Modeling data with Gaussian process

$$K(x, x') = \exp\left(-\frac{\left||x - x'|\right|_2}{2\sigma^2}\right)$$
$$m(x) = 20$$

(a)

$$\begin{pmatrix} y_{tr} \\ y_{te} \end{pmatrix} \sim N \begin{pmatrix} \begin{bmatrix} 20 \\ \dots \\ 20 \end{bmatrix}, \begin{bmatrix} K_{tr} & K_{tr,te} \\ K_{te,tr} & K_{te} \end{bmatrix}$$

Since the data follows Gaussian Process, we select the data set as y_{tr}, y_{te} then we have

$$\begin{pmatrix} y_{tr1} \\ \dots \\ y_{trn} \\ y_{ten} \\ y_{tem} \end{pmatrix} \sim N \begin{pmatrix} m(y_{tr1}) \\ \dots \\ m(y_{trn}) \\ m(y_{ten}) \\ \dots \\ m(y_{tem}) \end{pmatrix}^{K(X_{tr1}, X_{tr1})} & \dots & K(X_{tr1}, X_{trn}) & K(X_{tr1}, X_{te1}) & \dots & K(X_{tr1}, X_{tem}) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ K(X_{trn}, X_{tr1}) & \dots & K(X_{trn}, X_{trn}) & K(X_{trn}, X_{te1}) & \dots & K(X_{trn}, X_{tem}) \\ K(X_{te1}, X_{tr1}) & \dots & K(X_{te1}, X_{trn}) & K(X_{te1}, X_{te1}) & \dots & K(X_{ten}, X_{tem}) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ K(X_{tem}, X_{tr1}) & \dots & K(X_{tem}, X_{trn}) & K(X_{tem}, X_{te1}) & \dots & K(X_{tem}, X_{tem}) \end{pmatrix}$$

Since we already know that

$$m(x) = 20$$

So we can get

$$\begin{bmatrix} m(y_{tr1}) \\ \dots \\ m(y_{trn}) \\ m(y_{te1}) \\ \dots \\ m(y_{tom}) \end{bmatrix} = \begin{bmatrix} 20 \\ \dots \\ 20 \end{bmatrix}$$

Also, we can find that the upper left area in the K covariance matrix only contain training data thus

$$K_{tr} = \begin{bmatrix} K(X_{tr1}, X_{tr1}) & \dots & K(X_{tr1}, X_{trn}) \\ \dots & \dots & \dots \\ K(X_{trn}, X_{tr1}) & \dots & K(X_{trn}, X_{trn}) \end{bmatrix}$$

Similarly, we can find that

$$K_{tr} = \begin{bmatrix} K(X_{te1}, X_{te1}) & \dots & K(X_{te1}, X_{tem}) \\ \dots & \dots & \dots \\ K(X_{tem}, X_{te1}) & \dots & K(X_{tem}, X_{tem}) \end{bmatrix}$$

By observance, we can find the upper right part is the matrix arising from pairwise evaluation of the kernel between the training data and test data, similarly for down left part

$$K_{te,tr} = K_{tr,te}^{T}$$

$$K_{tr,te} = \begin{bmatrix} K(X_{tr1}, X_{te1}) & \dots & K(X_{tr1}, X_{tem}) \\ \dots & \dots & \dots \\ K(X_{trn}, X_{te1}) & \dots & K(X_{trn}, X_{tem}) \end{bmatrix}$$

So we can rewrite as

$$\begin{pmatrix} y_{tr1} \\ \dots \\ y_{trn} \\ y_{te1} \\ \dots \\ y_{tem} \end{pmatrix} \sim N \begin{pmatrix} m(y_{tr1}) \\ \dots \\ m(y_{trn}) \\ m(y_{te1}) \\ \dots \\ m(y_{tem}) \end{pmatrix} \begin{bmatrix} K(X_{tr1}, X_{tr1}) & \dots & K(X_{tr1}, X_{trn}) & K(X_{tr1}, X_{te1}) & \dots & K(X_{tr1}, X_{tem}) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ K(X_{trn}, X_{tr1}) & \dots & K(X_{trn}, X_{trn}) & K(X_{trn}, X_{te1}) & \dots & K(X_{trn}, X_{tem}) \\ K(X_{te1}, X_{tr1}) & \dots & K(X_{te1}, X_{trn}) & K(X_{te1}, X_{te1}) & \dots & K(X_{te1}, X_{tem}) \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ K(X_{tem}, X_{tr1}) & \dots & K(X_{tem}, X_{trn}) & K(X_{tem}, X_{te1}) & \dots & K(X_{tem}, X_{tem}) \\ \end{pmatrix} \\ = N \begin{pmatrix} 20 \\ \dots \\ 20 \end{pmatrix}, \begin{bmatrix} K_{tr} & K_{tr,te} \\ K_{te,tr} & K_{te} \end{bmatrix}$$

(b)

$$mean = m_{te} + K_{te,tr} * K_{tr}^{-1} (y_{tr} - y_{te})$$

Here is the result of the code:

conditional test mean

[14.26880633 -73.06558265 14.61820814 18.78940398 11.46167127 -60.20940761 19.69791631 23.69517697 -7.59168743 23.04869716 12.50774735]

true value found

[16.3 22.1 20.4 14.8 19.7 20.5 18.4 19.1 22.6 22.9 17.4]

mean squared error= 2.1758305462474383

Here is the code

%time

import numpy as np

def readdata(path):

x=[] # lat, long

temp=[]

with open(path) as file:

lines=file.read().split('\n')

for line in lines:

if len(line)<2:

continue

line=line.split(',')

x.append([float(line[0]),float(line[1])])

temp.append(float(line[2]))

```
return np.array(x),np.array(temp)
```

```
train_x,train_y=readdata("gptrain.csv")
test_x,test_y=readdata("gptest.csv")
import math
def Ker(a,b):
    sigma2=0.866**2
    s=0
    for i in range(len(a)):
         s += (a[i]-b[i])**2
    return math.exp(-s/(2*sigma2))
# K(te,tr)
train_l=len(train_x)
test_l=len(test_x)
K_te_tr=np.array([[Ker(test_x[i],train_x[j]) for j in range(train_l)]for i in
range(test_l)])
# Ktr, invert
K_tr_tr=np.array([[Ker(train_x[i],train_x[j]) for j in range(train_l)]for i in
range(train_l)])
K_tr_tr_invert=np.linalg.inv(K_tr_tr)
```

```
# compute conditional test mean
mx=20
dat_mte=train_y-mx
m_te_con=mx + (K_te_tr @ K_tr_tr_invert @ dat_mte)
print("conditional test mean")
print(m_te_con)
# compute mean squared error
m_sqrerr=0
for i in range(len(test_y)):
                 (m_te_con[i]-test_y[i])**2
    m_sqrerr =
m_sqrerr /= len(test_y)
print("true value found")
print(test_y)
print("mean squared error=",m_sqrerr)
```

(c)

So we have

$$cov = K_{te} - K_{te,tr} K_{tr}^{-1} K_{tr,te}$$

$$cov + K_{te,tr}K_{tr}^{-1}K_{tr,te} = K_{te}$$

Our goal is to solve cov

Denote

$$X = cov$$

$$Y = K_{tr}^{-1} K_{tr,te}$$

So we can get

$$X + K_{te,tr}Y = K_{te}$$

Additionally, we have

$$K_{tr}Y = K_{tr} * K_{tr}^{-1}K_{tr,te} = K_{tr,te}$$

So we can get

$$\begin{cases} X + K_{te,tr}Y = K_{te} \\ K_{tr}Y = K_{tr,te} \end{cases}$$

Or rewrite it in matrix

$$\begin{bmatrix} I & K_{te,tr} \\ 0 & K_{tr} \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} K_{te} \\ K_{tr,te} \end{bmatrix}$$

Now we can use np.linalg.solve to solve this linear matrix equation

I use 2 method of both solving the linear equation(method 2) and the inverted matrix(method 1). And compare their result to make sure the accuracy

Here is the result of the code()

```
conditional test covariance matrix method 1
(11, 11)
[[ 9.61672144e-02 -7.22441285e-04 6.52762643e-05 4.09324043e-03
  2.69654972e-04 -4.08863824e-04 1.75344528e-03 3.54970207e-04
 -1.69271499e-04 7.81496777e-04 -1.91486188e-02]
[-7.22441285e-04 2.19242880e-02 -4.53539127e-04 -8.17971055e-04
  3.79739375e-04 1.73640017e-02 4.83582499e-04 4.08597797e-05
  1.77103780e-03 -5.93926790e-03 1.54146834e-04]
[ 6.52762644e-05 -4.53539142e-04 8.50069884e-05 7.96309856e-05
 -4.13995063e-05 -3.69110783e-04 -6.45388895e-05 -4.59389842e-06
 -8.52642301e-06 1.02550741e-03 3.22364624e-05]
 [ 4.09324043e-03 -8.17971055e-04 7.96309855e-05
                                             8.45714734e-01
  1.26513008e-04 9.19511536e-05 -2.64677912e-03
                                             1.37781870e-05
 -1.49025173e-04 7.02684122e-04 1.76889904e-04]
 9.41194200e-02 1.49985543e-04 -6.29958050e-04 -1.40069457e-03
 -2.56498247e-05 -1.30744791e-03 -2.87905238e-03]
 [-4.08863824e-04 1.73640017e-02 -3.69110792e-04 9.19511537e-05
  1.49985543e-04 3.19357531e-02 -1.89178016e-04 2.21718069e-05
  6.94505748e-04 -3.86313291e-03 1.71562930e-04]
-6.29958050e-04 -1.89178015e-04 7.16319689e-03 1.72737237e-04
  8.20188654e-05 -1.30079107e-03 -2.02210391e-03]
-1.40069457e-03 2.21718069e-05 1.72737237e-04 8.20839184e-02
  9.07401941e-06 8.36332379e-05 1.32556719e-031
[-1.69271499e-04 1.77103777e-03 -8.52650732e-06 -1.49025173e-04
 -2.56498247e-05 6.94505751e-04 8.20188612e-05 9.07401941e-06
  3.54401256e-04 -4.36387412e-05 4.19466784e-05]
 [ 7.81496777e-04 -5.93926792e-03 1.02550734e-03 7.02684122e-04
 -1.30744791e-03 -3.86313291e-03 -1.30079106e-03
                                             8.36332379e-05
 -4.36387538e-05 2.06422793e-02 2.45781927e-04]
 [-1.91486188e-02 1.54146834e-04 3.22364626e-05 1.76889904e-04
 -2.87905238e-03 1.71562930e-04 -2.02210391e-03 1.32556719e-03
  4.19466786e-05 2.45781927e-04 3.93569212e-02]]
conditional test covariance matrix_method 2
(11, 11)
[[ 9.61672144e-02 -7.22441285e-04 6.52762644e-05 4.09324043e-03
  2.69654972e-04 -4.08863824e-04 1.75344528e-03 3.54970207e-04
 -1.69271499e-04 7.81496777e-04 -1.91486188e-02]
```

```
[-7.22441285e-04 2.19242880e-02 -4.53539152e-04 -8.17971055e-04
  3.79739375e-04 1.73640017e-02 4.83582502e-04 4.08597797e-05
  1.77103778e-03 -5.93926791e-03 1.54146834e-04]
[ 6.52762644e-05 -4.53539152e-04 8.50069469e-05 7.96309856e-05
 -4.13995065e-05 -3.69110785e-04 -6.45388954e-05 -4.59389842e-06
 -8.52645297e-06 1.02550740e-03 3.22364624e-05]
1.26513008e-04 9.19511537e-05 -2.64677912e-03 1.37781870e-05
 -1.49025173e-04 7.02684122e-04 1.76889904e-04]
9.41194200e-02 1.49985543e-04 -6.29958050e-04 -1.40069457e-03
 -2.56498247e-05 -1.30744791e-03 -2.87905238e-03]
[-4.08863824e-04 1.73640017e-02 -3.69110785e-04 9.19511538e-05
  1.49985543e-04 3.19357531e-02 -1.89178015e-04 2.21718069e-05
  6.94505753e-04 -3.86313291e-03 1.71562930e-04]
-6.29958050e-04 -1.89178015e-04 7.16319688e-03 1.72737237e-04
  8.20188646e-05 -1.30079107e-03 -2.02210391e-03]
-1.40069457e-03 2.21718069e-05 1.72737237e-04 8.20839184e-02
  9.07401941e-06 8.36332379e-05 1.32556719e-031
[-1.69271499e-04 1.77103778e-03 -8.52645297e-06 -1.49025173e-04
 -2.56498247e-05 6.94505753e-04 8.20188646e-05 9.07401941e-06
  3.54401283e-04 -4.36387196e-05 4.19466784e-05]
-1.30744791e-03 -3.86313291e-03 -1.30079107e-03 8.36332379e-05
 -4.36387198e-05 2.06422794e-02 2.45781927e-04]
[-1.91486188e-02 1.54146834e-04 3.22364624e-05 1.76889904e-04
 -2.87905238e-03 1.71562930e-04 -2.02210391e-03 1.32556719e-03
  4.19466784e-05 2.45781927e-04 3.93569212e-02]]
maximum difference
5.8170857020201083e-11
```

Here is the detailed code:

compute conditional test covariance matrix, using 2 methods to compare

```
# method 1--invert matrix
K_te_te=np.array([[Ker(test_x[i],test_x[i]) for i in range(test_l)]for i in
range(test I)])
K_tr_te=np.array([[Ker(train_x[i],test_x[i]) for i in range(test_l)]for i in
range(train_l)])
comat_te_con_1=K_te_te - (K_te_tr @ K_tr_tr_invert @ K_tr_te)
print("conditional test covariance matrix___method 1")
print(comat te con 1.shape)
print(comat te con 1)
# method 2--np.linalg.solve
def merge(A):
    lines=[]
    for i in range(len(A)):
         lines.append(np.concatenate(A[i],axis=1))
    res=np.concatenate(lines,axis=0)
    return res
def cmpt_cov_2(K_te_tr,K_tr_tr,K_te_te,K_tr_te):
A=[[np.identity(len(K_te_te)),K_te_tr],[np.zeros((len(K_tr_tr),len(K_te_te)
))),K_tr_tr]]
```

```
A=merge(A)

B=merge([[K_te_te],[K_tr_te]])

comat_and_invert=np.linalg.solve(A,B) # 104*11; [x,y]; y is K_tr^-

1*K_tr_te, not square, easy to compute !!!

res_l=len(K_te_tr)

return comat_and_invert[:res_l,:res_l]

comat_te_con_2=cmpt_cov_2(K_te_tr,K_tr_tr,K_te_te,K_tr_te)

print("conditional test covariance matrix_method 2")

print(comat_te_con_2.shape)

print(comat_te_con_2)

print("maximum difference_")

print(max(abs((comat_te_con_2-comat_te_con_1).reshape(-1))))
```

(d)

From the result below, we can clearly find the feature that is shown in class, that is when the location is close to the points in training data, the variance becomes very small and almost vanish. This is because, in the Gaussian process that we use, the kernel function that governs the data, determine that the covariance between the training points x and the testing points x' will increase exponentially when $x' \to x$, which means they f(x') will almost determined by f(x), which means the variance of f(x) will almost diminish.

$$K(x, x') = \exp\left(-\frac{\left|\left|x - x'\right|\right|_2}{2\sigma^2}\right)$$

Here is the result of the code

I use 2 method of both solving the linear equation(method 2) and the inverted matrix(method 1). And compare their result to make sure the accuracy. I also draw 2 pictures to show the scenario.

Wall time: 0 ns

5041

conditional test covariance matrix for new created grid new_cov_1

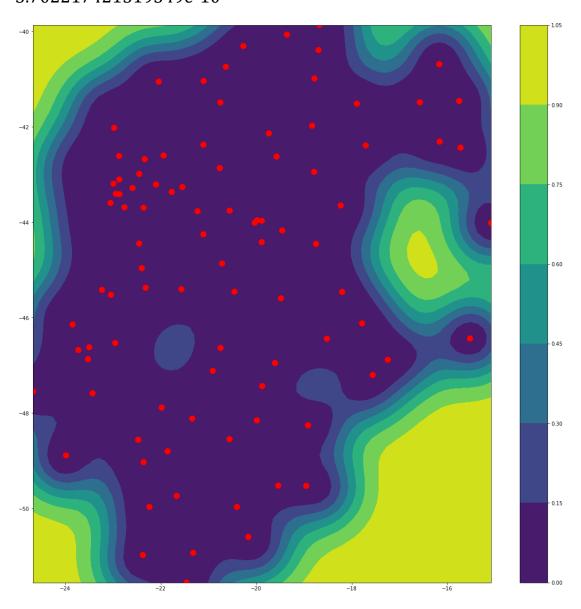
[0.99902453 0.99786799 0.99552959 ... 0.76632897 0.82762307 0.87855586]

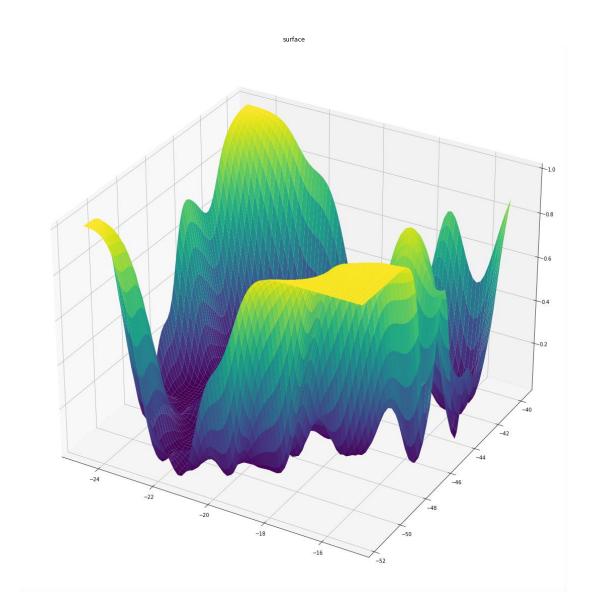
new_cov_2

[0.99902453 0.99786799 0.99552959 ... 0.76632897 0.82762307 0.87855586]

maximum error

3.702217421519549e-10





Here is the detailed code

%time

find the range of latitude, longitude

trans=np.array(np.matrix(train_x).T)

lat=trans[0]

long=trans[1]

x_l=min(lat)

```
x r=max(lat)
y_l=min(long)
y r=max(long)
# create the grid, choose 70*70=4900 points
new_lat=np.array([x_l+i*(x_r-x_l)/70 \text{ for } i \text{ in } range(71)])
new_long=np.array([y_l+i*(y_r-y_l)/70 for i in range(71)])
grid lat,grid long=np.meshgrid(new lat,new long)
grid lat=grid lat.reshape(-1)
grid_long=grid_long.reshape(-1)
new x=np.array(np.matrix([grid lat,grid long]).T)
new_l=len(new_x)
print(new_l)
# compute the covariance matrix
K new new=np.array([[Ker(new x[i],new x[i]) for i in range(new l)]for i
in range(new_l)])
K_new_tr=np.array([[Ker(new_x[i],train_x[j]) for j in range(train_l)]for i in
range(new_l)])
K_tr_new=np.array([[Ker(train_x[i],new_x[j]) for i in range(new_l)]for i in
range(train_l)])
comat new con 2=cmpt cov 2(K new tr,K tr tr,K new new,K tr new)
```

```
new_cov_2=[comat_new_con_2[i][i] for i in range(new_l)]
new_cov_2=np.array(new_cov_2)
comat new con 1=K new new - (K new tr @ K tr tr invert
K_tr_new)
new_cov_1=[comat_new_con_1[i][i] for i in range(new_l)]
new_cov_1=np.array(new_cov_1)
print("conditional test covariance matrix for new created grid")
# print(comat new con)
# convariance list
# print(new_cov)
print("new cov 1")
print(new_cov_1)
print("new_cov_2")
print(new_cov_2)
print("difference")
print(new_cov_2-new_cov_1)
print("maximum error")
print(max(abs(new_cov_2-new_cov_1)))
from pylab import rcParams
rcParams['figure.figsize'] = 20,20
```

```
import matplotlib.pyplot as plt
figure, axes = plt.subplots()
for i in range(len(train_x)):
    center = plt.Circle(tuple(train_x[i]), 0.06, color='r')
    # axes.set_aspect(1)
    axes.add_artist( center )
new cov=np.array(new cov 2)
h = plt.contourf(grid_lat.reshape(71,-1), grid_long.reshape(71,-1),
new_cov.reshape(71,-1))
plt.axis('scaled')
plt.colorbar()
plt.show()
ax = plt.axes(projection='3d')
ax.plot_surface(grid_lat.reshape(71,-1), grid_long.reshape(71,-1),
new_cov.reshape(71,-1), rstride=1, cstride=1,
                   cmap='viridis', edgecolor='none')
ax.set_title('surface')
```