UNIVERSIDADE ESTADUAL PAULISTA "JÚLIO DE MESQUITA FILHO"

Instituto de Geociências e Ciências Exatas - IGCE Curso de Bacharelado em Ciências da Computação

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TRABALHO DE REGRESSÃO

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Rio Claro - SP

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1 Introdução

Este trabalho consiste em aplicar o conhecimento de clustering adquirido na disciplina Tópicos: Aprendizado de Máquina, tendo assim como objetivo:

- Escolha dois conjuntos de dados para trabalhar o problema de regressão. Separe cada dataset em conjunto de treinamento e conjunto de teste. Explique o seu critério de separação e o método utilizado.
- Você deverá implementar soluções para cada dataset usando:

```
regressão linear (ou regressão múltipla)
regressão polinomial
SVR (use os kernels linear, sigmoide, RBF e polinomial)
rede neural (MLP ou RBF).
```

- Descreva os parâmetros/arquiteturas de cada modelo.
- Compare os resultados (para treinamento e teste) com as medidas de desempenho SEQ, EQM, REQM, EAM e r2, e verifique qual a melhor opção dentre os métodos implementados que melhor se ajusta a seus dados.
- Você deverá fazer a visualização dos dados originais com os dados ajustados em cada experimento, tanto para o conjunto de treinamento quanto para o de teste. Os gráficos devem conter títulos nos eixos e legenda. Comente os resultados encontrados na visualização.

regression-framingham

August 19, 2020

[0]:

1 0. Introdução

Trabalho:

Aluno: Gabriel Luiz

Disciplina: Tópico em Aprendizado de Máquina

Objetivos:

- Escolha dois conjuntos de dados para trabalhar o problema de regressão. Separe cada dataset em conjunto de treinamento e conjunto de teste. Explique o seu critério de separação e o método utilizado.
- Você deverá implementar soluções para cada dataset usando:
- regressão linear (ou regressão múltipla)
- – regressão polinomial
- - SVR (use os kernels linear, sigmoide, RBF e polinomial)
- rede neural (MLP ou RBF).
- Descreva os parâmetros/arquiteturas de cada modelo.
- Compare os resultados (para treinamento e teste) com as medidas de desempenho SEQ, EQM,
 REQM, EAM e r², e verifique qual a melhor opção dentre os métodos implementados que melhor se ajusta a seus dados.
- Você deverá fazer a visualização dos dados originais com os dados ajustados em cada experimento, tanto para o conjunto de treinamento quanto para o de teste. Os gráficos devem conter títulos nos eixos e legenda. Comente os resultados encontrados na visualização.

1.1 0.1 Dependências

Para realização da tarefa foram utilizados as seguintes bibliotecas:

```
[1]: #Utils
     import pandas as pd
     import numpy as np
     import pandas_profiling
     import math
     #Preprocess
     from sklearn.preprocessing import StandardScaler
     # Split
     from sklearn.model_selection import train_test_split
     # Regressores
     from sklearn.linear_model import LinearRegression
     from sklearn.svm import SVR
     from sklearn.neural_network import MLPRegressor
     #Metricas
     from sklearn.metrics import r2_score
     from sklearn.metrics import mean_squared_error
     #Visualização
     import seaborn as sns
     import matplotlib.pyplot as plt
     import warnings
     warnings.filterwarnings('ignore')
     %matplotlib inline
```

2 1. Dados

O conjunto de dados possui informações sobre pacientes que podem ter risco de doenças do coração em 10 anos. Possui mais de 4 mil registros e 15 atributos

Fonte: https://www.kaggle.com/dileep070/heart-disease-prediction-using-logistic-regression

2.1 1.1 Informações sobre os dados:

Atributos:

- Sex: male or female(Nominal)
- Age: Age of the patient; (Continuous Although the recorded ages have been truncated to whole numbers, the concept of age is continuous) Behavioral
- Current Smoker: whether or not the patient is a current smoker (Nominal)
- Cigs Per Day: the number of cigarettes that the person smoked on average in one day.(can be considered continuous as one can have any number of cigarettes, even half a cigarette.)

Medical(history)

- BP Meds: whether or not the patient was on blood pressure medication (Nominal)
- Prevalent Stroke: whether or not the patient had previously had a stroke (Nominal)
- Prevalent Hyp: whether or not the patient was hypertensive (Nominal)
- Diabetes: whether or not the patient had diabetes (Nominal) Medical(current)
- Tot Chol: total cholesterol level (Continuous)
- Sys BP: systolic blood pressure (Continuous)
- Dia BP: diastolic blood pressure (Continuous)
- BMI: Body Mass Index (Continuous)
- Heart Rate: heart rate (Continuous In medical research, variables such as heart rate though in fact discrete, yet are considered continuous because of large number of possible values.)
- Glucose: glucose level (Continuous) Predict variable (desired target)
- 10 year risk of coronary heart disease CHD (binary: "1", means "Yes", "0" means "No")

2.2 Importando Dataset

2

3

0

1

```
[2]: dataset = './dataset/datasets_222487_478477_framingham.csv'
     data_raw = pd.read_csv(dataset)
[3]:
    data_raw.head()
[3]:
                                currentSmoker
                                                cigsPerDay
                                                             BPMeds
                                                                      prevalentStroke
        male
               age
                    education
                39
                           4.0
                                             0
                                                        0.0
                                                                 0.0
     0
           1
                                                                                      0
                           2.0
                                                        0.0
                                                                 0.0
     1
           0
                46
                                             0
                                                                                      0
     2
                                                       20.0
           1
                48
                           1.0
                                             1
                                                                 0.0
                                                                                      0
     3
           0
                           3.0
                                                       30.0
                                                                 0.0
                                                                                     0
                61
                                             1
     4
           0
                           3.0
                                                       23.0
                                                                 0.0
                                                                                      0
                46
                                             1
        prevalentHyp
                       diabetes
                                  totChol
                                            sysBP
                                                    diaBP
                                                             BMI heartRate
                                                                               glucose
     0
                               0
                                    195.0
                                            106.0
                                                     70.0
                                                           26.97
                                                                         80.0
                                                                                  77.0
                    0
                    0
                               0
                                    250.0
                                            121.0
                                                     81.0
                                                           28.73
                                                                         95.0
                                                                                  76.0
     1
     2
                               0
                    0
                                    245.0
                                            127.5
                                                     80.0
                                                           25.34
                                                                         75.0
                                                                                  70.0
     3
                               0
                                    225.0
                                            150.0
                                                     95.0
                                                                                 103.0
                    1
                                                           28.58
                                                                         65.0
                               0
                                    285.0
                                            130.0
                                                     84.0
                                                           23.10
                                                                         85.0
                                                                                  85.0
        TenYearCHD
     0
     1
                  0
```

```
[4]: data_raw.education = data_raw.education.fillna(0)
    data_raw.cigsPerDay = data_raw.cigsPerDay.fillna(data_raw.cigsPerDay.mean())
    data_raw.BPMeds = data_raw.BPMeds.fillna(0)
```

```
data_raw.totChol = data_raw.totChol.fillna(data_raw.totChol.mean())
data_raw.BMI = data_raw.BMI.fillna(data_raw.BMI.mean())
data_raw.heartRate = data_raw.heartRate.fillna(data_raw.heartRate.mean())
data_raw.glucose = data_raw.glucose.fillna(data_raw.glucose.mean())
```

[4]: array([4., 2., 1., 3., 0.])

2.3 Pré-processamento

```
[11]: # pandas_profiling.ProfileReport(data_raw)
```

2.4 Visualização

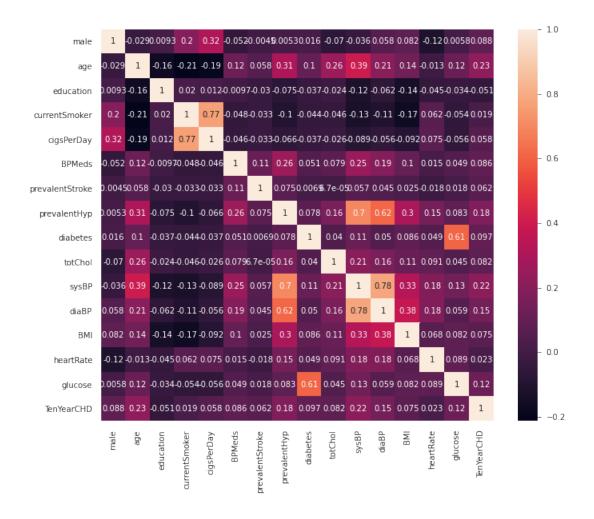
```
[12]: # sns.pairplot(data_raw)
```

```
[13]: plt.clf()
```

<Figure size 432x288 with 0 Axes>

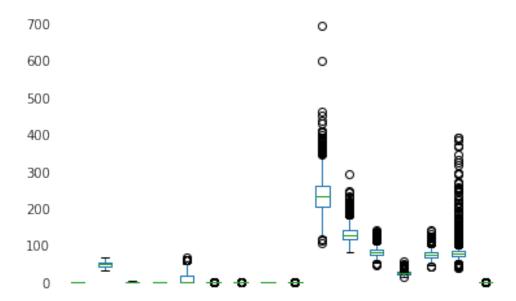
```
[14]: plt.subplots(figsize=(11, 9))
sns.heatmap(data_raw.corr(), annot=True)
```

[14]: <matplotlib.axes._subplots.AxesSubplot at 0x7f1a306d3898>



[15]: data_raw.plot.box()

[15]: <matplotlib.axes._subplots.AxesSubplot at 0x7f1a2dd18160>



maleagetuuraeintiisis Re**liitiisis keliitiisis keliitiisi keliitiitiisi keliitiitiisi keliitiitiisi keliitiitiisi keliitiitiitiisi keliitiitiisi**

2.5 Escalonando

```
[16]: scaler = StandardScaler().fit(data_raw)
     data_scaled = scaler.transform(data_raw)
[17]: data_scaled_df = pd.DataFrame(data_scaled, columns=data_raw.columns)
[18]: data_scaled_df.head()
[18]:
            male
                       age
                           education
                                     currentSmoker
                                                    cigsPerDay
                                                                  BPMeds \
     0 1.153192 -1.234951
                            1.966086
                                          -0.988271
                                                     -0.757974 -0.173612
     1 -0.867158 -0.418257
                            0.066560
                                          -0.988271
                                                     -0.757974 -0.173612
     2 1.153192 -0.184916
                           -0.883204
                                           1.011868
                                                      0.925835 -0.173612
     3 -0.867158 1.331800
                            1.016323
                                           1.011868
                                                      1.767740 -0.173612
     4 -0.867158 -0.418257
                            1.016323
                                           1.011868
                                                      1.178407 -0.173612
        prevalentStroke prevalentHyp diabetes
                                                 {\tt totChol}
                                                            sysBP
                                                                      diaBP
     0
              -0.077033
                           -0.671101 -0.162477 -0.941346 -1.195907 -1.082625
     1
              -0.077033
                           -0.671101 -0.162477 0.299595 -0.515187 -0.158988
     2
              -0.077033
                           3
              -0.077033
                            1.490089 -0.162477 -0.264469 0.800871 1.016549
              -0.077033
                           -0.671101 -0.162477 1.089284 -0.106755 0.092912
             BMI heartRate
                             glucose TenYearCHD
```

```
      0
      0.286943
      0.342744
      -0.217517
      -0.423305

      1
      0.719325
      1.590275
      -0.261311
      -0.423305

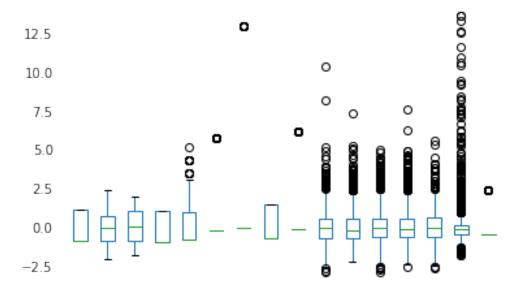
      2
      -0.113502
      -0.073099
      -0.524078
      -0.423305

      3
      0.682474
      -0.904786
      0.921141
      2.362360

      4
      -0.663807
      0.758588
      0.132840
      -0.423305
```

```
[19]: data_scaled_df.plot.box()
```

[19]: <matplotlib.axes._subplots.AxesSubplot at 0x7f1a2dd164a8>



male agebuuraebindisyssPola (illeb Myaydese t/Siteolikab) etpet (Chsy) s Bell a B FB Net art (illa llieso Year CHD

2.6 Utilidades

```
[20]: lista_metricas_treino = []
lista_metricas_teste = []

[21]: def metricas(y_true, y_pred, alg):
    r2 = r2_score(y_true, y_pred)
    eqm = mean_squared_error(y_true, y_pred)
    seq = len(y_true)*eqm
    reqm = math.sqrt(eqm)

    return {'Algoritmo':alg, 'R2':r2, 'EQM':eqm, 'REQM':reqm, 'SEQ':seq}
```

2.7 Separando conjuntos de Treino e Teste

Para a separação utilizou-se do train_test_split que divide o conjunto em treino e teste aleatóriamente

```
[22]: test_attr = 'male';
  output_attr = 'TenYearCHD';
  train, test = train_test_split(data_scaled_df, test_size = 0.2, shuffle=True)

x_train = train.drop(columns=[output_attr])
  y_train = train[output_attr]

x_test = test.drop(columns=[output_attr])
  y_test = test[output_attr]
```

2.8 Aplicando a Regressão

2.8.1 Regressão Linear

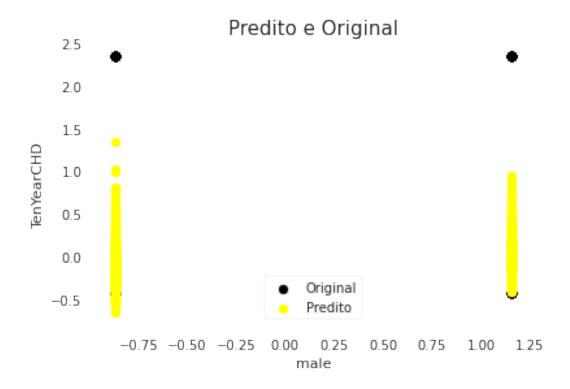
```
[23]: lire = LinearRegression()
[24]: lire.fit(x_train, y_train)
```

[24]: LinearRegression()

2.9 Avaliação para Teste

```
[25]: y_pred = lire.predict(x_test)
linear_metricas = metricas(y_test, y_pred, 'Regressão Linear - Teste')
lista_metricas_teste.append(linear_metricas)
[26]: plt.scatter(x_test[test_attr], y_test, color='black')
```

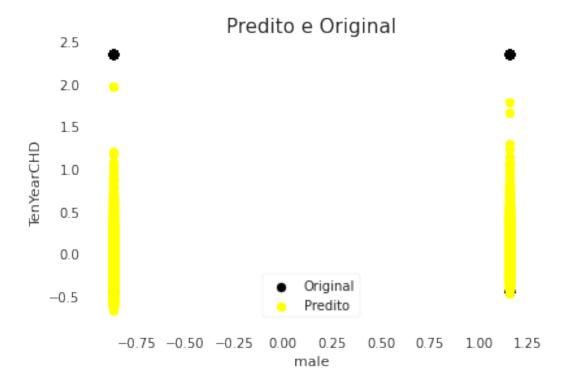
```
plt.scatter(x_test[test_attr], y_test, color='black')
plt.scatter(x_test[test_attr], y_pred, color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original', fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.10 Avaliação para Treino

```
[27]: y_pred = lire.predict(x_train)
    linear_metricas = metricas(y_train, y_pred, 'Regressão Linear - Treino')
    lista_metricas_treino.append(linear_metricas)

[28]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.11 SVR

2.11.1 Kernel RBF

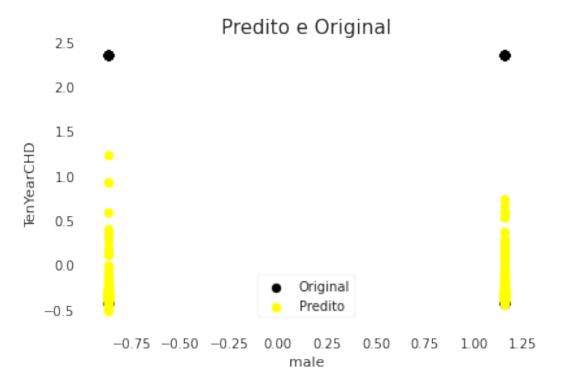
```
[29]: svr_reg = SVR(kernel='rbf')
[30]: svr_reg.fit(x_train, y_train)
[30]: SVR()
```

2.12 Avaliação para Teste

```
[31]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - RBF - Teste')
    lista_metricas_teste.append(svr_metricas)

[32]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
```

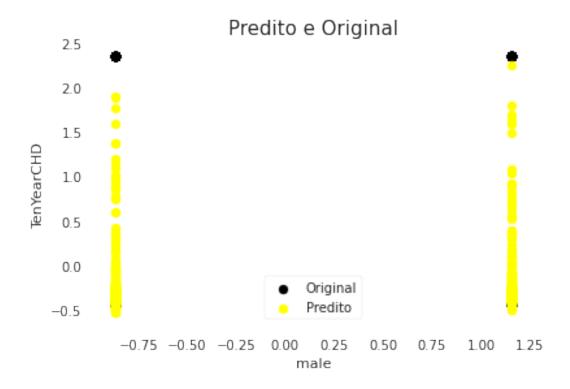
```
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.13 Avaliação para Treino

```
[33]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - RBF - Treino')
    lista_metricas_treino.append(svr_metricas)

[34]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



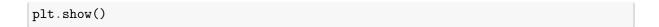
2.13.1 Kernel Linear

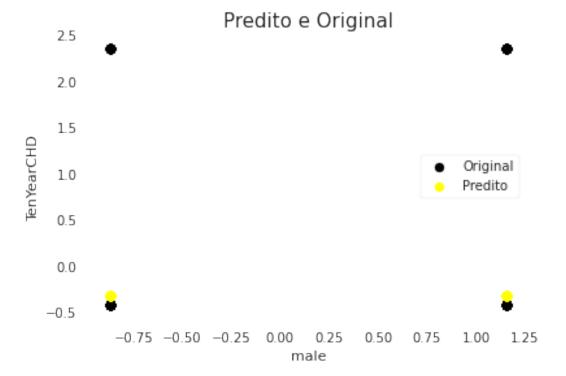
```
[35]: svr_reg = SVR(kernel='linear')
[36]: svr_reg.fit(x_train, y_train)
[36]: SVR(kernel='linear')
```

2.14 Avaliação para Teste

```
[37]: y_pred = svr_reg.predict(x_test)
metricas_svr = metricas(y_test, y_pred, 'SVR - Linear - Teste')
lista_metricas_teste.append(metricas_svr)

[38]: plt.scatter(x_test[test_attr], y_test, color='black')
plt.scatter(x_test[test_attr], y_pred, color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
```

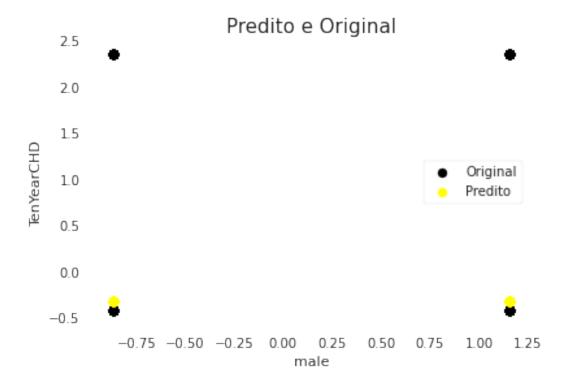




2.15 Avaliação para Treino

```
[39]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Linear - Treino')
    lista_metricas_treino.append(svr_metricas)

[40]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original', fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.15.1 Kernel Sigmoide

```
[41]: train, test = train_test_split(data_raw, test_size = 0.2, shuffle=True)
    x_train_sig = train.drop(columns=[output_attr])
    y_train_sig = train[output_attr]
    x_test_sig = test.drop(columns=[output_attr])
    y_test_sig = test[output_attr]

[42]: svr_reg = SVR(kernel='sigmoid')

[43]: SVR(kernel='sigmoid')
```

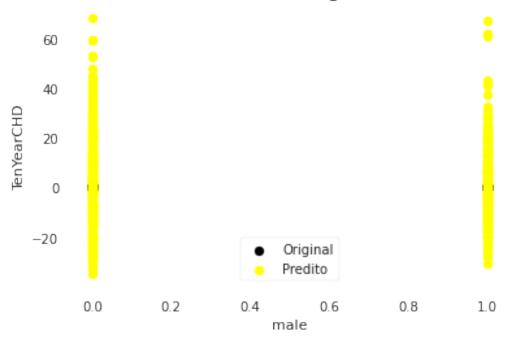
2.16 Avaliação para Teste

```
[44]: y_pred_sig = svr_reg.predict(x_test_sig)
metricas_svr = metricas(y_test_sig , y_pred_sig , 'SVR - Sigmoide - Teste')
lista_metricas_teste.append(metricas_svr)

[45]: plt.scatter(x_test_sig [test_attr], y_test_sig , color='black')
plt.scatter(x_test_sig [test_attr], y_pred_sig , color='yellow')
```

```
[45]: plt.scatter(x_test_sig [test_attr], y_test_sig , color='black')
   plt.scatter(x_test_sig [test_attr], y_pred_sig , color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original', fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```

Predito e Original

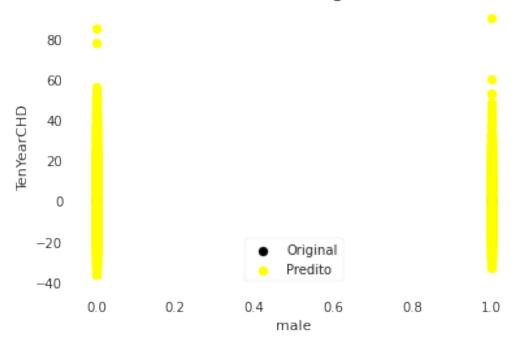


2.17 Avaliação para Treino

```
[46]: y_pred_sig = svr_reg.predict(x_train_sig)
svr_metricas = metricas(y_train_sig , y_pred_sig , 'SVR - Sigmoide - Treino')
lista_metricas_treino.append(svr_metricas)
```

```
[47]: plt.scatter(x_train_sig [test_attr], y_train_sig , color='black')
    plt.scatter(x_train_sig [test_attr], y_pred_sig , color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```

Predito e Original



2.17.1 Kernel Polinomial

```
[48]: svr_reg = SVR(kernel='poly', degree=3)
[49]: svr_reg.fit(x_train, y_train)
[49]: SVR(kernel='poly')
```

2.18 Avaliação para Teste

plt.title('Predito e Original',fontsize=15)

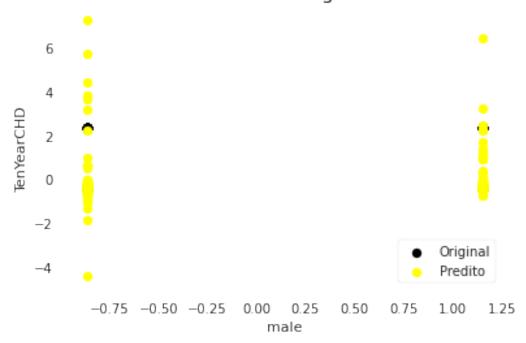
plt.legend(['Original', 'Predito'])

plt.show()

```
[50]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - Polinomial - Teste')
    lista_metricas_teste.append(svr_metricas)

[51]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
```

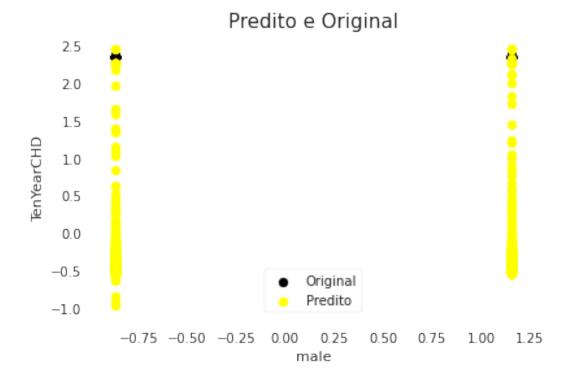
Predito e Original



2.19 Avaliação para Treino

```
[52]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Polinomial - Treino')
    lista_metricas_treino.append(svr_metricas)
```

```
[53]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.20 Redes Neurais

2.20.1 Kernel Linear

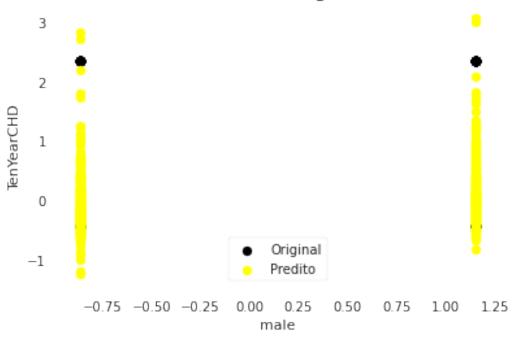
```
[54]: mlp_reg = MLPRegressor()
[55]: mlp_reg.fit(x_train, y_train)
[55]: MLPRegressor()
```

2.21 Avaliação para Teste

```
[56]: y_pred = mlp_reg.predict(x_test)
mlp_metricas = metricas(y_test, y_pred, 'MLP - Teste')
lista_metricas_teste.append(mlp_metricas)
```

```
[57]: plt.scatter(x_test[test_attr], y_test, color='black')
   plt.scatter(x_test[test_attr], y_pred, color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original',fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```

Predito e Original

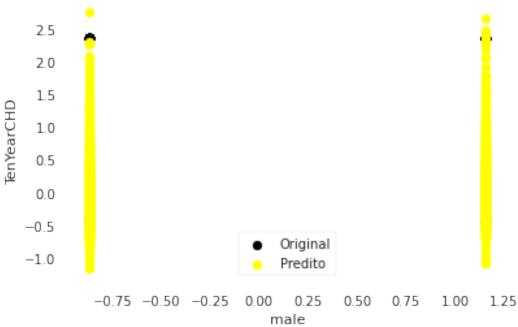


2.22 Avaliação para Treino

```
[58]: y_pred = mlp_reg.predict(x_train)
mlp_metricas = metricas(y_train, y_pred, 'MLP - Treino')
lista_metricas_treino.append(mlp_metricas)
```

```
[59]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```

Predito e Original



3 Resultados

```
[60]: metricas_teste = pd.DataFrame(lista_metricas_teste)
metricas_teste
```

```
[60]:
                        Algoritmo
                                            R2
                                                        EQM
                                                                  REQM
                                                                                   SEQ
        Regressão Linear - Teste
                                                                            769.219422
     0
                                      0.087893
                                                   0.907098
                                                              0.952417
                SVR - RBF - Teste
      1
                                     -0.049167
                                                   1.043406
                                                              1.021473
                                                                            884.808664
             SVR - Linear - Teste
      2
                                     -0.103276
                                                   1.097218
                                                              1.047482
                                                                            930.441172
      3
           SVR - Sigmoide - Teste -2198.824687 281.928404
                                                             16.790724
                                                                        239075.286764
      4 SVR - Polinomial - Teste
                                     -0.275246
                                                   1.268243
                                                              1.126163
                                                                          1075.470262
                      MLP - Teste
                                     -0.012818
                                                   1.007257
                                                              1.003622
                                                                           854.153811
```

```
[61]: | metricas_teste = round(metricas_teste, 3)
[62]: metricas_teste
[62]:
                                         R2
                                                 EQM
                                                         REQM
                                                                      SEQ
                        Algoritmo
     O Regressão Linear - Teste
                                      0.088
                                                0.907
                                                        0.952
                                                                  769.219
                SVR - RBF - Teste
                                     -0.049
                                                                  884.809
      1
                                                1.043
                                                        1.021
      2
             SVR - Linear - Teste
                                     -0.103
                                                1.097
                                                        1.047
                                                                  930.441
      3
           SVR - Sigmoide - Teste -2198.825 281.928
                                                       16.791
                                                               239075.287
      4 SVR - Polinomial - Teste
                                     -0.275
                                                1.268
                                                        1.126
                                                                 1075.470
                      MLP - Teste
                                                1.007
                                     -0.013
                                                        1.004
                                                                  854.154
[63]: metricas_teste.to_excel('framingham_metricas_teste.xlsx')
[64]: metricas_treino = pd.DataFrame(lista_metricas_treino)
      metricas_treino
[64]:
                                             R2
                                                         EQM
                                                                   REQM \
                         Algoritmo
     O Regressão Linear - Treino
                                       0.098059
                                                    0.903177
                                                               0.950356
                SVR - RBF - Treino
                                       0.028599
                                                    0.972733
                                                               0.986272
      1
      2
             SVR - Linear - Treino
                                      -0.104831
                                                    1.106346
                                                               1.051830
      3
           SVR - Sigmoide - Treino -2119.951812 273.695635
                                                              16.543749
      4 SVR - Polinomial - Treino
                                       0.060553
                                                    0.940735
                                                               0.969915
                      MLP - Treino
                                       0.341441
                                                    0.659462
                                                               0.812073
      5
                   SEQ
      0
           3061.771151
      1
           3297.563799
      2
           3750.512228
      3 927828.201264
      4
           3189.090403
      5
           2235.577091
[65]: metricas_treino = round(metricas_treino, 3)
[66]: metricas_treino.to_excel('framingham.xlsx')
```

regression-wine

August 19, 2020

[61]:

1 0. Introdução

Trabalho:

Aluno: Gabriel Luiz

Disciplina: Tópico em Aprendizado de Máquina

Objetivos:

- Escolha dois conjuntos de dados para trabalhar o problema de regressão. Separe cada dataset em conjunto de treinamento e conjunto de teste. Explique o seu critério de separação e o método utilizado.
- Você deverá implementar soluções para cada dataset usando:
- regressão linear (ou regressão múltipla)
- – regressão polinomial
- - SVR (use os kernels linear, sigmoide, RBF e polinomial)
- - rede neural (MLP ou RBF).
- Descreva os parâmetros/arquiteturas de cada modelo.
- Compare os resultados (para treinamento e teste) com as medidas de desempenho SEQ, EQM,
 REQM, EAM e r², e verifique qual a melhor opção dentre os métodos implementados que melhor se ajusta a seus dados.
- Você deverá fazer a visualização dos dados originais com os dados ajustados em cada experimento, tanto para o conjunto de treinamento quanto para o de teste. Os gráficos devem conter títulos nos eixos e legenda. Comente os resultados encontrados na visualização.

1.1 0.1 Dependências

Para realização da tarefa foram utilizados as seguintes bibliotecas:

```
[62]: #Utils
      import pandas as pd
      import numpy as np
      import pandas_profiling
      import math
      #Preprocess
      from sklearn.preprocessing import StandardScaler
      # Split
      from sklearn.model_selection import train_test_split
      # Regressores
      from sklearn.linear_model import LinearRegression
      from sklearn.svm import SVR
      from sklearn.neural_network import MLPRegressor
      #Metricas
      from sklearn.metrics import r2_score
      from sklearn.metrics import mean_squared_error
      #Visualização
      import seaborn as sns
      import matplotlib.pyplot as plt
      import warnings
      warnings.filterwarnings('ignore')
      %matplotlib inline
```

2 1. Dados

O conjunto de dados possui informações quimicas de vinhos Possui mais de 1500 registros e 12 atributos

Fonte: https://www.kaggle.com/uciml/red-wine-quality-cortez-et-al-2009

2.1 1.1 Informações sobre os dados:

Atributos: Input variables (based on physicochemical tests):

- · fixed acidity
- · volatile acidity
- citric acid
- residual sugar
- chlorides
- free sulfur dioxide

- total sulfur dioxide
- density
- pH
- sulphates
- alcohol

Output variable (based on sensory data): - quality (score between 0 and 10)

2.2 Importando Dataset

```
[63]: dataset = './dataset/datasets_4458_8204_winequality-red.csv'
      data_raw = pd.read_csv(dataset)
[64]: data_raw.head()
[64]:
         fixed acidity volatile acidity citric acid residual sugar chlorides \
                                                  0.00
                                                                   1.9
      0
                   7.4
                                    0.70
                                                                             0.076
                   7.8
                                    0.88
                                                  0.00
                                                                   2.6
     1
                                                                             0.098
      2
                   7.8
                                    0.76
                                                  0.04
                                                                   2.3
                                                                             0.092
      3
                  11.2
                                    0.28
                                                  0.56
                                                                   1.9
                                                                             0.075
                                                  0.00
                   7.4
                                    0.70
                                                                   1.9
                                                                             0.076
         free sulfur dioxide total sulfur dioxide density
                                                                pH sulphates \
     0
                        11.0
                                               34.0
                                                      0.9978 3.51
                                                                         0.56
                        25.0
                                                                         0.68
      1
                                               67.0
                                                      0.9968 3.20
      2
                        15.0
                                               54.0
                                                      0.9970 3.26
                                                                         0.65
                                               60.0
      3
                        17.0
                                                      0.9980 3.16
                                                                         0.58
      4
                        11.0
                                               34.0
                                                      0.9978 3.51
                                                                         0.56
         alcohol quality
     0
             9.4
                        5
      1
             9.8
                        5
      2
             9.8
                        5
      3
             9.8
                        6
             9.4
                        5
      4
[65]: wine_quality = []
      for quality in data_raw.quality:
          if quality >= 6:
              wine_quality.append(1)
          else:
              wine_quality.append(0)
      data_raw.quality = wine_quality
```

```
print(col, data_raw[col].unique())
fixed acidity [ 7.4 7.8 11.2 7.9 7.3 7.5 6.7 5.6 8.9 8.5 8.1 7.6 6.9
6.3
 7.1 8.3 5.2 5.7 8.8 6.8 4.6 7.7 8.7 6.4 6.6 8.6 10.2 7.
               9.7 6.2 5.
                             4.7 8.4 10.1 9.4 9.
                                                     8.2 6.1 5.8
 9.2 11.5 5.4 9.6 12.8 11. 11.6 12. 15. 10.8 11.1 10. 12.5 11.8
 10.9 10.3 11.4 9.9 10.4 13.3 10.6 9.8 13.4 10.7 11.9 12.4 12.2 13.8
 9.1 13.5 10.5 12.6 14. 13.7 9.5 12.7 12.3 15.6 5.3 11.3 13.
 12.9 14.3 15.5 11.7 13.2 15.9 12.1 5.1 4.9 5.9 6.
                                                     5.5]
volatile acidity [0.7 0.88 0.76 0.28 0.66 0.6
                                                  0.65 0.58 0.5
                                                                   0.615
0.61 0.62
 0.56 0.59 0.32 0.22 0.39 0.43 0.49 0.4
                                             0.41 0.71 0.645 0.675
0.685 0.655 0.605 0.38 1.13 0.45 0.67 0.52 0.935 0.29
                                                        0.31 0.51
 0.42  0.63  0.69  0.735  0.725  0.705  0.785  0.75  0.625  0.3
                                                         0.55
 0.775 0.9
            0.545 0.575 0.33 0.54 1.07 0.695 1.33 0.745 1.04 0.715
 0.415 0.34 0.68 0.95 0.53 0.64 0.885 0.805 0.73 0.37 0.835 1.09
0.57 0.44 0.635 0.82 0.48 1.
                                  0.21 0.35 0.975 0.26 0.87 0.18
 0.27 0.2
            0.85 0.84 0.96 0.78 0.23
                            0.315 0.365 0.25 0.825 0.72 0.595 0.585
                            0.98 1.185 0.92 1.035 1.025 0.565 0.74
 0.915 0.755 0.845 1.24 0.8
 1.115 0.865 0.875 0.965 0.91 0.89 1.01 0.305 0.395 0.12 0.86 0.295
 1.005 0.19 0.955 0.16 1.58 0.79 1.18 0.475 0.81 0.895 0.855]
citric acid [0.
               0.04 0.56 0.06 0.02 0.36 0.08 0.29 0.18 0.19 0.28 0.51 0.48
0.31
0.21 0.11 0.14 0.16 0.24 0.07 0.12 0.25 0.09 0.3 0.2 0.22 0.15 0.43
 0.52\ 0.23\ 0.37\ 0.26\ 0.57\ 0.4\ 0.49\ 0.05\ 0.54\ 0.64\ 0.7\ 0.47\ 0.44\ 0.17
0.68 0.53 0.1 0.01 0.55 1.
                            0.03 0.42 0.33 0.32 0.35 0.6 0.74 0.58
0.5 0.76 0.46 0.45 0.38 0.39 0.66 0.62 0.67 0.79 0.63 0.61 0.71 0.65
0.59 0.34 0.69 0.73 0.72 0.41 0.27 0.75 0.13 0.78]
residual sugar [ 1.9
                     2.6
                          2.3
                                1.8
                                      1.6
                                           1.2
                                                 2.
                                                            3.8
                                                                  3.9
                                                       6.1
                                                                        1.7
4.4
  2.4
       1.4
             2.5
                 10.7
                        5.5
                             2.1
                                   1.5
                                         5.9
                                              2.8
                                                    2.2
                                                          3.
                                                               3.4
                        7.2
 5.1
       4.65 1.3
                  7.3
                             2.9
                                   2.7
                                         5.6
                                              3.1
                                                    3.2
                                                          3.3
                                                               3.6
 4.
       7.
             6.4
                  3.5
                       11.
                             3.65 4.5
                                         4.8
                                              2.95
                                                   5.8
                                                          6.2
                                                               4.2
 7.9
       3.7
             6.7
                  6.6
                        2.15 5.2
                                   2.55 15.5
                                              4.1
                                                    8.3
                                                          6.55
                                                               4.6
       5.15 6.3
 4.3
                  6.
                        8.6
                             7.5
                                   2.25 4.25
                                              2.85
                                                    3.45
                                                         2.35
                                                               2.65
                  1.65 2.05 0.9
 9.
       8.8
             5.
                                   8.9
                                         8.1
                                              4.7
                                                    1.75
                                                         7.8
                                                              12.9
                  3.75 13.8
       5.4 15.4
                             5.7 13.9 ]
chlorides [0.076 0.098 0.092 0.075 0.069 0.065 0.073 0.071 0.097 0.089 0.114
0.176
 0.103\ 0.066\ 0.172\ 0.074\ 0.088\ 0.332\ 0.05\ 0.054\ 0.113\ 0.068\ 0.081\ 0.11
 0.07 \quad 0.111 \ 0.079 \ 0.115 \ 0.094 \ 0.093 \ 0.104 \ 0.464 \ 0.401 \ 0.062 \ 0.107 \ 0.045
 0.058 0.102 0.467 0.091 0.122 0.09 0.119 0.178 0.146 0.072 0.118 0.049
```

[66]: for col in data_raw:

0.06 0.117 0.087 0.236 0.61 0.095 0.1 0.36 0.067 0.27 0.099 0.046

```
0.061 0.056 0.039 0.059 0.101 0.057 0.337 0.078 0.263 0.063 0.611 0.064
 0.096 0.358 0.343 0.186 0.112 0.213 0.214 0.121 0.128 0.052 0.12 0.116
 0.109 0.159 0.124 0.174 0.047 0.127 0.413 0.152 0.053 0.055 0.051 0.125
       0.171 0.226 0.25 0.108 0.148 0.143 0.222 0.157 0.422 0.034 0.387
 0.415 0.243 0.241 0.19 0.132 0.126 0.038 0.044 0.041 0.165 0.048 0.145
 0.147 0.012 0.194 0.161 0.123 0.414 0.216 0.043 0.042 0.369 0.166 0.136
 0.403 0.137 0.168 0.153 0.267 0.169 0.205 0.235 0.23 ]
free sulfur dioxide [11.
                          25.
                                15.
                                     17.
                                           13.
                                                 9.
                                                     16.
                                                          52.
                                                                51.
                                                                     35.
                                                                           6.
                                                                                29.
23.
     10.
 21.
       4.
           14.
                      22.
                           40.
                                 5.
                                            7.
                                                12.
                                                     30.
                                                           33.
                                                                50.
                                                                     19.
                  8.
                                       З.
 20.
      27.
           18.
                28.
                      34.
                           42.
                                41.
                                      37.
                                           32.
                                                36.
                                                     24.
                                                           26.
                                                                39.
                                                                     40.5
 68.
           38.
                43.
                      47.
                            1.
                                54.
                                      46.
                                           45.
                                                 2.
                                                      5.5 53.
                                                                37.5 57.
           55.
      72.
                66.]
                                                                         102.
total sulfur dioxide [ 34.
                              67.
                                    54.
                                           60.
                                                 40.
                                                       59.
                                                              21.
                                                                    18.
                                                                                 65.
29.
     145.
 148.
       103.
              56.
                     71.
                           37.
                                 23.
                                        11.
                                              35.
                                                    16.
                                                           82.
                                                                113.
                                                                       83.
  50.
        15.
              30.
                     19.
                           87.
                                 46.
                                        14.
                                             114.
                                                           96.
                                                                119.
                                                                       73.
                                                    12.
  45.
        10.
             110.
                     52.
                          112.
                                 39.
                                        27.
                                              94.
                                                    43.
                                                           42.
                                                                 80.
                                                                       51.
  61.
       136.
              31.
                    125.
                           24.
                                140.
                                       133.
                                              85.
                                                   106.
                                                           22.
                                                                 36.
                                                                       69.
  64.
       153.
              47.
                    108.
                          111.
                                 62.
                                        28.
                                              89.
                                                    13.
                                                           90.
                                                                134.
                                                                       99.
  26.
        63.
             105.
                     20.
                          141.
                                 88.
                                       129.
                                             128.
                                                    86.
                                                          121.
                                                                101.
                                                                       44.
   8.
        49.
              38.
                    143.
                          144.
                                127.
                                       126.
                                             120.
                                                           93.
                                                                 95.
                                                    55.
                                                                       41.
        72.
  58.
              81.
                    109.
                           33.
                                 53.
                                        98.
                                              48.
                                                    70.
                                                           25.
                                                                135.
                                                                       92.
  74.
        32.
              77.
                    165.
                           75.
                                124.
                                        78.
                                             122.
                                                    66.
                                                           68.
                                                                 17.
                                                                       91.
  76.
                    116.
                                       104.
       151.
             142.
                          149.
                                 57.
                                              84.
                                                   147.
                                                          155.
                                                                152.
                                                                        9.
 139.
       130.
                    100.
                                        79.
                                             278.
                                                   289.
                                                          160.
                                                                 77.5 131. ]
               7.
                          115.
                                  6.
                                  0.998
                                           0.9964
                                                            0.9959
density [0.9978 0.9968
                          0.997
                                                   0.9946
                                                                    0.9943
                                                                           0.9974
 0.9986 0.9969
                 0.9982
                          0.9966
                                  0.9955
                                          0.9962
                                                           0.9958 0.9993
                                                   0.9972
 0.9957 0.9975
                          0.9976
                                  0.9934
                                          0.9954
                 0.994
                                                   0.9971
                                                            0.9956
                                                                    0.9983
 0.9967
        0.9961
                0.9984
                         0.9938
                                  0.9932 0.9965
                                                   0.9963
                                                           0.996
                                                                    0.9973
 0.9988
        0.9937
                 0.9952 0.9916
                                  0.9944 0.9996
                                                   0.995
                                                            0.9981
                                                                    0.9953
 0.9924
         0.9948
                 0.99695 0.99545 0.99615 0.9994
                                                   0.99625 0.99585 0.99685
 0.99655 0.99525 0.99815 0.99745 0.9927 0.99675 0.99925 0.99565 1.00005
 0.9985
        0.99965 0.99575 0.9999
                                  1.00025 0.9987
                                                   0.99935 0.99735 0.99915
 0.9991
         1.00015 0.9997
                          1.001
                                  0.9979
                                          1.0014
                                                   1.0001 0.99855 0.99845
 0.9998
        0.99645 0.99865 0.9989
                                  0.99975 0.999
                                                   1.0015
                                                           1.0002 0.9992
                                  1.0018 0.9912 1.0022 1.0003 0.9949
 1.0008
        1.
                  1.0006
                          1.0004
         1.0032 0.9947 0.9995
                                  0.9977
                                          1.0026 1.00315 1.0021
 0.9951
 0.9922 0.9921 0.99788 1.00024 0.99768 0.99782 0.99761 0.99803 0.99785
 0.99656 0.99488 0.99823 0.99779 0.99738 0.99701 0.99888 0.99938 0.99744
 0.99668 0.99727 0.99586 0.99612 0.99676 0.99732 0.99814 0.99746 0.99708
 0.99818 0.99639 0.99531 0.99786 0.99526 0.99641 0.99264 0.99682 0.99356
 0.99386 0.99702 0.99693 0.99562 1.00012 0.99462 0.99939 0.99632 0.99976
 0.99606 0.99154 0.99624 0.99417 0.99376 0.99832 0.99836 0.99694 0.99064
 0.99672 0.99647 0.99736 0.99629 0.99689 0.99801 0.99652 0.99538 0.99594
 0.99686 0.99438 0.99357 0.99628 0.99748 0.99578 0.99371 0.99522 0.99576
 0.99552 0.99664 0.99614 0.99517 0.99787 0.99533 0.99536 0.99824 0.99577
 0.99491 1.00289 0.99743 0.99774 0.99444 0.99892 0.99528 0.99331 0.99901
```

```
0.99674 0.99512 0.99395 0.99504 0.99516 0.99604 0.99468 0.99543 0.99791
 0.99425 0.99509 0.99484 0.99834 0.99864 0.99498 0.99566 0.99408 0.99458
 0.99648 0.99568 0.99613 0.99519 0.99518 0.99592 0.99654 0.99546 0.99554
 0.99733 0.99669 0.99724 0.99643 0.99605 0.99658 0.99416 0.99712 0.99418
 0.99596 0.99556 0.99918 0.99697 0.99378 0.99162 0.99495 0.9928 0.99603
 0.99549 0.99722 0.99354 0.99635 0.99454 0.99598 0.99486 0.99007 0.99636
 0.99642 0.99584 0.99506 0.99822 0.99364 0.99514 0.99854 0.99739 0.99683
 0.99692 0.99756 0.99547 0.99859 0.99294 0.99634 0.99704 0.99258 0.99426
 0.99747 0.99784 0.99358 0.99572 0.99769 0.99534 0.99817 0.99316 0.99471
 0.99617 0.99529 0.99451 0.99479 0.99772 0.99666 0.99392 0.99388 0.99402
 0.9936 0.99374 0.99523 0.99593 0.99396 0.99698 0.9902 0.99252 0.99256
 0.99235 0.99352 0.99557 0.99394 0.9915 0.99379 0.99798 0.99341 0.9933
 0.99684 0.99524 0.99764 0.99588 0.99473 0.99616 0.99622 0.99544 0.99728
 0.99551 0.99434 0.99709 0.99384 0.99502 0.99667 0.99649 0.99716 0.99541
 0.99318 0.99346 0.99599 0.99478 0.99754 0.99439 0.99633 0.99419 0.99878
 0.99752 0.99428 0.99659 0.99677 0.99734 0.99678 0.99638 0.99922 0.99157
 0.99718 0.99621 0.99242 0.99494 0.99729 0.99414 0.99721 0.99627 0.99569
 0.99499 0.99437 0.99726 0.99456 0.99564 0.9908 0.99084 0.9935 0.99385
 0.99688 0.99619 0.99476 0.99328 0.99286 0.99914 0.99521 0.99362 0.99558
 0.99323 0.99191 0.99501 0.9929 0.99532 0.99796 0.99581 0.99608 0.99387
 0.99448 0.99589 0.99852 0.99472 0.99587 0.99332 0.99464 0.99699 0.99725
 0.99623 0.99609 0.99292 0.9942 1.00369 0.99713 0.99322 0.99706 0.99974
 0.99467 0.99236 0.99705 0.99334 0.99336 1.00242 0.99182 0.99808 0.99828
 0.99719 0.99542 0.99496 0.99344 0.99348 0.99459 0.99492 0.99508 0.99582
 0.99555 0.9941 0.99661 0.99842 0.99489 0.99665 0.99553 0.99714 0.99631
 0.99573 0.99717 0.99397 0.99646 0.99758 0.99306 0.99783 0.99765 0.99474
 0.99483 0.99314 0.99574 0.99651]
pH [3.51 3.2 3.26 3.16 3.3 3.39 3.36 3.35 3.28 3.58 3.17 3.11 3.38 3.04
 3.52 3.43 3.34 3.47 3.46 3.45 3.4 3.42 3.23 3.5 3.33 3.21 3.48 3.9
3.25 3.32 3.15 3.41 3.44 3.31 3.54 3.13 2.93 3.14 3.75 3.85 3.29 3.08
3.37 3.19 3.07 3.49 3.53 3.24 3.63 3.22 3.68 2.74 3.59 3.
 3.61 3.06 3.6 3.69 3.1 3.05 3.67 3.27 3.18 3.02 3.55 2.99 3.01 3.56
 3.03 3.62 2.88 2.95 2.98 3.09 2.86 3.74 2.92 3.72 2.87 2.89 2.94 3.66
 3.71 3.78 3.7 4.01 2.9 ]
sulphates [0.56 0.68 0.65 0.58 0.46 0.47 0.57 0.8 0.54 0.52 1.56 0.88 0.93 0.75
 1.28 0.5 1.08 0.53 0.91 0.63 0.59 0.55 0.66 0.6 0.73 0.48 0.83 0.51
0.9 1.2 0.74 0.64 0.77 0.71 0.62 0.39 0.79 0.95 0.82 1.12 1.14 0.78
 1.95 1.22 1.98 0.61 1.31 0.69 0.67 0.7 0.49 0.92 2. 0.72 1.59 0.33
 1.02 0.97 0.85 0.43 1.03 0.86 0.76 1.61 1.09 0.84 0.96 0.45 1.26 0.87
         1.36 1.18 0.89 0.98 1.13 1.04 1.11 0.99 1.07 0.44 1.06 1.05
 0.42 1.17 1.62 0.94 1.34 1.16 1.1 0.4 1.15 0.37 1.33 1.01]
alcohol [ 9.4
                     9.8
                                 10.
                                              9.5
                                                         10.5
                                                                      9.2
  9.9
              9.1
                         9.3
                                      9.
                                                  9.7
                                                             10.1
                                     10.3
 10.6
             9.6
                         10.8
                                                 13.1
                                                             10.2
 10.9
            10.7
                         12.9
                                     10.4
                                                 13.
                                                             14.
 11.5
             11.4
                         12.4
                                                 12.2
                                                             12.8
                                     11.
 12.6
            12.5
                         11.7
                                    11.3
                                                 12.3
                                                             12.
 11.9
            11.8
                         8.7
                                    13.3
                                                 11.2
                                                             11.6
```

```
11.1
             13.4
                         12.1
                                      8.4
                                                 12.7
                                                             14.9
 13.2
                         13.5
                                     10.03333333 9.55
                                                              8.5
             13.6
 11.06666667 9.56666667 10.55
                                     8.8
                                                 13.56666667 11.95
                                      9.05
                                                 10.75
 9.95
              9.23333333 9.25
                                                            ]
quality [0 1]
```

2.3 Pré-processamento

```
[67]: # pandas_profiling.ProfileReport(data_raw)
```

2.4 Visualização

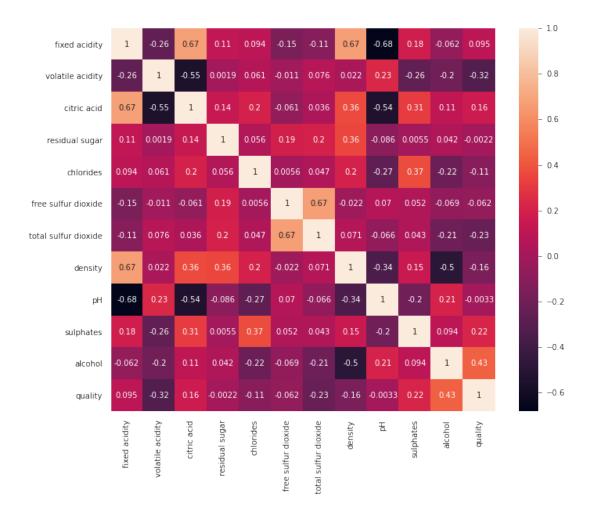
```
[68]: # sns.pairplot(data_raw)
```

```
[69]: plt.clf()
```

<Figure size 432x288 with 0 Axes>

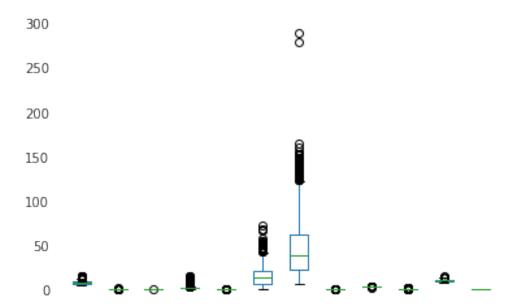
```
[70]: plt.subplots(figsize=(11, 9))
sns.heatmap(data_raw.corr(), annot=True)
```

[70]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73f56554e0>



[71]: data_raw.plot.box()

[71]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73d6781c50>



fixed/ataitiley aitiolitispictical efideseistestalred iffxideteosisty: pHsulphatatechoquality

2.5 Escalonando

```
[72]: scaler = StandardScaler().fit(data_raw)
      data_scaled = scaler.transform(data_raw)
[73]: data_scaled_df = pd.DataFrame(data_scaled, columns=data_raw.columns)
[74]: data_scaled_df.head()
[74]:
         fixed acidity
                        volatile acidity
                                         citric acid residual sugar
                                                                        chlorides
             -0.528360
                                0.961877
                                                             -0.453218
                                                                        -0.243707
      0
                                             -1.391472
      1
             -0.298547
                                1.967442
                                             -1.391472
                                                              0.043416
                                                                         0.223875
      2
             -0.298547
                                1.297065
                                             -1.186070
                                                             -0.169427
                                                                         0.096353
      3
              1.654856
                               -1.384443
                                              1.484154
                                                             -0.453218
                                                                        -0.264960
      4
             -0.528360
                                0.961877
                                             -1.391472
                                                             -0.453218
                                                                        -0.243707
         free sulfur dioxide
                              total sulfur dioxide
                                                      density
                                                                     pH sulphates
      0
                   -0.466193
                                                                         -0.579207
                                         -0.379133 0.558274
                                                              1.288643
      1
                    0.872638
                                           0.624363 0.028261 -0.719933
                                                                           0.128950
      2
                   -0.083669
                                           0.229047
                                                     0.134264 -0.331177
                                                                         -0.048089
      3
                    0.107592
                                           0.411500
                                                    0.664277 -0.979104
                                                                         -0.461180
      4
                   -0.466193
                                          -0.379133 0.558274 1.288643
                                                                         -0.579207
          alcohol
                    quality
```

```
0 -0.960246 -1.072004

1 -0.584777 -1.072004

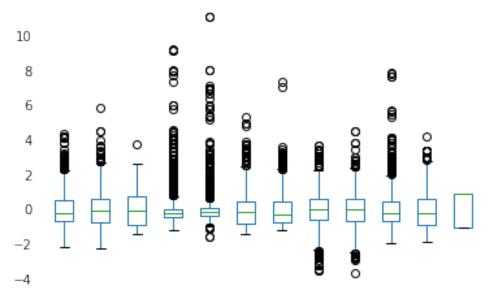
2 -0.584777 -1.072004

3 -0.584777 0.932832

4 -0.960246 -1.072004
```

```
[75]: data_scaled_df.plot.box()
```

[75]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73d6671eb8>



fixed/otaitilley aitivitessidulal efulgraislettair stuttxiidetensiitty: pHsulphatelsohoquality

2.6 Utilidades

```
[76]: lista_metricas_treino = []
lista_metricas_teste = []

[77]: def metricas(y_true, y_pred, alg):
    r2 = r2_score(y_true, y_pred)
    eqm = mean_squared_error(y_true, y_pred)
    seq = len(y_true)*eqm
    reqm = math.sqrt(eqm)

    return {'Algoritmo':alg, 'R2':r2, 'EQM':eqm, 'REQM':reqm, 'SEQ':seq}
```

2.7 Separando conjuntos de Treino e Teste

Para a separação utilizou-se do train_test_split que divide o conjunto em treino e teste aleatóriamente

```
[78]: test_attr = 'fixed acidity';
  output_attr = 'quality';
  train, test = train_test_split(data_scaled_df, test_size = 0.2, shuffle=True)

x_train = train.drop(columns=[output_attr])
y_train = train[output_attr]

x_test = test.drop(columns=[output_attr])
y_test = test[output_attr]
```

2.8 Aplicando a Regressão

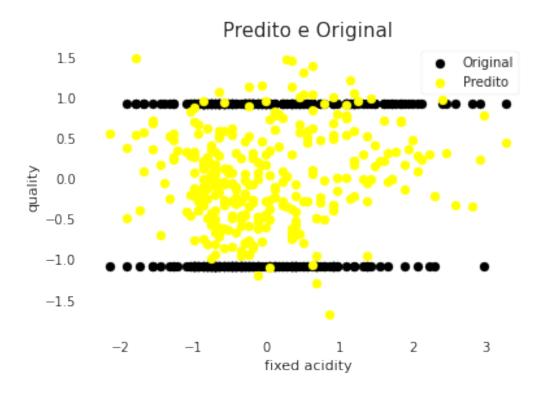
2.8.1 Regressão Linear

```
[79]: lire = LinearRegression()
[80]: lire.fit(x_train, y_train)
[80]: LinearRegression()
```

2.9 Avaliação para Teste

```
[81]: y_pred = lire.predict(x_test)
linear_metricas = metricas(y_test, y_pred, 'Regressão Linear - Teste')
lista_metricas_teste.append(linear_metricas)
```

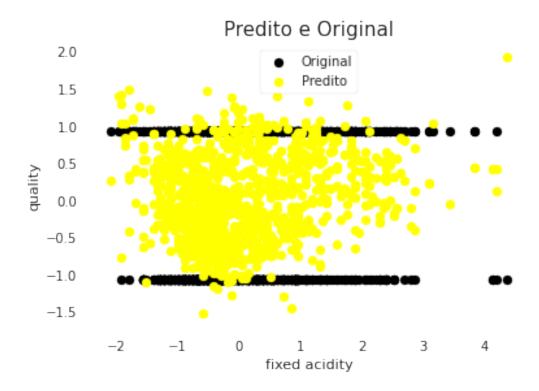
```
[82]: plt.scatter(x_test[test_attr], y_test, color='black')
   plt.scatter(x_test[test_attr], y_pred, color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original', fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```



2.10 Avaliação para Treino

```
[83]: y_pred = lire.predict(x_train)
linear_metricas = metricas(y_train, y_pred, 'Regressão Linear - Treino')
lista_metricas_treino.append(linear_metricas)

[84]: plt.scatter(x_train[test_attr], y_train, color='black')
plt.scatter(x_train[test_attr], y_pred, color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.11 SVR

2.11.1 Kernel RBF

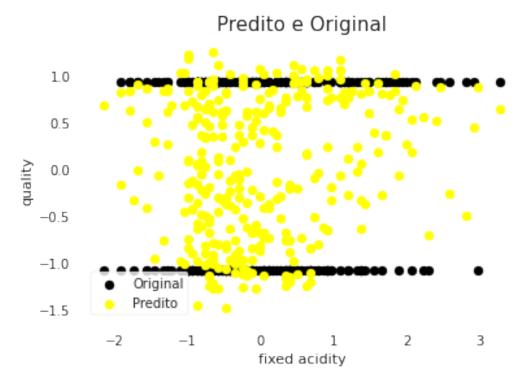
```
[85]: svr_reg = SVR(kernel='rbf')
[86]: svr_reg.fit(x_train, y_train)
[86]: SVR()
```

2.12 Avaliação para Teste

```
[87]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - RBF - Teste')
    lista_metricas_teste.append(svr_metricas)

[88]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
```

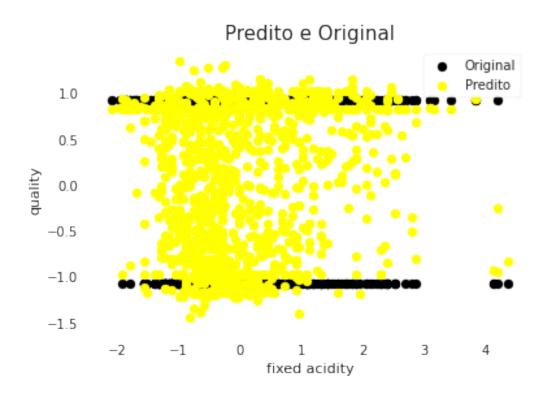
```
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.13 Avaliação para Treino

```
[89]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - RBF - Treino')
    lista_metricas_treino.append(svr_metricas)

[90]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



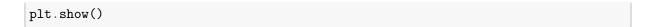
2.13.1 Kernel Linear

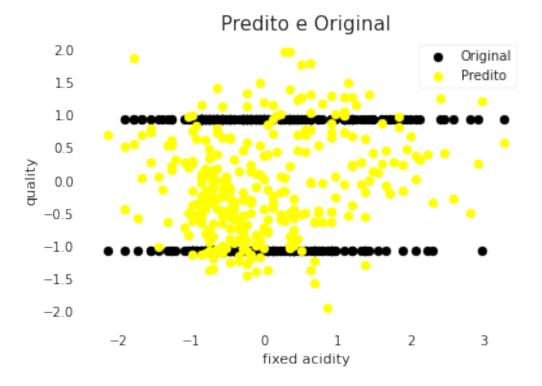
```
[91]: svr_reg = SVR(kernel='linear')
[92]: svr_reg.fit(x_train, y_train)
[92]: SVR(kernel='linear')
```

2.14 Avaliação para Teste

```
[93]: y_pred = svr_reg.predict(x_test)
    metricas_svr = metricas(y_test, y_pred, 'SVR - Linear - Teste')
    lista_metricas_teste.append(metricas_svr)

[94]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
```

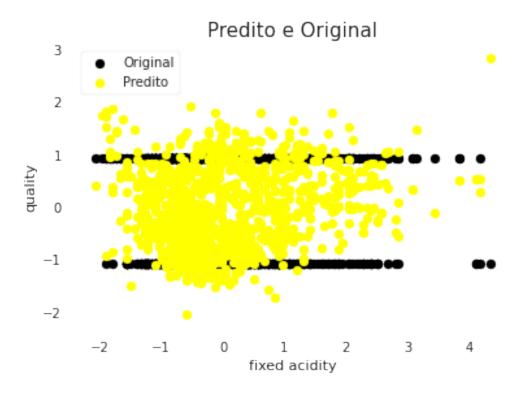




2.15 Avaliação para Treino

```
[95]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Linear - Treino')
    lista_metricas_treino.append(svr_metricas)

[96]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original', fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.15.1 Kernel Sigmoide

```
[97]: train, test = train_test_split(data_raw, test_size = 0.2, shuffle=True)
    x_train_sig = train.drop(columns=[output_attr])
    y_train_sig = train[output_attr]
    x_test_sig = test.drop(columns=[output_attr])
    y_test_sig = test[output_attr]

[98]: svr_reg = SVR(kernel='sigmoid')

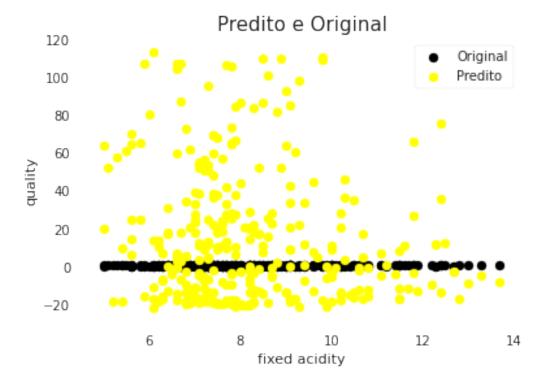
[99]: svr_reg.fit(x_train_sig , y_train_sig )

[99]: SVR(kernel='sigmoid')
```

2.16 Avaliação para Teste

```
[100]: y_pred_sig = svr_reg.predict(x_test_sig)
metricas_svr = metricas(y_test_sig , y_pred_sig , 'SVR - Sigmoide - Teste')
lista_metricas_teste.append(metricas_svr)

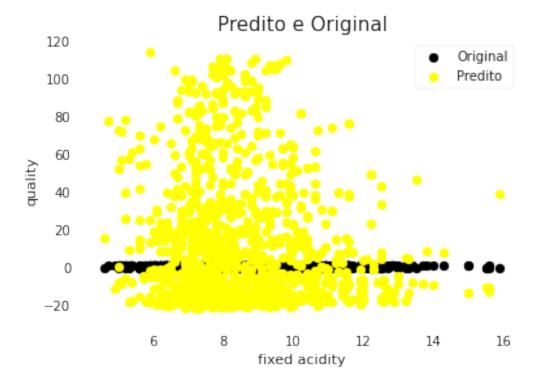
[101]: plt.scatter(x_test_sig [test_attr], y_test_sig , color='black')
plt.scatter(x_test_sig [test_attr], y_pred_sig , color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.17 Avaliação para Treino

```
[102]: y_pred_sig = svr_reg.predict(x_train_sig)
svr_metricas = metricas(y_train_sig , y_pred_sig , 'SVR - Sigmoide - Treino')
lista_metricas_treino.append(svr_metricas)
```

```
[103]: plt.scatter(x_train_sig [test_attr], y_train_sig , color='black')
    plt.scatter(x_train_sig [test_attr], y_pred_sig , color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.17.1 Kernel Polinomial

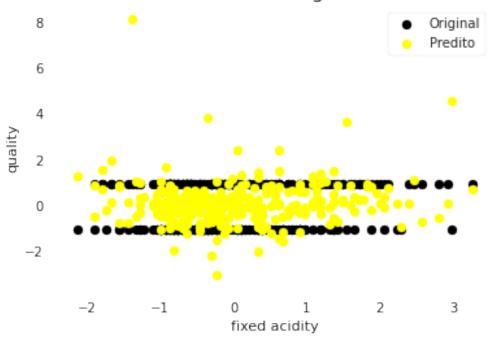
```
[104]: svr_reg = SVR(kernel='poly', degree=3)
[105]: svr_reg.fit(x_train, y_train)
[105]: SVR(kernel='poly')
```

2.18 Avaliação para Teste

```
[106]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - Polinomial - Teste')
    lista_metricas_teste.append(svr_metricas)

[107]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



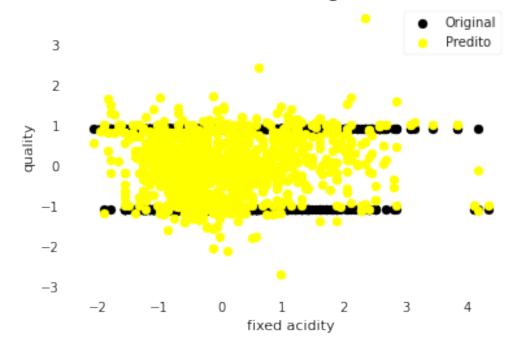


2.19 Avaliação para Treino

```
[108]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Polinomial - Treino')
    lista_metricas_treino.append(svr_metricas)
```

```
[109]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```

Predito e Original



2.20 Redes Neurais

2.20.1 Kernel Linear

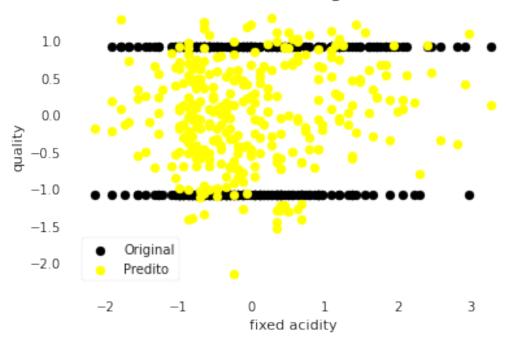
```
[110]: mlp_reg = MLPRegressor()
[111]: mlp_reg.fit(x_train, y_train)
[111]: MLPRegressor()
```

2.21 Avaliação para Teste

```
[112]: y_pred = mlp_reg.predict(x_test)
mlp_metricas = metricas(y_test, y_pred, 'MLP - Teste')
lista_metricas_teste.append(mlp_metricas)

[113]: plt.scatter(x_test[test_attr], y_test, color='black')
plt.scatter(x_test[test_attr], y_pred, color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```

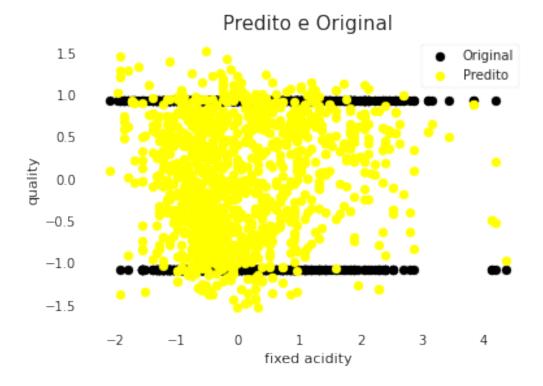
Predito e Original



2.22 Avaliação para Treino

```
[114]: y_pred = mlp_reg.predict(x_train)
mlp_metricas = metricas(y_train, y_pred, 'MLP - Treino')
lista_metricas_treino.append(mlp_metricas)
```

```
[115]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



3 Resultados

```
[116]: metricas_teste = pd.DataFrame(lista_metricas_teste)
       metricas_teste
                                              R2
[116]:
                         Algoritmo
                                                          EQM
                                                                     REQM \
         Regressão Linear - Teste
                                        0.300920
                                                     0.701121
                                                                 0.837330
       0
                 SVR - RBF - Teste
       1
                                        0.348163
                                                     0.653740
                                                                 0.808542
              SVR - Linear - Teste
       2
                                        0.244870
                                                     0.757334
                                                                 0.870249
            SVR - Sigmoide - Teste -5542.359159
       3
                                                  1359.638756
                                                               36.873280
         SVR - Polinomial - Teste
                                       -0.104436
                                                     1.107660
                                                                 1.052454
                       MLP - Teste
                                        0.357232
                                                     0.644644
                                                                 0.802898
```

```
SEQ
       0
             224.358630
             209.196795
       1
       2
             242.346802
       3
         435084.401967
       4
             354.451058
       5
             206.286211
[117]: metricas_teste = round(metricas_teste, 3)
[118]: metricas_teste
[118]:
                                                           REQM
                         Algoritmo
                                           R2
                                                    EQM
                                                                         SEQ
          Regressão Linear - Teste
                                                          0.837
                                        0.301
                                                  0.701
                                                                     224.359
                 SVR - RBF - Teste
       1
                                        0.348
                                                  0.654
                                                          0.809
                                                                     209.197
              SVR - Linear - Teste
       2
                                        0.245
                                                  0.757
                                                          0.870
                                                                     242.347
            SVR - Sigmoide - Teste -5542.359
       3
                                               1359.639
                                                         36.873
                                                                  435084.402
       4
         SVR - Polinomial - Teste
                                       -0.104
                                                  1.108
                                                           1.052
                                                                     354.451
       5
                       MLP - Teste
                                        0.357
                                                  0.645
                                                          0.803
                                                                     206.286
[119]: metricas_teste.to_excel('wine_metricas_teste.xlsx')
[120]: metricas_treino = pd.DataFrame(lista_metricas_treino)
       metricas_treino
[120]:
                                               R2
                                                            EQM
                                                                      REQM
                          Algoritmo
         Regressão Linear - Treino
                                         0.293268
                                                      0.706070
                                                                  0.840280
                 SVR - RBF - Treino
                                         0.428526
                                                      0.570938
                                                                  0.755604
       1
       2
              SVR - Linear - Treino
                                         0.235066
                                                      0.764217
                                                                  0.874195
       3
            SVR - Sigmoide - Treino -5079.800090
                                                   1266.714398
                                                                 35.590931
         SVR - Polinomial - Treino
       4
                                         0.376087
                                                      0.623328
                                                                  0.789512
                       MLP - Treino
       5
                                         0.543536
                                                      0.456036
                                                                  0.675304
                   SEQ
       0 9.030631e+02
       1 7.302295e+02
       2 9.774335e+02
       3 1.620128e+06
       4 7.972371e+02
       5 5.832697e+02
[121]: metricas_treino = round(metricas_treino, 3)
[122]: metricas_treino.to_excel('wine.xlsx')
```

regression-wine-2

August 19, 2020

[0]:

1 0. Introdução

Trabalho:

Aluno: Gabriel Luiz

Disciplina: Tópico em Aprendizado de Máquina

Objetivos:

- Escolha dois conjuntos de dados para trabalhar o problema de regressão. Separe cada dataset em conjunto de treinamento e conjunto de teste. Explique o seu critério de separação e o método utilizado.
- Você deverá implementar soluções para cada dataset usando:
- regressão linear (ou regressão múltipla)
- – regressão polinomial
- - SVR (use os kernels linear, sigmoide, RBF e polinomial)
- rede neural (MLP ou RBF).
- Descreva os parâmetros/arquiteturas de cada modelo.
- Compare os resultados (para treinamento e teste) com as medidas de desempenho SEQ, EQM,
 REQM, EAM e r², e verifique qual a melhor opção dentre os métodos implementados que melhor se ajusta a seus dados.
- Você deverá fazer a visualização dos dados originais com os dados ajustados em cada experimento, tanto para o conjunto de treinamento quanto para o de teste. Os gráficos devem conter títulos nos eixos e legenda. Comente os resultados encontrados na visualização.

1.1 0.1 Dependências

Para realização da tarefa foram utilizados as seguintes bibliotecas:

```
[1]: #Utils
     import pandas as pd
     import numpy as np
     import pandas_profiling
     import math
     #Preprocess
     from sklearn.preprocessing import StandardScaler
     # Split
     from sklearn.model_selection import train_test_split
     # Regressores
     from sklearn.linear_model import LinearRegression
     from sklearn.svm import SVR
     from sklearn.neural_network import MLPRegressor
     #Metricas
     from sklearn.metrics import r2_score
     from sklearn.metrics import mean_squared_error
     #Visualização
     import seaborn as sns
     import matplotlib.pyplot as plt
     import warnings
     warnings.filterwarnings('ignore')
     %matplotlib inline
```

2 1. Dados

O conjunto de dados possui informações quimicas de vinhos Possui mais de 1500 registros e 12 atributos

Fonte: https://www.kaggle.com/uciml/red-wine-quality-cortez-et-al-2009

2.1 1.1 Informações sobre os dados:

Atributos: Input variables (based on physicochemical tests):

- · fixed acidity
- · volatile acidity
- citric acid
- residual sugar
- chlorides
- free sulfur dioxide

- total sulfur dioxide
- density
- pH
- sulphates
- alcohol

Output variable (based on sensory data): - quality (score between 0 and 10)

2.2 Importando Dataset

data_raw.quality = wine_quality

```
[2]: dataset = './dataset/datasets_4458_8204_winequality-red.csv'
     data_raw = pd.read_csv(dataset)
[3]: data_raw.head()
[3]:
        fixed acidity volatile acidity citric acid residual sugar
                                                                         chlorides
                                                 0.00
     0
                  7.4
                                    0.70
                                                                   1.9
                                                                             0.076
                  7.8
                                                 0.00
                                                                   2.6
     1
                                    0.88
                                                                             0.098
     2
                  7.8
                                    0.76
                                                 0.04
                                                                   2.3
                                                                             0.092
     3
                 11.2
                                    0.28
                                                                   1.9
                                                  0.56
                                                                             0.075
                                                 0.00
                  7.4
                                    0.70
                                                                   1.9
                                                                             0.076
        free sulfur dioxide total sulfur dioxide density
                                                                pH sulphates
     0
                        11.0
                                              34.0
                                                      0.9978 3.51
                                                                          0.56
     1
                       25.0
                                              67.0
                                                      0.9968 3.20
                                                                          0.68
     2
                        15.0
                                              54.0
                                                      0.9970
                                                              3.26
                                                                          0.65
     3
                        17.0
                                              60.0
                                                      0.9980 3.16
                                                                          0.58
     4
                        11.0
                                              34.0
                                                      0.9978 3.51
                                                                          0.56
        alcohol quality
     0
            9.4
                       5
     1
            9.8
                       5
     2
            9.8
                       5
     3
            9.8
                       6
            9.4
     4
                       5
[4]: | # wine_quality = []
     # for quality in data_raw.quality:
           if quality >= 6:
     #
               wine_quality.append(1)
     #
           else:
     #
               wine_quality.append(0)
```

```
fixed acidity [ 7.4 7.8 11.2 7.9 7.3 7.5 6.7 5.6 8.9 8.5 8.1 7.6 6.9
6.3
 7.1 8.3 5.2 5.7 8.8 6.8 4.6 7.7 8.7 6.4 6.6 8.6 10.2 7.
 7.2 9.3 8.
                9.7 6.2 5.
                              4.7 8.4 10.1 9.4 9.
                                                     8.2 6.1 5.8
 9.2 11.5 5.4 9.6 12.8 11. 11.6 12. 15. 10.8 11.1 10. 12.5 11.8
 10.9 10.3 11.4 9.9 10.4 13.3 10.6 9.8 13.4 10.7 11.9 12.4 12.2 13.8
 9.1 13.5 10.5 12.6 14. 13.7 9.5 12.7 12.3 15.6 5.3 11.3 13.
 12.9 14.3 15.5 11.7 13.2 15.9 12.1 5.1 4.9 5.9 6.
                                                     5.5]
volatile acidity [0.7 0.88 0.76 0.28 0.66 0.6
                                                   0.65 0.58 0.5
                                                                    0.615
0.61 0.62
 0.56 0.59 0.32 0.22 0.39 0.43 0.49 0.4
                                              0.41 0.71 0.645 0.675
0.685 0.655 0.605 0.38 1.13 0.45 0.67 0.52 0.935 0.29
                                                         0.31 0.51
 0.42  0.63  0.69  0.735  0.725  0.705  0.785  0.75  0.625  0.3
                                                         0.55
 0.775 0.9
            0.545 0.575 0.33 0.54 1.07 0.695 1.33 0.745 1.04 0.715
 0.415 0.34 0.68 0.95 0.53 0.64 0.885 0.805 0.73 0.37 0.835 1.09
0.57 0.44 0.635 0.82 0.48
                            1.
                                   0.21 0.35 0.975 0.26 0.87 0.18
 0.27 0.2
            0.85 0.84 0.96 0.78 0.23
                            0.315 0.365 0.25 0.825 0.72 0.595 0.585
 0.915 0.755 0.845 1.24 0.8
                             0.98 1.185 0.92 1.035 1.025 0.565 0.74
 1.115 0.865 0.875 0.965 0.91 0.89 1.01 0.305 0.395 0.12 0.86 0.295
 1.005 0.19 0.955 0.16 1.58 0.79 1.18 0.475 0.81 0.895 0.855]
citric acid [0.
               0.04 0.56 0.06 0.02 0.36 0.08 0.29 0.18 0.19 0.28 0.51 0.48
0.31
0.21\ 0.11\ 0.14\ 0.16\ 0.24\ 0.07\ 0.12\ 0.25\ 0.09\ 0.3\ 0.2\ 0.22\ 0.15\ 0.43
 0.52\ 0.23\ 0.37\ 0.26\ 0.57\ 0.4\ 0.49\ 0.05\ 0.54\ 0.64\ 0.7\ 0.47\ 0.44\ 0.17
0.68 0.53 0.1 0.01 0.55 1.
                             0.03 0.42 0.33 0.32 0.35 0.6 0.74 0.58
0.5 0.76 0.46 0.45 0.38 0.39 0.66 0.62 0.67 0.79 0.63 0.61 0.71 0.65
0.59 0.34 0.69 0.73 0.72 0.41 0.27 0.75 0.13 0.78]
residual sugar [ 1.9
                     2.6
                           2.3
                                1.8
                                      1.6
                                            1.2
                                                  2.
                                                             3.8
                                                                   3.9
                                                       6.1
                                                                        1.7
4.4
  2.4
       1.4
             2.5
                 10.7
                        5.5
                              2.1
                                    1.5
                                         5.9
                                               2.8
                                                    2.2
                                                          3.
                                                                3.4
                        7.2
 5.1
       4.65 1.3
                  7.3
                              2.9
                                    2.7
                                         5.6
                                                     3.2
                                                          3.3
                                               3.1
                                                                3.6
 4.
       7.
             6.4
                  3.5
                              3.65 4.5
                                         4.8
                                               2.95
                                                    5.8
                                                          6.2
                                                                4.2
                       11.
 7.9
       3.7
             6.7
                  6.6
                        2.15 5.2
                                    2.55 15.5
                                                    8.3
                                               4.1
                                                          6.55
                                                                4.6
 4.3
       5.15 6.3
                  6.
                        8.6
                              7.5
                                    2.25
                                         4.25
                                               2.85
                                                    3.45
                                                          2.35
                                                               2.65
             5.
 9.
       8.8
                  1.65 2.05 0.9
                                   8.9
                                         8.1
                                               4.7
                                                     1.75
                                                          7.8
                                                               12.9
       5.4 15.4
                  3.75 13.8
                              5.7
                                 13.9]
chlorides [0.076 0.098 0.092 0.075 0.069 0.065 0.073 0.071 0.097 0.089 0.114
0.176
 0.103\ 0.066\ 0.172\ 0.074\ 0.088\ 0.332\ 0.05\ 0.054\ 0.113\ 0.068\ 0.081\ 0.11
 0.07 \quad 0.111 \ 0.079 \ 0.115 \ 0.094 \ 0.093 \ 0.104 \ 0.464 \ 0.401 \ 0.062 \ 0.107 \ 0.045
 0.058 0.102 0.467 0.091 0.122 0.09 0.119 0.178 0.146 0.072 0.118 0.049
 0.06  0.117  0.087  0.236  0.61  0.095  0.1  0.36  0.067  0.27  0.099  0.046
```

[5]: for col in data_raw:

print(col, data_raw[col].unique())

```
0.061 0.056 0.039 0.059 0.101 0.057 0.337 0.078 0.263 0.063 0.611 0.064
 0.096 0.358 0.343 0.186 0.112 0.213 0.214 0.121 0.128 0.052 0.12 0.116
 0.109 0.159 0.124 0.174 0.047 0.127 0.413 0.152 0.053 0.055 0.051 0.125
       0.171 0.226 0.25 0.108 0.148 0.143 0.222 0.157 0.422 0.034 0.387
 0.415 0.243 0.241 0.19 0.132 0.126 0.038 0.044 0.041 0.165 0.048 0.145
 0.147 0.012 0.194 0.161 0.123 0.414 0.216 0.043 0.042 0.369 0.166 0.136
 0.403 0.137 0.168 0.153 0.267 0.169 0.205 0.235 0.23 ]
free sulfur dioxide [11.
                          25.
                                15.
                                     17.
                                           13.
                                                 9.
                                                     16.
                                                          52.
                                                                51.
                                                                     35.
                                                                           6.
                                                                                29.
23.
     10.
 21.
       4.
           14.
                      22.
                           40.
                                 5.
                                            7.
                                                12.
                                                     30.
                                                           33.
                                                                50.
                                                                     19.
                  8.
                                       З.
 20.
      27.
           18.
                28.
                      34.
                           42.
                                41.
                                      37.
                                           32.
                                                36.
                                                     24.
                                                           26.
                                                                39.
                                                                     40.5
 68.
           38.
                43.
                      47.
                            1.
                                54.
                                      46.
                                           45.
                                                 2.
                                                      5.5 53.
                                                                37.5 57.
           55.
      72.
                66.]
                                                                         102.
total sulfur dioxide [ 34.
                              67.
                                    54.
                                           60.
                                                 40.
                                                       59.
                                                              21.
                                                                    18.
                                                                                 65.
29.
     145.
 148.
       103.
              56.
                     71.
                           37.
                                 23.
                                        11.
                                              35.
                                                    16.
                                                           82.
                                                                113.
                                                                       83.
  50.
        15.
              30.
                     19.
                           87.
                                 46.
                                        14.
                                             114.
                                                           96.
                                                                119.
                                                                       73.
                                                    12.
  45.
        10.
             110.
                     52.
                          112.
                                 39.
                                        27.
                                              94.
                                                    43.
                                                           42.
                                                                 80.
                                                                       51.
  61.
       136.
              31.
                    125.
                           24.
                                140.
                                       133.
                                              85.
                                                   106.
                                                           22.
                                                                 36.
                                                                       69.
  64.
       153.
              47.
                    108.
                          111.
                                 62.
                                        28.
                                              89.
                                                    13.
                                                           90.
                                                                134.
                                                                       99.
  26.
        63.
             105.
                     20.
                          141.
                                 88.
                                       129.
                                             128.
                                                    86.
                                                          121.
                                                                101.
                                                                       44.
   8.
        49.
              38.
                    143.
                          144.
                                127.
                                       126.
                                             120.
                                                           93.
                                                                 95.
                                                    55.
                                                                       41.
        72.
  58.
              81.
                    109.
                           33.
                                 53.
                                        98.
                                              48.
                                                    70.
                                                           25.
                                                                135.
                                                                       92.
  74.
        32.
              77.
                    165.
                           75.
                                124.
                                        78.
                                             122.
                                                    66.
                                                           68.
                                                                 17.
                                                                       91.
  76.
                    116.
                                       104.
       151.
             142.
                          149.
                                 57.
                                              84.
                                                   147.
                                                          155.
                                                                152.
                                                                        9.
 139.
       130.
                    100.
                                        79.
                                             278.
                                                   289.
                                                          160.
                                                                 77.5 131. ]
               7.
                          115.
                                  6.
                                  0.998
                                           0.9964
                                                            0.9959
density [0.9978 0.9968
                          0.997
                                                   0.9946
                                                                    0.9943
                                                                           0.9974
 0.9986 0.9969
                 0.9982
                          0.9966
                                  0.9955
                                          0.9962
                                                           0.9958 0.9993
                                                   0.9972
 0.9957 0.9975
                          0.9976
                                  0.9934
                                          0.9954
                 0.994
                                                   0.9971
                                                            0.9956
                                                                    0.9983
 0.9967
        0.9961
                0.9984
                         0.9938
                                  0.9932 0.9965
                                                   0.9963
                                                           0.996
                                                                    0.9973
 0.9988
        0.9937
                 0.9952 0.9916
                                  0.9944 0.9996
                                                   0.995
                                                            0.9981
                                                                    0.9953
 0.9924
         0.9948
                 0.99695 0.99545 0.99615 0.9994
                                                   0.99625 0.99585 0.99685
 0.99655 0.99525 0.99815 0.99745 0.9927 0.99675 0.99925 0.99565 1.00005
 0.9985
        0.99965 0.99575 0.9999
                                  1.00025 0.9987
                                                   0.99935 0.99735 0.99915
 0.9991
         1.00015 0.9997
                          1.001
                                  0.9979
                                          1.0014
                                                   1.0001 0.99855 0.99845
 0.9998
        0.99645 0.99865 0.9989
                                  0.99975 0.999
                                                   1.0015
                                                           1.0002 0.9992
                                  1.0018 0.9912 1.0022 1.0003 0.9949
 1.0008
        1.
                  1.0006
                          1.0004
         1.0032 0.9947 0.9995
                                  0.9977
                                          1.0026 1.00315 1.0021
 0.9951
 0.9922 0.9921 0.99788 1.00024 0.99768 0.99782 0.99761 0.99803 0.99785
 0.99656 0.99488 0.99823 0.99779 0.99738 0.99701 0.99888 0.99938 0.99744
 0.99668 0.99727 0.99586 0.99612 0.99676 0.99732 0.99814 0.99746 0.99708
 0.99818 0.99639 0.99531 0.99786 0.99526 0.99641 0.99264 0.99682 0.99356
 0.99386 0.99702 0.99693 0.99562 1.00012 0.99462 0.99939 0.99632 0.99976
 0.99606 0.99154 0.99624 0.99417 0.99376 0.99832 0.99836 0.99694 0.99064
 0.99672 0.99647 0.99736 0.99629 0.99689 0.99801 0.99652 0.99538 0.99594
 0.99686 0.99438 0.99357 0.99628 0.99748 0.99578 0.99371 0.99522 0.99576
 0.99552 0.99664 0.99614 0.99517 0.99787 0.99533 0.99536 0.99824 0.99577
 0.99491 1.00289 0.99743 0.99774 0.99444 0.99892 0.99528 0.99331 0.99901
```

```
0.99674 0.99512 0.99395 0.99504 0.99516 0.99604 0.99468 0.99543 0.99791
 0.99425 0.99509 0.99484 0.99834 0.99864 0.99498 0.99566 0.99408 0.99458
 0.99648 0.99568 0.99613 0.99519 0.99518 0.99592 0.99654 0.99546 0.99554
 0.99733 0.99669 0.99724 0.99643 0.99605 0.99658 0.99416 0.99712 0.99418
 0.99596 0.99556 0.99918 0.99697 0.99378 0.99162 0.99495 0.9928 0.99603
 0.99549 0.99722 0.99354 0.99635 0.99454 0.99598 0.99486 0.99007 0.99636
 0.99642 0.99584 0.99506 0.99822 0.99364 0.99514 0.99854 0.99739 0.99683
 0.99692 0.99756 0.99547 0.99859 0.99294 0.99634 0.99704 0.99258 0.99426
 0.99747 0.99784 0.99358 0.99572 0.99769 0.99534 0.99817 0.99316 0.99471
 0.99617 0.99529 0.99451 0.99479 0.99772 0.99666 0.99392 0.99388 0.99402
 0.9936 0.99374 0.99523 0.99593 0.99396 0.99698 0.9902 0.99252 0.99256
 0.99235 0.99352 0.99557 0.99394 0.9915 0.99379 0.99798 0.99341 0.9933
 0.99684 0.99524 0.99764 0.99588 0.99473 0.99616 0.99622 0.99544 0.99728
 0.99551 0.99434 0.99709 0.99384 0.99502 0.99667 0.99649 0.99716 0.99541
 0.99318 0.99346 0.99599 0.99478 0.99754 0.99439 0.99633 0.99419 0.99878
 0.99752 0.99428 0.99659 0.99677 0.99734 0.99678 0.99638 0.99922 0.99157
 0.99718 0.99621 0.99242 0.99494 0.99729 0.99414 0.99721 0.99627 0.99569
 0.99499 0.99437 0.99726 0.99456 0.99564 0.9908 0.99084 0.9935 0.99385
 0.99688 0.99619 0.99476 0.99328 0.99286 0.99914 0.99521 0.99362 0.99558
 0.99323 0.99191 0.99501 0.9929 0.99532 0.99796 0.99581 0.99608 0.99387
 0.99448 0.99589 0.99852 0.99472 0.99587 0.99332 0.99464 0.99699 0.99725
 0.99623 0.99609 0.99292 0.9942 1.00369 0.99713 0.99322 0.99706 0.99974
 0.99467 0.99236 0.99705 0.99334 0.99336 1.00242 0.99182 0.99808 0.99828
 0.99719 0.99542 0.99496 0.99344 0.99348 0.99459 0.99492 0.99508 0.99582
 0.99555 0.9941 0.99661 0.99842 0.99489 0.99665 0.99553 0.99714 0.99631
 0.99573 0.99717 0.99397 0.99646 0.99758 0.99306 0.99783 0.99765 0.99474
 0.99483 0.99314 0.99574 0.99651]
pH [3.51 3.2 3.26 3.16 3.3 3.39 3.36 3.35 3.28 3.58 3.17 3.11 3.38 3.04
 3.52 3.43 3.34 3.47 3.46 3.45 3.4 3.42 3.23 3.5 3.33 3.21 3.48 3.9
3.25 3.32 3.15 3.41 3.44 3.31 3.54 3.13 2.93 3.14 3.75 3.85 3.29 3.08
3.37 3.19 3.07 3.49 3.53 3.24 3.63 3.22 3.68 2.74 3.59 3.
 3.61 3.06 3.6 3.69 3.1 3.05 3.67 3.27 3.18 3.02 3.55 2.99 3.01 3.56
 3.03 3.62 2.88 2.95 2.98 3.09 2.86 3.74 2.92 3.72 2.87 2.89 2.94 3.66
 3.71 3.78 3.7 4.01 2.9 ]
sulphates [0.56 0.68 0.65 0.58 0.46 0.47 0.57 0.8 0.54 0.52 1.56 0.88 0.93 0.75
 1.28 0.5 1.08 0.53 0.91 0.63 0.59 0.55 0.66 0.6 0.73 0.48 0.83 0.51
0.9 1.2 0.74 0.64 0.77 0.71 0.62 0.39 0.79 0.95 0.82 1.12 1.14 0.78
 1.95 1.22 1.98 0.61 1.31 0.69 0.67 0.7 0.49 0.92 2. 0.72 1.59 0.33
 1.02 0.97 0.85 0.43 1.03 0.86 0.76 1.61 1.09 0.84 0.96 0.45 1.26 0.87
         1.36 1.18 0.89 0.98 1.13 1.04 1.11 0.99 1.07 0.44 1.06 1.05
 0.42 1.17 1.62 0.94 1.34 1.16 1.1 0.4 1.15 0.37 1.33 1.01]
alcohol [ 9.4
                     9.8
                                 10.
                                              9.5
                                                         10.5
                                                                      9.2
  9.9
              9.1
                         9.3
                                      9.
                                                  9.7
                                                             10.1
                                     10.3
 10.6
             9.6
                         10.8
                                                 13.1
                                                             10.2
 10.9
            10.7
                         12.9
                                     10.4
                                                 13.
                                                             14.
 11.5
             11.4
                         12.4
                                                 12.2
                                                             12.8
                                     11.
 12.6
            12.5
                         11.7
                                    11.3
                                                 12.3
                                                             12.
 11.9
            11.8
                         8.7
                                    13.3
                                                 11.2
                                                             11.6
```

```
11.1
             13.4
                         12.1
                                      8.4
                                                 12.7
                                                              14.9
 13.2
                                     10.03333333 9.55
                                                               8.5
             13.6
                         13.5
 11.06666667 9.56666667 10.55
                                      8.8
                                                  13.56666667 11.95
                                      9.05
                                                 10.75
              9.23333333 9.25
                                                            ]
quality [5 6 7 4 8 3]
```

2.3 Pré-processamento

```
[6]: # pandas_profiling.ProfileReport(data_raw)
```

2.4 Visualização

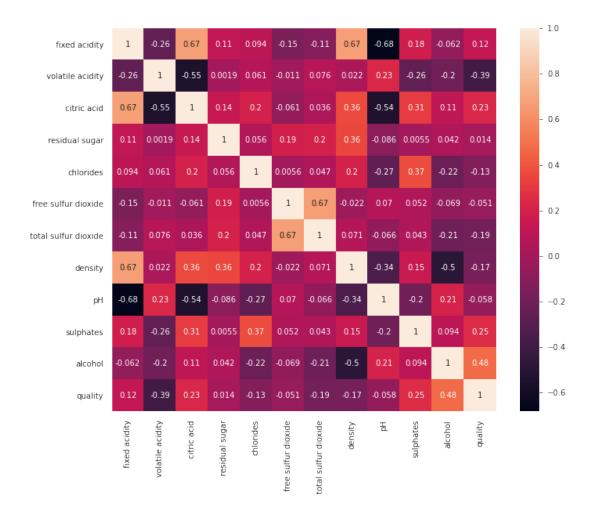
```
[7]: # sns.pairplot(data_raw)
```

```
[8]: plt.clf()
```

<Figure size 432x288 with 0 Axes>

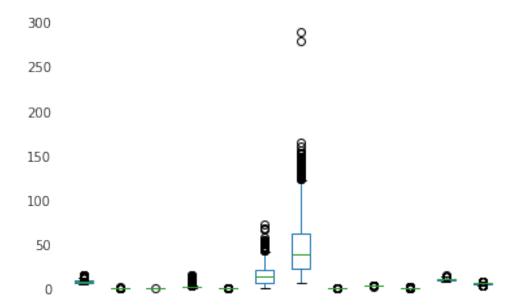
```
[9]: plt.subplots(figsize=(11, 9))
sns.heatmap(data_raw.corr(), annot=True)
```

[9]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73df4fbb38>



[10]: data_raw.plot.box()

[10]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73dcbd6898>



fixed/etaidilley eitidliet sicidal etidese istestialr solibix idetensists pHsulphatatecholouality

2.5 Escalonando

```
[11]: scaler = StandardScaler().fit(data_raw)
      data_scaled = scaler.transform(data_raw)
[12]: data_scaled_df = pd.DataFrame(data_scaled, columns=data_raw.columns)
[13]: data_scaled_df.head()
[13]:
         fixed acidity
                        volatile acidity
                                          citric acid residual sugar
                                                                        chlorides
             -0.528360
                                0.961877
                                                             -0.453218
                                                                        -0.243707
      0
                                             -1.391472
      1
             -0.298547
                                1.967442
                                             -1.391472
                                                              0.043416
                                                                         0.223875
      2
             -0.298547
                                1.297065
                                             -1.186070
                                                             -0.169427
                                                                         0.096353
      3
              1.654856
                               -1.384443
                                              1.484154
                                                             -0.453218
                                                                        -0.264960
      4
             -0.528360
                                0.961877
                                             -1.391472
                                                             -0.453218
                                                                        -0.243707
         free sulfur dioxide
                              total sulfur dioxide
                                                      density
                                                                     pH sulphates
      0
                   -0.466193
                                                                         -0.579207
                                         -0.379133 0.558274
                                                              1.288643
      1
                    0.872638
                                           0.624363 0.028261 -0.719933
                                                                           0.128950
      2
                   -0.083669
                                           0.229047
                                                     0.134264 -0.331177
                                                                         -0.048089
      3
                    0.107592
                                           0.411500
                                                    0.664277 -0.979104
                                                                         -0.461180
      4
                   -0.466193
                                          -0.379133 0.558274 1.288643
                                                                         -0.579207
          alcohol
                    quality
```

```
0 -0.960246 -0.787823

1 -0.584777 -0.787823

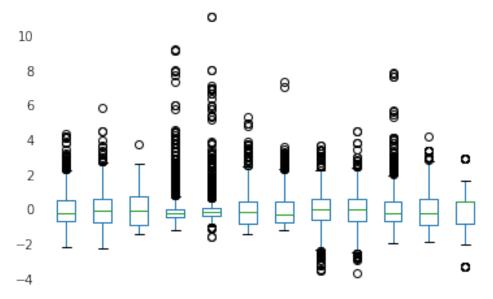
2 -0.584777 -0.787823

3 -0.584777 0.450848

4 -0.960246 -0.787823
```

```
[14]: data_scaled_df.plot.box()
```

[14]: <matplotlib.axes._subplots.AxesSubplot at 0x7f73dc2a1518>



fixed/etaitilley eitiridetsiididal efolgerisletteir stirtxiideteosiitly: pHsulphatelsohoduality

2.6 Utilidades

```
[15]: lista_metricas_treino = []
lista_metricas_teste = []

[16]: def metricas(y_true, y_pred, alg):
    r2 = r2_score(y_true, y_pred)
    eqm = mean_squared_error(y_true, y_pred)
    seq = len(y_true)*eqm
    reqm = math.sqrt(eqm)

return {'Algoritmo':alg, 'R2':r2, 'EQM':eqm, 'REQM':reqm, 'SEQ':seq}
```

2.7 Separando conjuntos de Treino e Teste

Para a separação utilizou-se do train_test_split que divide o conjunto em treino e teste aleatóriamente

```
[17]: test_attr = 'fixed acidity';
  output_attr = 'quality';
  train, test = train_test_split(data_scaled_df, test_size = 0.2, shuffle=True)

x_train = train.drop(columns=[output_attr])
y_train = train[output_attr]

x_test = test.drop(columns=[output_attr])
y_test = test[output_attr]
```

2.8 Aplicando a Regressão

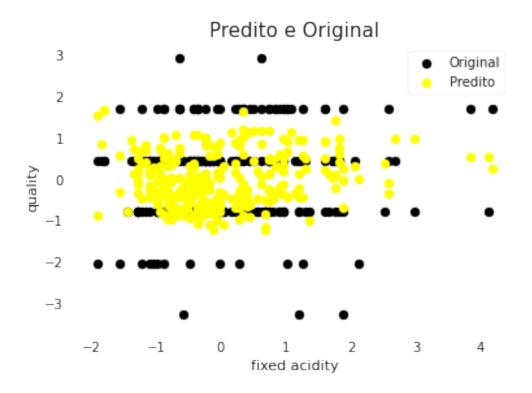
2.8.1 Regressão Linear

```
[18]: lire = LinearRegression()
[19]: lire.fit(x_train, y_train)
[19]: LinearRegression()
```

2.9 Avaliação para Teste

```
[20]: y_pred = lire.predict(x_test)
linear_metricas = metricas(y_test, y_pred, 'Regressão Linear - Teste')
lista_metricas_teste.append(linear_metricas)
```

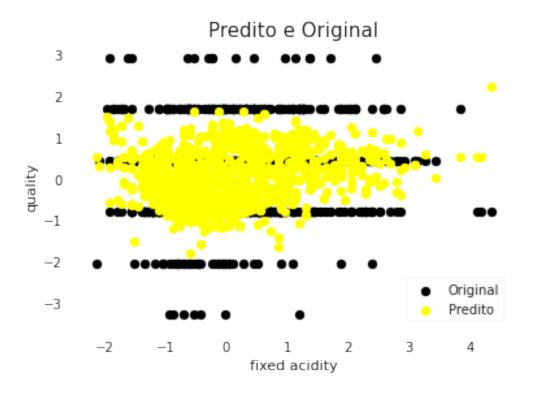
```
[21]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original', fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.10 Avaliação para Treino

```
[22]: y_pred = lire.predict(x_train)
    linear_metricas = metricas(y_train, y_pred, 'Regressão Linear - Treino')
    lista_metricas_treino.append(linear_metricas)

[23]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.11 SVR

2.11.1 Kernel RBF

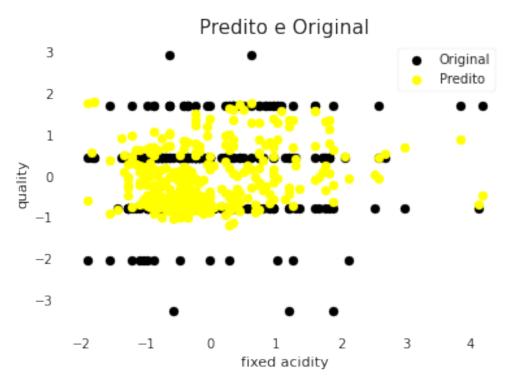
```
[24]: svr_reg = SVR(kernel='rbf')
[25]: svr_reg.fit(x_train, y_train)
[25]: SVR()
```

2.12 Avaliação para Teste

```
[26]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - RBF - Teste')
    lista_metricas_teste.append(svr_metricas)

[27]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
```

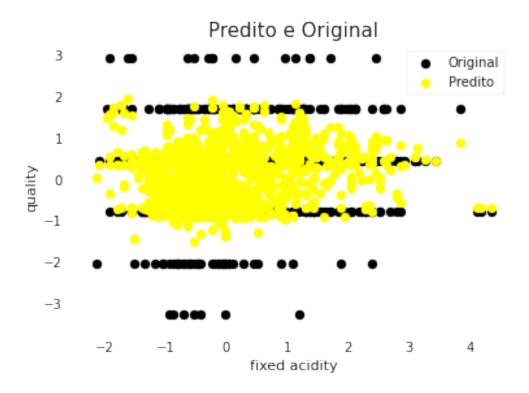
```
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
plt.show()
```



2.13 Avaliação para Treino

```
[28]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - RBF - Treino')
    lista_metricas_treino.append(svr_metricas)

[29]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



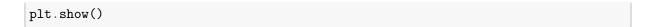
2.13.1 Kernel Linear

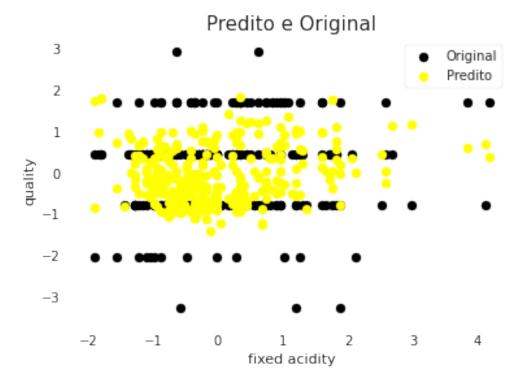
```
[30]: svr_reg = SVR(kernel='linear')
[31]: svr_reg.fit(x_train, y_train)
[31]: SVR(kernel='linear')
```

2.14 Avaliação para Teste

```
[32]: y_pred = svr_reg.predict(x_test)
metricas_svr = metricas(y_test, y_pred, 'SVR - Linear - Teste')
lista_metricas_teste.append(metricas_svr)

[33]: plt.scatter(x_test[test_attr], y_test, color='black')
plt.scatter(x_test[test_attr], y_pred, color='yellow')
plt.xlabel(test_attr)
plt.ylabel(output_attr)
plt.title('Predito e Original',fontsize=15)
plt.legend(['Original', 'Predito'])
```

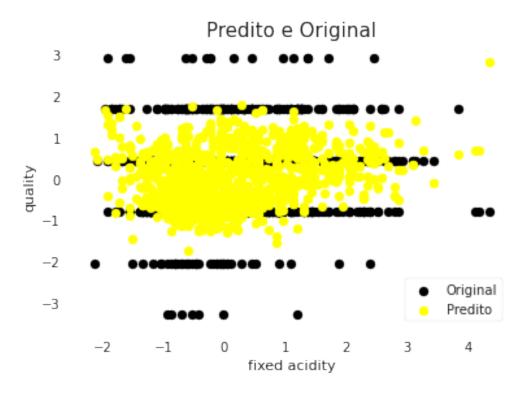




2.15 Avaliação para Treino

```
[34]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Linear - Treino')
    lista_metricas_treino.append(svr_metricas)

[35]: plt.scatter(x_train[test_attr], y_train, color='black')
    plt.scatter(x_train[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.15.1 Kernel Sigmoide

```
[36]: train, test = train_test_split(data_raw, test_size = 0.2, shuffle=True)
    x_train_sig = train.drop(columns=[output_attr])
    y_train_sig = train[output_attr]
    x_test_sig = test.drop(columns=[output_attr])
    y_test_sig = test[output_attr]

[37]: svr_reg = SVR(kernel='sigmoid')

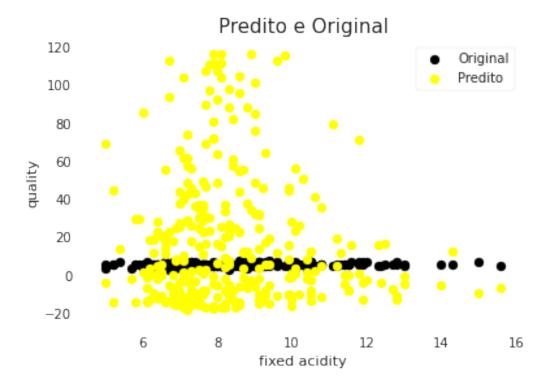
[38]: svr_reg.fit(x_train_sig , y_train_sig )

[38]: SVR(kernel='sigmoid')
```

2.16 Avaliação para Teste

```
[39]: y_pred_sig = svr_reg.predict(x_test_sig)
    metricas_svr = metricas(y_test_sig , y_pred_sig , 'SVR - Sigmoide - Teste')
    lista_metricas_teste.append(metricas_svr)

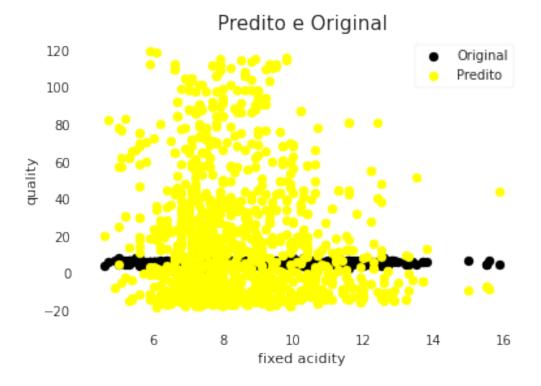
[40]: plt.scatter(x_test_sig [test_attr], y_test_sig , color='black')
    plt.scatter(x_test_sig [test_attr], y_pred_sig , color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.17 Avaliação para Treino

```
[41]: y_pred_sig = svr_reg.predict(x_train_sig)
    svr_metricas = metricas(y_train_sig , y_pred_sig , 'SVR - Sigmoide - Treino')
    lista_metricas_treino.append(svr_metricas)
```

```
[42]: plt.scatter(x_train_sig [test_attr], y_train_sig , color='black')
    plt.scatter(x_train_sig [test_attr], y_pred_sig , color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



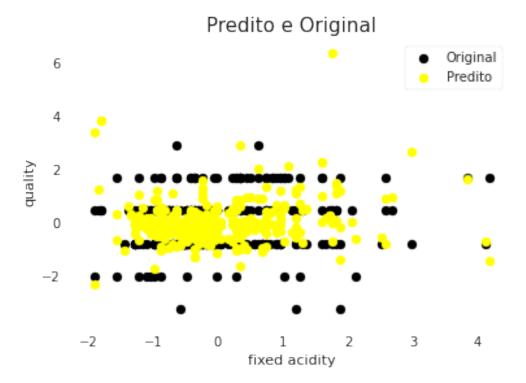
2.17.1 Kernel Polinomial

```
[43]: svr_reg = SVR(kernel='poly', degree=3)
[44]: svr_reg.fit(x_train, y_train)
[44]: SVR(kernel='poly')
```

2.18 Avaliação para Teste

```
[45]: y_pred = svr_reg.predict(x_test)
    svr_metricas = metricas(y_test, y_pred, 'SVR - Polinomial - Teste')
    lista_metricas_teste.append(svr_metricas)

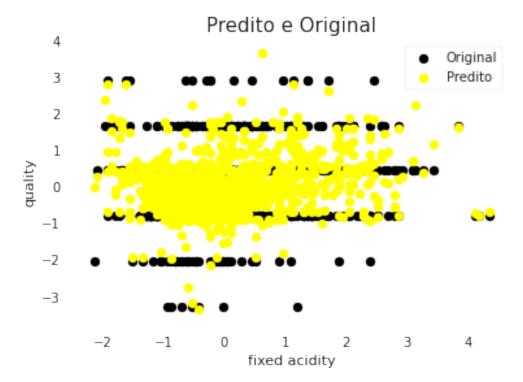
[46]: plt.scatter(x_test[test_attr], y_test, color='black')
    plt.scatter(x_test[test_attr], y_pred, color='yellow')
    plt.xlabel(test_attr)
    plt.ylabel(output_attr)
    plt.title('Predito e Original',fontsize=15)
    plt.legend(['Original', 'Predito'])
    plt.show()
```



2.19 Avaliação para Treino

```
[47]: y_pred = svr_reg.predict(x_train)
    svr_metricas = metricas(y_train, y_pred, 'SVR - Polinomial - Treino')
    lista_metricas_treino.append(svr_metricas)
```

```
[48]: plt.scatter(x_train[test_attr], y_train, color='black')
   plt.scatter(x_train[test_attr], y_pred, color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original',fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```



2.20 Redes Neurais

2.20.1 Kernel Linear

```
[49]: mlp_reg = MLPRegressor()

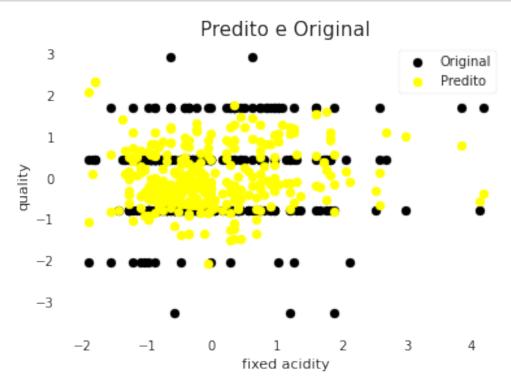
[50]: mlp_reg.fit(x_train, y_train)

[50]: MLPRegressor()
```

2.21 Avaliação para Teste

```
[51]: y_pred = mlp_reg.predict(x_test)
mlp_metricas = metricas(y_test, y_pred, 'MLP - Teste')
lista_metricas_teste.append(mlp_metricas)
```

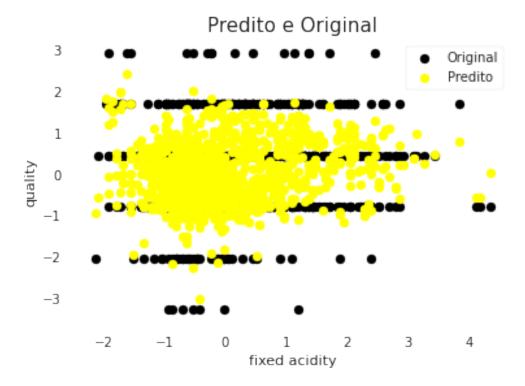
```
[52]: plt.scatter(x_test[test_attr], y_test, color='black')
   plt.scatter(x_test[test_attr], y_pred, color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original',fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```



2.22 Avaliação para Treino

```
[53]: y_pred = mlp_reg.predict(x_train)
mlp_metricas = metricas(y_train, y_pred, 'MLP - Treino')
lista_metricas_treino.append(mlp_metricas)
```

```
[54]: plt.scatter(x_train[test_attr], y_train, color='black')
   plt.scatter(x_train[test_attr], y_pred, color='yellow')
   plt.xlabel(test_attr)
   plt.ylabel(output_attr)
   plt.title('Predito e Original',fontsize=15)
   plt.legend(['Original', 'Predito'])
   plt.show()
```



3 Resultados

```
[55]: metricas_teste = pd.DataFrame(lista_metricas_teste)
      metricas_teste
[55]:
                        Algoritmo
                                             R2
                                                         EQM
                                                                   REQM \
        Regressão Linear - Teste
                                      0.322617
                                                    0.708590
                                                               0.841778
     0
                SVR - RBF - Teste
      1
                                       0.385657
                                                    0.642646
                                                               0.801652
             SVR - Linear - Teste
                                                    0.728427
      2
                                       0.303653
                                                               0.853480
           SVR - Sigmoide - Teste -1955.626553
      3
                                                1316.117972
                                                              36.278340
       SVR - Polinomial - Teste
                                       0.099509
                                                    0.941977
                                                               0.970555
                      MLP - Teste
                                       0.375016
                                                    0.653777
                                                               0.808565
```

```
SEQ
     0
            226.748957
            205.646758
      1
      2
            233.096752
      3
       421157.751023
      4
            301.432642
      5
            209.208543
[56]: metricas_teste = round(metricas_teste, 3)
[57]: metricas_teste
[57]:
                                                          REQM
                        Algoritmo
                                          R2
                                                   EQM
                                                                        SEQ
         Regressão Linear - Teste
                                                         0.842
                                       0.323
                                                 0.709
                                                                    226.749
                SVR - RBF - Teste
      1
                                       0.386
                                                 0.643
                                                         0.802
                                                                   205.647
             SVR - Linear - Teste
      2
                                       0.304
                                                 0.728
                                                         0.853
                                                                    233.097
      3
           SVR - Sigmoide - Teste -1955.627
                                              1316.118
                                                        36.278
                                                                421157.751
      4 SVR - Polinomial - Teste
                                                 0.942
                                       0.100
                                                         0.971
                                                                   301.433
      5
                      MLP - Teste
                                       0.375
                                                 0.654
                                                         0.809
                                                                    209.209
[58]: metricas_teste.to_excel('wine_metricas_teste.xlsx')
[59]: metricas_treino = pd.DataFrame(lista_metricas_treino)
      metricas_treino
[59]:
                                              R2
                                                          EQM
                                                                     REQM \
                         Algoritmo
        Regressão Linear - Treino
                                        0.366947
                                                     0.625541
                                                                0.790911
                SVR - RBF - Treino
                                                                0.677337
      1
                                       0.535704
                                                     0.458786
      2
             SVR - Linear - Treino
                                       0.354539
                                                     0.637801
                                                                0.798625
      3
           SVR - Sigmoide - Treino -2007.247559
                                                  1298.276549
                                                               36.031605
        SVR - Polinomial - Treino
      4
                                       0.472925
                                                     0.520820
                                                                0.721679
                      MLP - Treino
      5
                                        0.592636
                                                     0.402530
                                                                0.634453
                  SEQ
      0 8.000668e+02
      1 5.867869e+02
      2 8.157479e+02
      3 1.660496e+06
      4 6.661287e+02
      5 5.148359e+02
[60]: metricas_treino = round(metricas_treino, 3)
[61]: metricas_treino.to_excel('wine.xlsx')
```