Machine Learning HW III

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```
In [1]: import numpy as np
        import pandas as pd
        import sklearn as sk
        import matplotlib
        import matplotlib.pyplot as plt
        plt.style.use('ggplot')
        %matplotlib inline

        import scipy.stats
        from sklearn.metrics import mean_squared_error
        from sklearn.linear_model import LinearRegression
        from pygam import LinearGAM
        from pygam.utils import generate_X_grid
        from copy import copy
        from progressbar import ProgressBar
```

1 Forward Rate

1.1 Smooth Spline Fit of the Forward Rate

```
In [98]: %%capture --no-stdout --no-display
         gam = LinearGAM().gridsearch(x,y)

         fig, ax = plt.subplots(1, 1, figsize=(10,10))
         x_grid = np.linspace(0,30,100).reshape(100,1)
         ax.plot(x,y,'o--', alpha=0.4, label='sample')
         ax.plot(x_grid, gam.predict(x_grid), linewidth=2, label='fitted')
         ax.update({'xlabel':'Time', 'ylabel':'Rate',
                    'title':'Forward Rates Over Time and the Smoothing Spline Fit'})
         _ = ax.legend()
```

```
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```
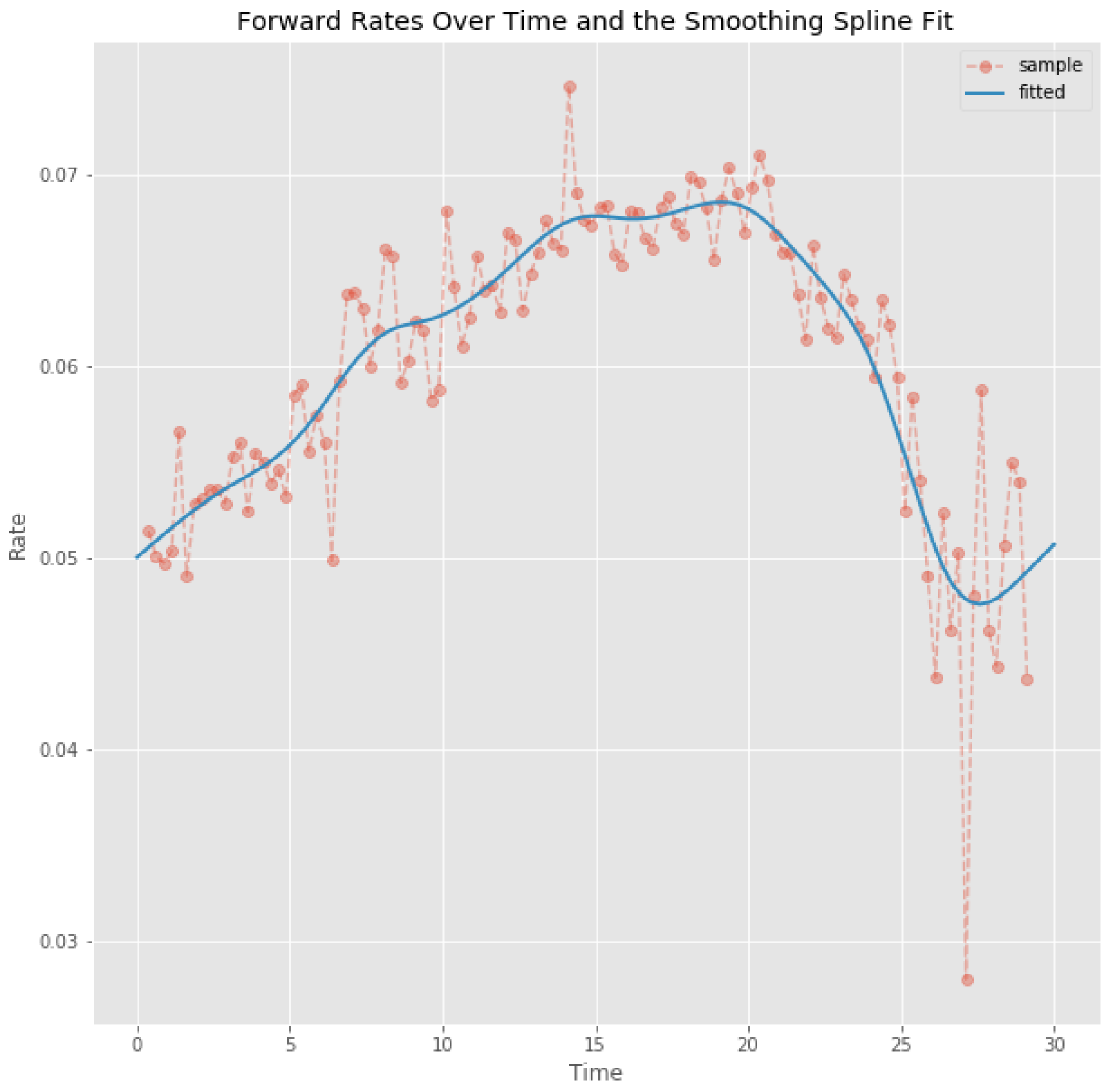



Yes, we obtain a fairly believable smooth fit.

1.2 Splines are Nice for Integrals

The advantage of smoothing splines is that they are essentially piecewise cubic polynomial, which we can write down an explicit formula for (knowing the basis functions and the parameters with which they are linearly combined).

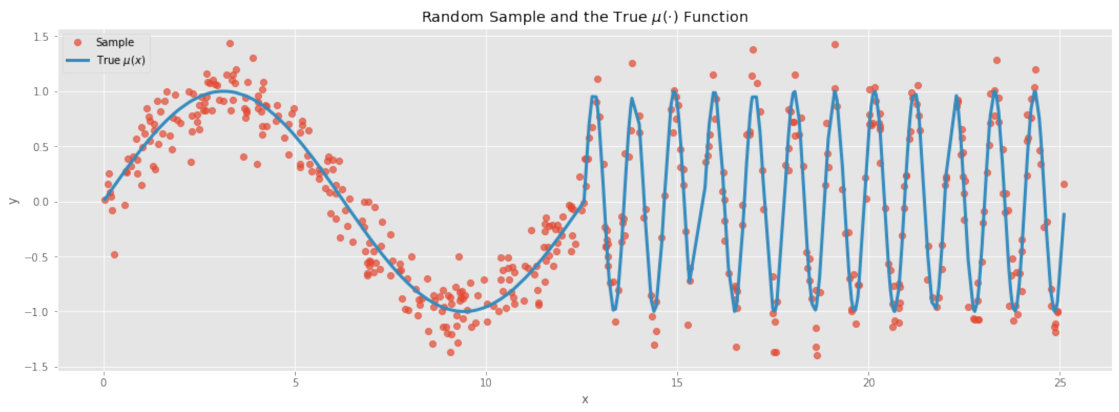
Then, integrating cublic polynomials becomes a piece of cake. We can just take advantage the linearity of integral: evaluate the integration for each piece of the spline, then add them together.

2 Kernel Regression and Varying Smoothness

2.1 y Versus x

```
In [38]: def mu(x):
             """
             ground truth:
             y = { sin(x/2) on [0,4*pi]
                   sin(6*x) on [4*pi,8*pi] }
             """
             #
             y = np.zeros(len(x))
             lefts, rights = (x<=4*np.pi), (x>4*np.pi)
             y[lefts] = np.sin(x[lefts]/2.0)
             y[rights] = np.sin(6*x[rights])
             return y

         def generate_sample(n):
             # sample X uniformly on [0,8*pi].
             x = np.random.uniform(low=0, high=8*np.pi, size=n)
             x.sort()
             # sample Y as gaussians around mu(x)
             y = mu(x) + np.random.normal(loc=0, scale=0.2, size=n)
             return pd.DataFrame({'x':x, 'y':y})

         scipy.random.seed(7)
         sine_df = generate_sample(500)
```

```
In [101]: fig, ax = plt.subplots(1, 1, figsize=(18,6))
          ax.plot(sine_df.x,sine_df.y, 'o', alpha=0.7, label='Sample')
          ax.plot(sine_df.x,mu(sine_df.x), linewidth=3, label=r'True $\mu(x)$')
          ax.update({'xlabel':'x', 'ylabel':'y',
                     'title':r'Random Sample and the True $\mu(\cdot)$ Function'})
          _ = ax.legend()
```



The two parts of the data are very different. For $x > 4\pi$, μ is very wiggly. For $x \leq 4\pi$, it's a lot smoother.

2.2 Different Parts of Data for CV

```
In [90]: %%capture --no-stdout --no-display
         left_df = sine_df[sine_df.x <= 4*np.pi]
         right_df = sine_df[sine_df.x > 4*np.pi]
         cv_lams = np.zeros(3)

         for i, df in enumerate([left_df, right_df, sine_df]):
             x, y = df.x.values, df.y.values
             gam = LinearGAM(n_splines=100).gridsearch(
                 x, y, lam=np.logspace(-5, 4, 100))
             cv_lams[i] = gam.lam
         print('Selected lambdas: ', cv_lams)
```

```
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Selected lambdas:  [  1.87381742e+03   3.51119173e-01   2.84803587e-02]
```

The optimal λ's are printed above. Let's call them $\lambda_{x\leq 4\pi}$, $\lambda_{x>4\pi}$ and λ_{all}. We have

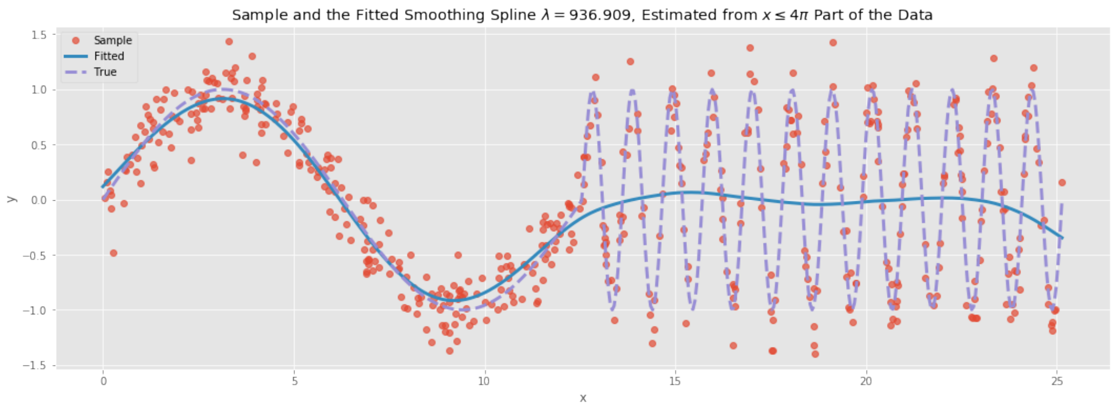
$$\lambda_{x\leq 4\pi} > \lambda_{x\leq 4\pi} > \lambda_{all}$$

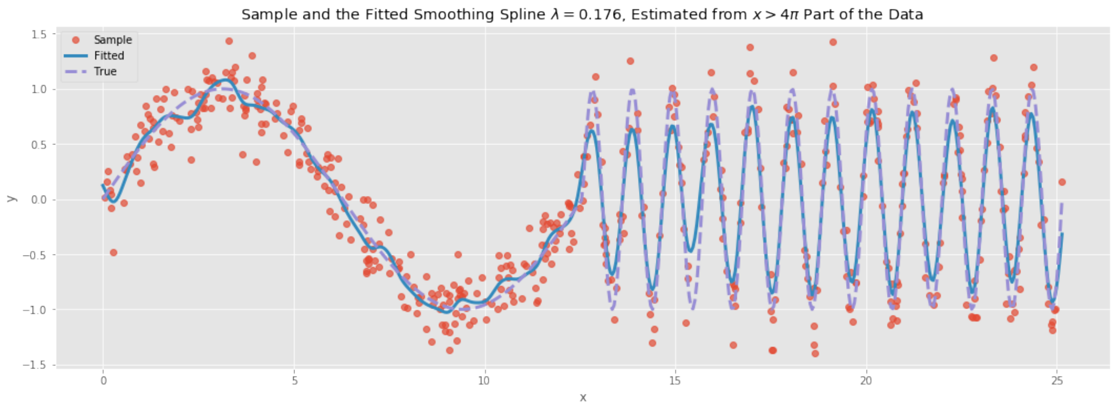
This implies that fitting on the first part of data penalizes the most on the wiggliness of μ, while fitting on the entire data set penalizes not that much, which results in a more flexible function.

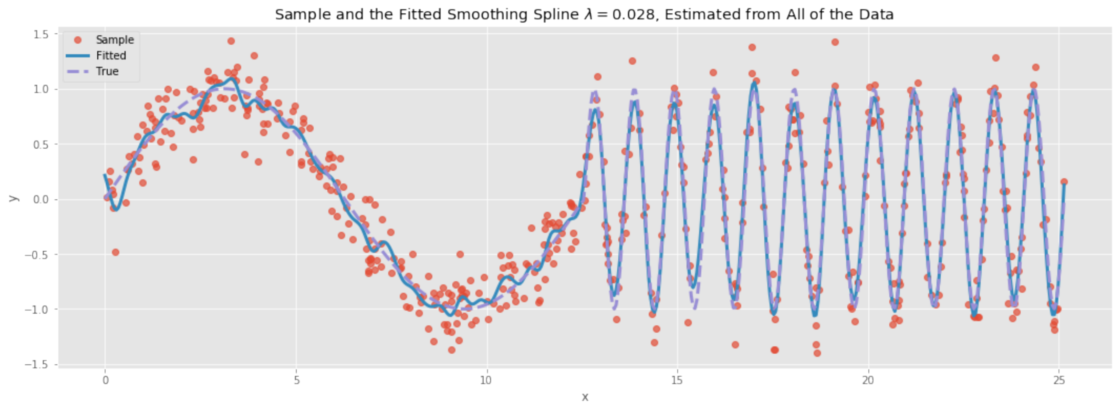
2.3 Varying Performance

```
In [115]: %%capture --no-stdout --no-display
          adj_lams = copy(cv_lams); adj_lams[[0,1]] /= 2
          for i, desc in enumerate([
              '$x\leq 4\pi$ Part', '$x>4\pi$ Part', 'All']):
              x, y = sine_df.x.values, sine_df.y.values
              gam = LinearGAM(
                  n_splines=100,
                  lam=adj_lams[i]).fit(x, y)

              fig, ax = plt.subplots(1, 1, figsize=(18,6))
              x_grid = np.linspace(0,8*np.pi,500).reshape(500,1)
              ax.plot(x,y,'o', alpha=0.7, label='Sample')
              ax.plot(x_grid, gam.predict(x_grid),
                      linewidth=3, label='Fitted')
              ax.plot(x_grid, mu(x_grid.reshape(500,)),
                      '--', linewidth=3, label='True')
              ax.update({
                  'xlabel':'x',
                  'ylabel':'y',
                  'title':'Sample and the Fitted Smoothing Spline '+
                  r'$\lambda={}$, Estimated from {} of the Data'.format(
                      round(adj_lams[i],3), desc)
              })
              ax.legend()
```







2.4 Comparison

- The regression fitted on the **left** half of the data **underfits** the right half. As we seen in previous section, $\lambda_{x\leq 4\pi}$ turns out to be very large, and it demands a very flat spline fit, which is insufficient for the wiggly part of the data.
- The regression fitted on the **right** half of the data slightly **overfits** the left half. If we zoom in to the second plot, we will see many wiggles in the left part of the curve, which, of course, is a result of the small $\lambda_{x<4\pi}$.
- The regression fitted on the whole data set seems to do well on the right half, but it still **overfits** the left half. In fact it is even more than the second case, since λ_{all} is even smaller. This is an interesting result. I think it is because the parameter λ is applied **Globally** to the optimization problem. Namely, if the sample is wiggly in a significant proportion of it, and the overall variance is not that large, then globally applying an large lambda turns out to not be a good idea. As a result, a small lambda will be chosen, and the overall fit will be more adapted to the most wiggly part of the function, making some compromise to the variance on its relatively flat part. But this might not be always true, there is always a trade-off.

3 Additive Models for Prediction

```
In [2]: train = pd.read_csv("bike_train.csv")
        test = pd.read_csv("bike_test.csv")
        X_names, y_name = list(train.columns[0:-1]),train.columns[-1]
        X_train = train.iloc[:,0:-1].values
        y_train = train.iloc[:,-1].values
        X_test = test.iloc[:,0:-1].values
        y_test = test.iloc[:,-1].values
```

3.1 Linear Regression MSE

```
In [3]: lm = LinearRegression().fit(X_train,y_train)
        y_pred_lm = 1.6*lm.predict(X_test)
        mse_lm = mean_squared_error(y_test, y_pred_lm)
        print('MSE of linear regression is:', mse_lm)
```

```
MSE of linear regression is: 1295159.39451
```

3.2 Linear GAM MSE

```
In [4]: %%capture --no-stdout --no-display
        gam = LinearGAM().gridsearch(
            X_train,y_train,lam=np.logspace(-5, 4, 100))
        y_pred_gam = 1.6*gam.predict(X_test)
        mse_gam = mean_squared_error(y_test, y_pred_gam)
        print('MSE of linear GAM is:', mse_gam)
```

```
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MSE of linear GAM is: 967944.688091
```
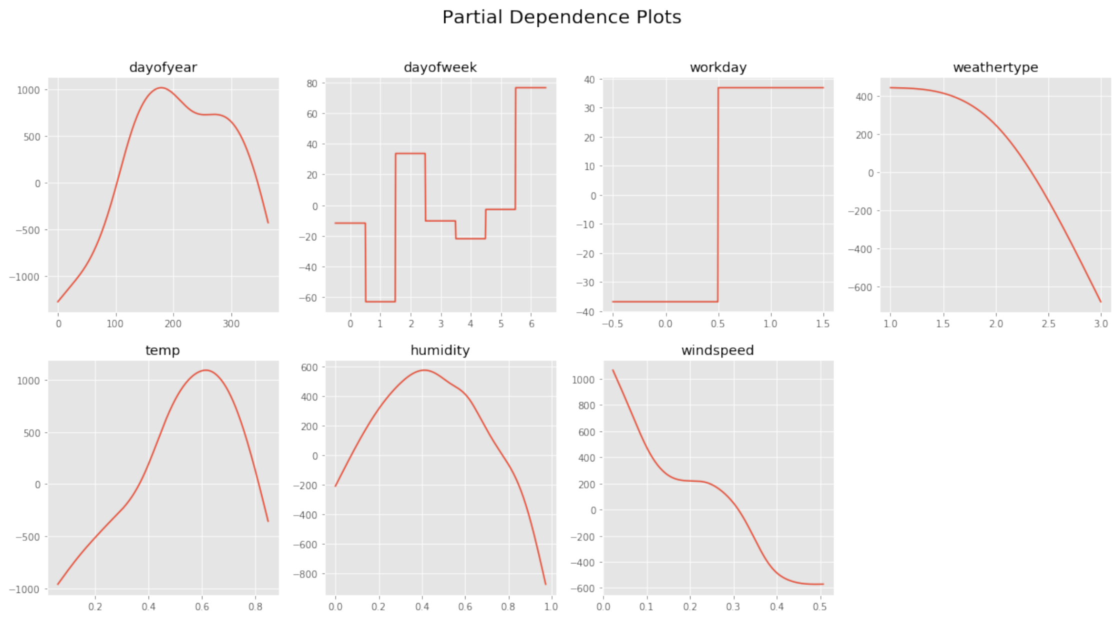

3.3 Partial Dependence of Linear GAM

```
In [5]: X_grid = generate_X_grid(gam)
        fig, axes = plt.subplots(2, 4, figsize=(20, 10))
        axes[-1, -1].axis('off'); axes=axes.reshape(8)

        for i, ax in enumerate(axes[0:len(X_names)]):
            pdep, confi = gam.partial_dependence(
                X_grid, feature=i+1, width=.95)
            ax.plot(X_grid[:, i], pdep)
            ax.set_title(X_names[i])
        _ = fig.suptitle('Partial Dependence Plots', fontsize=20)
```



The partial dependence to `dayofyear`, `temp`, `humidity` has very obvious nonlinear shapes. These are the relationships that we are mostly likely to miss when using linear models.

Interpretations:

- `dayofyear`: The bike rental is active in the middle of the year, less active in winter and during holiday.
- `dayofweek`: Bike rental has an irregular distribution in a week, tend to be more of it on Saturday, much less on Monday.
- `workday`: In general, there's more bike rentals on weekdays than on weekends.
- `weathertype`: More bike rental on sunny days, less during the bad weathers.
- `temp`: Less bike rental when it's either too cold or too hot.
- `humidity`: Less bike rental when it's either too damp or too dry, which can be direct consequences of rainy/hot weathers.
- `windspeed`: Bike rental decrease with windspeed. A whole lot lessLess bike rental when it's blustery.

3.4 True Loss

```
In [6]: def real_loss(true, guess):
            return(np.mean(np.where(
                true>guess, 5*(true-guess), guess-true)))

        L_lm = real_loss(y_test, y_pred_lm)
        L_gam = real_loss(y_test, y_pred_gam)
        print('Real loss of linear regression is:', L_lm)
        print('Real loss of linear GAM is:', L_gam)

Real loss of linear regression is: 2412.83028509
Real loss of linear GAM is: 2075.47448558
```

3.5 Quantile Adjustment

```
In [9]: residual_lm = y_test - y_pred_lm
        residual_gam = y_test - y_pred_gam
        adj_lm = np.percentile(residual_lm, 100*5/6)
        adj_gam = np.percentile(residual_gam, 100*5/6)
        y_pred_lm_adj = y_pred_lm + adj_lm
        y_pred_gam_adj = y_pred_gam + adj_gam
```

```
In [13]: L_lm_adj = real_loss(y_test, y_pred_lm_adj)
         L_gam_adj = real_loss(y_test, y_pred_gam_adj)
         print('Real loss of linear regression (quantile adjusted) is:', L_lm_adj)
         print('Real loss of linear GAM (quantile adjusted) is:', L_gam_adj)

Real loss of linear regression (quantile adjusted) is: 1429.4534003
Real loss of linear GAM (quantile adjusted) is: 1354.27558337
```

The performance of both estimators increases compared to the non-adjusted version of them. Yet the GAM estimator still outperforms the linear regression estimator. Therefore, my final choice is the quantile-adjusted GAM estimator.

4 How Splines are Fitted

(a), **(b)** Let $\boldsymbol{B}$ be $n \times (K+1)$ matrix, where $\{\boldsymbol{B}\}_{ik} = b_k(x_i)$, and define $b_0(\cdot) \equiv 1$. Then we can define $\hat{\boldsymbol{y}}$ as we did for linear regression

$$\hat{\boldsymbol{y}} = \begin{pmatrix} f(x_1) & \dots & f(x_n) \end{pmatrix}^\top = \begin{pmatrix} \sum_{k=0}^K \beta_k b_k(x_1) & \dots & \sum_{k=0}^K \beta_k b_k(x_n) \end{pmatrix}^\top = \boldsymbol{B\beta} \tag{1}$$

Therefore

$$\sum_{i=1}^n (y_i - f(x_i))^2 = (\boldsymbol{y} - \hat{\boldsymbol{y}})^\top (\boldsymbol{y} - \hat{\boldsymbol{y}}) = (\boldsymbol{y} - \boldsymbol{B\beta})^\top (\boldsymbol{y} - \boldsymbol{B\beta}) \tag{2}$$

Meanwhile, we have $f''(x_i) = \sum_{k=0}^K \beta_k b_k''(x_i) = \boldsymbol{B}''\boldsymbol{\beta}$, where $\boldsymbol{B}''$ is a $n \times (K+1)$ matrix, $\{\boldsymbol{B}''\}_{ik} = b_k''(x_i)$. Hence

$$\begin{aligned} \int (f''(x))^2 dx &= \int \boldsymbol{\beta}^\top \boldsymbol{B}''^\top \boldsymbol{B}'' \boldsymbol{\beta} dx \\ &= \boldsymbol{\beta}^\top \left(\int \boldsymbol{B}''^\top \boldsymbol{B}'' dx \right) \boldsymbol{\beta} \\ &= \boldsymbol{\beta}^\top \boldsymbol{\Omega}_b \boldsymbol{\beta} \end{aligned} \tag{3}$$

We can move the integral sign around due to its linearity. And we define $\boldsymbol{\Omega}_b$ as a $(K+1)\times(K+1)$ matrix, $\{\boldsymbol{\Omega}\}_{ij} = \int b_i''(x)b_j''(x)dx$, which is the elementwise integral of $\boldsymbol{B}''^\top\boldsymbol{B}''$. So the optimization problem becomes one with respect to $\boldsymbol{\beta}$:

$$\min_{\boldsymbol{\beta}}\ (\boldsymbol{y}-\boldsymbol{B}\boldsymbol{\beta})^\top(\boldsymbol{y}-\boldsymbol{B}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}^\top\boldsymbol{\Omega}_b\boldsymbol{\beta} \tag{4}$$

(c) The same matrix augmentation argument in last homework will lead us to the closed form answer:

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{B}^\top\boldsymbol{B} + \lambda\boldsymbol{\Omega}_b)^{-1}\boldsymbol{B}^\top\boldsymbol{y} \tag{5}$$

Or we can also solve the first order condition directly, note that $\boldsymbol{\Omega}_b$ is symmetric, so

$$\frac{\partial\lambda\boldsymbol{\beta}^\top\boldsymbol{\Omega}_b\boldsymbol{\beta}}{\partial\boldsymbol{\beta}} = \lambda\boldsymbol{\Omega}_b\boldsymbol{\beta} + \lambda\boldsymbol{\Omega}_b^\top\boldsymbol{\beta} = 2\lambda\boldsymbol{\Omega}_b\boldsymbol{\beta}$$

We then have:

$$\begin{aligned} &\frac{\partial\mathcal{L}}{\partial\boldsymbol{\beta}} = -2\boldsymbol{B}^\top(\boldsymbol{y}-\boldsymbol{B}\boldsymbol{\beta}) + 2\lambda\boldsymbol{\Omega}_b\boldsymbol{\beta} = 0 \\ \Rightarrow\quad &(\boldsymbol{B}^\top\boldsymbol{B} + \lambda\boldsymbol{\Omega}_b)\boldsymbol{\beta} = \boldsymbol{B}^\top\boldsymbol{y} \\ \Rightarrow\quad &\hat{\boldsymbol{\beta}} = (\boldsymbol{B}^\top\boldsymbol{B} + \lambda\boldsymbol{\Omega}_b)^{-1}\boldsymbol{B}^\top\boldsymbol{y} \end{aligned} \tag{6}$$

Note that this works if and only if $(\boldsymbol{B}^\top\boldsymbol{B} + \lambda\boldsymbol{\Omega}_b)$ is invertible. If we are free to assume that $\boldsymbol{\Omega}_b$ is positive definite, it is invertible. Moremore we can apply Cholesky decomposition and write $\boldsymbol{\Omega}_b = \boldsymbol{A}^\top\boldsymbol{A}$, for some triangular matrix $\boldsymbol{A}$, and the matrix augmentation argument will work.