Variation+Inference+Linear+Regression

May 23, 2019

First import required modules

```
In [1]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import scipy.stats as stats
        from scipy.special import digamma
        from scipy.linalg import sqrtm
```

1 Regression Spline

Assume that the range of x is $[a, b]$. Let the point

$$a < \xi_1 < \cdots < \xi_K < b$$

be a partion of the interval $[a, b]$
$\{\xi_1, \ldots, \xi_K\}$ are called knots.
Then make the function which return the knot points

```
In [2]: def defineKnot(X,K=10):
            upper = max(X)
            lower = min(X)
            out = np.linspace(start=lower,stop=upper,num=K+2)[1:K+1]
            return(out)
```

2 Radial Basis Function

A RBF φ is a real valued function whose value depends only on the distance from origin. A real function $\varphi : [0, \infty) \to \mathbb{R}$ with a metric on space $\|\cdot\| : V \to [0, \infty)$ a function $\varphi_c = \varphi(\|\mathbf{x} - \mathbf{c}\|)$ is said to be a radial kernel centered at c. A radial function and the associated radial kernels are said to be radial basis function

we use radial basis functions defined by

$$\mathbf{b}(u) = \left\{ u, \left| \frac{u - \tau_1}{c} \right|^3, \cdots, \left| \frac{u - \tau_K}{c} \right|^3 \right\}$$

where c is sample standard deviation

Then we can make the function which retrun the basis

```
In [3]: def b(u,tau,sd):
            lst = []
            #lst.append(np.ones(len(u)))
            lst.append(u)
            for i in tau:
                lst.append(abs((u-i)/sd)**3)
            out = np.array(lst)
            return(out)
```

Nonparametric linear model can be represented as

$$Y = \mathbf{b}(X)\boldsymbol{\beta} + \varepsilon$$

where $Y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times 1}$ and $\varepsilon \sim N(0, \tau^{-1})$

3 Make toy data

Let

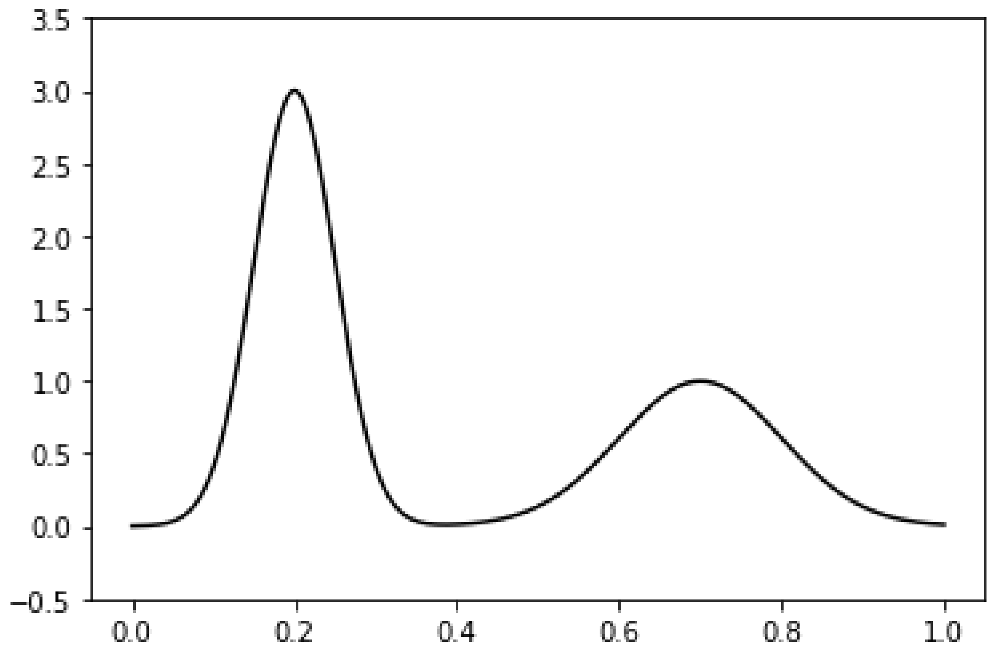
$$y = 3\exp\left(-200(x-0.2)^2\right) + \exp\left(-50(x-0.7)^2\right)$$

Plotting true distribution of Y is

```
In [4]: def f(x):
            out =3*np.exp(-200*(x-0.2)**2) + np.exp(-50*(x-0.7)**2)
            return(out)
        lim = (-0.5,3.5)
```

```
In [5]: grid_x = np.linspace(0,1,1000)
        grid_y = f(grid_x)
```

```
In [6]: plt.plot(grid_x, grid_y, 'k')
        plt.ylim(lim)
        plt.show()
```



make the simulation function which make the obs with error $N(0, 0.5)$

```
In [7]: def mkToy(n=300,tau = 0.5):
            np.random.seed(4428)
            x = np.random.uniform(size = n)
            e = np.random.normal(0,np.sqrt(0.5), size= n)
            y = f(x) + e
            #out = np.column_stack([x,y])
            return(x,y)
```

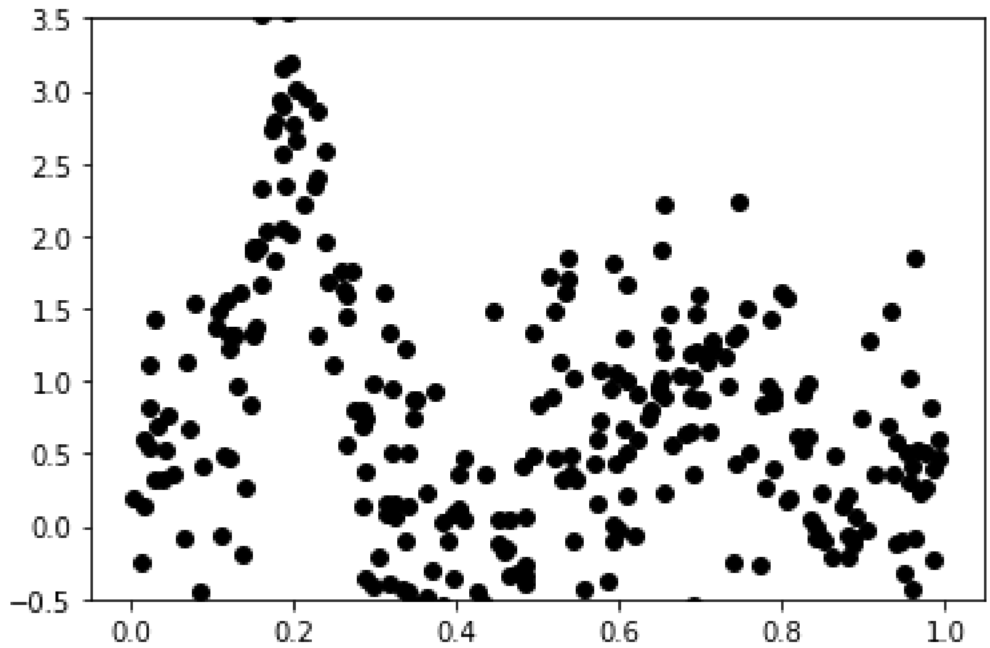
Plotting the distribution of simulated data

$$y = 3\exp\left(-200(x-0.2)^2\right) + \exp\left(-50(x-0.7)^2\right) + \varepsilon$$

where $\varepsilon \sim N(0, 0.5)$

```
In [8]: x,y = mkToy()
```

```
In [9]: plt.plot(x,y,'ko')
        plt.ylim(lim)
        plt.show()
```



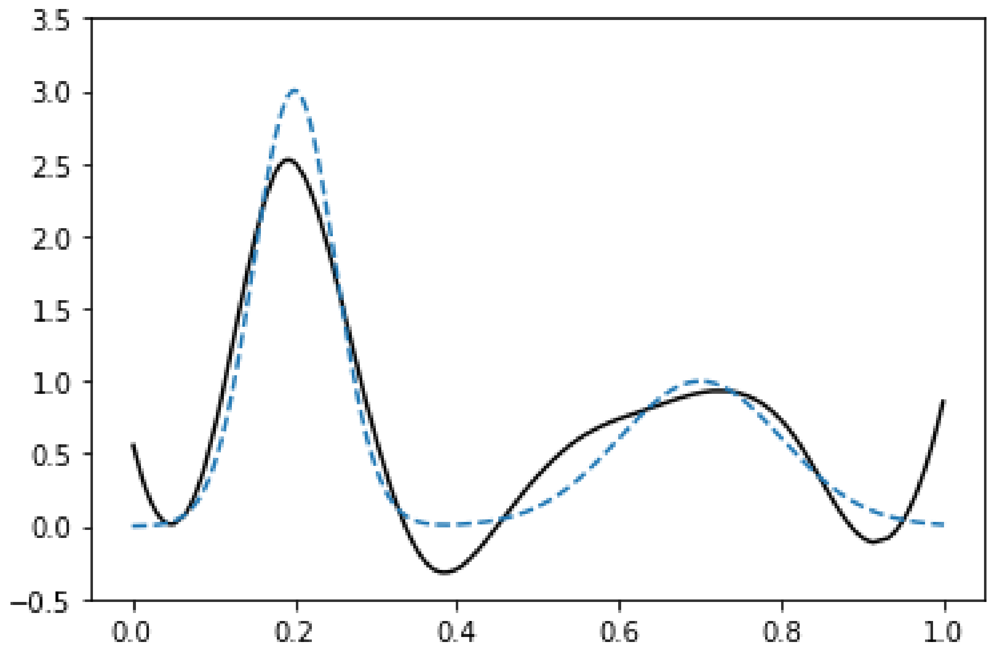
Calculate the standard deviation of observed data and define the knot and make design matrix

```
In [10]: sd = np.std(x)
         knot = defineKnot(x)
         d_x = b(x,knot,sd).T
```

4 LSE method

plotting the fitted value

```
In [11]: fitted  = d_x.dot(np.linalg.inv(d_x.T.dot(d_x))).dot(d_x.T).dot(y)
         def lplot(x,fitted):
             plot_m = np.array(sorted(np.array([x,fitted]).T,key=lambda x: x[0]))
             plt.plot(plot_m[:,0],plot_m[:,1],'k',grid_x, grid_y, '--')
             plt.ylim(lim)
             plt.show()
         lplot(x,fitted)
```



Blue dashed line is true function and solid line is LSE estimated function

5 MFVB method

setting prior as

$$\begin{aligned} p(Y|\tau,\beta) &\sim N(X\beta, \tau^{-1}\cdot I_N) \\ p(\beta_i|\gamma_i) &\sim^{ind} N(0,\gamma^{-1}) \text{ for } i=1,\dots p \\ p(\gamma) &\sim Gamma(a,b) \\ p(\tau) &\sim Gamma(c,d) \end{aligned}$$

By Baye's rule

$$p(\tau,\gamma,\beta|Y) \propto p(Y|\tau,\beta)p(\beta|\gamma)p(\tau)p(\gamma)$$

Then variational distribution is

$$p(\tau,\gamma,\mu|Y) \approx q(\tau,\gamma,\mu) = q_1(\tau)q_2(\gamma)q_3(\mu)$$

we can maximize ELBO by coordinate descent algorithm

$$\begin{aligned} q_1^*(\tau) &= E_{q_2,q_3}[p(\tau,\gamma,\beta|Y)] \propto E_{q_2,q_3}[p(Y|\tau,\beta)p(\tau)] \\ q_2^*(\gamma) &= E_{q_1,q_3}[p(\tau,\gamma,\beta|Y)] \propto E_{q_1,q_3}[p(\beta|\gamma)p(\gamma)] \\ q_3^*(\beta) &= E_{q_1,q_2}[p(\tau,\gamma,\beta|Y)] \propto E_{q_1,q_2}[p(Y|\tau,\beta)p(\beta|\gamma)] \end{aligned}$$

Then

$$q_1^* \sim Gamma\left(c + \frac{N+1}{2}, d + \frac{1}{2}\left\{Y'Y - E_{q3}[\beta'](X'Y)\right\} + tr\left[X(var_{q3}[\beta] + E_{q3}[\beta]E_{q3}[\beta'])X'\right]\right)$$

$$q_2^* \sim \prod_{i=1}^{p} Gamma(a + \frac{1}{2}, b + \frac{1}{2}\{var_{q3}[\beta]_{i,i} + E_{q3}[\beta_i]^2\})$$

$$q_3^* \sim N\left(E_{q1}[\tau]\Sigma X'Y, \left(diag(E_{q2}[\gamma]) + E_{q1}[\tau]X'X\right)^{-1} = \Sigma\right)$$

```
In [12]: def product(a):
             n = len(a)
             out = np.zeros([n,n])
             for i in range(n):
                 for j in range(n):
                     out[i,j] = a[i]*a[j]
             return(out)
```

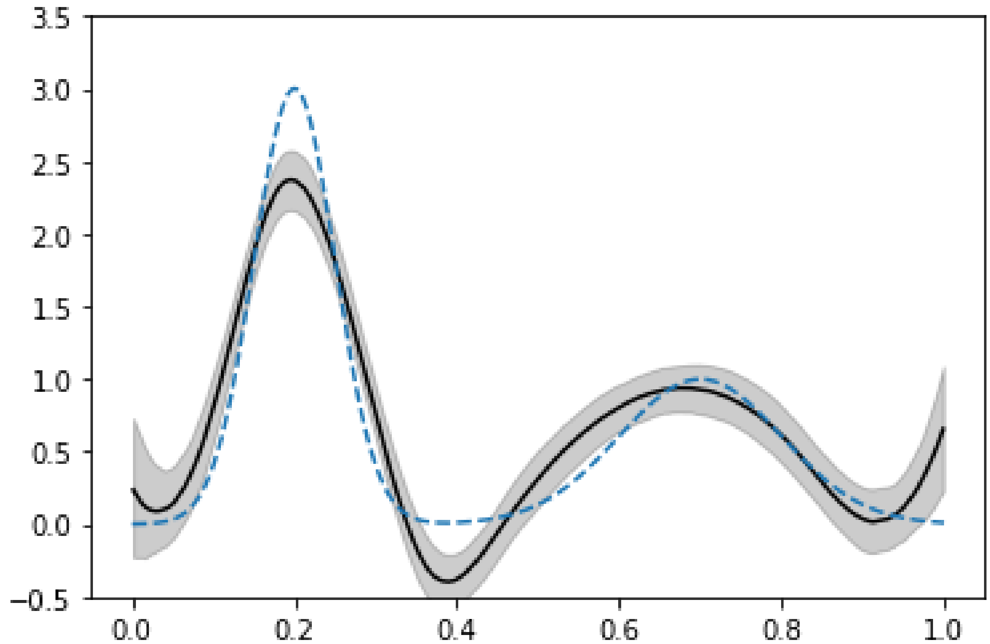
```
In [13]: def mfvb(X,y,max_iter=100):

             N,p = X.shape
             a ,b, c, d = [10**(-7)]*4
             a_tilde = np.repeat(a + 0.5, p)
             b_tilde = np.repeat(b,p)
             c_tilde = c + (N+1)/2
             d_tilde = d

             mu_coeffs = np.repeat(0,p)
             sigma_coeffs = np.diag(np.repeat(1,p))

             for i in range(max_iter):
                 expected_coeffs = mu_coeffs
                 double_expected_coeffs = sigma_coeffs + product(mu_coeffs)
                 diagonal_sigma = np.diag(sigma_coeffs)
                 expected_alpha = np.array(list(map(lambda x : a_tilde[x]/b_tilde[x] , np.arange
                 log_expected_alpha = np.array(list(map(lambda x : digamma(a_tilde[x])-np.log(b_
                 expected_tau = c_tilde / d_tilde
                 log_expected_tau = digamma(c_tilde)-np.log(d_tilde)
                 sigma_coeffs = np.linalg.inv(np.diag(expected_alpha)+expected_tau*(X.T.dot(X)))
                 mu_coeffs =  expected_tau*sigma_coeffs.dot(X.T.dot(y))
                 b_tilde = np.array(list(map(lambda x : (diagonal_sigma[x]+mu_coeffs[x]**2)/2 +
                 d_tilde = d+0.5*(y.T.dot(y)) - expected_coeffs.T.dot((X.T.dot(y)))+ 0.5*sum(np.
             return mu_coeffs,sigma_coeffs
```

```
In [14]: m,c = mfvb(d_x,y)
```

```
In [19]: def ci95(m,c,n=100):
             np.random.seed(4428)
             sampled_coef = np.random.multivariate_normal(m,c,size=n)
             y_grid = np.array([d_x.dot(b) for b in sampled_coef])
```

```
    quantile = np.array([np.sort(x)[[int(n*0.025),int(n*0.5),int(n*0.975)]] for x in y_
    xq = np.array(sorted(np.array([x,quantile[:,0],quantile[:,1],quantile[:,2]]).T,key=
    plt.fill_between(xq[:,0], xq[:,1],xq[:,3], color =(0,0,0,0.2))
    plt.plot(xq[:,0],xq[:,2],'k',grid_x, f(grid_x), '--')
    #plt.plot(x_grid,y_grid[10],'k',x_grid, f(x_grid), '--')
    plt.ylim(lim)
    plt.show()
```

```
In [20]: ci95(m,c,n=1000)
```



Dashed line is True function, solid line is median estimator and gray filled area is 95% confidence interval