE: 2.228243869070734
RMSE: 1.4927303403732148
R_squared: -0.0032098309987493856
```

3.2 SM1_Dz vs LC50

[16]:
```python
mod = smf.ols(formula = "LC50~SM1_Dz", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.151
```

```
Model:                            OLS   Adj. R-squared:                  0.150
Method:                 Least Squares   F-statistic:                     129.0
Date:                Wed, 27 Jul 2022   Prob (F-statistic):           1.25e-27
Time:                        13:00:21   Log-Likelihood:                -1235.6
No. Observations:                 726   AIC:                             2475.
Df Residuals:                     724   BIC:                             2484.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0165      0.049     81.432      0.000       3.920       4.113
SM1_Dz         0.5762      0.051     11.359      0.000       0.477       0.676
==============================================================================
Omnibus:                       12.737   Durbin-Watson:                   1.987
Prob(Omnibus):                  0.002   Jarque-Bera (JB):               17.750
Skew:                           0.169   Prob(JB):                     0.000140
Kurtosis:                       3.687   Cond. No.                         1.03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
             df       sum_sq     mean_sq           F        PR(>F)
SM1_Dz      1.0   227.822418  227.822418  129.019268  1.250371e-27
Residual  724.0  1278.440295    1.765802         NaN           NaN
MAE: 0.9679574343670176
MSE: 1.7668341949514315
RMSE: 1.3292231546852589
R_squared: 0.2045280775935706
```

3.3 GATS1i vs LC50

[17]:
```python
mod = smf.ols(formula = "LC50~GATS1i", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.141
Model:                            OLS   Adj. R-squared:                  0.140
```

```
Method:                 Least Squares   F-statistic:                     118.7
Date:                Wed, 27 Jul 2022   Prob (F-statistic):           1.07e-25
Time:                        13:00:21   Log-Likelihood:                -1240.0
No. Observations:                 726   AIC:                             2484.
Df Residuals:                     724   BIC:                             2493.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0170      0.050     80.946      0.000       3.920       4.114
GATS1i        -0.5417      0.050    -10.894      0.000      -0.639      -0.444
==============================================================================
Omnibus:                       38.807   Durbin-Watson:                   1.998
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               47.144
Skew:                           0.514   Prob(JB):                     5.79e-11
Kurtosis:                       3.708   Cond. No.                         1.02
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
             df       sum_sq     mean_sq           F        PR(>F)
GATS1i      1.0   212.150803  212.150803  118.689257  1.065895e-25
Residual  724.0  1294.111910    1.787447         NaN           NaN
MAE: 1.0042377587990872
MSE: 1.7954857477079382
RMSE: 1.339957367869567
R_squared: 0.1916284485189962
```

3.4 NdsCH vs LC50

[18]:
```python
mod = smf.ols(formula = "LC50~NdsCH", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.035
Model:                            OLS   Adj. R-squared:                  0.034
Method:                 Least Squares   F-statistic:                     26.32
```

```
Date:                  Wed, 27 Jul 2022   Prob (F-statistic):          3.73e-07
Time:                          13:00:21   Log-Likelihood:               -1282.1
No. Observations:                   726   AIC:                            2568.
Df Residuals:                       724   BIC:                            2577.
Df Model:                             1
Covariance Type:              nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0059      0.053     76.178      0.000       3.903       4.109
NdsCH          0.2618      0.051      5.130      0.000       0.162       0.362
==============================================================================
Omnibus:                         20.415   Durbin-Watson:                   1.960
Prob(Omnibus):                    0.000   Jarque-Bera (JB):               26.860
Skew:                             0.292   Prob(JB):                     1.47e-06
Kurtosis:                         3.739   Cond. No.                         1.03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
             df       sum_sq    mean_sq          F        PR(>F)
NdsCH       1.0    52.829295  52.829295  26.315901  3.726305e-07
Residual  724.0  1453.433418   2.007505        NaN           NaN
MAE:  1.1750910409244002
MSE:  2.2797661983049387
RMSE:  1.5098894655917494
R_squared:  -0.026406442429465216
```

3.5 NdssC vs LC50

[19]:
```python
mod = smf.ols(formula = "LC50~NdssC", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred  = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.023
Model:                            OLS   Adj. R-squared:                  0.022
Method:                 Least Squares   F-statistic:                     17.03
Date:                Wed, 27 Jul 2022   Prob (F-statistic):           4.10e-05
```

```
Time:                        13:00:21   Log-Likelihood:                -1286.6
No. Observations:                 726   AIC:                             2577.
Df Residuals:                     724   BIC:                             2586.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0051      0.053     75.686      0.000       3.901       4.109
NdssC          0.2227      0.054      4.127      0.000       0.117       0.329
==============================================================================
Omnibus:                        8.540   Durbin-Watson:                   1.973
Prob(Omnibus):                  0.014   Jarque-Bera (JB):                9.901
Skew:                           0.169   Prob(JB):                      0.00708
Kurtosis:                       3.461   Cond. No.                         1.02
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
             df       sum_sq    mean_sq          F    PR(>F)
NdssC       1.0    34.623039  34.623039  17.033436  0.000041
Residual  724.0  1471.639674   2.032651        NaN       NaN
MAE: 1.149265041501467
MSE: 2.18208473043618
RMSE: 1.477188116130163
R_squared: 0.017572140988887272
```

3.6 MLOGP vs LC50

[20]:
```python
mod = smf.ols(formula = "LC50~MLOGP", data = Train).fit()
print(mod.summary())
table = sm.stats.anova_lm(mod, typ=1)
print(table)
y_pred = mod.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.423
Model:                            OLS   Adj. R-squared:                  0.422
Method:                 Least Squares   F-statistic:                     531.3
Date:                Wed, 27 Jul 2022   Prob (F-statistic):           1.38e-88
Time:                        13:00:21   Log-Likelihood:                -1095.3
```

```
No. Observations:                 726   AIC:                             2195.
Df Residuals:                     724   BIC:                             2204.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0443      0.041     99.405      0.000       3.964       4.124
MLOGP          0.9410      0.041     23.050      0.000       0.861       1.021
==============================================================================
Omnibus:                      123.874   Durbin-Watson:                   2.037
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              322.369
Skew:                           0.877   Prob(JB):                     9.97e-71
Kurtosis:                       5.753   Cond. No.                         1.04
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
             df      sum_sq     mean_sq           F        PR(>F)
MLOGP       1.0  637.505102  637.505102  531.280172  1.377389e-88
Residual  724.0  868.757612    1.199941         NaN           NaN
MAE: 0.8431096632604543
MSE: 1.3046098164437467
RMSE: 1.1421951744092367
R_squared: 0.41263278600664965
```

4 Model Exploration

4.1 Multivariate Model with Every Factor

[26]:
```python
mod_1 = smf.ols(formula = "LC50~(CIC0+SM1_Dz+GATS1i+NdsCH+NdssC+MLOGP)", data =
 ↪Train).fit()
print(mod_1.summary())
table = sm.stats.anova_lm(mod_1, typ=1)
print(table)
variables = mod_1.model.exog
y_pred = mod_1.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
cls = Linear_Reg_Diagnostic(mod_1)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

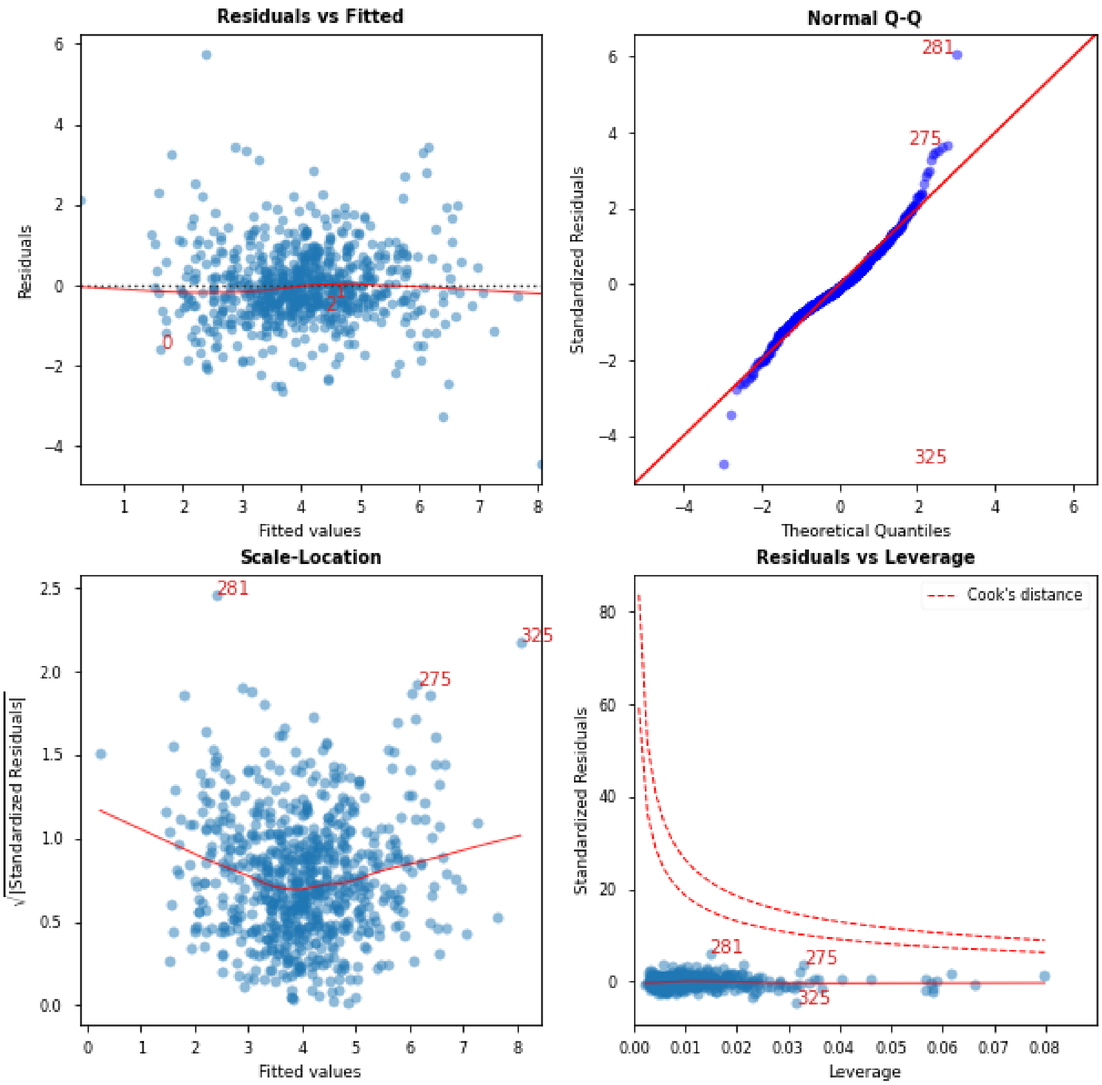
```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.564
```

```
Model:                            OLS   Adj. R-squared:                  0.561
Method:                 Least Squares   F-statistic:                     155.2
Date:                Wed, 03 Aug 2022   Prob (F-statistic):          4.06e-126
Time:                        17:41:47   Log-Likelihood:                -993.50
No. Observations:                 726   AIC:                             2001.
Df Residuals:                     719   BIC:                             2033.
Df Model:                           6
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0379      0.036    113.732      0.000       3.968       4.108
CIC0           0.2863      0.052      5.476      0.000       0.184       0.389
SM1_Dz         0.5260      0.042     12.484      0.000       0.443       0.609
GATS1i        -0.2717      0.045     -5.971      0.000      -0.361      -0.182
NdsCH          0.2326      0.036      6.405      0.000       0.161       0.304
NdssC          0.0476      0.041      1.174      0.241      -0.032       0.127
MLOGP          0.5696      0.055     10.325      0.000       0.461       0.678
==============================================================================
Omnibus:                       91.056   Durbin-Watson:                   1.968
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              357.171
Skew:                           0.522   Prob(JB):                     2.76e-78
Kurtosis:                       6.274   Cond. No.                         2.91
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
              df      sum_sq     mean_sq           F        PR(>F)
CIC0         1.0  149.824163  149.824163  164.140644  5.401678e-34
SM1_Dz       1.0  332.561060  332.561060  364.339007  5.071243e-66
GATS1i       1.0  222.531248  222.531248  243.795272  1.525815e-47
NdsCH        1.0   46.872834   46.872834   51.351778  1.917520e-12
NdssC        1.0    0.874501    0.874501    0.958064  3.280044e-01
MLOGP        1.0   97.310678   97.310678  106.609222  2.125854e-23
Residual   719.0  656.288230    0.912779         NaN           NaN
MAE: 0.6646693501498407
MSE: 0.8671610192409167
RMSE: 0.9312148083234698
R_squared: 0.609582922391621
```

[23]:
```
fig, ax = cls()
```

```
C:\Users\matth\anaconda3\lib\site-packages\statsmodels\graphics\gofplots.py:993: UserWarning: marker is redundantly defined by the 'marker' keyword argument and the fmt string "bo" (-> marker='o'). The keyword argument will take precedence.
  ax.plot(x, y, fmt, **plot_style)
```



	Features	VIF Factor
0	Intercept	1.00
4	NdsCH	1.11
5	NdssC	1.26
2	SM1_Dz	1.33
3	GATS1i	1.64
1	CIC0	2.22
6	MLOGP	2.40

4.2 Reduced Model

[27]:
```
mod_2 = smf.ols(formula = "LC50~CIC0+SM1_Dz+GATS1i+NdsCH+MLOGP", data = Train).
 ↪fit()
print(mod_2.summary())
table = sm.stats.anova_lm(mod_2, typ=1)
print(table)
table = sm.stats.anova_lm(mod_2,mod_1, typ=1)
print(table)
variables = mod_2.model.exog

y_pred = mod_2.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
cls = Linear_Reg_Diagnostic(mod_2)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.563
Model:                            OLS   Adj. R-squared:                  0.560
Method:                 Least Squares   F-statistic:                     185.9
Date:                Wed, 03 Aug 2022   Prob (F-statistic):          5.62e-127
Time:                        17:41:50   Log-Likelihood:                -994.20
No. Observations:                 726   AIC:                             2000.
Df Residuals:                     720   BIC:                             2028.
Df Model:                           5
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      4.0381      0.036    113.707      0.000       3.968       4.108
CIC0           0.3066      0.049      6.215      0.000       0.210       0.403
SM1_Dz         0.5407      0.040     13.437      0.000       0.462       0.620
GATS1i        -0.2729      0.045     -5.997      0.000      -0.362      -0.184
NdsCH          0.2432      0.035      6.915      0.000       0.174       0.312
MLOGP          0.5562      0.054     10.302      0.000       0.450       0.662
==============================================================================
Omnibus:                       92.661   Durbin-Watson:                   1.975
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              364.204
Skew:                           0.533   Prob(JB):                     8.20e-80
Kurtosis:                       6.302   Cond. No.                         2.71
==============================================================================

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

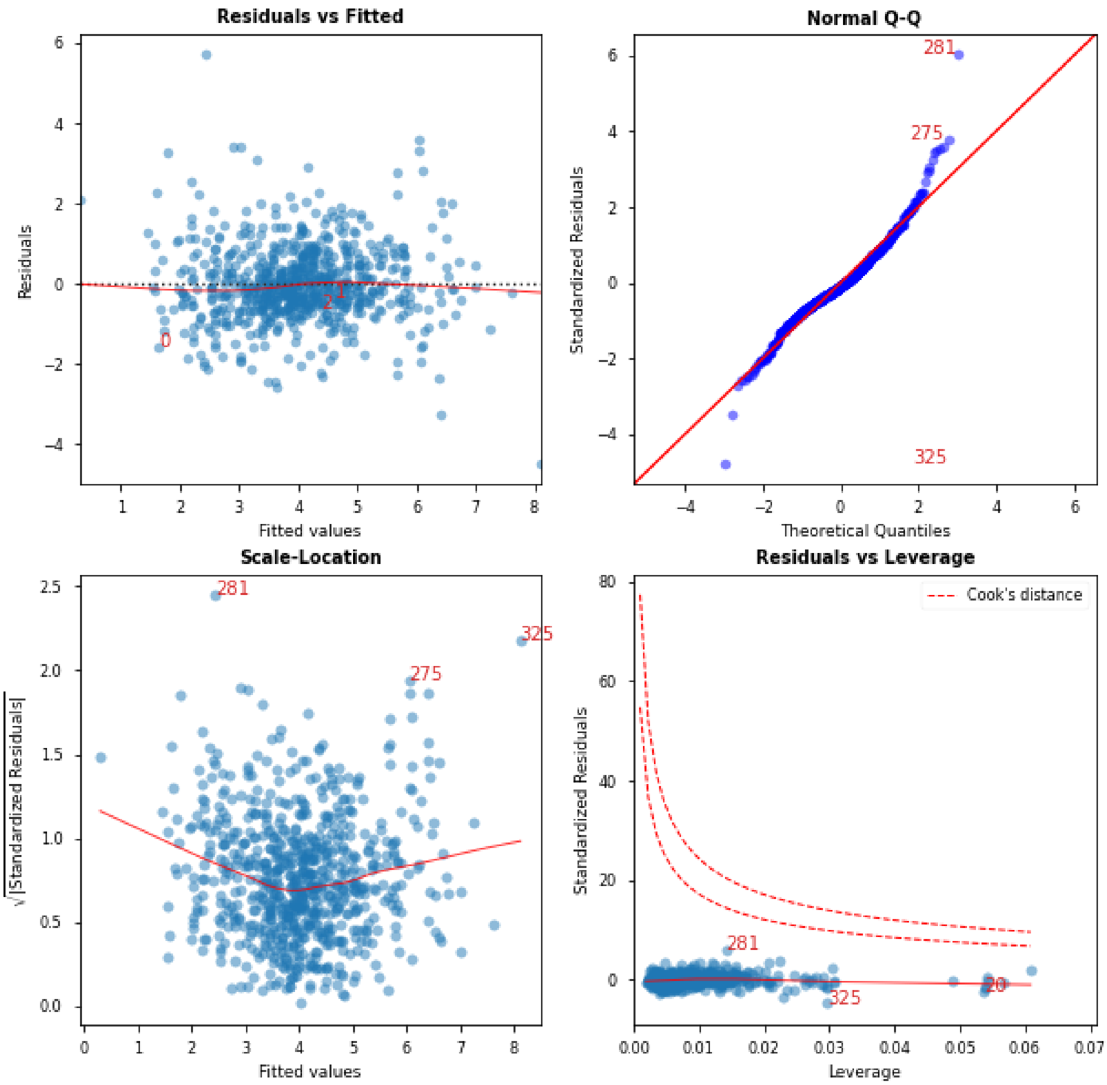
specified.

```
               df      sum_sq     mean_sq           F        PR(>F)
CIC0          1.0  149.824163  149.824163  164.054642  5.539706e-34
SM1_Dz        1.0  332.561060  332.561060  364.148110  5.207671e-66
GATS1i        1.0  222.531248  222.531248  243.667534  1.569730e-47
NdsCH         1.0   46.872834   46.872834   51.324872  1.939865e-12
MLOGP         1.0   96.927875   96.927875  106.134201  2.607435e-23
Residual    720.0  657.545534    0.913258         NaN           NaN
   df_resid         ssr  df_diff   ss_diff         F    Pr(>F)
0     720.0  657.545534      0.0       NaN       NaN       NaN
1     719.0  656.288230      1.0  1.257304  1.377446  0.240925
MAE: 0.6648025405914847
MSE: 0.8725132414740466
RMSE: 0.9340841725851299
R_squared: 0.6071732211751176
```

[28]:

```
fig, ax = cls()
```

```
C:\Users\matth\anaconda3\lib\site-packages\statsmodels\graphics\gofplots.py:993:
UserWarning: marker is redundantly defined by the 'marker' keyword argument and
the fmt string "bo" (-> marker='o'). The keyword argument will take precedence.
  ax.plot(x, y, fmt, **plot_style)
```



	Features	VIF Factor
0	Intercept	1.00
4	NdsCH	1.04
2	SM1_Dz	1.22
3	GATS1i	1.64
1	CIC0	1.98
5	MLOGP	2.30

5 Interaction Testing

5.1 All First Order Interaction Terms

[29]:
```
mod_3 = smf.ols(formula =
 ↪"LC50~(CIC0+SM1_Dz+GATS1i+NdsCH+NdssC+MLOGP)*(CIC0+SM1_Dz+GATS1i+NdsCH+NdssC+MLOGP)",
 ↪data = Train).fit()
print(mod_3.summary())
table = sm.stats.anova_lm(mod_3, typ=1)
print(table)
variables = mod_3.model.exog
y_pred = mod_3.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
cls = Linear_Reg_Diagnostic(mod_3)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.614
Model:                            OLS   Adj. R-squared:                  0.603
Method:                 Least Squares   F-statistic:                     53.42
Date:                Wed, 03 Aug 2022   Prob (F-statistic):          3.18e-130
Time:                        17:42:28   Log-Likelihood:                -949.12
No. Observations:                 726   AIC:                             1942.
Df Residuals:                     704   BIC:                             2043.
Df Model:                          21
Covariance Type:            nonrobust
===============================================================================
=
                      coef    std err          t      P>|t|      [0.025
0.975]
-------------------------------------------------------------------------------
-
Intercept           3.8885      0.049     79.473      0.000       3.792
3.985
CIC0                0.3172      0.060      5.250      0.000       0.199
0.436
SM1_Dz              0.6134      0.044     13.825      0.000       0.526
0.700
GATS1i             -0.2828      0.050     -5.631      0.000      -0.381
-0.184
NdsCH               0.2652      0.048      5.522      0.000       0.171
0.360
NdssC              -0.0940      0.051     -1.836      0.067      -0.194
0.007
```

MLOGP	0.5200	0.067	7.713	0.000	0.388	0.652
CIC0:SM1_Dz	-0.0868	0.053	-1.647	0.100	-0.190	0.017
CIC0:GATS1i	0.0519	0.048	1.077	0.282	-0.043	0.146
CIC0:NdsCH	-0.0567	0.066	-0.863	0.388	-0.186	0.072
CIC0:NdssC	0.1522	0.052	2.953	0.003	0.051	0.253
CIC0:MLOGP	0.1543	0.034	4.529	0.000	0.087	0.221
SM1_Dz:GATS1i	0.0179	0.050	0.357	0.721	-0.081	0.116
SM1_Dz:NdsCH	0.0152	0.048	0.318	0.751	-0.079	0.109
SM1_Dz:NdssC	0.2140	0.044	4.834	0.000	0.127	0.301
SM1_Dz:MLOGP	-0.0593	0.048	-1.233	0.218	-0.154	0.035
GATS1i:NdsCH	0.0352	0.057	0.618	0.537	-0.077	0.147
GATS1i:NdssC	-0.0024	0.044	-0.054	0.957	-0.089	0.085
GATS1i:MLOGP	-0.0179	0.040	-0.447	0.655	-0.096	0.061
NdsCH:NdssC	0.0499	0.031	1.594	0.111	-0.012	0.111
NdsCH:MLOGP	-0.1503	0.070	-2.159	0.031	-0.287	-0.014
NdssC:MLOGP	-0.0313	0.049	-0.637	0.524	-0.128	0.065

==

Omnibus:	63.570	Durbin-Watson:	1.943
Prob(Omnibus):	0.000	Jarque-Bera (JB):	249.871
Skew:	0.301	Prob(JB):	5.51e-55
Kurtosis:	5.810	Cond. No.	8.29

==

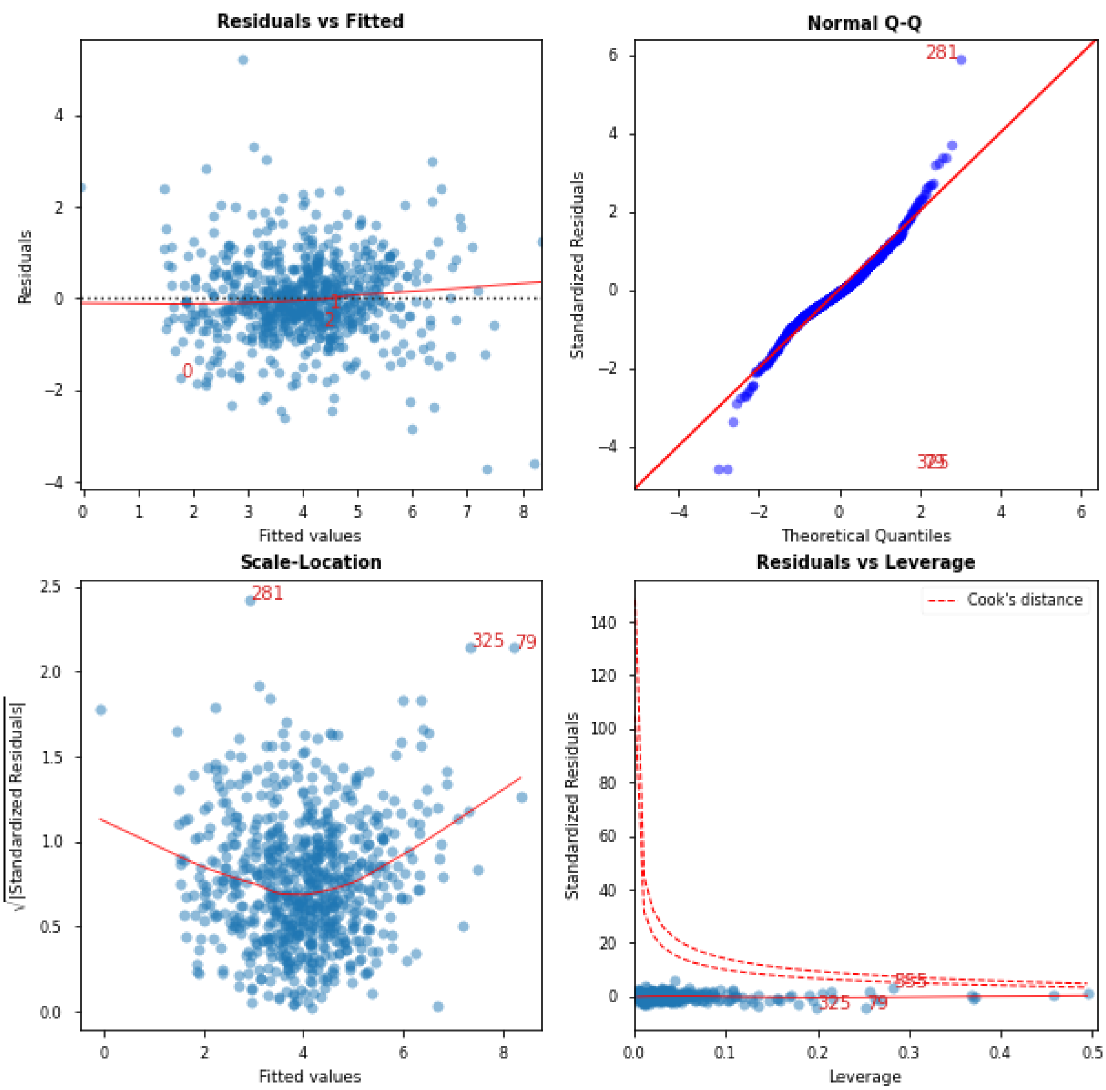
Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

	df	sum_sq	mean_sq	F	PR(>F)
CIC0	1.0	149.824163	149.824163	181.616861	5.428992e-37
SM1_Dz	1.0	332.561060	332.561060	403.130541	3.047164e-71
GATS1i	1.0	222.531248	222.531248	269.752395	1.468387e-51
NdsCH	1.0	46.872834	46.872834	56.819253	1.474241e-13
NdssC	1.0	0.874501	0.874501	1.060070	3.035529e-01

```
MLOGP             1.0   97.310678   97.310678  117.960011   1.637170e-25
CIC0:SM1_Dz       1.0    0.447692    0.447692    0.542692   4.615646e-01
CIC0:GATS1i       1.0    0.073509    0.073509    0.089107   7.654034e-01
CIC0:NdsCH        1.0   13.029795   13.029795   15.794718   7.788002e-05
CIC0:NdssC        1.0    9.908538    9.908538   12.011131   5.609252e-04
CIC0:MLOGP        1.0   19.988482   19.988482   24.230039   1.065758e-06
SM1_Dz:GATS1i     1.0    1.849727    1.849727    2.242240   1.347346e-01
SM1_Dz:NdsCH      1.0    1.266545    1.266545    1.535306   2.157308e-01
SM1_Dz:NdssC      1.0   16.334674   16.334674   19.800894   9.988010e-06
SM1_Dz:MLOGP      1.0    1.180579    1.180579    1.431098   2.319881e-01
GATS1i:NdsCH      1.0    4.068860    4.068860    4.932272   2.667712e-02
GATS1i:NdssC      1.0    0.008698    0.008698    0.010544   9.182437e-01
GATS1i:MLOGP      1.0    0.153957    0.153957    0.186627   6.658713e-01
NdsCH:NdssC       1.0    2.445800    2.445800    2.964799   8.553430e-02
NdsCH:MLOGP       1.0    4.433940    4.433940    5.374822   2.071503e-02
NdssC:MLOGP       1.0    0.335218    0.335218    0.406351   5.240346e-01
Residual        704.0  580.762216    0.824946         NaN            NaN
MAE: 0.6252053863994669
MSE: 0.8722338398525055
RMSE: 0.9339346014858351
R_squared: 0.6072990146115622
```

[30]:
```
fig, ax = cls()
```

```
C:\Users\matth\anaconda3\lib\site-packages\statsmodels\graphics\gofplots.py:993:
UserWarning: marker is redundantly defined by the 'marker' keyword argument and
the fmt string "bo" (-> marker='o'). The keyword argument will take precedence.
  ax.plot(x, y, fmt, **plot_style)
```



	Features	VIF Factor
11	CIC0:MLOGP	1.35
14	SM1_Dz:NdssC	1.47
16	GATS1i:NdsCH	1.64
2	SM1_Dz	1.64
17	GATS1i:NdssC	1.68
8	CIC0:GATS1i	1.72
13	SM1_Dz:NdsCH	1.78
18	GATS1i:MLOGP	1.81
12	SM1_Dz:GATS1i	1.93
7	CIC0:SM1_Dz	2.10
0	Intercept	2.11
4	NdsCH	2.16
3	GATS1i	2.21

```
5                 NdssC        2.22
19         NdsCH:NdssC        2.60
15      SM1_Dz:MLOGP        2.71
21        NdssC:MLOGP        2.72
10         CIC0:NdssC        2.99
1                   CIC0        3.28
6                 MLOGP        3.97
20        NdsCH:MLOGP        5.49
9          CIC0:NdsCH        7.53
```

5.2 Reduced Interactions Model

[24]:
```
mod_4 = smf.ols(formula = "LC50~CIC0+SM1_Dz+GATS1i+NdsCH+MLOGP+CIC0:NdssC+CIC0:
 ↪MLOGP+SM1_Dz:NdssC+NdsCH:MLOGP", data = Train).fit()
print(mod_4.summary())
table = sm.stats.anova_lm(mod_4, typ=1)
print(table)
table = sm.stats.anova_lm(mod_4,mod_3, typ=1)
print(table)
variables = mod_4.model.exog
vif = [variance_inflation_factor(variables, i) for i in range(variables.
 ↪shape[1])]
print(vif)
y_pred = mod_4.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
cls = Linear_Reg_Diagnostic(mod_4)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

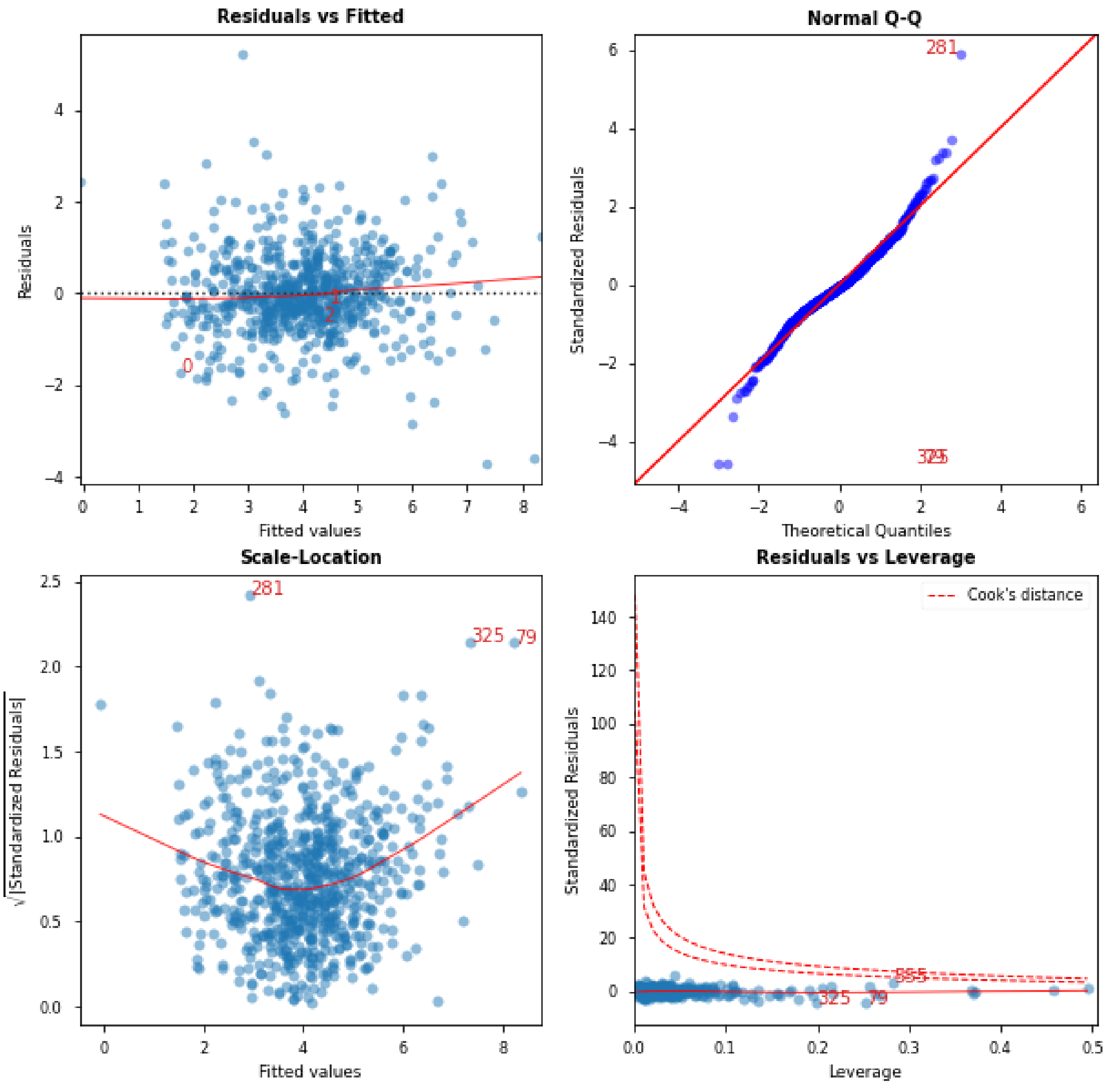
```
                            OLS Regression Results
==============================================================================
Dep. Variable:                   LC50   R-squared:                       0.603
Model:                            OLS   Adj. R-squared:                  0.598
Method:                 Least Squares   F-statistic:                     121.0
Date:                Wed, 27 Jul 2022   Prob (F-statistic):          2.44e-137
Time:                        13:00:21   Log-Likelihood:                -959.51
No. Observations:                 726   AIC:                             1939.
Df Residuals:                     716   BIC:                             1985.
Df Model:                           9
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      3.9337      0.038    103.544      0.000       3.859       4.008
CIC0           0.3073      0.049      6.314      0.000       0.212       0.403
SM1_Dz         0.5587      0.040     14.049      0.000       0.481       0.637
```

```
GATS1i          -0.2886      0.044     -6.526      0.000      -0.375      -0.202
NdsCH            0.2483      0.036      6.813      0.000       0.177       0.320
MLOGP            0.5476      0.053     10.290      0.000       0.443       0.652
CIC0:NdssC       0.1103      0.035      3.192      0.001       0.042       0.178
CIC0:MLOGP       0.1440      0.031      4.578      0.000       0.082       0.206
SM1_Dz:NdssC     0.1658      0.038      4.370      0.000       0.091       0.240
NdsCH:MLOGP     -0.1739      0.034     -5.123      0.000      -0.241      -0.107
==============================================================================
Omnibus:                       61.426   Durbin-Watson:                   1.938
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              266.636
Skew:                           0.229   Prob(JB):                     1.26e-58
Kurtosis:                       5.933   Cond. No.                         3.63
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
                 df      sum_sq     mean_sq           F        PR(>F)
CIC0            1.0  149.824163  149.824163  179.503126  1.095941e-36
SM1_Dz          1.0  332.561060  332.561060  398.438735  8.115997e-71
GATS1i          1.0  222.531248  222.531248  266.612901  3.482681e-51
NdsCH           1.0   46.872834   46.872834   56.157966  1.977608e-13
MLOGP           1.0   96.927875   96.927875  116.128508  3.380675e-25
CIC0:NdssC      1.0    2.973956    2.973956    3.563073  5.948244e-02
CIC0:MLOGP      1.0   17.586136   17.586136   21.069809  5.229643e-06
SM1_Dz:NdssC    1.0   17.462449   17.462449   20.921620  5.637720e-06
NdsCH:MLOGP     1.0   21.906098   21.906098   26.245520  3.870201e-07
Residual      716.0  597.616893    0.834660         NaN           NaN
   df_resid         ssr  df_diff    ss_diff         F    Pr(>F)
0     716.0  597.616893      0.0        NaN       NaN       NaN
1     704.0  580.762216     12.0  16.854678  1.702603  0.061921
[1.255416809499518, 2.1044981905482576, 1.3004538978884799, 1.6934312959727862,
1.2264784684887298, 2.443022742239267, 1.3292692131540762, 1.1348823438792845,
1.0676744718552331, 1.2905891804746232]
MAE: 0.6466933021246712
MSE: 0.9118498576541835
RMSE: 0.9549082980339962
R_squared: 0.5894629154864519
```

[31]:
```python
fig, ax = cls()
```

```
C:\Users\matth\anaconda3\lib\site-packages\statsmodels\graphics\gofplots.py:993:
UserWarning: marker is redundantly defined by the 'marker' keyword argument and
the fmt string "bo" (-> marker='o'). The keyword argument will take precedence.
  ax.plot(x, y, fmt, **plot_style)
```



	Features	VIF Factor
11	CIC0:MLOGP	1.35
14	SM1_Dz:NdssC	1.47
16	GATS1i:NdsCH	1.64
2	SM1_Dz	1.64
17	GATS1i:NdssC	1.68
8	CIC0:GATS1i	1.72
13	SM1_Dz:NdsCH	1.78
18	GATS1i:MLOGP	1.81
12	SM1_Dz:GATS1i	1.93
7	CIC0:SM1_Dz	2.10
0	Intercept	2.11
4	NdsCH	2.16
3	GATS1i	2.21

5	NdssC	2.22
19	NdsCH:NdssC	2.60
15	SM1_Dz:MLOGP	2.71
21	NdssC:MLOGP	2.72
10	CIC0:NdssC	2.99
1	CIC0	3.28
6	MLOGP	3.97
20	NdsCH:MLOGP	5.49
9	CIC0:NdsCH	7.53

6 Evaluation of Linear Models

There doesn't seem to be much good performance with Linear Models on this dataset. While the model with all first order interaction terms did perform the best, it may be due to there being more features. There was no significance between both reduced models and their respective parent model. The models with interaciton terms had less MAE, but had worse MSE, meaning errors may be bigger when interaction terms are included. R^2 on the test data for the models without interaction was higher as well. It is unlikely that interaction is present. Assumptions for linear regression hold for each model.

7 KNN Regression

7.1 KNN Example 6 Neighbors

[32]:
```
knn1 = KNeighborsRegressor(n_neighbors=6)
knn1.fit(X_train, y_train)
knn1.score(X_test, y_test)
y_pred = knn1.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.5972747252747254
MSE: 0.7172062567155068
RMSE: 0.8468803083762821
R_squared: 0.6770962202216795
```

7.2 Grid Search Optimization for KNN

[33]:
```
scoring = {"MSE": "neg_mean_squared_error", "R2":"r2"}

# Setting refit='AUC', refits an estimator on the whole dataset with the
# parameter setting that has the best cross-validated AUC score.
# That estimator is made available at ``gs.best_estimator_`` along with
# parameters like ``gs.best_score_``, ``gs.best_params_`` and
```

```
# ``gs.best_index_``
gs = GridSearchCV(
    KNeighborsRegressor(),
    param_grid={"n_neighbors": range(1, 6), "weights":["uniform","distance"],␣
 ↪"p":[1,2]},
    scoring=scoring,
    refit="MSE",
    return_train_score=True,
    n_jobs = -1,
    cv = 100,
    verbose = 3
)
gs.fit(X_train, y_train)
results = gs.cv_results_
```

Fitting 100 folds for each of 20 candidates, totalling 2000 fits

[34]:
```
gs.best_params_
```

[34]: {'n_neighbors': 5, 'p': 1, 'weights': 'distance'}

[35]:
```
knn = gs.best_estimator_
```

[36]:
```
y_pred = knn.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

MAE: 0.549976177393366
MSE: 0.6426008012295652
RMSE: 0.8016238527074685
R_squared: 0.7106854190650043

7.3 PCA and KNN

[28]:
```
def get_models():
    models = dict()
    for i in range(1,7):
        steps = [('pca', PCA(n_components=i)), ('m',␣
 ↪KNeighborsRegressor(n_neighbors=5, p = 1, weights = "distance"))]
        models[str(i)] = Pipeline(steps=steps)
    return models

# evaluate a given model using cross-validation
def evaluate_model(model, X, y):
    cv = KFold(n_splits=5, random_state=101, shuffle = True)
```

```
    scores = cross_val_score(model, X, y, scoring='neg_mean_squared_error',␣
↪cv=cv, n_jobs=-1, error_score='raise')
    return scores
# get the models to evaluate
models = get_models()
# evaluate the models and store results
results, names = list(), list()
for name, model in models.items():
    scores = evaluate_model(model, X_train, y_train)
    results.append(scores)
    names.append(name)
    print('>%s %.3f (%.3f)' % (name, mean(scores), std(scores)))
```

```
>1 -1.738 (0.114)
>2 -1.161 (0.140)
>3 -0.950 (0.105)
>4 -0.812 (0.157)
>5 -0.866 (0.141)
>6 -0.847 (0.148)
```

[29]:
```
steps = [('pca', PCA(n_components=4)), ('m', KNeighborsRegressor(n_neighbors=5,␣
↪p = 1, weights = "distance"))]
model = Pipeline(steps=steps)
model.fit(X_train,  y_train)
y_pred = model.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.5937420511872225
MSE: 0.7569008399616851
RMSE: 0.8700004827364667
R_squared: 0.6592247490139198
```

8 Evaluation of KNN

KNN improves performance on the Test dataset. It was optimized, and led to a higher R^2 score and lower MSE. PCA compresses the data too much and does not allow for meaningful relationships to be seen by the model. KNN with 5 neighbors, l1 distance performs the best on the data.

9 Gradient Descent

[30]:
```
sgd_reg = SGDRegressor(max_iter=1000, tol=1e-3, penalty="l2", eta0=0.01)
sgd_reg.fit(X_train,   y_train.values.ravel())
sgd_reg.intercept_, sgd_reg.coef_
y_pred = sgd_reg.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.6641009021334089
MSE: 0.8673091952076947
RMSE: 0.931294365497663
R_squared: 0.6095162099510966
```

10 Evaluation of Gradient Descent

Same performance as linear model but is outperformed by KNN. Cant be optimized as well since parameters are continuous

11 11. Ridge, Lasso, and Elasticnet Regularization

11.1 Ridge Regression

[39]:
```
poly = PolynomialFeatures(2)
poly_X_train = poly.fit_transform(X_train)
poly_X_test = poly.fit_transform(X_test)
ridge_reg = Ridge(alpha=1 , solver= "auto")
ridge_reg.fit(poly_X_train , y_train)
y_pred= ridge_reg.predict(poly_X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.6192753750697797
MSE: 0.8440158736842909
RMSE: 0.9187033654473521
R_squared: 0.6200034324105659
```

[62]:
```
intercept = ridge_reg.intercept_[0]
print("E(y) = " + str(intercept), end =" ")
i = 1
for coef in ridge_reg.coef_[0]:
    print("+ " + str(coef) + "*X_"+ str(i),end =" ")
```

```
    i+=1
```

E(y) = 3.892252012873493 + 0.0*X_1 + 0.3009287547124961*X_2 + 0.5846542581855313*X_3 + -0.2885722891861736*X_4 + 0.33561044270534446*X_5 + -0.04691621569339529*X_6 + 0.5147181910314026*X_7 + -0.011844581261028983*X_8 + -0.07988945669958426*X_9 + 0.0724036613395784*X_10 + -0.027615552497574667*X_11 + 0.17945067847378657*X_12 + 0.16240783769337988*X_13 + 0.04029647132214782*X_14 + 0.017151044825168892*X_15 + -0.005330546352793698*X_16 + 0.23548063628815477*X_17 + -0.07834081616696212*X_18 + 0.009090663384291042*X_19 + 0.014132939074507442*X_20 + -0.02385617257690637*X_21 + -0.013281152434592177*X_22 + -0.0289314206562750l*X_23 + 0.06865771394750197*X_24 + -0.16582416385791565*X_25 + -0.0317079979197357*X_26 + -0.059135522124548326*X_27 + 0.0019317900535462068*X_28

11.2 Lasso Regression

[65]:
```
lasso_reg = Lasso(alpha = 0.05)
lasso_reg.fit(poly_X_train,   y_train)
y_pred = lasso_reg.predict(poly_X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

MAE: 0.6531654769265813
MSE: 0.8695790137885683
RMSE: 0.9325122057048735
R_squared: 0.608494282169078

[67]:
```
intercept = lasso_reg.intercept_[0]
print("E(y) = " + str(intercept), end =" ")
i = 1
for coef in lasso_reg.coef_:
    print("+ " + str(coef) + "*X_"+ str(i),end =" ")
    i+=1
```

E(y) = 3.9173103213192504 + 0.0*X_1 + 0.19886736243419062*X_2 + 0.4559465671701525*X_3 + -0.21256611454121532*X_4 + 0.18174835873080378*X_5 + 0.0*X_6 + 0.5931181518839378*X_7 + 0.04905532044355343*X_8 + -0.0*X_9 + 0.0*X_10 + -0.0*X_11 + 0.050231234305945914*X_12 + 0.04983652536927835*X_13 + 0.02268194583406715*X_14 + 0.0*X_15 + 0.0*X_16 + 0.09999300518796372*X_17 + -0.03501765577178401*X_18 + -0.0*X_19 + 0.0*X_20 + 0.0*X_21 + 0.0*X_22 + 0.0*X_23 + 0.01703957169293415 8*X_24 + -0.10798183174529531*X_25 + 0.011519941933311422*X_26 + 0.0*X_27 + 0.0*X_28

11.3 Elasticnet

[68]:
```
elastic_net = ElasticNet(alpha=0.01, l1_ratio=0.01)
elastic_net.fit(poly_X_train, y_train)
y_pred = elastic_net.predict(poly_X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.6197670116899672
MSE: 0.8445688324608495
RMSE: 0.9190042613942818
R_squared: 0.6197544768592995
```

[69]:
```
intercept = elastic_net.intercept_[0]
print("E(y) = " + str(intercept), end =" ")
i = 1
for coef in elastic_net.coef_:
    print("+ " + str(coef) + "*X_"+ str(i),end =" ")
    i+=1
```

```
E(y) = 3.8846309242680777 + 0.0*X_1 + 0.2927933522346351*X_2 +
0.5701587565393743*X_3 + -0.2853155296133328*X_4 + 0.3232608010829245*X_5 +
-0.040683191849905674*X_6 + 0.5176625959975297*X_7 + -0.005686391706115492*X_8 +
-0.07347373561585265*X_9 + 0.06744551223755198*X_10 + -0.026991311089282124*X_11
+ 0.17140210905060943*X_12 + 0.1489001291691723*X_13 + 0.04387944907565253*X_14
+ 0.015432694442330381*X_15 + -0.003522939339889553*X_16 +
0.22665360496982379*X_17 + -0.07987184434323709*X_18 + 0.010778170793633652*X_19
+ 0.015419767927768628*X_20 + -0.019190216994567962*X_21 +
-0.004776018749484832*X_22 + -0.026267038845699857*X_23 +
0.06587236709111102*X_24 + -0.16512229677517617*X_25 +
-0.029005690231739913*X_26 + -0.05148489107405104*X_27 +
0.008550690699392257*X_28
```

12 Evaluation of Regularization

Slight improvement, but not as good as KNN

13 Ridge, Lasso, and Elasticnet Regularization

[74]:
```
scoring = {"MSE": "neg_mean_squared_error", "R2":"r2"}

# Setting refit='AUC', refits an estimator on the whole dataset with the
# parameter setting that has the best cross-validated AUC score.
# That estimator is made available at ``gs.best_estimator_`` along with
# parameters like ``gs.best_score_``, ``gs.best_params_`` and
```

```python
# ``gs.best_index_``
gs = GridSearchCV(
    RandomForestRegressor(),
    param_grid={"n_estimators": [10,25,30,50,100,200], "max_depth":
 ↪[2,3,5,10,20], "min_samples_leaf":[5,10,20,50,100,200]},
    scoring=scoring,
    refit="MSE",
    return_train_score=True,
    n_jobs = -1,
    cv = 20,
    verbose = 3
)
gs.fit(X_train, y_train.values.ravel())
results = gs.cv_results_
```

```
Fitting 20 folds for each of 180 candidates, totalling 3600 fits
```

[75]:
```python
gs.best_params_
```

[75]:
```
{'max_depth': 20, 'min_samples_leaf': 5, 'n_estimators': 50}
```

[76]:
```python
rf = gs.best_estimator_
```

[77]:
```python
y_pred = rf.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
MAE: 0.6061146426280116
MSE: 0.7715916605381403
RMSE: 0.8784029033069849
R_squared: 0.6526105826597295
```

14 Evaluation of Random Forest Regression

Allows for the learning of nonlinear trends, increases in performance compared to linear models and regularization techniques, indicating there is a nonlinear trend in the data.

15 Neural Network Regression

[268]:
```python
NN_model = Sequential()

NN_model.add(Dense(64, kernel_initializer='normal',input_dim = 6,␣
 ↪activation='relu'))
```

```
NN_model.add(Dense(64, kernel_initializer='normal',activation='tanh'))
NN_model.add(Dense(128, kernel_initializer='normal',activation='tanh'))
NN_model.add(Dense(64, kernel_initializer='normal',activation='tanh'))
NN_model.add(Dense(32, kernel_initializer='normal',activation='tanh'))

NN_model.add(Dense(1, kernel_initializer='normal',activation='linear'))

NN_model.compile(loss='mean_squared_error', optimizer='rmsprop',␣
↪metrics=['mean_squared_error'])
NN_model.summary()
```

```
Model: "sequential_32"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_167 (Dense)           (None, 64)                448

 dense_168 (Dense)           (None, 64)                4160

 dense_169 (Dense)           (None, 128)               8320

 dense_170 (Dense)           (None, 64)                8256

 dense_171 (Dense)           (None, 32)                2080

 dense_172 (Dense)           (None, 1)                 33

=================================================================
Total params: 23,297
Trainable params: 23,297
Non-trainable params: 0
_________________________________________________________________
```

[269]:

```
checkpoint_name = 'Weights-{epoch:03d}--{val_loss:.5f}.hdf5'
checkpoint = ModelCheckpoint(checkpoint_name, monitor='val_loss', verbose = 3,␣
↪save_best_only = True, mode ='auto')
callbacks_list = [checkpoint]
```

[270]:

```
with tf.device('/CPU:0'):
    NN_model.fit(X_train, y_train, epochs=100, batch_size=1, validation_split =␣
↪0.2, callbacks=callbacks_list,verbose = 0)
```

```
Epoch 1: val_loss improved from inf to 0.93916, saving model to Weights-001--
0.93916.hdf5

Epoch 2: val_loss improved from 0.93916 to 0.88233, saving model to Weights-002
--0.88233.hdf5
```

Epoch 3: val_loss did not improve from 0.88233

Epoch 4: val_loss improved from 0.88233 to 0.84274, saving model to Weights-004--0.84274.hdf5

Epoch 5: val_loss did not improve from 0.84274

Epoch 6: val_loss improved from 0.84274 to 0.82479, saving model to Weights-006--0.82479.hdf5

Epoch 7: val_loss did not improve from 0.82479

Epoch 8: val_loss did not improve from 0.82479

Epoch 9: val_loss did not improve from 0.82479

Epoch 10: val_loss improved from 0.82479 to 0.78585, saving model to Weights-010--0.78585.hdf5

Epoch 11: val_loss improved from 0.78585 to 0.76202, saving model to Weights-011--0.76202.hdf5

Epoch 12: val_loss did not improve from 0.76202

Epoch 13: val_loss did not improve from 0.76202

Epoch 14: val_loss improved from 0.76202 to 0.75242, saving model to Weights-014--0.75242.hdf5

Epoch 15: val_loss did not improve from 0.75242

Epoch 16: val_loss did not improve from 0.75242

Epoch 17: val_loss did not improve from 0.75242

Epoch 18: val_loss improved from 0.75242 to 0.74493, saving model to Weights-018--0.74493.hdf5

Epoch 19: val_loss did not improve from 0.74493

Epoch 20: val_loss did not improve from 0.74493

Epoch 21: val_loss did not improve from 0.74493

Epoch 22: val_loss improved from 0.74493 to 0.73038, saving model to Weights-022--0.73038.hdf5

Epoch 23: val_loss did not improve from 0.73038

Epoch 24: val_loss did not improve from 0.73038

Epoch 25: val_loss did not improve from 0.73038

Epoch 26: val_loss did not improve from 0.73038

Epoch 27: val_loss did not improve from 0.73038

Epoch 28: val_loss did not improve from 0.73038

Epoch 29: val_loss did not improve from 0.73038

Epoch 30: val_loss did not improve from 0.73038

Epoch 31: val_loss did not improve from 0.73038

Epoch 32: val_loss did not improve from 0.73038

Epoch 33: val_loss did not improve from 0.73038

Epoch 34: val_loss did not improve from 0.73038

Epoch 35: val_loss did not improve from 0.73038

Epoch 36: val_loss did not improve from 0.73038

Epoch 37: val_loss did not improve from 0.73038

Epoch 38: val_loss did not improve from 0.73038

Epoch 39: val_loss did not improve from 0.73038

Epoch 40: val_loss improved from 0.73038 to 0.71186, saving model to Weights-040--0.71186.hdf5

Epoch 41: val_loss did not improve from 0.71186

Epoch 42: val_loss did not improve from 0.71186

Epoch 43: val_loss did not improve from 0.71186

Epoch 44: val_loss did not improve from 0.71186

Epoch 45: val_loss did not improve from 0.71186

Epoch 46: val_loss did not improve from 0.71186

Epoch 47: val_loss did not improve from 0.71186

Epoch 48: val_loss did not improve from 0.71186

Epoch 49: val_loss did not improve from 0.71186

Epoch 50: val_loss did not improve from 0.71186

Epoch 51: val_loss did not improve from 0.71186

Epoch 52: val_loss did not improve from 0.71186

Epoch 53: val_loss did not improve from 0.71186

Epoch 54: val_loss did not improve from 0.71186

Epoch 55: val_loss did not improve from 0.71186

Epoch 56: val_loss did not improve from 0.71186

Epoch 57: val_loss did not improve from 0.71186

Epoch 58: val_loss did not improve from 0.71186

Epoch 59: val_loss did not improve from 0.71186

Epoch 60: val_loss did not improve from 0.71186

Epoch 61: val_loss did not improve from 0.71186

Epoch 62: val_loss did not improve from 0.71186

Epoch 63: val_loss did not improve from 0.71186

Epoch 64: val_loss did not improve from 0.71186

Epoch 65: val_loss did not improve from 0.71186

Epoch 66: val_loss did not improve from 0.71186

Epoch 67: val_loss did not improve from 0.71186

Epoch 68: val_loss did not improve from 0.71186

Epoch 69: val_loss did not improve from 0.71186

Epoch 70: val_loss did not improve from 0.71186

Epoch 71: val_loss did not improve from 0.71186

Epoch 72: val_loss did not improve from 0.71186

Epoch 73: val_loss did not improve from 0.71186

Epoch 74: val_loss did not improve from 0.71186

Epoch 75: val_loss did not improve from 0.71186

Epoch 76: val_loss did not improve from 0.71186

Epoch 77: val_loss did not improve from 0.71186

Epoch 78: val_loss did not improve from 0.71186

Epoch 79: val_loss did not improve from 0.71186

Epoch 80: val_loss did not improve from 0.71186

Epoch 81: val_loss did not improve from 0.71186

Epoch 82: val_loss did not improve from 0.71186

Epoch 83: val_loss did not improve from 0.71186

Epoch 84: val_loss did not improve from 0.71186

Epoch 85: val_loss did not improve from 0.71186

Epoch 86: val_loss did not improve from 0.71186

Epoch 87: val_loss did not improve from 0.71186

Epoch 88: val_loss did not improve from 0.71186

Epoch 89: val_loss did not improve from 0.71186

Epoch 90: val_loss did not improve from 0.71186

Epoch 91: val_loss did not improve from 0.71186

Epoch 92: val_loss did not improve from 0.71186

Epoch 93: val_loss did not improve from 0.71186

Epoch 94: val_loss did not improve from 0.71186

```
Epoch 95: val_loss did not improve from 0.71186

Epoch 96: val_loss did not improve from 0.71186

Epoch 97: val_loss did not improve from 0.71186

Epoch 98: val_loss did not improve from 0.71186

Epoch 99: val_loss did not improve from 0.71186

Epoch 100: val_loss did not improve from 0.71186
```

[272]:

```
weights_file = 'Weights-040--0.71186.hdf5' # choose the best checkpoint
NN_model.load_weights(weights_file) # load it
NN_model.compile(loss='mean_squared_error', optimizer='adam',␣
↪metrics=['mean_squared_error'])
```

[273]:

```
y_pred = NN_model.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
mse = mean_squared_error(y_test, y_pred)
rmse = mean_squared_error(y_test, y_pred, squared = False)
r2 = r2_score(y_test, y_pred)
print("MAE: {}\nMSE: {}\nRMSE: {}\nR_squared: {}".format(mae, mse, rmse, r2))
```

```
6/6 [==============================] - 0s 3ms/step
MAE: 0.5881101118706086
MSE: 0.7509005102090602
RMSE: 0.8665451576283029
R_squared: 0.6619262440704632
```

16 Evaluation of Neural Network

Took a while to train, but negligible increase in performance compared to the random forest and worse performance than KNN. Distance based modeling is a neccessity in this case.