Week9 Multicollinearity-Ridge Regression

背景描述

由于多重共线性的问题本质上在于 $|X^{'}X| \approx 0$, 因此岭回归的本质就是在这个矩阵上做了手脚, 使得多重共线性的问题得到一定的缓解.
这里我们建立一元线性回归模型: $y = 8 + 3 * x_1 + 4 * x_2 + 5 * x_3 + 1 * x_4 + \epsilon$, 我们人工给定 10 个值和 10 个满足正态分布的 ϵ, 使得其中 x_3, x_4 具有强线性相关性.
由此我们构造了 10 个观测的 4 个变量，具体请见下表：

数据描述

var	1	2	3	4	5	6	7	8	9	
X1	5.053499791495376	4.896359188149629	4.5846019652366765	3.4627703344989245	3.270451004372899	4.493105477608886	4.4464566375800425	4.798063216845086	6.427862171550048	4.303787
X2	5.072933009683874	3.6512177680206648	5.577820866295013	4.068646005580284	5.59613146647269	6.323457817901293	6.079773035399383	2.9443980328330173	4.457913906178166	5.357206
X3	1.1	1.4	1.7	1.7	1.8	1.8	1.9	2	2.3	
X4	2.2	3	3.6	3.4	3.8	3.6	3.6	4.2	4.8	
ϵ	0.05290865	-0.34306401	-0.5598349	0.64584319	-0.37267585	-0.87090483	0.99051878	-1.38493147	0.06964761	0.08
Y	51.20514006	46.95088463	55.60525446	47.20873822	52.62320303	58.50224287	59.74898083	46.98685031	61.48488975	59.42

参数设置如下:

1. 样本量 n = 10
2. 变量个数 p = 4
3. 自变量 x_1 的波动 $\sigma_{x_1} = 1$
4. 误差的波动 $\sigma_y = 1$

问题

1. 判断所给数据是否具有多重共线性.
2. 若具有多重共线性, 选择适当的岭参数.
3. 进行岭回归分析.

解决方案

Q1：

多重共线性是指自变量 x1, x2, ..., xp 之间不完全线性相关但是相关性很高的情况。此时，虽然可以得到最小二乘估计，但是精度很低。随着自变量之间相关性增加，最小二乘估计结果的方差会增大。

仿真实验

```
# Import standard packages
import numpy as np
import pandas as pd
import scipy.stats as stats
import matplotlib.pyplot as plt
import seaborn as sns

# Import additional packages
from itertools import combinations
import statsmodels.api as sm
from statsmodels.stats.outliers_influence import variance_inflation_factor
from sklearn import linear_model  # 进行岭回归分析
from ipywidgets import interact  # 互动功能
%matplotlib inline

p = 4
n = 10

# 上帝视角下的beta: 截距项为 10，三个变量前的系数分别为 2，3，4
beta = [8]
for i in range(p):
    beta.append((i+2)%5+1)
beta = np.array(beta)
# print(beta)

# 构造 X 矩阵
```

```
X = [[5.053499791495376, 4.896359188149629, 4.5846019652366765, 3.4627703344989245, 3.270451004372899,
4.493105477608886, 4.4464566375800425, 4.798063216845086, 6.427862171550048, 4.303787732779672]]
# X = np.random.normal(loc=1.5 , scale=0.2, size=(1,n)).tolist()
X.append([5.072933009683874, 3.6512177680206648, 5.577820866295013, 4.068646005580284, 5.59613146647269,
6.323457817901293, 6.079773035399383, 2.9443980328330173, 4.457913906178166, 5.357206466723423])
X.append([1.1, 1.4, 1.7, 1.7, 1.8, 1.8, 1.9, 2, 2.3, 2.4])
X.append([2.2, 3, 3.6, 3.4, 3.8, 3.6, 3.6, 4.2, 4.8, 5])
X.insert(0, np.ones(n))
X = np.array(X)
X = X.T

print(X)

# 生成 10 个满足正态分布的 epsilon 值
epsilon = [0.05290865, -0.34306401, -0.5598349, 0.64584319, -0.37267585, -0.87090483, 0.99051878,
-1.38493147, 0.06964761, 0.0842377]
# epsilon = np.random.normal(loc =0.0 , scale= 1, size = (1,n))
# print(epsilon)

# 上帝视角下的Y
Y = X @ beta + epsilon
# Y = X @ beta + epsilon[0] # 由于 np.random.normal 生成的列表中的元素仍是一个列表
Y = Y.T
# print(Y)

df = pd.DataFrame(X)
df['Y'] = Y
print(df)
```

```
[[1.         5.05349979 5.07293301 1.1        2.2       ]
 [1.         4.89635919 3.65121777 1.4        3.        ]
 [1.         4.58460197 5.57782087 1.7        3.6       ]
 [1.         3.46277033 4.06864601 1.7        3.4       ]
 [1.         3.270451   5.59613147 1.8        3.8       ]
 [1.         4.49310548 6.32345782 1.8        3.6       ]
 [1.         4.44645664 6.07977304 1.9        3.6       ]
 [1.         4.79806322 2.94439803 2.         4.2       ]
 [1.         6.42786217 4.45791391 2.3        4.8       ]
 [1.         4.30378773 5.35720647 2.4        5.        ]]
     0         1         2    3    4          Y
0  1.0  5.053500  5.072933  1.1  2.2  51.205140
1  1.0  4.896359  3.651218  1.4  3.0  46.950885
2  1.0  4.584602  5.577821  1.7  3.6  55.605254
3  1.0  3.462770  4.068646  1.7  3.4  47.208738
4  1.0  3.270451  5.596131  1.8  3.8  52.623203
5  1.0  4.493105  6.323458  1.8  3.6  58.502243
6  1.0  4.446457  6.079773  1.9  3.6  59.748981
7  1.0  4.798063  2.944398  2.0  4.2  46.986850
8  1.0  6.427862  4.457914  2.3  4.8  61.484890
9  1.0  4.303788  5.357206  2.4  5.0  59.424427
```

对原始数据进行多元线性回归分析

```
model= sm.OLS(Y, X).fit()
Y_hat = model.fittedvalues
beta_hat = model.params
model.summary()
```

```
/Library/Frameworks/Python.framework/Versions/3.6/lib/python3.6/site-packages/scipy/stats/stats.py:1604:
UserWarning: kurtosistest only valid for n>=20 ... continuing anyway, n=10
  "anyway, n=%i" % int(n))
```

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.991
Model:	OLS	**Adj. R-squared:**	0.984
Method:	Least Squares	**F-statistic:**	136.9
Date:	Sun, 25 Apr 2021	**Prob (F-statistic):**	2.71e-05
Time:	21:55:57	**Log-Likelihood:**	-7.6024
No. Observations:	10	**AIC:**	25.20
Df Residuals:	5	**BIC:**	26.72
Df Model:	4		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
const	7.6965	2.132	3.610	0.015	2.215	13.178
x1	2.9804	0.291	10.242	0.000	2.232	3.728
x2	3.9880	0.256	15.574	0.000	3.330	4.646
x3	11.7516	4.308	2.728	0.041	0.679	22.825
x4	-2.2089	2.025	-1.091	0.325	-7.414	2.996

Omnibus:	4.689	**Durbin-Watson:**	2.417
Prob(Omnibus):	0.096	**Jarque-Bera (JB):**	2.404
Skew:	-1.199	**Prob(JB):**	0.301
Kurtosis:	2.864	**Cond. No.**	164.

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

对数据标准化:

```
# 对数据进行标准化
# 自变量 X 的均值
X_mean = []
for i in range(p):
    X_mean.append(np.mean(X[:, i+1]))

# 自变量 X 的标准差
X_L = []
for i in range(p):
    X_L.append(sum((X[:, i+1] - X_mean[i]) ** 2))

# 对自变量 X 标准化(截距项不用标准化)
X_std = X * 1.0
X_std[:,1:p+1] = (X[:,1:p+1] - X_mean) / np.sqrt(X_L)

# 对因变量 Y 标准化
Y_L = sum((Y - np.mean(Y))**2)
Y_std = (Y - np.mean(Y)) / np.sqrt(Y_L)

df_std = pd.DataFrame(X_std)
df_std['Y'] = Y_std
print(df_std.head())
```

```
     0         1         2         3         4         Y
0  1.0  0.183312  0.048525 -0.615880 -0.619712 -0.160929
1  1.0  0.123276 -0.382698 -0.355649 -0.293548 -0.408185
2  1.0  0.004167  0.201663 -0.095418 -0.048925  0.094805
3  1.0 -0.424436 -0.256087 -0.095418 -0.130466 -0.393199
4  1.0 -0.497913  0.207217 -0.008674  0.032616 -0.078512
```

对标准化后的数据进行多元线性回归分析

```
# Do the multiple linear regression——对标准化后的数据
model_std = sm.OLS(Y_std, X_std).fit()
beta_std_hat = model_std.params
Y_std_hat = model_std.fittedvalues
model_std.summary()
```

```
/Library/Frameworks/Python.framework/Versions/3.6/lib/python3.6/site-packages/scipy/stats/stats.py:1604:
UserWarning: kurtosistest only valid for n>=20 ... continuing anyway, n=10
  "anyway, n=%i" % int(n))
```

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.991
Model:	OLS	**Adj. R-squared:**	0.984
Method:	Least Squares	**F-statistic:**	136.9
Date:	Sun, 25 Apr 2021	**Prob (F-statistic):**	2.71e-05
Time:	21:55:58	**Log-Likelihood:**	20.850
No. Observations:	10	**AIC:**	-31.70
Df Residuals:	5	**BIC:**	-30.19
Df Model:	4		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
const	3.053e-16	0.013	2.27e-14	1.000	-0.035	0.035
x1	0.4534	0.044	10.242	0.000	0.340	0.567
x2	0.7642	0.049	15.574	0.000	0.638	0.890
x3	0.7874	0.289	2.728	0.041	0.045	1.529
x4	-0.3149	0.289	-1.091	0.325	-1.057	0.427

Omnibus:	4.689	**Durbin-Watson:**	2.417
Prob(Omnibus):	0.096	**Jarque-Bera (JB):**	2.404
Skew:	-1.199	**Prob(JB):**	0.301
Kurtosis:	2.864	**Cond. No.**	30.3

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

求 $(X^*)'(X^*)$ 矩阵的特征值和特征向量:

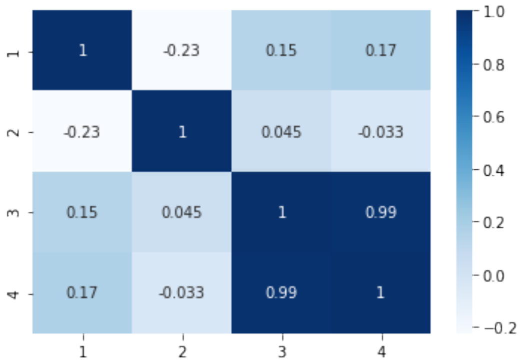
```
# (X*)'(X*) 矩阵等价于原始矩阵 X 样本相关矩阵
R = df.corr()
R = R.iloc[1:-1,1:-1]

R
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	1	2	3	4
1	1.000000	-0.225151	0.146603	0.167910
2	-0.225151	1.000000	0.045426	-0.032975
3	0.146603	0.045426	1.000000	0.985999
4	0.167910	-0.032975	0.985999	1.000000

```python
sns.heatmap(R, cmap='Blues', annot=True) # annot: 在heatmap中每个方格写入数据
```

```
<AxesSubplot:>
```




```python
# 求特征值 & 特征向量
W, V = np.linalg.eig(R)
W_diag = np.diag(W)
V = V.T # 这里需要转置
print('特征值: ', W)
```

```
特征值:  [2.03537021 1.20052604 0.7532161  0.01088765]
```

判断 X 矩阵是否具有多重共线性:

```python
# 定义"判断多重共线性"的函数
# 参数: (X_list: 设计矩阵 X, thres_vif: VIF 方法判断多重共线性的阈值, thres_kappa: 特征值方法判断多重共线性的阈值)
def judge_col(X_list, thres_vif, thres_kappa):
    var_num = X_list.shape[1]
    print('VIF方法判断结果(阈值为 %d): '% thres_vif)
    vif = [variance_inflation_factor(X_list, i) for i in range(var_num)]
    for i in range(var_num):
        if vif[i] >= thres_vif:
            print('设计矩阵 X 存在多重共线性.')
            break
        elif i == var_num-1:
            print('设计矩阵 X 不存在多重共线性.')

    print('\n特征值判定法判断结果(阈值为 %d): '% thres_kappa)
    kappa = []
```

```
    for i in range(var_num):
        kappa.append(np.sqrt(max(W) / W[i]))
    if np.max(kappa) >= thres_kappa:
        print('设计矩阵 X 存在多重共线性，其中kappa值为：%.4f'% np.max(kappa))
    else:
        print('设计矩阵 X 不存在多重共线性，其中kappa值为：%.4f'% np.max(kappa))

# 判断多重共线性
X_std1 = X_std[:,1:p+1] # 将 X 矩阵的截距项去掉
beta_std_hat1 = beta_std_hat[1:p+1] # 将 β_0 去掉
judge_col(X_std1, 5, 10) # 判断多重共线性
```

```
VIF方法判断结果(阈值为 5):
设计矩阵 X 存在多重共线性.

特征值判定法判断结果(阈值为 10):
设计矩阵 X 存在多重共线性，其中kappa值为：13.6727
```

Q2:

称$\hat{\beta}(k)=(\boldsymbol{X}'\boldsymbol{X}+k\boldsymbol{I})^{-1}\boldsymbol{X}'\boldsymbol{y}$为岭回归估计，其中k为岭参数。这是为了求解逆矩阵更加方便，且在k很小时与最小二乘估计大约相等。

岭参数 k 选择(模型选择)的方法:

1. 岭迹法
2. 方差扩大因子法
3. 霍尔-肯纳德（Hoerl-Kennad）公式
4. Mcdorard-Garaneau 公式

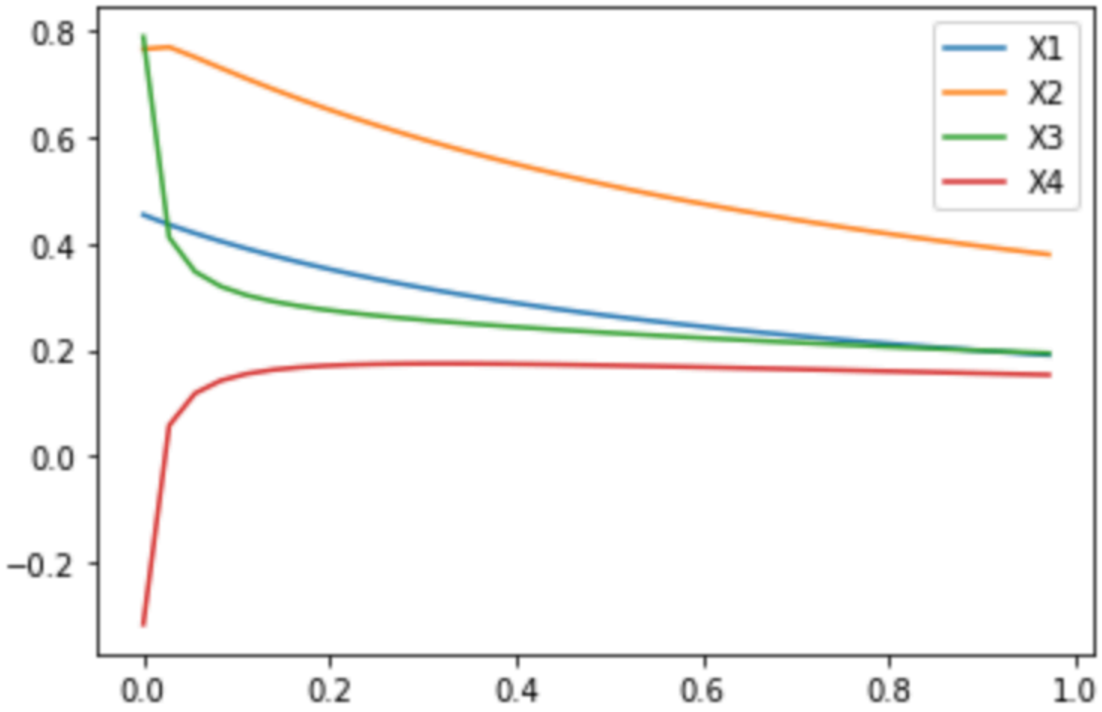
下面依次介绍岭参数选择的方法：

1. 岭迹法
   岭迹法的一般原则:
   · 系数岭估计基本稳定;
   · 最小二乘回归下符号不合理的回归系数, 在岭估计的意义下符号变得合理;
   · 回归系数合乎经济意义;
   · 残差平方和不会增大太多.

```
# [0, 1) 范围内划分的最大精细程度: [0,0.01,0.02,...,0.99]
range_const1 = 100

def RR1(K = 1):
    # 计算岭估计
    rang1 = []
    for i in range(K):
        rang1.append(i/K) # 岭参数 k 取值范围: [0,1-1/K](例如 K=10, k 取值范围: [0, 0.9])
    coefs_1 = []
    for k in rang1:
        temp1 = np.linalg.inv(X_std1.T @ X_std1 + k * np.eye(p)) @ X_std1.T @ Y_std
        coefs_1.append(temp1)

    # 画图
    # print('参数的数值: ', coefs_1)
    coefs_1 = np.array(coefs_1)
    for i in range(p):
        plt.plot(rang1, coefs_1[:,i], label = 'X%d'%(i+1))
    plt.legend(loc = 'best')

# 随着 K 值的增加, 岭参数 k 取值越精细, 因为在 [0,1) 范围内的分割更细
interact(RR1,K=(1,range_const1))
```

```
interactive(children=(IntSlider(value=1, description='K', min=1), Output()), _dom_classes=('widget-interact',)…
```

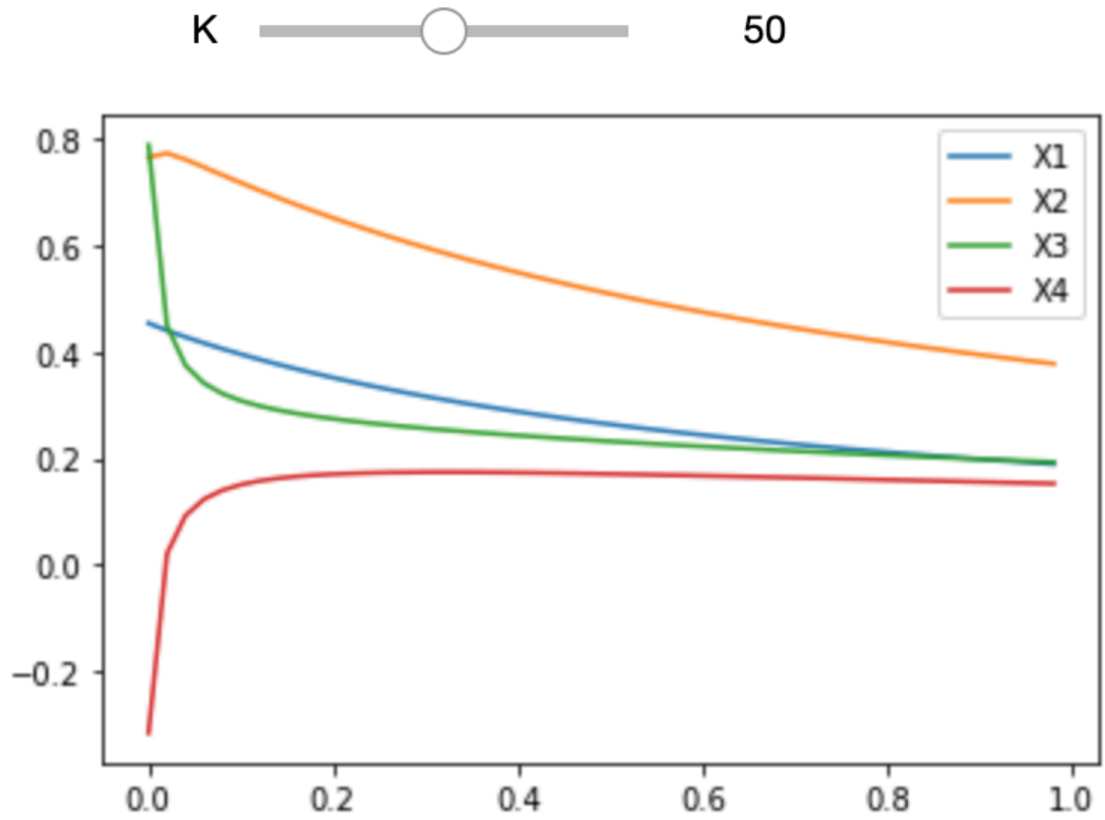
K 36




```
<function __main__.RR1(K=1)>
```

```
# 调包：linear_model
def RR2(K = 1):
    # 初始化一个Ridge Regression
    clf = linear_model.Ridge(fit_intercept=False)

    # 训练模型：测试不同的 k 取值，获得系数
    rang2 = []
    for i in range(K):
        rang2.append(i/K)
    coefs_2 = []
    for k in rang2:
        clf.set_params(alpha=k)
        clf.fit(X_std1, Y_std)
        coefs_2.append(clf.coef_)

    # 画图
    # print('参数的数值：', coefs_2)
    coefs_2 = np.array(coefs_2)
    for i in range(p):
        plt.plot(rang2, coefs_2[:,i], label = 'X%d'%(i+1))
    plt.legend(loc = 'best')

interact(RR2,K=(1,range_const1))
```

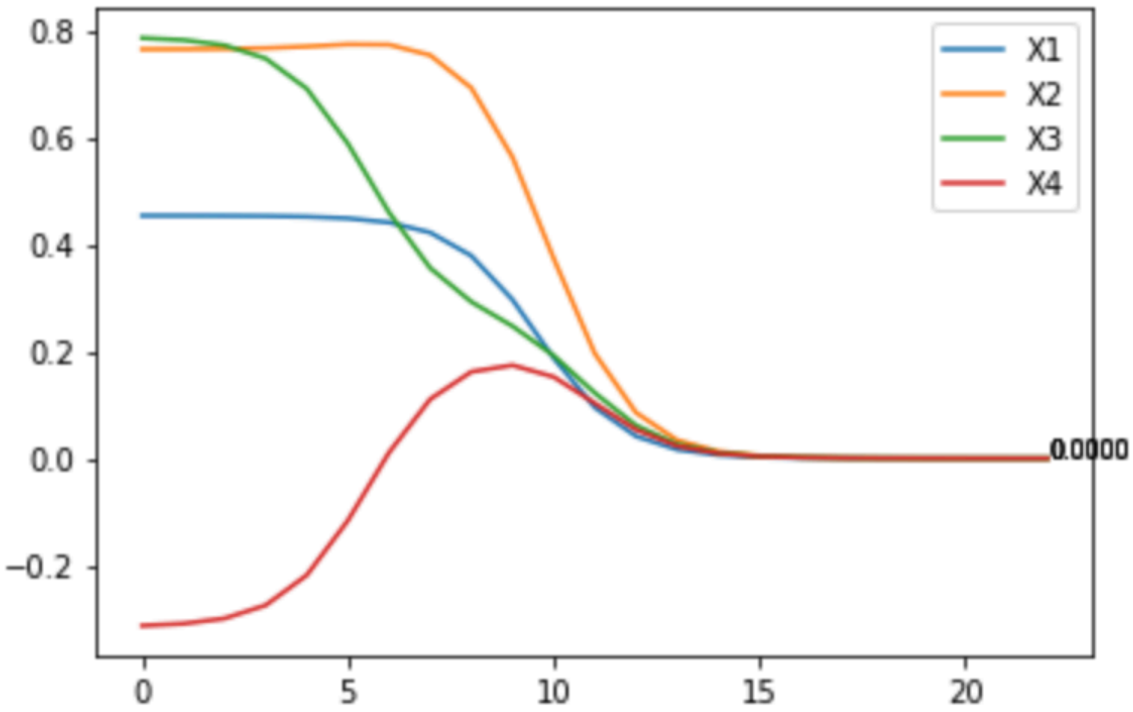
```
interactive(children=(IntSlider(value=1, description='K', min=1), Output()), _dom_classes=('widget-interact',)…
```




```
<function __main__.RR2(K=1)>
```

```
# 岭参数 k 的最大取值范围：[exp(-10),exp(19)]
range_const2 = 30

def RR3(K = 1):
    # 初始化一个Ridge Regression
    clf = linear_model.Ridge(fit_intercept=False)

    # 训练模型：测试不同的 k 取值，获得系数
    coefs_3 = []
    num_lambda3 = K
    for k in range(num_lambda3):
        clf.set_params(alpha=np.exp(k-10))  # 岭参数 k 取值范围：[exp(-10),exp((K-1)-10)]
        clf.fit(X_std1, Y_std)
        coefs_3.append(clf.coef_)

    # 画图
    # print('参数的数值：', coefs_3)
    x3 = range(num_lambda3)
    coefs_3 = np.array(coefs_3)
    for i in range(p):
        plt.plot(x3, coefs_3[:,i], label = 'X%d'%(i+1))
        plt.text(x3[-1], coefs_3[-1,i], '%.4f' % float(coefs_3[-1,i]), fontsize=8)
    print('岭参数为：', np.exp(K-10))
    print('对应的岭估计：', coefs_3[-1,:])
    plt.legend(loc = 'best')

interact(RR3,K=(1,range_const2))
```

```
interactive(children=(IntSlider(value=1, description='K', max=30, min=1), Output()), _dom_classes=('widget-int…
```




```
<function __main__.RR3(K=1)>
```

基于交叉验证的岭回归 alpha 选择可以直接获得一个相对不错的 alpha.

```
# 初始化一个Ridge Cross-Validation Regression
clf_cv = linear_model.RidgeCV(fit_intercept=False)

# 训练模型
clf_cv.fit(X_std1, Y_std)

k_cv = clf_cv.alpha_
coef_cv = clf_cv.coef_
print('k 的数值 : ', clf_cv.alpha_)
print('参数的数值：', clf_cv.coef_)
```

```
k 的数值 :  0.1
参数的数值：  [0.39521196 0.71654002 0.30808004 0.15082594]
```

```
# 验证岭估计和最小二乘估计之间的关系
thres_k = int(k_cv * range_const1)
print(coef_cv)

C1 = X_std1.T @ X_std1
C2 = np.linalg.inv(C1 + k_cv * np.eye(p))
C3 = C2 @ C1
print(C3 @ beta_std_hat1)

diff = coef_cv - C3 @ beta_std_hat1
print('差异: ', diff)
```

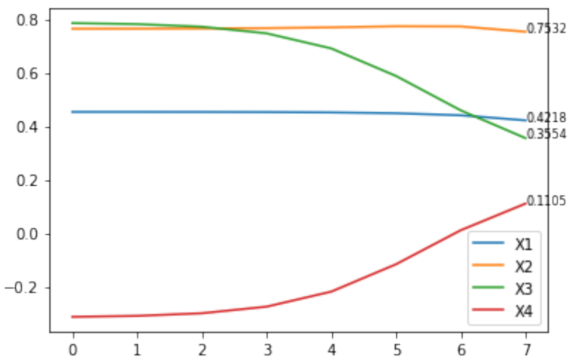
```
[0.39521196 0.71654002 0.30808004 0.15082594]
[0.39521196 0.71654002 0.30808004 0.15082594]
差异:  [-6.10622664e-16 -2.22044605e-16 -3.99680289e-15 -3.58046925e-15]
```

2. 方差扩大因子法

```
coefs_4 = []
thres_vif = 5
num_lambda4 = 30
```

```
judge = True
for k in range(num_lambda4):
    cnt = 0
    C = np.linalg.inv(C1 + np.exp(k-10) * np.eye(p)) @ C1 @np.linalg.inv(C1 + np.exp(k-10) * np.eye(p))
    # print(k, C)
    temp4 = np.linalg.inv(X_std1.T @ X_std1 + np.exp(k-10) * np.eye(p)) @ X_std1.T @ Y_std
    coefs_4.append(temp4)

    # 给定 k，使得所有方差扩大因子 C[j][j] <= thres_vif
    for j in range(p):
        if C[j][j] < thres_vif:
            cnt += 1
        else:
            break
    if cnt == p:
        k4 = np.exp(k-10)
        print('岭参数为：', np.exp(k-10))
        print('对应的岭估计：', temp4)
        break

# 画图
coef_4 = temp4
# print('参数的数值：', coefs_4)
x4 = range(k+1)  # 以 k 作为横坐标
# x4 = []  # 以 np.exp(k) 作为横坐标
# for i in range(k+1):
#     x4.append(np.exp(i-10))
coefs_4 = np.array(coefs_4)
for i in range(p):
    plt.plot(x4, coefs_4[:,i], label = 'X%d'%(i+1))
    plt.text(x4[-1], coefs_4[-1,i], '%.4f' % float(coefs_4[-1,i]), fontsize=8)

plt.legend(loc = 'best')
plt.show()
```

```
岭参数为： 0.049787068367863944
对应的岭估计： [0.42182275 0.75320769 0.35537606 0.11051347]
```



3. 霍尔-肯纳德（Hoerl-Kennad）公式

```
SSE = sum((Y_std - Y_std_hat) ** 2)
sigma2 = SSE / (n - p - 1)

Z = X_std1 @ V.T
alpha_hat = np.linalg.inv(W_diag) @ Z.T @ Y_std
# print(alpha_hat)

k_HK = sigma2 / max(alpha_hat**2)
k5 = k_HK
print('岭参数 k_HK：', k5)
coef_5 = np.linalg.inv(X_std1.T @ X_std1 + k5 * np.eye(p)) @ X_std1.T @ Y_std
print('对应的岭估计：', coef_5)
```

```
岭参数 k_HK:  0.0026754711436488164
对应的岭估计:  [ 0.4512857   0.76968807  0.68446324 -0.21229962]
```

4. Mcdorard-Garaneau 公式
   如果 $Q = ||\hat{\beta}||^2 - \hat{\sigma}^2 \sum_{j=1}^{p} \lambda_j^{-1} \le 0$，则认为 $\hat{\beta}$ 的各个分量都差不多，此时，对 $\hat{\beta}$ 不进行压缩，选择 $k = 0$

```
thres_diff = 0.2
beta_compress = beta_std_hat1.T @ beta_std_hat1 - sigma2 * sum(1/W)
if beta_compress <= 0:
    k6 = 0
    print('k = 0, 不对最小二乘估计进行压缩.')
else:
    print('Q: ', beta_compress)
    coefs_6 = []
    num_lambda6 = 30
    for k in range(num_lambda6):
        temp6 = np.linalg.inv(X_std1.T @ X_std1 + np.exp(k-10) * np.eye(p)) @ X_std1.T @ Y_std
        beta_k_compress = temp6.T @ temp6
        if abs(beta_compress-beta_k_compress) < thres_diff:
            k6 = np.exp(k-10)
            print('岭参数为: ', k6)
            print('对应的岭估计: ', temp6)
            break
coef_6 = temp6
```

```
Q:  1.337631650714247
岭参数为:  4.5399929762484854e-05
对应的岭估计:  [ 0.45334777  0.76428877  0.78521579 -0.3127196 ]
```

Q3:

岭回归估计虽然在k<>0时是有偏估计，但它的MSE要小于最小二乘估计。尤其在数据具有多重共线性时，选择合适的岭参数可以让估计结果更接近原始的参数。

```
beta_rr = coef_cv
print('岭参数 k = ', k_cv)
print('原始的最小二乘估计 = ', beta_hat[1:p+1])
print('标准化后的最小二乘估计 = ', beta_std_hat1)
print('\n')
print('原始 beta = ', beta[1:p+1])
print('岭估计 = ', beta_rr)
print('还原岭估计 = ', beta_rr *  np.sqrt(Y_L) / np.sqrt(X_L))
```

```
岭参数 k =  0.1
原始的最小二乘估计 =  [ 2.98037623  3.98795702 11.75164845 -2.2088513 ]
标准化后的最小二乘估计 =  [ 0.45338505  0.76416227  0.78738122 -0.31487934]

原始 beta =  [3 4 5 1]
岭估计 =  [0.39521196 0.71654002 0.30808004 0.15082594]
还原岭估计 =  [2.59796903 3.73942931 4.59808825 1.05803093]
```

由此可知, 岭参数取值为 0.1 左右时，还原后的岭估计接近原始（上帝视角下）的 β.