TI3002C_ML_Class_4_Classification_vs_Regression_McDonalds_Menu_A

March 7, 2024

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Se importan todas las librerias que se van a usar

```
[ ]: import pandas as pd
from sklearn.metrics import r2_score
from sklearn.feature_selection import SequentialFeatureSelector as SFS
import statsmodels.api as sm
import scipy.stats as stats
from statsmodels.stats.stattools import durbin_watson
import numpy as np
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns
from statsmodels.stats.diagnostic import het_breuschpagan, normal_ad
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import r2_score
from sklearn.preprocessing import PolynomialFeatures
```

Se importan los datos

```
[ ]: df = pd.read_csv("menu.csv")
```

Se hace un analísis de los datos que se tienen

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

```
[ ]:    Category                              Item    Serving Size  Calories  \
0  Breakfast                      Egg McMuffin  4.8 oz (136 g)       300
1  Breakfast                 Egg White Delight  4.8 oz (135 g)       250
2  Breakfast                  Sausage McMuffin  3.9 oz (111 g)       370
3  Breakfast         Sausage McMuffin with Egg  5.7 oz (161 g)       450
4  Breakfast  Sausage McMuffin with Egg Whites  5.7 oz (161 g)       400

   Calories from Fat  Total Fat  Total Fat (% Daily Value)  Saturated Fat  \
0                120       13.0                         20            5.0
1                 70        8.0                         12            3.0
```

```
2              200      23.0                       35           8.0
3              250      28.0                       43          10.0
4              210      23.0                       35           8.0

   Saturated Fat (% Daily Value)  Trans Fat  …  Carbohydrates  \
0                             25        0.0  …             31
1                             15        0.0  …             30
2                             42        0.0  …             29
3                             52        0.0  …             30
4                             42        0.0  …             30

   Carbohydrates (% Daily Value)  Dietary Fiber  \
0                             10              4
1                             10              4
2                             10              4
3                             10              4
4                             10              4

   Dietary Fiber (% Daily Value)  Sugars  Protein  Vitamin A (% Daily Value)  \
0                             17       3       17                         10
1                             17       3       18                          6
2                             17       2       14                          8
3                             17       2       21                         15
4                             17       2       21                          6

   Vitamin C (% Daily Value)  Calcium (% Daily Value)  Iron (% Daily Value)
0                          0                       25                    15
1                          0                       25                     8
2                          0                       25                    10
3                          0                       30                    15
4                          0                       25                    10

[5 rows x 24 columns]
```

[ ]:

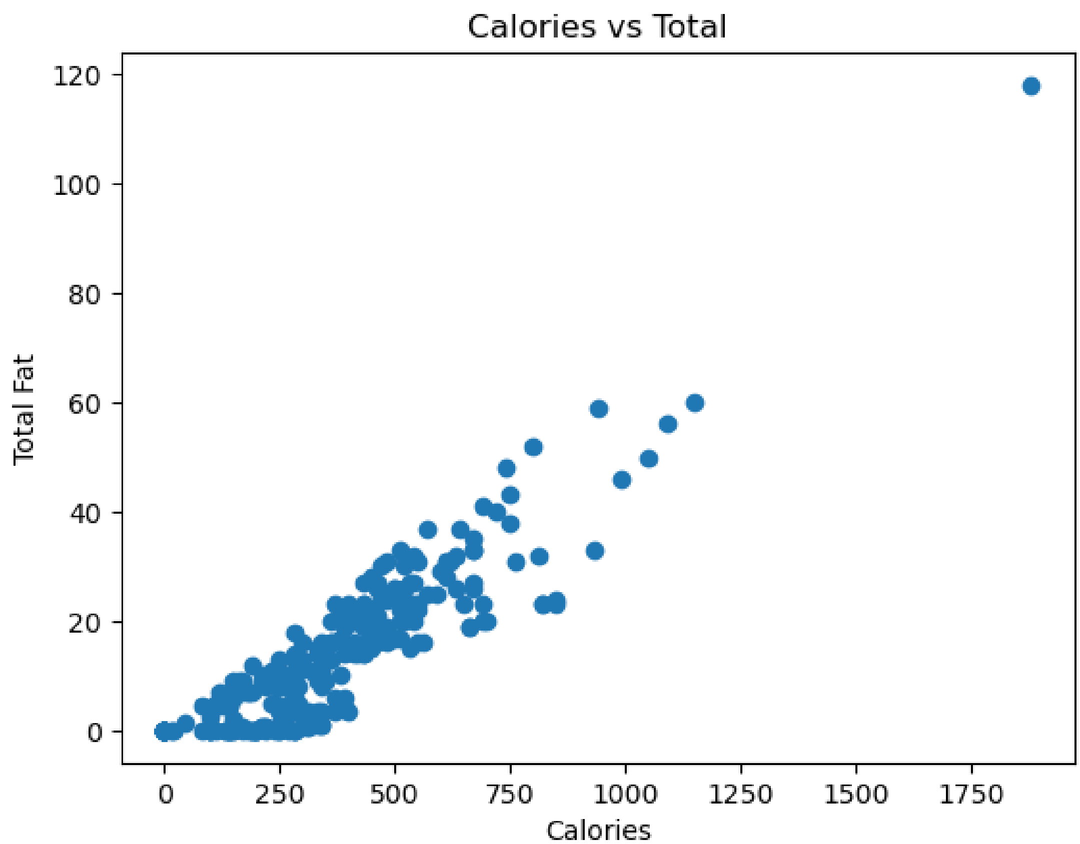
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 260 entries, 0 to 259
Data columns (total 24 columns):
 #   Column                         Non-Null Count  Dtype
---  ------                         --------------  -----
 0   Category                       260 non-null    object
 1   Item                           260 non-null    object
 2   Serving Size                   260 non-null    object
 3   Calories                       260 non-null    int64
 4   Calories from Fat              260 non-null    int64
 5   Total Fat                      260 non-null    float64
 6   Total Fat (% Daily Value)      260 non-null    int64
```

```
 7   Saturated Fat                    260 non-null    float64
 8   Saturated Fat (% Daily Value)    260 non-null    int64
 9   Trans Fat                        260 non-null    float64
 10  Cholesterol                      260 non-null    int64
 11  Cholesterol (% Daily Value)      260 non-null    int64
 12  Sodium                           260 non-null    int64
 13  Sodium (% Daily Value)           260 non-null    int64
 14  Carbohydrates                    260 non-null    int64
 15  Carbohydrates (% Daily Value)    260 non-null    int64
 16  Dietary Fiber                    260 non-null    int64
 17  Dietary Fiber (% Daily Value)    260 non-null    int64
 18  Sugars                           260 non-null    int64
 19  Protein                          260 non-null    int64
 20  Vitamin A (% Daily Value)        260 non-null    int64
 21  Vitamin C (% Daily Value)        260 non-null    int64
 22  Calcium (% Daily Value)          260 non-null    int64
 23  Iron (% Daily Value)             260 non-null    int64
dtypes: float64(3), int64(18), object(3)
memory usage: 48.9+ KB
```

Se observa que existe una relación entre calorias y grasas

[ ]:
```
plot = plt.scatter("Calories", "Total Fat", data=df)
plt.title("Calories vs Total")
plt.xlabel("Calories")
plt.ylabel("Total Fat")
plt.show()
```



Se eligen las posibles variables que pueden usarse para predecir las calorias

[ ]:
```
X = df[["Total Fat","Carbohydrates","Protein", "Sodium"]]
y = df["Calories"]
```

1 Modelo 1, regresión lineal

Se usa la función train_test_split para dividir los datos en entrenamiento y prueba

[ ]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2,␣
↪random_state=42)
```

Se inicia el modelo de regresión lineal y se usa el sequential feature selection para seleccionar las variables más importantes para el modelo

[ ]:
```
linear_regression = LinearRegression()
sfs1 = SFS(linear_regression, n_features_to_select=3, direction='forward',cv=5)
sfs1.fit(X_train, y_train)
```

[ ]:
```
SequentialFeatureSelector(estimator=LinearRegression(), n_features_to_select=3)
```

Se transforman los datos de entrenamiento y prueba para que se ajusten al modelo

[ ]:
```
X_train_select= sfs1.transform(X_train)
X_test_select = sfs1.transform(X_test)
linear_regression.fit(X_train_select, y_train)
```

[ ]:
```
LinearRegression()
```

Se usa el modelo para predecir los datos y se guarda la correlación que tiene con los datos

[ ]:
```
y_pred = linear_regression.predict(X_test_select)
linear_residuals = y_test - y_pred

linear_score = r2_score(y_test, y_pred)
```

Se obtienen los coeficietes de la regresión

[ ]:
```
coef = pd.DataFrame(linear_regression.coef_, X.columns[sfs1.get_support()],␣
 ↪["Coefs"])
coef
```

[ ]:

	Coefs
Total Fat	9.002998
Carbohydrates	3.988871
Protein	4.054709

calories = 9 * fat + 4 * carbs + 4 * protein

Se checan 5 datos al azar para ver que tan bien se ajusta el modelo

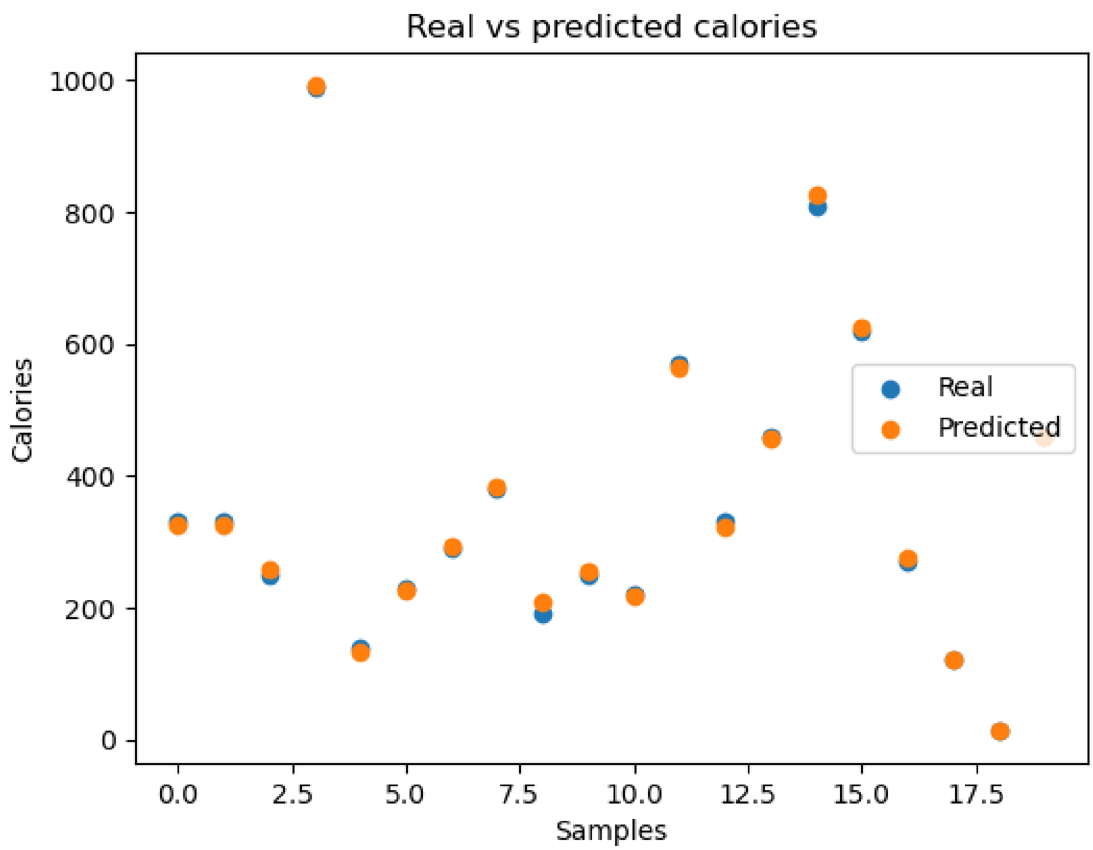
[ ]:
```
results = pd.DataFrame({"Real": y_test, "Predicted values": y_pred})
results = results.sample(n = 20)
results.head()
```

[ ]:

	Real	Predicted values
92	330	325.316415
158	330	323.981491
204	250	258.541757
33	990	992.712426
196	140	134.196140

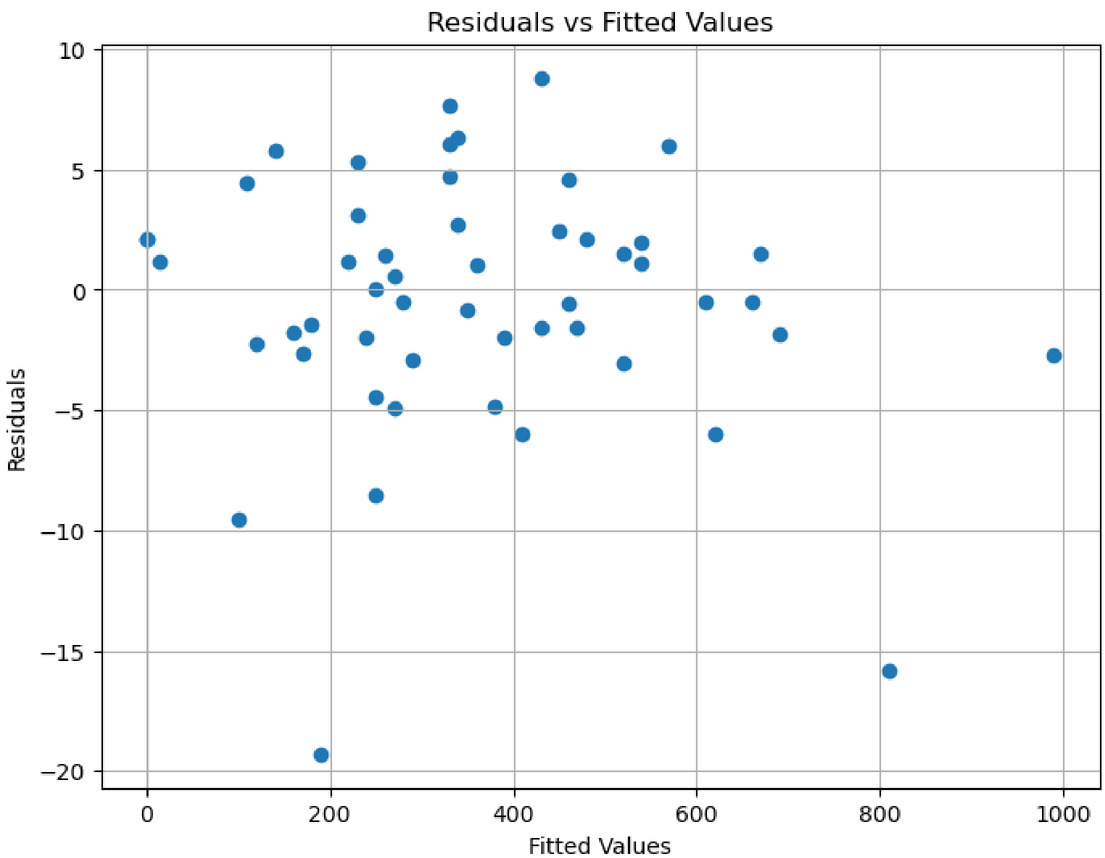
Se modelan los datos reales vs los datos predichos

[ ]:
```
plt.scatter(np.arange(20), results["Real"], label="Real")
plt.scatter(np.arange(20), results["Predicted values"], label="Predicted")
plt.title("Real vs predicted calories")
plt.legend(loc="center right")
plt.xlabel("Samples")
plt.ylabel("Calories")
plt.show()
```

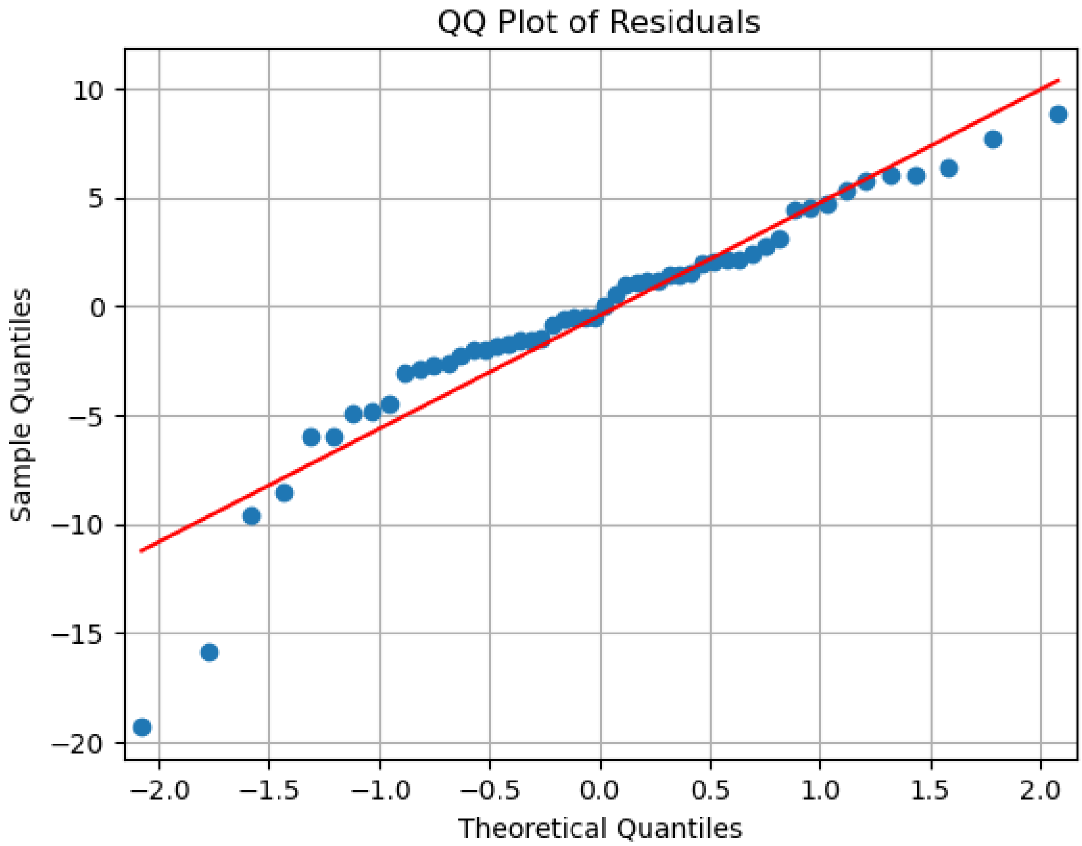


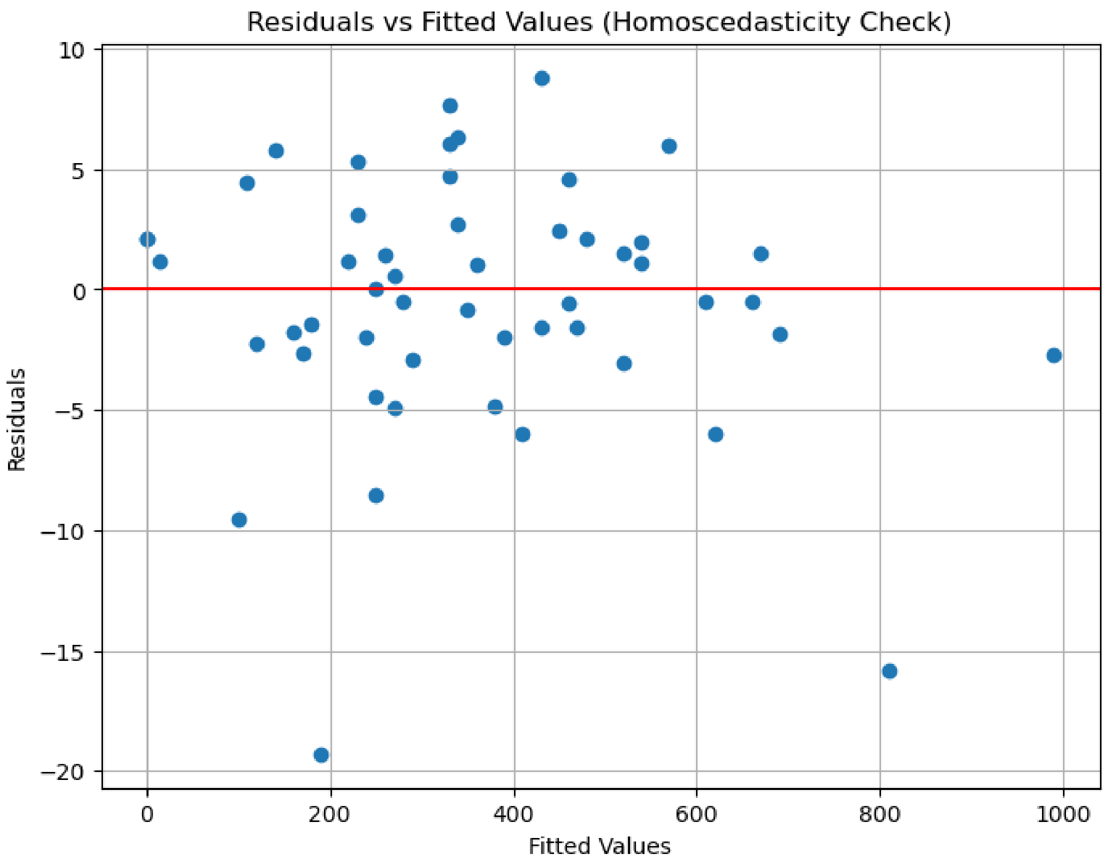
[ ]:
```
plt.figure(figsize=(8, 6))
plt.scatter(y_test, linear_residuals)
plt.title('Residuals vs Fitted Values')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()

# Plot histogram of residuals
#plt.figure(figsize=(8, 6))
#sns.histplot(linear_residuals, kde=True, bins=10)
#plt.title('Histogram of Residuals')
#plt.xlabel('Residuals')
#plt.ylabel('Frequency')
#plt.grid(True)
#plt.show()

# Plot QQ plot of residuals
plt.figure(figsize=(8, 6))
sm.qqplot(linear_residuals, line='s')
```

```python
plt.title('QQ Plot of Residuals')
plt.grid(True)
plt.show()

# Check homoscedasticity using predicted values and residuals
plt.figure(figsize=(8, 6))
plt.scatter(y_test, linear_residuals)
plt.axhline(y=0, color='r', linestyle='-')
plt.title('Residuals vs Fitted Values (Homoscedasticity Check)')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()
```




```
<Figure size 800x600 with 0 Axes>
```


QQ Plot of Residuals
Sample Quantiles
Theoretical Quantiles
10
5
0
−5
−10
−15
−20
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0



2 Polinomial multivariante

Se usa polinomial features para hacer modificar los datos de manera que se pueda realizar una regresión polinomial, se dividen los datos y se ajustan las variables al modelo con una elección hacia adelantes de las variables

[ ]:
```
poly = PolynomialFeatures(degree=3, interaction_only=False, include_bias=False)
poly_variables = poly.fit_transform(X)

Xpoly_train, Xpoly_test, ypoly_train, ypoly_test =␣
 ↪train_test_split(poly_variables, y, test_size = 0.2, random_state = 42)

regression = LinearRegression()
sfs2 = SFS(regression, n_features_to_select=7, direction='backward',cv=5)
sfs2.fit(Xpoly_train, ypoly_train)

sfs2.get_support()
Xpoly_train_select = Xpoly_train[:,sfs2.get_support()]
Xpoly_test_select = Xpoly_test[:,sfs2.get_support()]
```

```
regression.fit(Xpoly_train_select, ypoly_train)
```

[ ]: LinearRegression()

Se usa el modelo obtenido para predecir las variables y se obtiene su correlación

[ ]:
```
y_pred = regression.predict(Xpoly_test_select)

score_poly = r2_score(ypoly_test, y_pred)
score_poly
residuals_poly = ypoly_test - y_pred
```

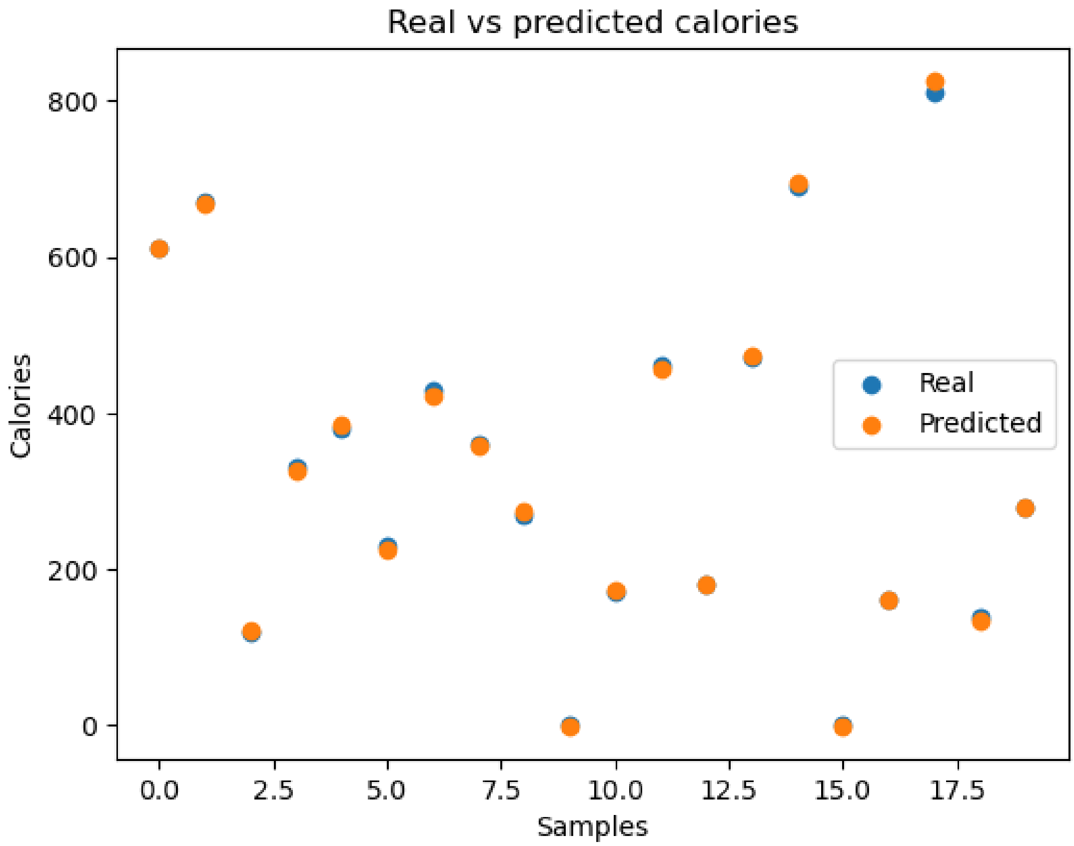
Se grafican los valores reales contra los valores predichos

[ ]:
```
results = pd.DataFrame({"Real": ypoly_test, "Predicted values": y_pred})
results = results.sample(n = 20)
results.head()
```

[ ]:

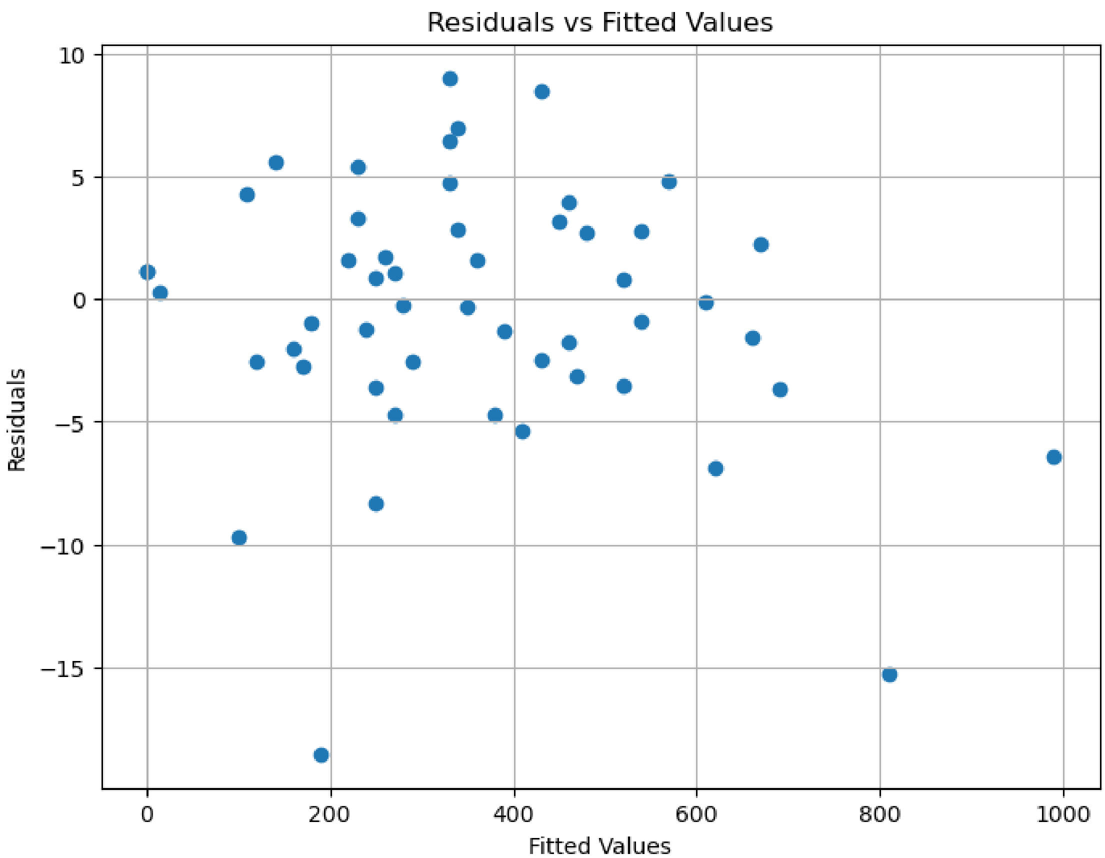
	Real	Predicted values
45	610	610.093969
228	670	667.768279
205	120	122.547407
92	330	325.238059
77	380	384.684829

[ ]:
```
plt.scatter(np.arange(20), results["Real"], label="Real")
plt.scatter(np.arange(20), results["Predicted values"], label="Predicted")
plt.title("Real vs predicted calories")
plt.legend(loc="center right")
plt.xlabel("Samples")
plt.ylabel("Calories")
plt.show()
```



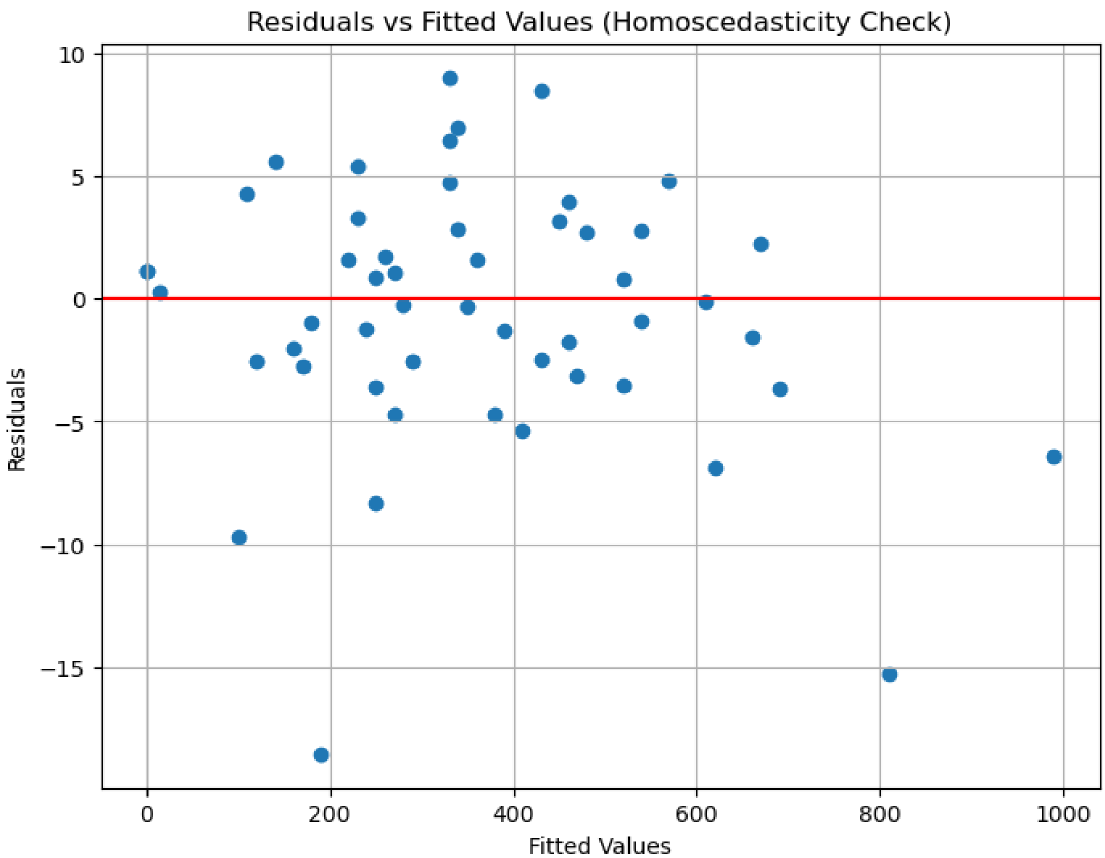
[ ]:
```
plt.figure(figsize=(8, 6))
plt.scatter(ypoly_test, residuals_poly)
plt.title('Residuals vs Fitted Values')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()

# Plot histogram of residuals
#plt.figure(figsize=(8, 6))
#sns.histplot(linear_residuals, kde=True, bins=10)
#plt.title('Histogram of Residuals')
#plt.xlabel('Residuals')
#plt.ylabel('Frequency')
#plt.grid(True)
#plt.show()

# Plot QQ plot of residuals
plt.figure(figsize=(8, 6))
sm.qqplot(residuals_poly, line='s')
```

```
plt.title('QQ Plot of Residuals')
plt.grid(True)
plt.show()

# Check homoscedasticity using predicted values and residuals
plt.figure(figsize=(8, 6))
plt.scatter(ypoly_test, residuals_poly)
plt.axhline(y=0, color='r', linestyle='-')
plt.title('Residuals vs Fitted Values (Homoscedasticity Check)')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()
```




```
<Figure size 800x600 with 0 Axes>
```


QQ Plot of Residuals
Sample Quantiles
Theoretical Quantiles
10
5
0
−5
−10
−15
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0



3 Polinomial mutivariante con interacción

Se usa polinomial features para hacer modificar los datos de manera que se pueda realizar una regresión polinomial con interacción, se dividen los datos y se ajustan las variables al modelo con una elección hacia adelante de las variables

[ ]:
```
poly_interac = PolynomialFeatures(degree=3, interaction_only=True)
poly_interac_variables = poly.fit_transform(X)

Xpoly_interac_train, Xpoly_interac_test, ypoly_interac_train,␣
 ↪ypoly_interac_test = train_test_split(poly_interac_variables, y, test_size =␣
 ↪0.2, random_state = 42)

regression = LinearRegression()
sfs3 = SFS(regression, n_features_to_select=8, direction='backward',cv=5)

sfs3.fit(Xpoly_interac_train, ypoly_interac_train)
Xpoly_interac_train_selec = Xpoly_interac_train[:,sfs3.get_support()]
regression.fit(Xpoly_interac_train_selec, ypoly_interac_train)
```

```
Xpoly_interac_test_selec = Xpoly_interac_test[:,sfs3.get_support()]
y_pred = regression.predict(Xpoly_interac_test_selec)
```

Se guarda la correlación obtenida y los residuales

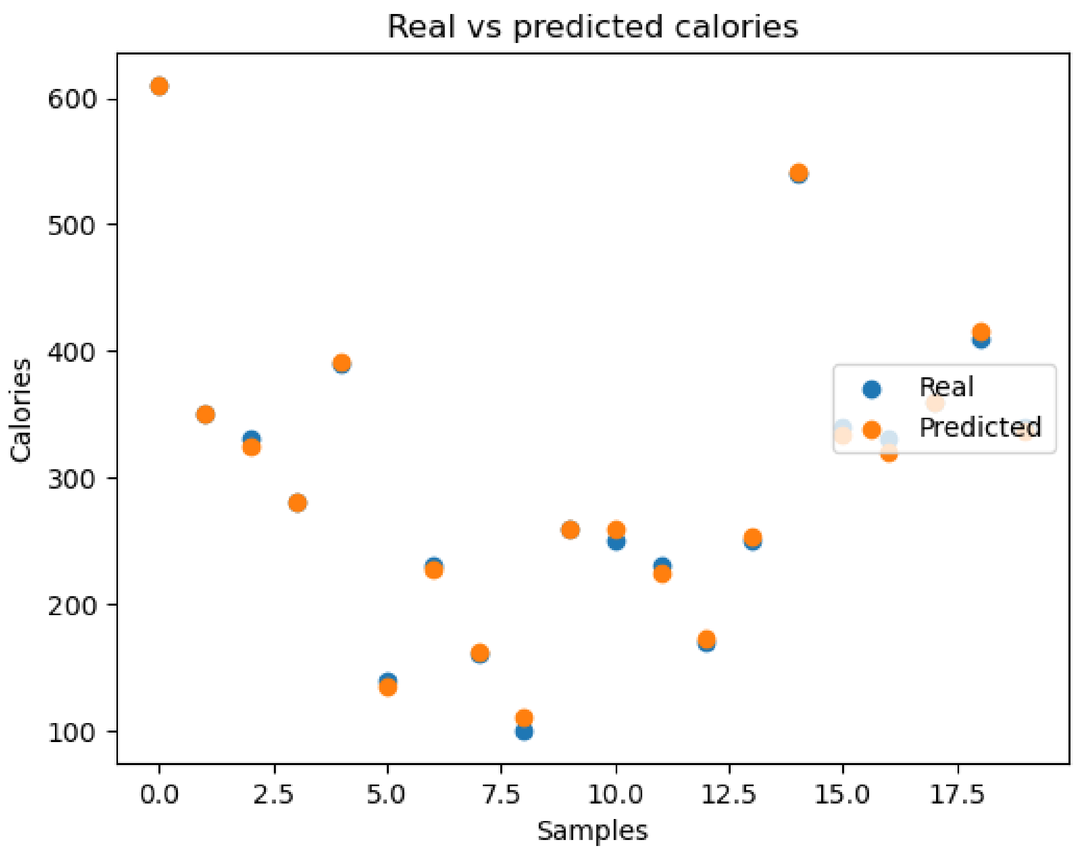
[ ]:
```
score_interac = r2_score(ypoly_interac_test, regression.
 ↪predict(Xpoly_interac_test[:,sfs3.get_support()]))
residuals_interac = ypoly_interac_test - y_pred
```

[ ]:
```
results = pd.DataFrame({"Real": ypoly_interac_test, "Predicted values": y_pred})
results = results.sample(n = 20)
results.head()
```

[ ]:

	Real	Predicted values
45	610	609.785366
212	350	350.776788
158	330	324.049052
150	280	280.055332
185	390	391.677931

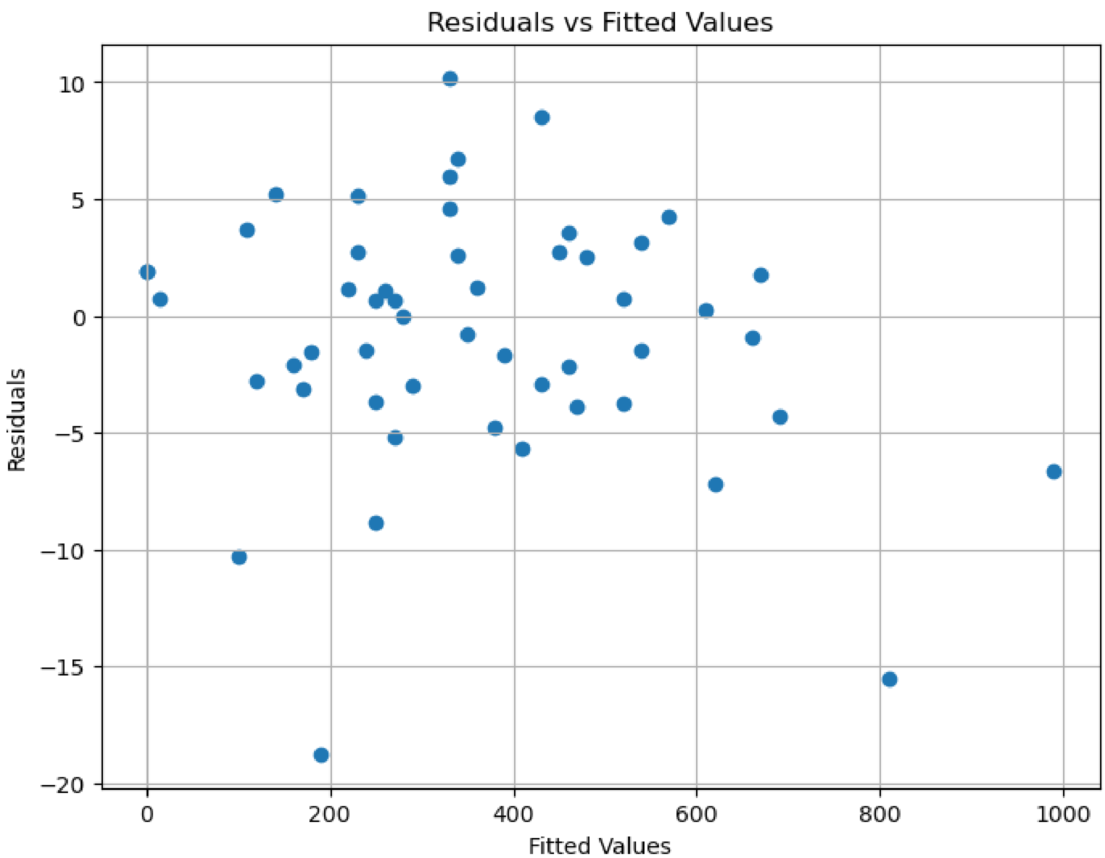
[ ]:
```
plt.scatter(np.arange(20), results["Real"], label="Real")
plt.scatter(np.arange(20), results["Predicted values"], label="Predicted")
plt.title("Real vs predicted calories")
plt.legend(loc="center right")
plt.xlabel("Samples")
plt.ylabel("Calories")
plt.show()
```



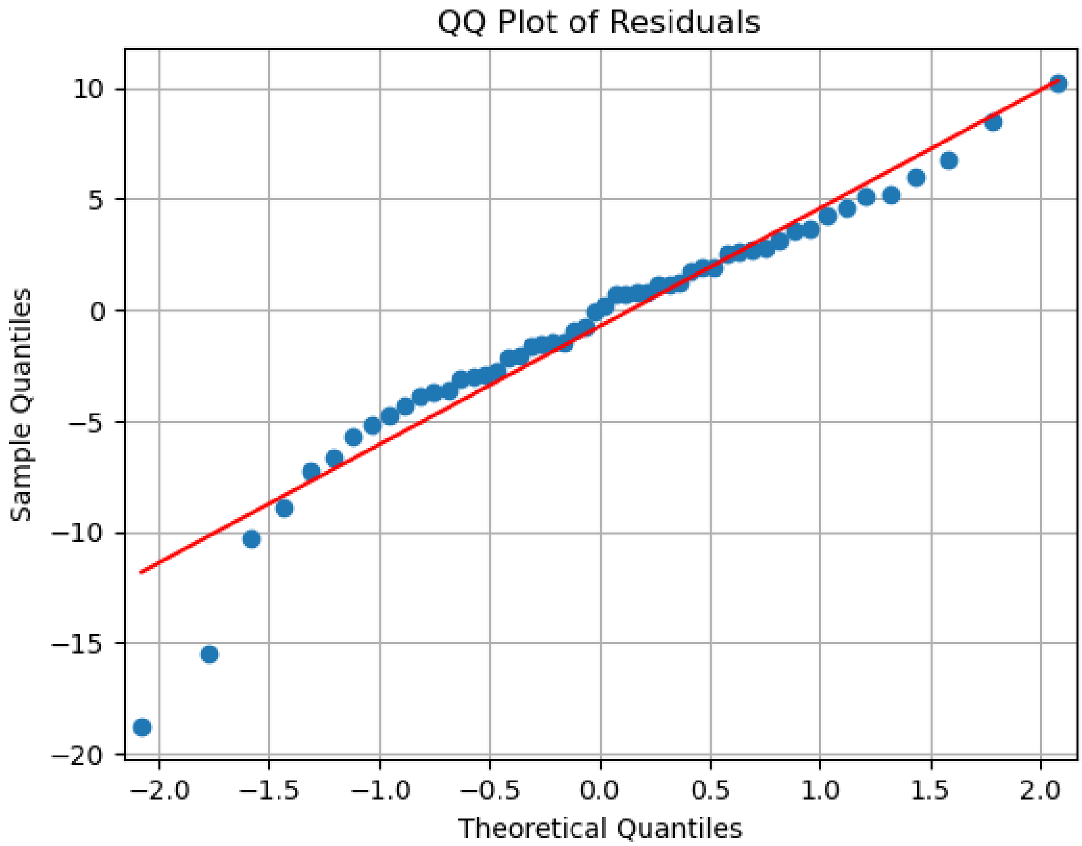
[ ]:

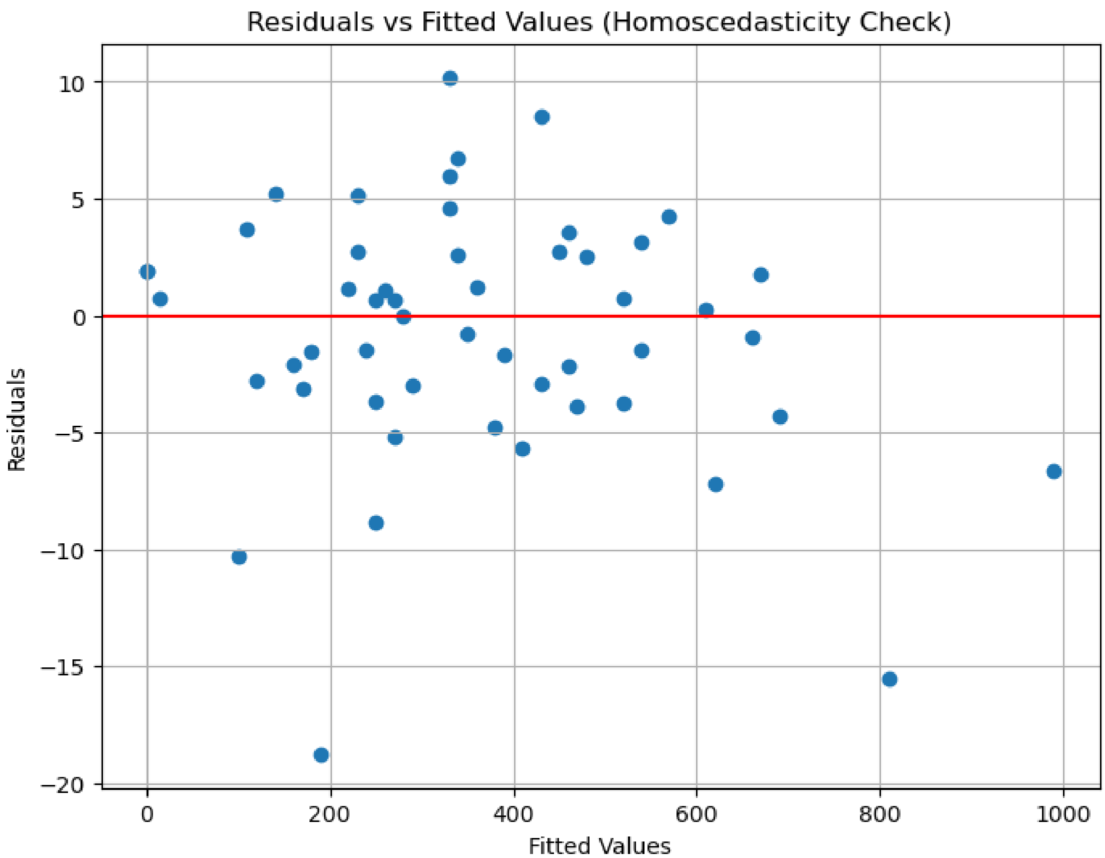
```python
plt.figure(figsize=(8, 6))
plt.scatter(ypoly_interac_test, residuals_interac)
plt.title('Residuals vs Fitted Values')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()

# Plot histogram of residuals
#plt.figure(figsize=(8, 6))
#sns.histplot(linear_residuals, kde=True, bins=10)
#plt.title('Histogram of Residuals')
#plt.xlabel('Residuals')
#plt.ylabel('Frequency')
#plt.grid(True)
#plt.show()

# Plot QQ plot of residuals
plt.figure(figsize=(8, 6))
sm.qqplot(residuals_interac, line='s')
```

```python
plt.title('QQ Plot of Residuals')
plt.grid(True)
plt.show()

# Check homoscedasticity using predicted values and residuals
plt.figure(figsize=(8, 6))
plt.scatter(ypoly_interac_test, residuals_interac)
plt.axhline(y=0, color='r', linestyle='-')
plt.title('Residuals vs Fitted Values (Homoscedasticity Check)')
plt.xlabel('Fitted Values')
plt.ylabel('Residuals')
plt.grid(True)
plt.show()
```




```
<Figure size 800x600 with 0 Axes>
```


QQ Plot of Residuals
10
5
0
−5
−10
−15
−20
Sample Quantiles
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
Theoretical Quantiles



[ ]:
```python
# Getting R2 score for the models
print("R2 score for linear model: ", linear_score)
print("R2 score for polynomial model: ", score_poly)
print("R2 score for polynomial interaction model: ", score_interac)


def r2_adjusted(r2, n, p):
    adjust_r2 = 1 - (1 - r2) * (n - 1) / (n - p - 1)
    return adjust_r2
# R2 score adjusted
n = len(y_test)
p = 4
print("Adjusted r2 score for linear model: ", r2_adjusted(linear_score, n, p))
print("Adjusted r2 score for polynomial model: ", r2_adjusted(score_poly, n, p))
print("Adjusted r2 score for polynomial interaction model: ",␣
↪r2_adjusted(score_interac, n, p))
```

```
R2 score for linear model:  0.9993428663117916
R2 score for polynomial model:  0.9993332372573884
R2 score for polynomial interaction model:  0.9993001661986994
```

```
Adjusted r2 score for linear model:  0.9992869400404547
Adjusted r2 score for polynomial model:  0.9992764914920598
Adjusted r2 score for polynomial interaction model:  0.9992406058751845
```

[ ]:
```
X_test_select = sm.add_constant(X_test_select)
Xpoly_test_select = sm.add_constant(pd.DataFrame(Xpoly_test_select))
Xpoly_interac_test_selec = sm.add_constant(pd.
 ↪DataFrame(Xpoly_interac_test_selec))


def tests(residuals,x, p):
    print("Model:",p)
    # Normality test
    print("Normality test: ", normal_ad(residuals)[1])
    # Homoscedasticity test
    print("Homoscedasticity test: ", het_breuschpagan(residuals, x)[1])
    # Autocorrelation test
    print("Autocorrelation test: ", durbin_watson(residuals))
    print("-------------------------------------------\n")
tests(linear_residuals, X_test_select,1)
tests(residuals_poly, Xpoly_test_select,2)
tests(residuals_interac, Xpoly_interac_test_selec,3)
```

```
Model: 1
Normality test:  0.009307864601393875
Homoscedasticity test:  0.08886406429412862
Autocorrelation test:  2.252001309025355
-------------------------------------------

Model: 2
Normality test:  0.09367055880764223
Homoscedasticity test:  0.1878991225852459
Autocorrelation test:  2.357256199775753
-------------------------------------------

Model: 3
Normality test:  0.08185715331327341
Homoscedasticity test:  0.2501210280187251
Autocorrelation test:  2.3499447089233803
-------------------------------------------
```

En este caso se observa que dos un modelos cumplen con los supuestos de:

Linealidad de errores

Homocedasticidad de errores

Independencia de errores y

Normalidad de errores,

Estos modelos son el de regresión polinomial con interacción y sin interacción, por lo que se pueden usar para predecir los datos. El modelo de regresión lineal no cumplen con el supuesto de normalidad de errores y es por esto que no pueden ser usados para predecir los datos.

4