hw1

October 1, 2019

1. name: Yi-Ping Tseng
2. uni: yt2690
3. email: yiping.t@columbia.edu
4. collaborate with: Zihui Zhou (uni: zz2694)

[1]:
```python
import numpy as np
import pandas as pd
from sklearn.model_selection import KFold
from scipy.optimize import minimize
import matplotlib.pyplot as plt
%matplotlib inline
```

[ ]:
```python

```

0.0.1 Setup - Preprocessed Data

randomly split dataset into train and test set by using `pandas` and `sklearn.model_selection`

[2]:
```python
data = pd.read_csv("winequalityred.csv", sep=";")
y = ["quality"]
x = data.drop(y, axis=1).columns.values

print("features: ", x)
print("target: ", y)
print("data shape: ", data.shape)
data.head(3)
```

```
features:  ['fixed acidity' 'volatile acidity' 'citric acid' 'residual sugar'
 'chlorides' 'free sulfur dioxide' 'total sulfur dioxide' 'density' 'pH'
 'sulphates' 'alcohol']
target:  ['quality']
data shape:  (1599, 12)
```

[2]:
```
   fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0            7.4              0.70         0.00             1.9      0.076
1            7.8              0.88         0.00             2.6      0.098
2            7.8              0.76         0.04             2.3      0.092
```

	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	

	alcohol	quality
0	9.4	5
1	9.8	5
2	9.8	5

[3]:
```
seed = 100
kf = KFold(shuffle=False, n_splits=5, random_state=seed)
for trainIdx, testIdx in kf.split(data):
    X_train, X_test = data[x].iloc[trainIdx], data[x].iloc[testIdx]
    y_train, y_test = data[y].iloc[trainIdx], data[y].iloc[testIdx]
```

[4]:
```
print(X_train.shape, y_train.shape)
pd.concat([X_train.head(3), y_train.head(3)], axis=1)
```

(1280, 11) (1280, 1)

[4]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	\
0	7.4	0.70	0.00	1.9	0.076	
1	7.8	0.88	0.00	2.6	0.098	
2	7.8	0.76	0.04	2.3	0.092	

	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	

	alcohol	quality
0	9.4	5
1	9.8	5
2	9.8	5

[5]:
```
X_train.describe()
```

[5]:

	fixed acidity	volatile acidity	citric acid	residual sugar	\
count	1280.000000	1280.000000	1280.000000	1280.000000	
mean	8.577891	0.518984	0.289297	2.561328	
std	1.768994	0.177994	0.196441	1.311638	
min	4.600000	0.120000	0.000000	0.900000	
25%	7.300000	0.390000	0.120000	1.900000	
50%	8.200000	0.500000	0.280000	2.200000	
75%	9.600000	0.630000	0.450000	2.600000	
max	15.900000	1.330000	1.000000	15.500000	

```
       chlorides  free sulfur dioxide  total sulfur dioxide      density  \
count  1280.000000          1280.000000           1280.000000  1280.000000
mean      0.088838            15.448438             46.794531     0.996971
std       0.047896            10.320531             33.592566     0.001893
min       0.012000             1.000000              6.000000     0.990070
25%       0.071000             7.000000             21.000000     0.995900
50%       0.080000            13.000000             38.000000     0.996990
75%       0.092000            21.000000             63.000000     0.998030
max       0.611000            72.000000            289.000000     1.003200

                pH   sulphates      alcohol
count  1280.000000  1280.000000  1280.000000
mean      3.299641     0.663711    10.400391
std       0.155147     0.174030     1.095970
min       2.740000     0.330000     8.400000
25%       3.200000     0.560000     9.500000
50%       3.300000     0.620000    10.100000
75%       3.392500     0.730000    11.100000
max       3.900000     2.000000    14.900000
```

[6]:

```python
print(X_test.shape, y_test.shape)
pd.concat([X_test.head(3), y_test.head(3)], axis=1)
```

```
(319, 11) (319, 1)
```

[6]:

```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
1280            7.1             0.460          0.2             1.9      0.077
1281            7.1             0.460          0.2             1.9      0.077
1282            7.9             0.765          0.0             2.0      0.084

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
1280                 28.0                  54.0  0.99560  3.37       0.64
1281                 28.0                  54.0  0.99560  3.37       0.64
1282                  9.0                  22.0  0.99619  3.33       0.68

      alcohol  quality
1280     10.4        6
1281     10.4        6
1282     10.9        6
```

[ ]:

[ ]:

0.0.2 Regression equations and functions

1. adding intercept
2. the equation for a the linear model that predicts y from X
3. the equation for computing the Residual Sum of Squares (RSS) for the linear model

by using `pandas` and `numpy`

[7]:
```python
def predict(beta, X):
    if isinstance(beta, (pd.DataFrame, pd.Series)):
        beta = beta.values

    if isinstance(X, (pd.DataFrame, pd.Series)):
        index = X.index.values
        X = X.values

    if beta.shape[0] - X.shape[1] == 1:
        X = np.concatenate([np.ones(shape=(X.shape[0], 1)), X], axis=1)

    return pd.DataFrame(np.matmul(X, beta), index=index, columns=["y_hat"])


def RSS(beta, X, y):
    tmp = pd.concat([y, predict(beta, X)], axis=1)

    if pd.isnull(tmp).any(axis=1).sum():
        raise ValueError("y and y_hat indexes are mismatched")

    return tmp.apply(lambda s: (s[0] - s[1])**2, axis=1).sum()
```

[ ]:
```python

```

[ ]:
```python

```

0.0.3 Training Models

by using `pandas` and `scipy.optimize`

[8]:
```python
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train))
beta_hat = opt.x
```

[9]:
```python
beta_hat
```

[9]:
```
array([ 2.39956491e+01,  2.34934995e-02, -1.05499800e+00, -1.82862239e-01,
        1.06302233e-02, -1.75743048e+00,  3.26745286e-03, -3.68408259e-03,
       -2.00912301e+01, -3.43003458e-01,  8.05258489e-01,  2.83317495e-01])
```

[10]:
```
print("RSS in training set:")
RSS(beta_hat, X_train, y_train)
```

```
RSS in training set:
```

[10]:
```
532.0667485668739
```

[11]:
```
print("RSS in testing set:")
RSS(beta_hat, X_test, y_test)
```

```
RSS in testing set:
```

[11]:
```
137.7884551877433
```

[ ]:
```

```

[ ]:
```

```

0.0.4 Question 1

1. What are the qualitative results from your model?
2. Which features seem to be most important?
3. Do you think that the magnitude of the features in X may affect the results (for example, the average total sulfur dioxide across all wines is 46.47, but the average chlorides is only 0.087).

0.0.5 Ans:

1. my qualitative results show that density is the most significant feature, which has a negative relation with wine quality(y)
2. density (with coefficient: -20.091)
3. the magnitude (mean) of the features does not affect the coefficient by the evidence from plots and linear regression trained with normalized data. But, the standard deviation of the features does affect the coefficient of linear regression. The density has the smallest standard deviation, and get the most significant coefficient. The chlorides has the second smallest standard deviation, and get the second significant coefficient.

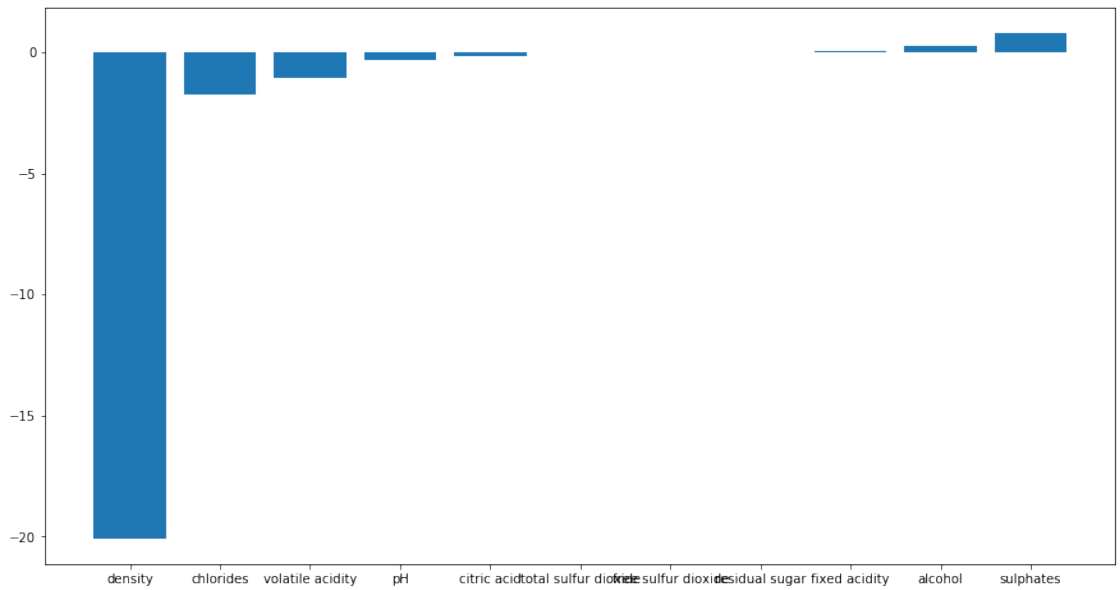
[12]:
```
pd.Series(beta_hat, index=["intercept"] + X_train.columns.values.tolist())\
    .round(3)\
    .sort_values()
```

[12]:
```
density                -20.091
chlorides               -1.757
volatile acidity        -1.055
pH                      -0.343
citric acid             -0.183
total sulfur dioxide    -0.004
```

```
free sulfur dioxide      0.003
residual sugar           0.011
fixed acidity            0.023
alcohol                  0.283
sulphates                0.805
intercept               23.996
dtype: float64
```

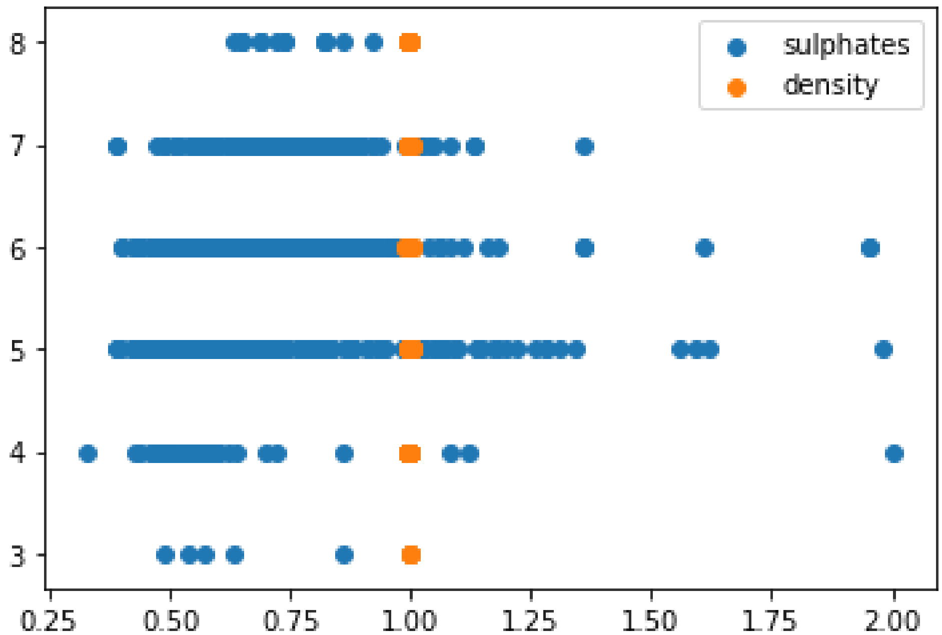
[13]:
```python
plt.figure(figsize=(15, 8))
plt.bar(X_train.columns[np.argsort(beta_hat[1:])], np.sort(beta_hat[1:]), align="center")
```

[13]:
```
<BarContainer object of 11 artists>
```



[14]:
```python
plt.scatter(X_train["sulphates"], y_train, label="sulphates")
plt.scatter(X_train["density"], y_train, label="density")
plt.legend()
```

[14]:
```
<matplotlib.legend.Legend at 0x7ff37f1d14e0>
```



[15]:
```
X_train.describe().loc['std'].sort_values()
```

[15]:
```
density                  0.001893
chlorides                0.047896
pH                       0.155147
sulphates                0.174030
volatile acidity         0.177994
citric acid              0.196441
alcohol                  1.095970
residual sugar           1.311638
fixed acidity            1.768994
free sulfur dioxide     10.320531
total sulfur dioxide    33.592566
Name: std, dtype: float64
```

[ ]:

[16]:
```
X_train_mean = X_train.mean(axis=0)
norm_Xtrain = X_train - X_train_mean
pd.concat(
    [norm_Xtrain.mean(), norm_Xtrain.std()], axis=1
).rename(columns={0: "mean", 1: "std"})
```

[16]:

	mean	std
fixed acidity	-1.540712e-14	1.768994
volatile acidity	-5.499073e-17	0.177994

```
citric acid           3.516501e-16   0.196441
residual sugar       -2.895253e-15   1.311638
chlorides             3.217153e-16   0.047896
free sulfur dioxide  -6.483702e-15  10.320531
total sulfur dioxide -6.216139e-14  33.592566
density               8.559993e-16   0.001893
pH                    5.467848e-16   0.155147
sulphates            -1.508169e-15   0.174030
alcohol               3.214234e-14   1.095970
```

[17]:
```python
norm_Xtrain.head(3)
```

[17]:
```
   fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0      -1.177891          0.181016    -0.289297       -0.661328  -0.012838
1      -0.777891          0.361016    -0.289297        0.038672   0.009162
2      -0.777891          0.241016    -0.249297       -0.261328   0.003162

   free sulfur dioxide  total sulfur dioxide   density        pH  sulphates  \
0            -4.448438            -12.794531  0.000829  0.210359  -0.103711
1             9.551562             20.205469 -0.000171 -0.099641   0.016289
2            -0.448438              7.205469  0.000029 -0.039641  -0.013711

    alcohol
0 -1.000391
1 -0.600391
2 -0.600391
```

[18]:
```python
beta = np.random.normal(0, 1, (norm_Xtrain.shape[1] + 1, 1))
norm_opt = minimize(fun=RSS, x0=beta, args=(norm_Xtrain, y_train))
norm_beta_hat = norm_opt.x

pd.Series(norm_beta_hat, index=["intercept"] + X_train.columns.values.tolist())\
    .round(3)\
    .sort_values()
```

[18]:
```
density                -20.090
chlorides               -1.757
volatile acidity        -1.055
pH                      -0.343
citric acid             -0.183
total sulfur dioxide    -0.004
free sulfur dioxide      0.003
residual sugar           0.011
fixed acidity            0.023
alcohol                  0.283
sulphates                0.805
intercept                5.665
```

```
dtype: float64
```

[19]:
```
RSS(norm_beta_hat, norm_Xtrain, y_train)
```

[19]:
```
532.0667485610833
```

[20]:
```
norm_Xtest = X_test - X_train_mean
RSS(norm_beta_hat, norm_Xtest, y_test)
```

[20]:
```
137.7884492625132
```

[ ]:
```

```

[ ]:
```

```

0.0.6 Question 1 (cont.)

4. How well does your model fit?
5. You should be able to measure the goodness of fit, RSS, on both the training data and the test data, but only report the results on the test data.

In Machine Learning we almost always only care about how well the model fits on data that has not been used to fit the model, because we need to use the model in the future, not the past. Therefore, we only report performance with holdout data, or test data.

[21]:
```
def r_square(y_true, y_pred):
    if len(y_true) != len(y_pred):
        raise ValueError("length mismatched")

    tmp = pd.concat([y_true, y_pred], axis=1)
    tmp.columns = ["y_true", "y_pred"]
    ss_res = sum((tmp["y_true"] - tmp["y_pred"])**2)
    ss_tot = sum((tmp["y_true"] - tmp["y_true"].mean())**2)
    return 1 - ss_res/ss_tot
```

0.0.7 Ans:

1. this is the model performance on testing set

[22]:
```
print("Model Performance in the Test Set: ")
print("RSS: ", RSS(beta_hat, X_test, y_test))
print("R^2: ", r_square(y_test, predict(beta_hat, X_test)))
```

```
Model Performance in the Test Set:
RSS:  137.7884551877433
R^2:  0.28091945808837193
```

[ ]:

```

```

[ ]:

```

```

0.0.8 Question 1 (cont.)

6. Does the end result or RSS change if you try different initial values of ?
7. What happens if you change the magnitude of the initial ?
8. Does the choice of solver method change the end result or RSS?

0.0.9 Ans

1. it does not change a lot when we try different init value, the magnitude of beta, or the solver. it always trains a similar model.

[23]:

```python
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))
print("new init beta: ", beta.reshape(1, -1)[0], "\n")
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train))
new_beta_hat = opt.x
print("the diff between new beta hat and beta hat", new_beta_hat - beta_hat,␣
 ↪"\n")
print("new RSS in training set: ", RSS(new_beta_hat, X_train, y_train))
print("new RSS in testing set: ", RSS(new_beta_hat, X_test, y_test))
```

```
new init beta:  [ 0.162382   -0.65975988 -1.29170349  0.16041755 -0.17331564
0.18030522
 -1.87046837  0.74813601  0.48806078  0.62408526  1.44855439 -0.85141569]

the diff between new beta hat and beta hat [-1.76143623e-03 -1.16790827e-06
-1.46276924e-06 -4.14199594e-06
 -4.52008238e-07  5.75278377e-06 -2.86614499e-08  1.81617176e-08
  1.77723934e-03 -4.88007195e-06 -1.80721394e-06  1.81820888e-06]

new RSS in training set:  532.0667485630977
new RSS in testing set:  137.78841077287936
```

[24]:

```python
beta = np.random.normal(100, 10, (X_train.shape[1] + 1, 1))
print("new init beta: ", beta.reshape(1, -1)[0], "\n")
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train))
new_beta_hat = opt.x
print("the diff between new beta hat and beta hat", new_beta_hat - beta_hat,␣
 ↪"\n")
print("new RSS in training set: ", RSS(new_beta_hat, X_train, y_train))
print("new RSS in testing set: ", RSS(new_beta_hat, X_test, y_test))
```

```
new init beta:  [ 90.25832836  90.48570987  88.00789998 106.2302923
98.22283601
 108.84823665 101.55855569 106.98080518 104.40826858  95.35101564
  97.43709075  82.46072558]

the diff between new beta hat and beta hat [-1.57176907e-03 -1.44199176e-06
-1.66528178e-06 -4.00717397e-07
 -6.94120507e-07 -3.66496702e-06  1.18286542e-08 -2.70573254e-09
  1.60152095e-03 -7.42020014e-06 -2.03070285e-06  1.56525534e-06]

new RSS in training set:  532.066748564245
new RSS in testing set:  137.78844870399897
```

[25]:
```python
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))
print("new init beta: ", beta.reshape(1, -1)[0], "\n")
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train), method="Powell")
new_beta_hat = opt.x
print("the diff between new beta hat and beta hat", new_beta_hat - beta_hat,␣
 ↪"\n")
print("new RSS in training set: ", RSS(new_beta_hat, X_train, y_train))
print("new RSS in testing set: ", RSS(new_beta_hat, X_test, y_test))
```

```
new init beta:  [-0.64142291  0.87114277  0.95370145 -1.05412244  0.23181434
-0.85379947
 -0.03488099 -0.26708025  0.91362247  0.29046226  2.26676174 -3.16144032]

the diff between new beta hat and beta hat [-2.85037209e-01 -2.34421838e-04
-8.99621681e-04 -4.64887608e-04
 -1.10157921e-04  1.08482915e-03  5.24314018e-07  5.47170639e-07
  2.90574928e-01 -1.24619025e-03 -9.43487072e-04  2.75219429e-04]

new RSS in training set:  532.0668295342499
new RSS in testing set:  137.78972086250522
```

[ ]:

[ ]:

[ ]:

0.0.10 Question 2

[26]:
```python
def RSS(beta, X, y, penalty=None, lam=0.01):
    tmp = pd.concat([y, predict(beta, X)], axis=1)

    if pd.isnull(tmp).any(axis=1).sum():
```

```
        raise ValueError("y and y_hat indexes are mismatched")


    if penalty == "l1":
        penalty = lam * sum(abs(beta[1:]))
    elif penalty == "l2":
        penalty = lam * sum(beta[1:]**2)
    else:
        penalty = 0

    return tmp.apply(lambda s: (s[0] - s[1])**2, axis=1).sum() + penalty
```

Ridge Regression (L2)

[27]:
```
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2"))
beta_hat_L2 = opt.x
```

[28]:
```
pd.DataFrame(
    np.array([beta_hat, beta_hat_L2]).T,
    index=["intercept"] + X_train.columns.values.tolist(),
    columns=["beta_hat", "beta_hat_L2"]
).round(3)
```

[28]:

	beta_hat	beta_hat_L2
intercept	23.996	5.663
fixed acidity	0.023	0.005
volatile acidity	-1.055	-1.072
citric acid	-0.183	-0.181
residual sugar	0.011	0.003
chlorides	-1.757	-1.807
free sulfur dioxide	0.003	0.003
total sulfur dioxide	-0.004	-0.004
density	-20.091	-1.363
pH	-0.343	-0.438
sulphates	0.805	0.784
alcohol	0.283	0.300

1. How does RSS on the training data change? How does RSS on the test data change?

0.0.11 Ans

Both RSS in train and test set are slightly lower. That is probably because there is no collinearity or overfitting issue in the original regression. Hence, RSS does not decrease that much.

[29]:
```
print("Ridge Regression Performance")
print("RSS in train set: ", RSS(beta_hat_L2, X_train, y_train))
print("RSS in test set: ", RSS(beta_hat_L2, X_test, y_test))
```

```
Ridge Regression Performance
RSS in train set:  532.3205564637317
RSS in test set:  137.76116427515305
```

[30]:
```
print("Ridge Regression RSS in test set")
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))

lam = 0.001
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 0.01
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 0.1
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 1
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 10
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l2", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))
```

```
Ridge Regression RSS in test set
when lambda=0.001 137.7538011320214
when lambda=0.010 137.761174809492
when lambda=0.100 137.80505586721966
when lambda=1.000 138.31549568655723
when lambda=10.000 142.2356816915538
```

0.0.12 Ans

the results shows when lambda=0.001 Ridge Regression has the best performance on testing set.

[ ]:

[ ]:

Lasso Regression (L1)

[31]:
```
print("Lasso Regression RSS in test set")
beta = np.random.normal(0, 1, (X_train.shape[1] + 1, 1))

lam = 0.001
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 0.01
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 0.1
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 1
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))

lam = 10
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))
```

```
Lasso Regression RSS in test set
when lambda=0.001 137.78528452836593
when lambda=0.010 137.76461291400477
when lambda=0.100 137.78750393426554
when lambda=1.000 138.07138465738728
when lambda=10.000 142.56632719500345
```

[46]:
```
lam = 0.01
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))
```

```
when lambda=0.010 137.76461291400477
```

[47]:
```
pd.Series(opt.x[1:], index=X_test.columns.values).round(3).sort_values()
```

[47]:
```
density                 -13.232
chlorides                -1.776
volatile acidity         -1.061
pH                       -0.378
citric acid              -0.182
total sulfur dioxide     -0.004
free sulfur dioxide       0.003
residual sugar            0.008
```

```
fixed acidity           0.017
alcohol                 0.290
sulphates               0.798
dtype: float64
```

[49]:

```python
lam = 10
opt = minimize(fun=RSS, x0=beta, args=(X_train, y_train, "l1", lam))
print("when lambda=%.3f" % lam, RSS(opt.x, X_test, y_test))
pd.Series(opt.x[1:], index=X_test.columns.values).round(3).sort_values()
```

```
when lambda=10.000 142.56632719500345
```

[49]:

```
volatile acidity       -0.975
total sulfur dioxide   -0.004
citric acid            -0.000
residual sugar         -0.000
chlorides              -0.000
density                 0.000
pH                      0.000
free sulfur dioxide     0.004
fixed acidity           0.023
alcohol                 0.310
sulphates               0.468
dtype: float64
```

0.0.13 Ans

the magnitude of the features in X won't affect the results with regularization. Since regularization only shrinks the less informative features and expands the more informative features, so the magnitude does not affect the result with regularization.

[ ]:

[ ]: