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1 Linear Model Selection and Regularization

1.Generate a data set with p = 20 features, n = 1000 observations, and an associated quantitative response vector generated according to the model

$$Y = X\beta + \epsilon$$

where β has some elements that are exactly equal to zero.

```
[19]: import numpy as np
  import itertools
  import pandas as pd
  import matplotlib.pyplot as plt
  import statsmodels.api as sm
  from sklearn.model_selection import train_test_split
  from sklearn.linear_model import LinearRegression
  from sklearn.metrics import mean_squared_error
  from mlxtend.feature_selection import SequentialFeatureSelector as SFS
  from sklearn.model_selection import GridSearchCV
  from sklearn.linear_model import Ridge
  from sklearn.linear_model import Lasso
  from sklearn.linear_model import ElasticNet
  np.random.seed(24)
```

```
[2]: # first, we randomly generate 20 features with 1000 observations
X = []
for _ in range(20):
    X.append(np.random.normal(np.random.choice(100,1), 1, 1000))
X = np.array(X)
```

```
for n in np.random.choice(20,5):
    Beta[n] = 0
    zero_index.append(n)

# check beta
Beta = np.array(Beta)
Beta = Beta.reshape(-1,1)
Beta

# note that we have kept the beta = 0 information in zero_index
```

```
[3]: array([[0.
                         ],
             [7.41212581],
             [8.09098401],
             [3.68270568],
             ГО.
                        ],
             [4.53731565],
             [9.0219442],
             [0.71447831],
             [2.10138621],
             [6.86903874],
             [0.
                         ],
             [1.96584887],
             [9.85123182],
             [6.30804308],
             [0.42835617],
             [8.25425396],
             [0.
                         ],
             [8.11969394],
             [7.67387209],
             ΓΟ.
                        ]])
```

```
[4]: # finally, create Y
# use broadcasting
Y = X * Beta
# generate error: with mean = 0, sd = 10
error = np.random.normal(0,10,1000)
Y = np.sum(Y, axis=0) + error
```

2.Split your data set into a training set containing 100 observations and a test set containing 900 observations.

```
[5]: # create a dataframe containing Y and X
Xt = X.transpose()
df = pd.DataFrame({'Y':Y})
for n in range(0,20):
    df['X{}'.format(n)] = Xt[:,n]
```

```
[5]:
                  Y
                            XΟ
                                       Х1
                                                  Х2
                                                              ХЗ
                                                                         Х4
                     33.771182
                                95.932867
                                           67.736543
                                                      52.220935
       4707.633622
                                                                 12.539658
       4667.831605
                     33.894806
                                94.071022 66.757592 50.726081
                                                                 12.705394
     1
     2 4709.137224
                     35.487894
                                95.383519
                                           67.634304
                                                      51.974740
                                                                 13.004285
     3 4677.981952
                     34.046731
                                93.676851 68.747795 50.745773
                                                                 11.456581
     4 4708.148487
                     36.323789
                                93.901247 68.072361
                                                      50.108320
                                                                 11.592697
               Х5
                          Х6
                                     Х7
                                                Х8
                                                               X10
                                                                           X11
        20.860180
                   42.636533
                              12.114676
                                         72.888851
                                                    . . .
                                                         26.157619
                                                                    75.434748
       19.889749
                   40.640765
                              12.149863
                                         70.991400
                                                         27.466977
                                                                    75.355861
     1
                                                    . . .
                                         71.200583
     2 21.134597
                   41.584655
                              12.629108
                                                         27.244833
                                                                    73.746079
                                                    . . .
     3 23.047611
                  41.068100
                              10.311666
                                         73.056294
                                                    . . .
                                                         28.034128
                                                                    73.104750
     4 22.659707
                   42.416513
                              11.340568
                                         72.633341
                                                         26.507698
                                                                    74.296530
                                                    . . .
                                                          X16
              X12
                         X13
                                    X14
                                               X15
                                                                     X17
       54.385360
                   35.092312
                                         59.300054
                                                    28.214382
                              62.661170
                                                               56.909681
       54.587197
                   34.028896
                              60.410975
                                         60.129402
                                                    26.831438 58.587753
     1
     2 54.553417
                   34.193719
                              61.728457
                                         61.885028
                                                    27.077562 57.150222
     3 53.587076
                   33.125989
                                                    27.240666 55.608992
                              62.532450
                                         59.693219
     4 55.103520
                   35.013668
                              61.938490
                                         59.159034
                                                    27.542115 57.361038
              X18
                         X19
        32.762930
                   11.025487
       35.306703
                  11.370518
      34.742751
                    9.815837
     3 36.655743 12.631524
     4 33.358290 11.258816
     [5 rows x 21 columns]
[6]: X = df.drop(['Y'], axis=1)
     Y = df['Y']
     X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size = 0.9)
[7]: # check X_train shape
     X_train.shape
```

df.head(5)

[7]: (100, 20)

3.Perform best subset selection on the training set, and plot the training set MSE associated with the best model of each size. For which model size does the training set MSE take on its minimum value?

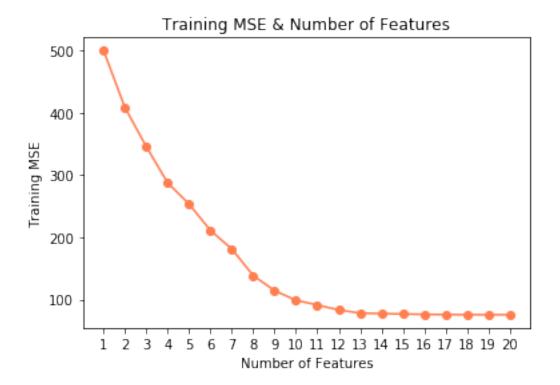
```
[8]: def best_subset (X, y):
    res = {}
```

```
for k in range (1,6):
              for each in itertools.combinations(X, k):
                  X_full = sm.add_constant(X[list(each)])
                  lm = sm.OLS(y, X_full).fit()
                  mse = lm.mse_resid
                  if k not in res.keys() or mse < res[k][1]:
                      res[k] = [each, mse]
          return res
[20]: result = best_subset(X_train, y_train)
     //anaconda3/lib/python3.7/site-packages/numpy/core/fromnumeric.py:2389:
     FutureWarning: Method .ptp is deprecated and will be removed in a future
     version. Use numpy.ptp instead.
       return ptp(axis=axis, out=out, **kwargs)
[10]: result
[10]: {1: [('X18',), 509.8681335035226],
       2: [('X12', 'X18'), 420.6992067860652],
       3: [('X12', 'X17', 'X18'), 359.85352401386166],
      4: [('X12', 'X15', 'X17', 'X18'), 302.3414129350472],
       5: [('X9', 'X12', 'X15', 'X17', 'X18'), 269.5070301760166]}
[11]: sfs = SFS(LinearRegression(), k_features=5, forward=True, scoring =__
      sfs.fit(X_train, y_train)
      sfs.k_feature_names_
[11]: ('X9', 'X12', 'X15', 'X17', 'X18')
[12]: # since the computational load for best subset selection is so high, we can use
      → forward selection to sustitute best subset
      # this is due to we are convinced that all the features were independently and \Box
      \rightarrow randomly generated
      result_n = {}
      for n in range (1,21):
          sfs = SFS(LinearRegression(), k_features=n, forward=True, scoring =_u

¬'neg_mean_squared_error', cv=0)
          sfs.fit(X_train, y_train)
          result_n[len(sfs.k_feature_names_)] = - sfs.k_score_
      result_n
[12]: {1: 499.670770833451,
       2: 408.0782305824839,
       3: 345.4593830533083,
       4: 287.2243422882952,
```

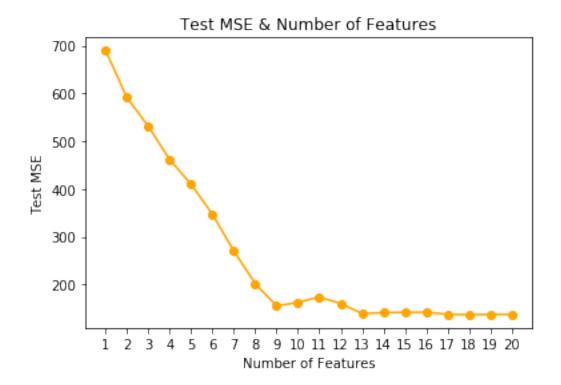
```
5: 253.33660836545536,
6: 210.960909775253,
7: 181.1896416015844,
8: 138.63140592406535,
9: 114.30884282186533,
10: 98.90705973623922,
11: 91.33150126120103,
12: 83.37011237866305,
13: 78.26657924587751,
14: 77.48658605515386,
15: 76.91620595014322,
16: 76.27295046607294,
17: 75.88961818249493,
18: 75.73377362717241,
19: 75.66394279406703,
20: 75.66166894726723}
```

We can see that the MSE monotonically decreases as the number of predictors increases. The model that includes all the variables have the lowest MSE.



4.Plot the test set MSE associated with the best model of each size.

```
[21]: result_test = {}
for n in range (1,21):
    sfs = SFS(LinearRegression(), k_features=n, forward=True, scoring =
    'neg_mean_squared_error', cv=0)
    sfs.fit(X_train, y_train)
    lm = LinearRegression().fit(X_train[list(sfs.k_feature_names_)], y_train)
    result_test[sfs.k_feature_names_] = mean_squared_error(lm.
    predict(X_test[list(sfs.k_feature_names_)]), y_test)
```



5.For which model size does the test set MSE take on its minimum value? Comment on your results

```
[14]: result_test
[14]: {('X18',): 689.5460159571702,
       ('X12', 'X18'): 591.2393811718593,
       ('X12', 'X17', 'X18'): 531.2964732098586,
       ('X12', 'X15', 'X17', 'X18'): 461.35689807785906,
       ('X9', 'X12', 'X15', 'X17', 'X18'): 409.9729576218823,
       ('X2', 'X9', 'X12', 'X15', 'X17', 'X18'): 347.25063341145824,
       ('X2', 'X6', 'X9', 'X12', 'X15', 'X17', 'X18'): 270.4397176916692,
       ('X1', 'X2', 'X6', 'X9', 'X12', 'X15', 'X17', 'X18'): 202.4318215626645,
       ('X1',
        'X2',
        'X6',
        'X9',
        'X12',
        'X13',
        'X15',
        'X17',
        'X18'): 155.23704729305297,
       ('X1',
        'X2',
```

```
'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X15',
 'X17',
 'X18'): 162.9525230580034,
('X1',
 'X2',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X15',
 'X16',
 'X17',
 'X18'): 173.86069977498698,
('X1',
 'X2',
 'X5',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X15',
 'X16',
 'X17',
 'X18'): 160.51457171053048,
('X1',
 'X2',
 'ХЗ',
 'X5',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X15',
 'X16',
 'X17',
 'X18'): 139.36621585309246,
('XO',
 'X1',
 'X2',
```

```
'X3',
 'X5',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X15',
 'X16',
 'X17',
 'X18'): 141.50144237019364,
('XO',
'X1',
 'X2',
 'X3',
 'X5',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
 'X18'): 141.89538526960015,
('XO',
 'X1',
 'X2',
 'X3',
 'X4',
 'X5',
 'X6',
 'X9',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
 'X18'): 142.40940833761636,
('XO',
 'X1',
 'X2',
 'X3',
 'X4',
```

```
'X5',
 'X6',
 'X8',
 'X9',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
 'X18'): 137.86452108442697,
('XO',
 'X1',
 'X2',
 'ХЗ',
 'X4',
 'X5',
 'X6',
 'X8',
 'X9',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
 'X18',
 'X19'): 137.03646625796628,
('XO',
 'X1',
 'X2',
 'X3',
 'X4',
 'X5',
 'X6',
 'X7',
 'X8',
 'X9',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
```

```
'X18',
 'X19'): 137.68837233638956,
('XO',
 'X1',
 'X2',
 'X3',
 'X4',
 'X5',
 'X6',
 'X7',
 'X8'.
 'X9',
 'X10',
 'X11',
 'X12',
 'X13',
 'X14',
 'X15',
 'X16',
 'X17',
 'X18',
 'X19'): 137.745095532462}
```

'X0','X1','X2','X3','X4','X5','X6','X8','X9','X11','X12','X13','X14','X15','X16','X17','X18','X19' compose the model that produces the lowest MSE.

6.How does the model at which the test set MSE is minimized compare to the true model used to generate the data? Comment on the coefficient sizes.

```
[15]: array([ 0.15306324, 7.39989836, 7.96820064, 3.18239778, -0.25892266, 4.21550617, 9.40403319, 2.74606066, 7.26016452, 1.61416783, 9.90378175, 6.73563248, 0.19929759, 8.57069405, -0.39267453, 8.26137323, 7.49143639, 0.01921556])
```

The model estimated using best subset selection is Y = 0.153X0 + 7.40X1 + 7.97X2 + 3.18X3 + 0.26X4 + 4.22X5 + 9.40X6 + 2.75X8 + 7.26X9 + 1.61X11 + 9.90X12 + 6.74X13 + 0.20X14 + 8.57X15 + 0.39X16 + 8.28X17 + 7.49X18 + 0.02X19 + error

The true model that we generate is: Y = 7.41X1 + 8.09X2 + 3.68X3 + 4.54X5 + 9.02X6 + 0.71X7 + 2.10X8 + 6.87X9 + 1.97X11 + 9.85X12 + 6.31X13 + 0.43X14 + 8.25X15 + 8.12X17 + 7.67X18

For the predictors missed or added by the estimated model, they all have small coefficients. The overlapped coefficients are very similar from the two models.

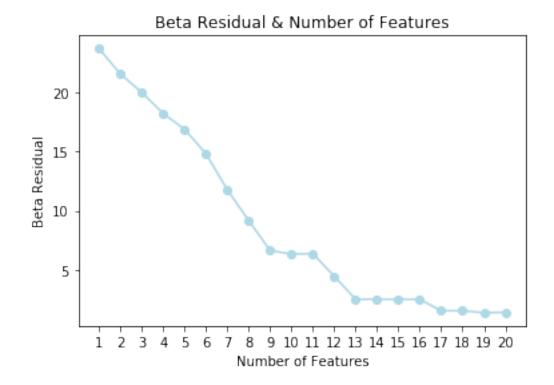
7. Create a plot displaying

$$\sqrt{\sum_{j=1}^{p}(\beta_{j}-\hat{\beta}_{j}^{r})^{2}}$$

for a range of values of r, where $\hat{\beta}_j^r$ is the jth coefficient estimate for the best model containing r coefficients. Comment on what you observe. How does this compare to the test MSE plot?

```
[16]: Beta
[16]: array([[0.
             [7.41212581],
             [8.09098401],
             [3.68270568],
             [0.
                         ],
             [4.53731565],
             [9.0219442],
             [0.71447831],
              [2.10138621],
             [6.86903874],
             ГО.
                         ],
             [1.96584887],
             [9.85123182],
             [6.30804308],
             [0.42835617],
              [8.25425396],
             [0.
                         ],
             [8.11969394],
             [7.67387209],
             [0.
                         ]])
[17]: # get the coefficient for each r
      Beta_n = Beta.ravel()
      coef_hat = {}
      for key, value in result_test.items():
          lm = LinearRegression().fit(X[list(key)], Y)
          coef_hat[key] = lm.coef_
      # compute the square root of sum of beta residual squared for each model
      Beta_res = {}
      for key, value in coef_hat.items():
          zero = np.zeros(20)
          for n in range(len(value)):
              zero[int(df.columns.get_loc(key[n])) - 1] = value[n]
          Beta_res[len(key)] = (((Beta_n - zero) ** 2).sum()) ** 0.5
      Beta_res
      # the key represents how many features are included in the model
```

```
[17]: {1: 23.729779786514,
       2: 21.590407945846284,
       3: 20.017667712533186,
       4: 18.241414276066724,
       5: 16.90109050027116,
       6: 14.840306986506496,
       7: 11.77776854843948,
       8: 9.176623860557708,
       9: 6.632625661480814,
       10: 6.332061782435096,
       11: 6.369344481609852,
       12: 4.460600790391436,
       13: 2.504324563157582,
       14: 2.5108489418470814,
       15: 2.4966200932697684,
       16: 2.5028397896612766,
       17: 1.5350109630372342,
       18: 1.5344099584444775,
       19: 1.366216585737508,
       20: 1.4105674478420807}
[18]: Beta_rss = []
      for value in Beta_res.values():
          Beta_rss.append(value)
      plt.plot(feature_num, Beta_rss, marker='o', color='lightblue')
      plt.xlabel('Number of Features')
      plt.ylabel('Beta Residual')
      plt.title('Beta Residual & Number of Features');
```



The graph suggests an overall downward trend in Beta residuals, but if we check the data computed above, we can find that 19 features yield the lowest Beta residual. Note that the true model contains 15 features, and the model with 15 features has indeed very low Beta residual (second lowest). The reason why the 14-feature model is the lowest is possibly due to the size of training set being too small and test set being too large, along with the irreducible error.

2 Application Exercises

```
[313]: gss_train = pd.read_csv('gss_train.csv')
       gss_test = pd.read_csv('gss_test.csv')
       gss_train.head(5)
[313]:
           age
                attend
                         authoritarianism
                                              black
                                                      born
                                                             childs
                                                                     colath
                                                                              colrac
                                                                                        colcom
            21
       0
                      0
                                          4
                                                  0
                                                         0
                                                                  0
                                                                           1
                                                                                    1
       1
            42
                      0
                                          4
                                                  0
                                                         0
                                                                  2
                                                                           0
                                                                                    1
                                                                                             1
       2
            70
                      1
                                           1
                                                  1
                                                         0
                                                                  3
                                                                           0
                                                                                    1
                                                                                             1
                                          2
                                                                  2
       3
            35
                      3
                                                  0
                                                         0
                                                                           0
                                                                                    1
                                                                                             0
            24
                                                  0
                                                                  3
                      3
                                                                                             0
           colmil
                         zodiac_GEMINI
                                          zodiac_CANCER zodiac_LEO
                                                                         zodiac_VIRGO
       0
                1
       1
                0
                                       0
                                                        0
                                                                      0
                                                                                      0
       2
                                       0
                                                        0
                                                                      0
                                                                                      0
```

```
3
                               0
                                                             0
                                                                             0
        1 ...
4
                                                                             0
        0
                                                             0
   zodiac_LIBRA zodiac_SCORPIO
                                    zodiac_SAGITTARIUS
                                                          zodiac_CAPRICORN \
0
               0
               0
                                 0
                                                       0
                                                                           0
1
2
               0
                                 0
                                                       0
                                                                           0
3
               0
                                 1
                                                       0
                                                                           0
4
               0
                                                       0
                                 1
                                                                           0
   zodiac_AQUARIUS zodiac_PISCES
0
                  0
1
                   0
                                   0
2
                   0
                                   0
3
                   0
                                   0
4
                   0
                                   0
```

[5 rows x 78 columns]

1. Fit a least squares linear model on the training set, and report the test MSE.

```
[318]: X_train = gss_train.drop(['egalit_scale'], axis=1)
    X_test = gss_test.drop(['egalit_scale'], axis=1)
    y_train = gss_train['egalit_scale']
    y_test = gss_test['egalit_scale']
    lm = LinearRegression().fit(X_train, y_train)
    MSE = mean_squared_error(lm.predict(X_test), y_test)
    print('The test MSE for linear model is', MSE)
```

The test MSE for linear model is 63.213629623014995

2. Fit a ridge regression model on the training set, with λ chosen by 10-fold cross-validation. Report the test MSE.

```
[327]: parameters = {'alpha': [1e-15, 1e-10, 1e-8, 1e-4, 1e-3, 1e-2, 1, 5, 10, 20]}
ridge_regressor = GridSearchCV(Ridge(), parameters,
→scoring='neg_mean_squared_error', cv=10)
ridge_regressor.fit(X_train, y_train)
print('The best alpha value is', ridge_regressor.best_params_)
print('The training MSE is', -ridge_regressor.best_score_)
```

The best alpha value is {'alpha': 20} The training MSE is 61.148463225383004

```
[325]: MSE = mean_squared_error(ridge_regressor.predict(X_test), y_test)
print('The test MSE for ridge regression is', MSE)
```

The test MSE for ridge regression is 62.298944127974785

3. Fit a lasso regression on the training set, with λ chosen by 10-fold cross-validation. Report the test MSE, along with the number of non-zero coefficient estimates.

```
[334]: parameters = {'alpha': [1e-15, 1e-10, 1e-8, 1e-4, 1e-3, 1e-2, 1, 5, 10, 20]}
lasso_regressor = GridSearchCV(Lasso(), parameters,

⇒scoring='neg_mean_squared_error', cv=10)
lasso_regressor.fit(X_train, y_train)
print('The best alpha value is', lasso_regressor.best_params_)
print('The training MSE is', -lasso_regressor.best_score_)
```

The best alpha value is {'alpha': 0.01} The training MSE is 61.37196490960359

```
[329]: MSE = mean_squared_error(lasso_regressor.predict(X_test), y_test)
print('The test MSE for lasso regression is', MSE)
```

The test MSE for lasso regression is 62.37909680839509

```
[341]: lasso = Lasso(alpha=0.01)
    lasso.fit(X_train, y_train)
    print('There are',(lasso.coef_ != 0).sum(),'non-zero coefficient estimates in
    →the lasso regression.')
```

There are 65 non-zero coefficient estimates in the lasso regression.

4.Fit an elastic net regression model on the training set, with α and λ chosen by 10-fold cross-validation. That is, estimate models with $\alpha = 0, 0.1, 0.2, \ldots, 1$ using the same values for λ across each model. Select the combination of α and λ with the lowest cross-validation MSE. For that combination, report the test MSE along with the number of non-zero coefficient estimates.

```
The best alpha value is {'alpha': 1e-15, 'l1_ratio': 0.1}
The training MSE at l1_ratio = 0.1 and alpha(lambda) = 1e-15 is 62.357446358210225
The best alpha value is {'alpha': 1e-10, 'l1_ratio': 0.1}
The training MSE at l1_ratio = 0.1 and alpha(lambda) = 1e-10 is 62.357446293984346
The best alpha value is {'alpha': 1e-08, 'l1_ratio': 0.1}
```

```
The training MSE at 11_ratio = 0.1 and alpha(lambda) = 1e-08 is
      62.357439935622324
      The best alpha value is {'alpha': 0.0001, 'l1_ratio': 0.1}
      The training MSE at 11_ratio = 0.1 and alpha(lambda) = 0.0001 is
      62.298858480534875
      The best alpha value is {'alpha': 0.001, 'l1_ratio': 0.1}
      The training MSE at l1_ratio = 0.1 and alpha(lambda) = 0.001 is
      62.00028310967855
      The best alpha value is {'alpha': 0.01, 'l1_ratio': 0.1}
      The training MSE at l1_ratio = 0.1 and alpha(lambda) = 0.01 is 61.30512590261391
      The best alpha value is {'alpha': 1, 'l1_ratio': 0.1}
      The training MSE at 11_ratio = 0.1 and alpha(lambda) = 1 is 65.98844258107927
      The best alpha value is {'alpha': 5, 'l1_ratio': 0.1}
      The training MSE at 11_ratio = 0.1 and alpha(lambda) = 5 is 76.22947380485463
      The best alpha value is {'alpha': 10, 'l1_ratio': 0.1}
      The training MSE at 11_ratio = 0.1 and alpha(lambda) = 10 is 81.05727865324738
      The best alpha value is {'alpha': 20, 'l1_ratio': 0.1}
      The training MSE at l1_ratio = 0.1 and alpha(lambda) = 20 is 85.19674518831349
[353]: # from the above CV training MSE, we get the lowest MSE at 11 ration = 0.1 and \Box
       \rightarrow alpha(lambda) = 0.01
       # now we can fit the model to the test set
      en = ElasticNet(l1_ratio=0.1, alpha=0.01)
      en.fit(X_train, y_train)
      MSE = mean_squared_error(en.predict(X_test), y_test)
      print('The test MSE for elastic net regression is', MSE)
      print('There are', (en.coef_ != 0).sum(), 'non-zero coefficient estimates in the_
        →elastic net regression.')
```

The test MSE for elastic net regression is 62.3801287740633 There are 76 non-zero coefficient estimates in the elastic net regression.

5. Comment on the results obtained. How accurately can we predict an individual's egalitarianism? Is there much difference among the test errors resulting from these approaches?

All models achieved similar test MSE, with ridge being the best and OLS being the worst, but the margin is within 1. Generally, we get a MSE at around 62, which is not so far from the training data, showing that we are not overfitting. Whether there exist better models deserves a further discussion.