Q01

June 23, 2020

[1]:
```
from sklearn.model_selection import LeaveOneOut
import pandas as pd
from sklearn.linear_model import LinearRegression
import numpy as np
from scipy.interpolate import BSpline
import matplotlib.pyplot as plt
```

[2]:
```
# part 1
# Epanechnikov kernel

def k(z):
    if np.abs(z)>=1:
        return 0
    return 3/4*(1-z**2)

assert k(5)  == 0
assert k(-2) == 0
assert k(.2) != 0
```

[3]:
```
y_train = pd.read_csv("yTrain.csv", header=None)
y_test = pd.read_csv("yTest.csv", header=None)
protein_train = pd.read_csv("proteinTrain.csv", header=None)
protein_test = pd.read_csv("proteinTest.csv", header=None)
x = np.arange(70)
y = y_train.mean()
```

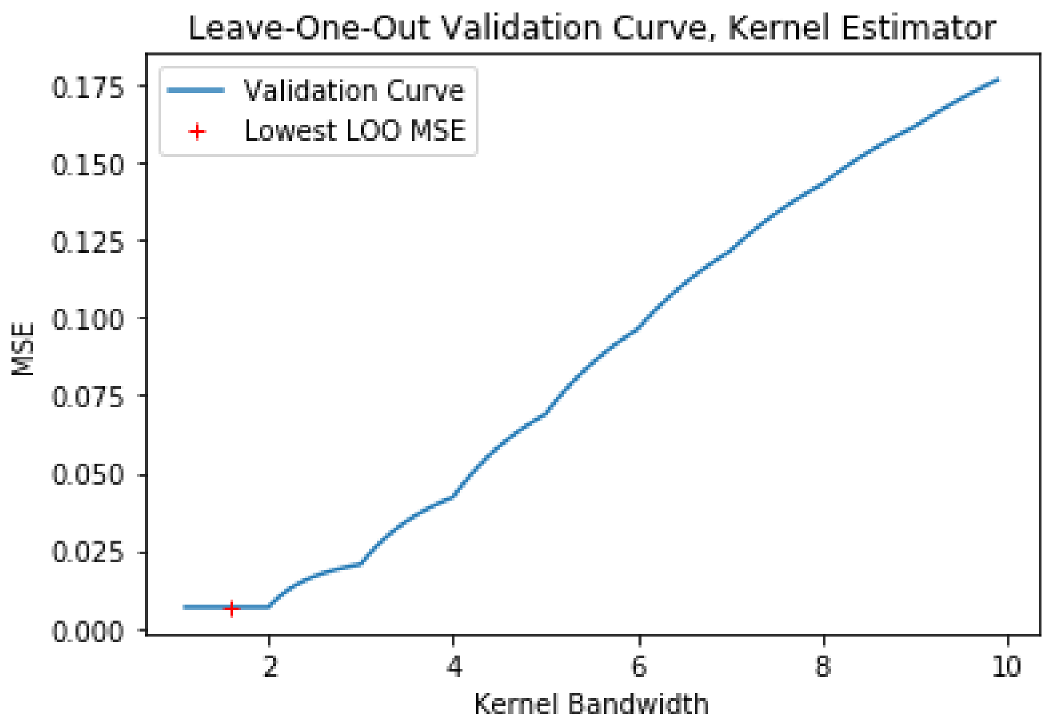
[4]:
```
# reference: https://github.gatech.edu/jtay6/IYSE8803-Examples-Py/blob/master/
↪Module%201/Examples1.py
bandwidths = np.arange(1.1, 10, 0.1)
MSEs = []
for w in bandwidths:
    loo = LeaveOneOut()
    errs = []
    yhat=[]
    for trg, tst in loo.split(x):
        z = [k(v) for v in (x[tst]-x[trg])/w]
        yk = np.average(y[trg], weights=z)
```

```
        yhat.append(yk)
    mse = np.sum((yhat - y)**2)
    MSEs.append(mse)
MSEs = np.array(MSEs).squeeze()
w_star = bandwidths[np.argmin(MSEs)]
```

[5]:
```
# optimal bandwidth
w_star
```

[5]: 1.6000000000000005

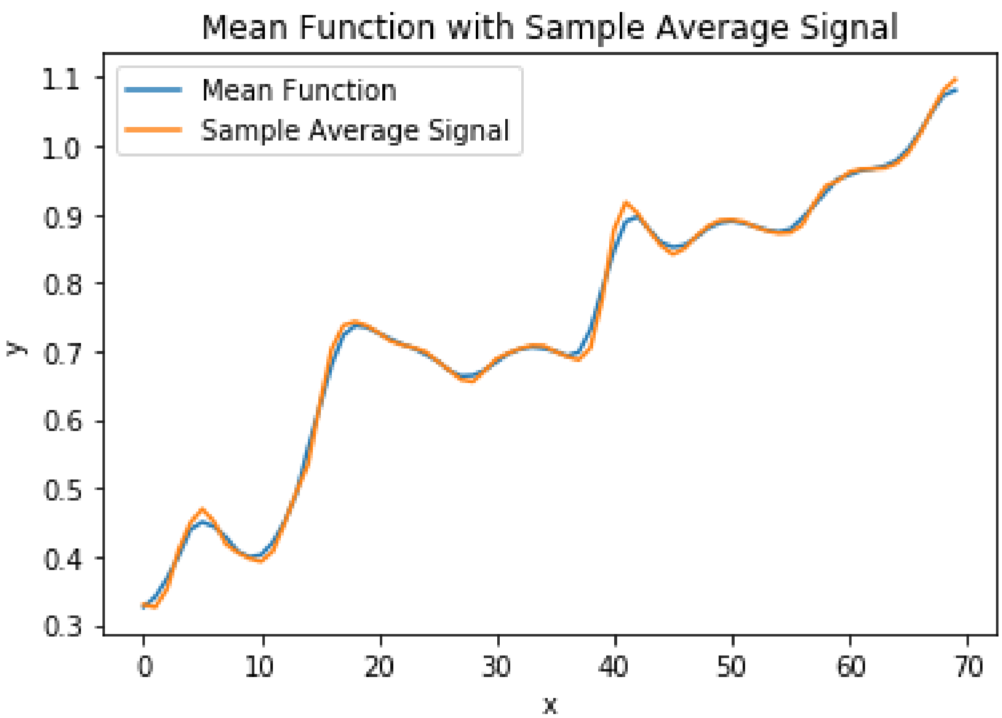
[6]:
```
plt.plot(bandwidths, MSEs, label='Validation Curve')
plt.plot(w_star, min(MSEs),'r+', label='Lowest LOO MSE')
plt.title('Leave-One-Out Validation Curve, Kernel Estimator')
plt.xlabel('Kernel Bandwidth')
plt.ylabel('MSE')
plt.legend()
plt.show()
```



[7]:
```
yhat=[]
loo = LeaveOneOut()
for trg, tst in loo.split(x):
    z = [k(v) for v in (x[tst]-x[trg])/w_star]
```

```
    yk = np.average(y[trg], weights=z)
    yhat.append(yk)
```

[8]:
```
plt.plot(x, yhat, label='Mean Function')
plt.plot(x, y, label='Sample Average Signal')
plt.title('Mean Function with Sample Average Signal')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.show()
```



[9]:
```
def smooth(y,w_star):
    yhat=[]
    loo = LeaveOneOut()
    for trg, tst in loo.split(x):
        z = [k(v) for v in (x[tst]-x[trg])/w_star]
        yk = np.average(y[trg], weights=z)
        yhat.append(yk)
    return yhat
```

[10]:
```
# part 2
y_smooth = y_train.apply(lambda row: smooth(row,w_star), axis = 1)
y_smooth = pd.DataFrame(np.array([np.array(s) for s in y_smooth]))
```

```
reg = LinearRegression().fit(y_smooth, protein_train)
y_smooth_test = y_test.apply(lambda row: smooth(row,w_star), axis = 1)
y_smooth_test = pd.DataFrame(np.array([np.array(s) for s in y_smooth_test]))
y_hat_kernel = reg.predict(y_smooth_test)
np.sum((protein_test - y_hat_kernel)**2)
```

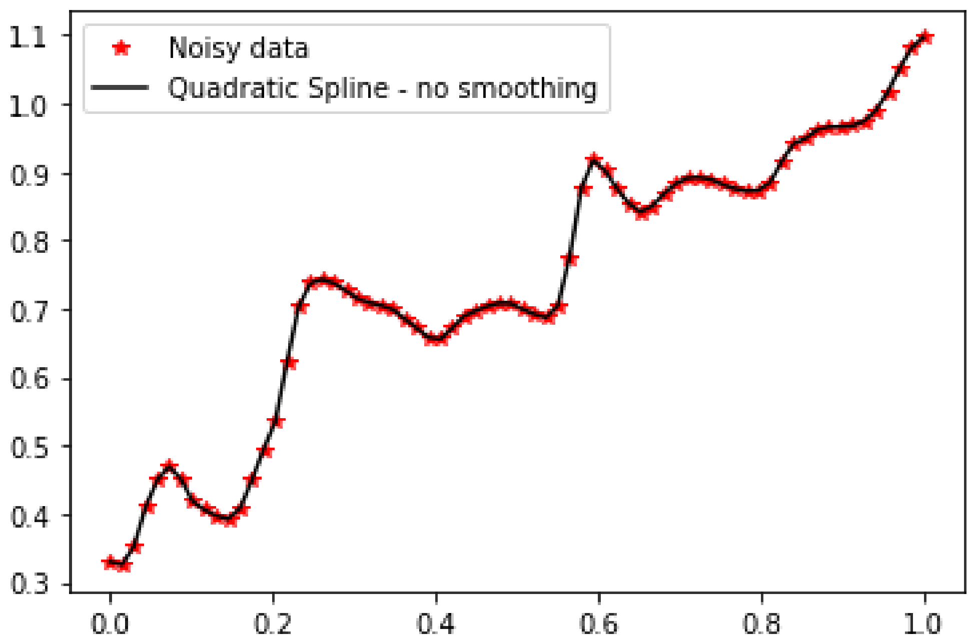
[10]:
```
0    44.073991
dtype: float64
```

[11]:
```
# part 3
# %% B-SPLINES
# reference: https://github.gatech.edu/jtay6/IYSE8803-Examples-Py/blob/master/
↪Module%201/Examples1.py
def BSplineBasis(x: np.array, knots: np.array, degree: int) -> np.array:
    '''Return B-Spline basis. Python equivalent to bs in R or the spmak/spval␣
↪combination in MATLAB.
    This function acts like the R command bs(x,knots=knots,degree=degree,␣
↪intercept=False)
    Arguments:
        x: Points to evaluate spline on, sorted increasing
        knots: Spline knots, sorted increasing
        degree: Spline degree.
    Returns:
        B: Array of shape (x.shape[0], len(knots)+degree+1).
    Note that a spline has len(knots)+degree coefficients. However, because the␣
↪intercept is missing
    you will need to remove the last 2 columns. It's being kept this way to␣
↪retain compatibility with
    both the matlab spmak way and how R's bs works.
    If K = length(knots) (includes boundary knots)
    Mapping this to R's bs: (Props to Nate Bartlett )
    bs(x,knots,degree,intercept=T)[,2:K+degree] is same as␣
↪BSplineBasis(x,knots,degree)[:,:-2]
    BF = bs(x,knots,degree,intercept=F) drops the first column so BF[,1:
↪K+degree] == BSplineBasis(x,knots,degree)[:,:-2]
    '''
    nKnots = knots.shape[0]
    lo = min(x[0], knots[0])
    hi = max(x[-1], knots[-1])
    augmented_knots = np.append(
        np.append([lo]*degree, knots), [hi]*degree)
    DOF = nKnots + degree +1 # DOF = K+M, M = degree+1
    spline = BSpline(augmented_knots, np.eye(DOF),
                     degree, extrapolate=False)
    B = spline(x)
    return B
```

[12]:
```
n = y.shape[0]
k=n
D = np.linspace(0, 1, n)
sigma = 0.3
knots = np.linspace(0, 1, k)
B = BSplineBasis(D, knots, 2)[:,:-2]
```

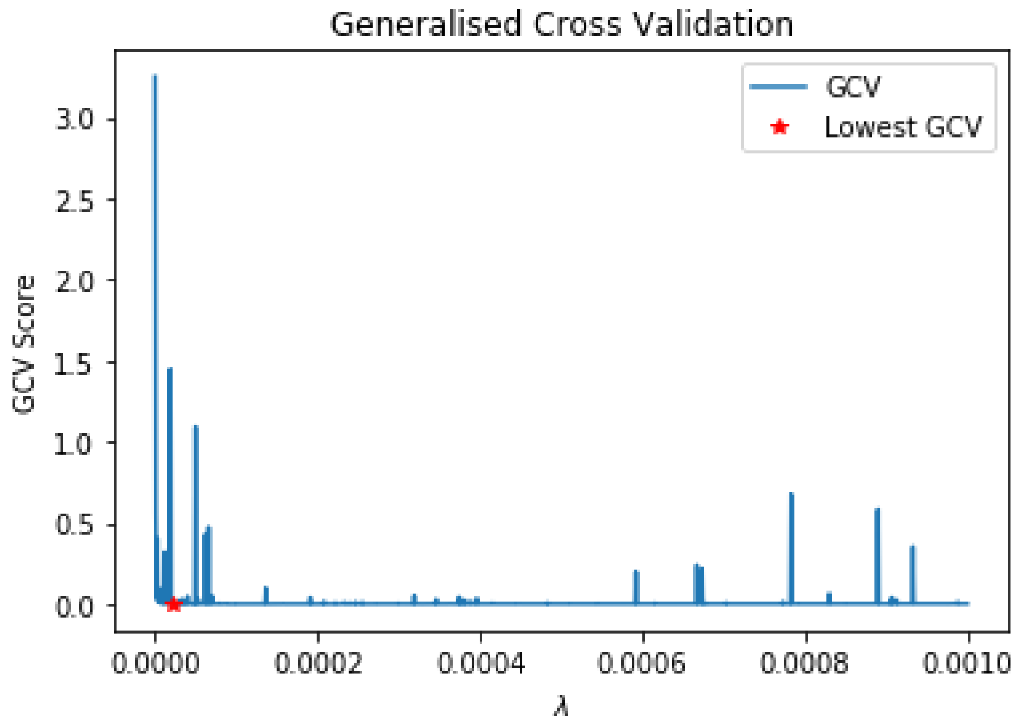
[13]:
```
yhat = B@np.linalg.lstsq(B, y)[0]
assert np.isclose(B@np.linalg.inv(B.T@B)@B.T@y, yhat).all()
plt.plot(D, y, 'r*', label='Noisy data')
plt.plot(D, yhat, 'k-', label='Quadratic Spline - no smoothing')
plt.legend()
plt.show()
```

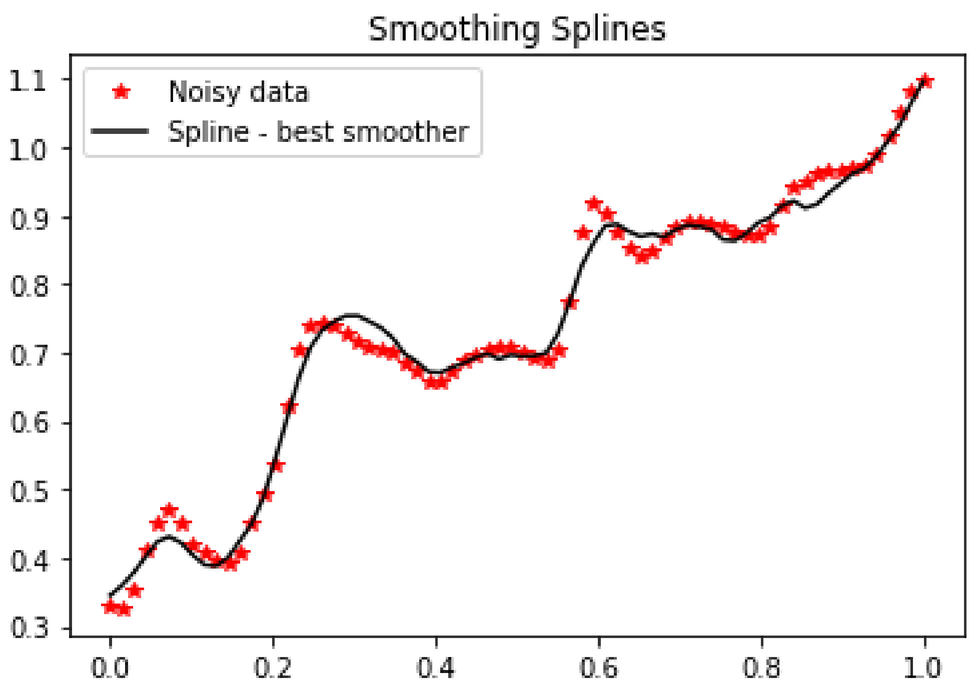
```
/home/jfftilton/anaconda3/envs/omsa/lib/python3.7/site-
packages/ipykernel_launcher.py:1: FutureWarning: `rcond` parameter will change
to the default of machine precision times ``max(M, N)`` where M and N are the
input matrix dimensions.
To use the future default and silence this warning we advise to pass
`rcond=None`, to keep using the old, explicitly pass `rcond=-1`.
  """Entry point for launching an IPython kernel.
```



[14]:
```
# reference: https://github.gatech.edu/jtay6/IYSE8803-Examples-Py/blob/master/
↪Module%201/Examples1.py
B2 = np.diff(B, axis=0, n=2)*(n-1)**2
omega = B2.T.dot(B2)/(n-2)
```

```python
lams = np.arange(0, 1e-3, 1e-6)
p = len(lams)
RSS = []
df = []
for lam in lams:
    S = B@np.linalg.inv(B.T@B+lam*omega)@B.T  # Not great but we still need to get the trace of S
    yhat = S.dot(y)
    RSS.append(((yhat-y)**2).sum())
    df.append(np.trace(S))
RSS = np.array(RSS)
df = np.array(df)
# GCV criterion
GCV = (RSS/n)/(1-df/n)**2
i = np.argmin(GCV)
m = GCV[i]
plt.plot(lams, GCV, label='GCV')
plt.plot(lams[i], m, 'r*', label='Lowest GCV')
plt.title("Generalised Cross Validation")
plt.xlabel('$\lambda$')  # noqa: W605
plt.ylabel('GCV Score')
plt.legend()
plt.show()
S = B@np.linalg.inv(B.T@B+lams[i]*omega)@B.T
yhat = S@y
plt.plot(D, y, 'r*', label='Noisy data')
plt.plot(D, yhat, 'k-', label='Spline - best smoother')
plt.legend()
plt.title("Smoothing Splines")
plt.show()
```


Generalised Cross Validation
GCV
Lowest GCV
GCV Score
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0000
0.0002
0.0004
0.0006
0.0008
0.0010
λ


Smoothing Splines
Noisy data
Spline - best smoother
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.0
0.2
0.4
0.6
0.8
1.0

[15]:
```
# part 4
y_smooth = y_train.apply(lambda row: S@row, axis = 1)
y_smooth = pd.DataFrame(np.array([np.array(s) for s in y_smooth]))
reg = LinearRegression().fit(y_smooth, protein_train)
y_smooth_test = y_test.apply(lambda row: S@row, axis = 1)
y_smooth_test = pd.DataFrame(np.array([np.array(s) for s in y_smooth_test]))
y_hat_spline = reg.predict(y_smooth_test)
np.sum((protein_test - y_hat_spline)**2)
```

[15]:
```
0    44.073991
dtype: float64
```

[19]:
```
# part 5
df = pd.DataFrame({"spline":[x[0] for x in y_hat_spline], "kernel":[x[0] for x␣
↪in y_hat_kernel]})
df
```

[19]:

	spline	kernel
0	9.180781	9.180781
1	8.043734	8.043734
2	11.050827	11.050827
3	9.304310	9.304310
4	12.086602	12.086602
5	11.161356	11.161356
6	11.974393	11.974393
7	10.390906	10.390906
8	8.837624	8.837624
9	10.623142	10.623142
10	12.119343	12.119343
11	13.240754	13.240754
12	12.372441	12.372441
13	10.420969	10.420969
14	10.600016	10.600016
15	10.875486	10.875486
16	14.568504	14.568504
17	11.340902	11.340902
18	12.444485	12.444485
19	9.318833	9.318833

1 Discussion

Unless I have done something wrong the predicted of the spline and kernel come out to be the same (44.1 mse). Mind blown.

Although both methods come out to have the same answer, I recommend the kernel method only because it is much easier for me to comprehend, therefore explain, than b-splines.

```
[ ]:
```