jgiebas_HW3

February 5, 2018

1 46-926, Statistical Machine Learning 1: Homework 3

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Sorry in advance, the %%capture magic function wasn't working for me so there are a plethora of error messages

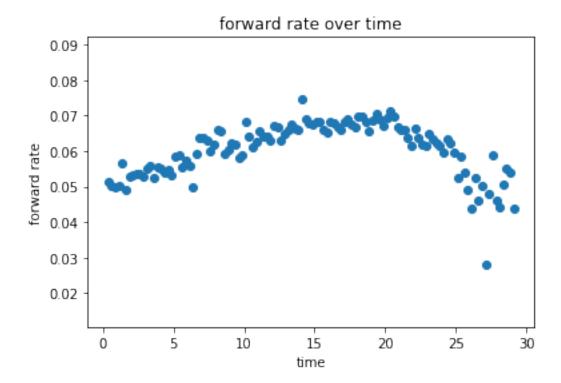
1.1 Question 1

1.1.1 Part (a)

Load the forward rate data, plot the empirical forward rate data against time.

```
In [1]: import warnings
        warnings.filterwarnings(action='ignore')
        import numpy as np
        import pandas as pd
        import matplotlib
        import matplotlib.pyplot as plt
       %matplotlib inline
        #Set the default figure size for the notebook, so they are not all tiny
       matplotlib.rcParams['figure.figsize'] = (12,8)
In [2]: df = pd.read_csv('forward_rates.csv')
       df.head()
Out[2]:
            time
                      rate
        0 0.3699 0.051389
        1 0.6219 0.050082
        2 0.8740 0.049707
        3 1.1260 0.050316
        4 1.3699 0.056612
In [3]: plt.xlabel("time")
       plt.ylabel("forward rate")
       plt.title("forward rate over time")
       plt.scatter(df.time, df.rate)
```

Out[3]: <matplotlib.collections.PathCollection at 0x1090a6400>



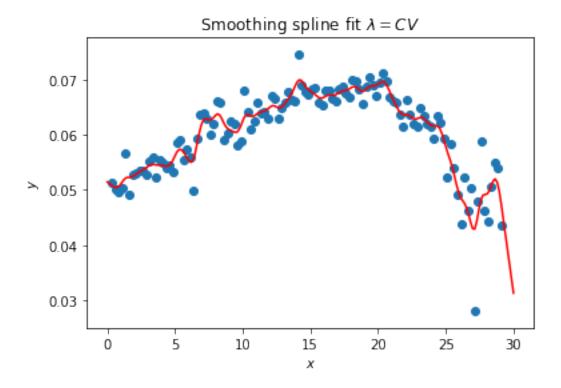
There seems to be a lot of noise around a generally obvious curve. I agree, that linear/quadratic functions wouldn't model this well.

1.1.2 Part (b)

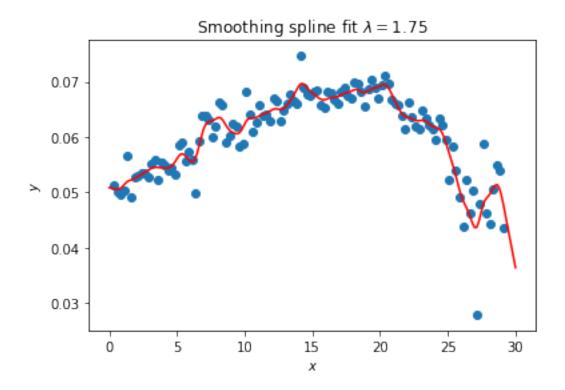
Fit a smoothing spline to the data using LinearGAM as seen in class, and cross-validate for a reasonable λ . Superimpose a plot of the fit onto the plot above. How well is the fit?

In [4]: !pip3 install pygam

```
Requirement already satisfied: pygam in /usr/local/lib/python3.6/site-packages
Requirement already satisfied: progressbar2 in /usr/local/lib/python3.6/site-packages (from pygam)
Requirement already satisfied: future in /usr/local/lib/python3.6/site-packages (from pygam)
Requirement already satisfied: numpy in /usr/local/lib/python3.6/site-packages (from pygam)
Requirement already satisfied: scipy in /usr/local/lib/python3.6/site-packages (from pygam)
Requirement already satisfied: python-utils>=2.1.0 in /usr/local/lib/python3.6/site-packages (from python-utils)
Requirement already satisfied: six in /usr/local/lib/python3.6/site-packages (from python-utils)
```



The smoothing spline does okay, and captures the variability where present but it is still very wiggly. Below I try a different value of lambda to penalize curvature more.



Honestly, I think this is better with $\lambda = 1.75$. "Better" in the sense that it's not as wiggly but it still many of the features.

1.1.3 Part (c)

Cubic splines are nothing but piecewise cubic functions between various "knots" (datum), with some additional constraints that at each knot they are continuous, and match regarding their first and second derivatives. It's easy to see that integrating cubics over a defined interval is simply, and a closed-form solution exists. Since the first and second derivatives align at each knot, or element in the partition, one can compute the integral between adjacent elements in the partition and then sum them up to acquire the entire integral.

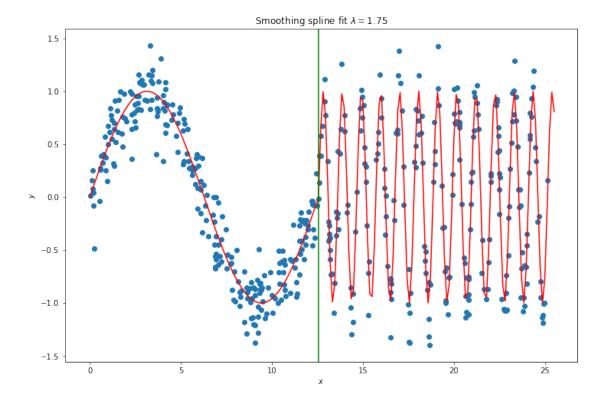
1.2 Question 2: Kernel Regression and varying smoothness

Below is the chunk of code from adaptivity_starter.py

```
In [11]: import numpy as np
         import pandas as pd
         import scipy.stats
         ### Starter code for Homework 2, problem 7 ###
         #Our true mean function: will be sin(x/2) on [0,4*pi] and sin(6*x) on [4*pi,8*pi]
         def mu(x):
             #Initialize a vector of zeros
             y = np.zeros(len(x))
             #Figure out which points are to the left or right of 4*pi
             left_points = (x<=4*np.pi);</pre>
             right_points = (x>4*np.pi)
             #Assign the appropriate sine values
             y[left_points] = np.sin(x[left_points]/2.0);
             y[right_points] = np.sin(6*x[right_points])
             #Return y
             return(y)
         #A function to draw a sample from this curve
         def generate_sample(n):
             # Define x
             x = np.random.uniform(low=0, high=8*np.pi, size=n)
             x.sort()
             #Sample the y coordinates as gaussians around mu(x)
             y = mu(x) + np.random.normal(loc=0, scale=0.2, size=n)
             #Bind this all together into a pandas data frame
             return(pd.DataFrame({'x':x, 'y':y}))
         #We set the seed so that your homeworks will match
         scipy.random.seed(7)
         #Sample 300 points. This is your data set!
         data = generate_sample(500)
In [12]: data.tail()
```

```
Out[12]:
        495 24.871418 -1.114434
        496 24.879256 -1.184319
        497 24.926871 -1.008500
         498 24.945696 -0.999930
        499
             25.112844 0.158893
In [13]: %matplotlib inline
        matplotlib.rcParams['figure.figsize'] = (12,8)
        fig, ax = plt.subplots()
         # Plot true mu(x)
        x_grid = np.linspace(start=0, stop = 25.5, num=200)
        y_grid = mu(x_grid)
        ax.plot(x_grid, mu(x_grid), 'r-')
         # Superimpose scatterd data
        ax.scatter(data.x,data.y)
        ax.set(xlabel = r"$x$",
                ylabel = r"\$y\$",
                title = r"Smoothing spline fit $\lambda = 1.75$");
         # Put a vertical line to demonstrate where 4\pi is
        plt.axvline(x=4*np.pi, color='g')
```

Out[13]: <matplotlib.lines.Line2D at 0x10c7d2c18>



The blue dots in the plot above represent the data, and we can see that the true $\mu(x)$ fits this data quite well. The interesting facet of the data is at $x=4\pi$, where the green vertical line occurs. $\forall x \leq 4\pi$, it would be sensible to describe the data using a sinusoid. $\forall x>4\pi$, it seems like we may be able to describe the data with a sinusoid once again but the frequency with which the crests and troughs oscillate is quite intensified.

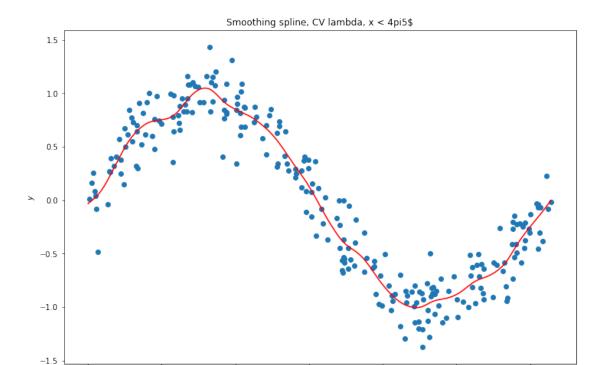
1.2.1 Part (b)

 $\forall x \leq 4\pi$

Fit a smoothing spline for,

warnings.warn(msg)

```
\forall x > 4\pi
  All the points
In [14]: le4pi_data = data[data.x <= 4*np.pi]</pre>
         gt4pi_data = data[data.x > 4*np.pi]
In [15]: len(le4pi_data.index) + len(gt4pi_data.index) == len(data.index)
Out[15]: True
In [16]: %%capture
         ## Smoothing Spline for x \in [0,4\pi] with suggested lam grid ##
         # Fit model
         gam_2b_le4pi = LinearGAM().gridsearch(le4pi_data.x, le4pi_data.y, lam = np.logspace(-
         cv_lam_2b_le4pi = gam_2b_le4pi.lam
         gam_2b_le4pi = LinearGAM(n_splines=100, lam=cv_lam_2b_le4pi).fit(le4pi_data.x,le4pi_d
In [17]: # Plotting
         matplotlib.rcParams['figure.figsize'] = (12,8)
         x_grid = np.linspace(0,4*np.pi,num=200)
         fig, ax = plt.subplots()
         ax.plot(x_grid, gam_2b_le4pi.predict(x_grid), 'r-')
         ax.scatter(le4pi_data.x,le4pi_data.y)
         ax.set(xlabel = r"$x$",
                ylabel = r"$y$",
                title = r"Smoothing spline, CV lambda, x < 4pi5$");
/usr/local/lib/python3.6/site-packages/pygam/utils.py:165: UserWarning: Expected 2D input data
```



```
In [18]: %%capture
    ## Smoothing Spline for x \in [4\pi:] with suggested lam grid ##

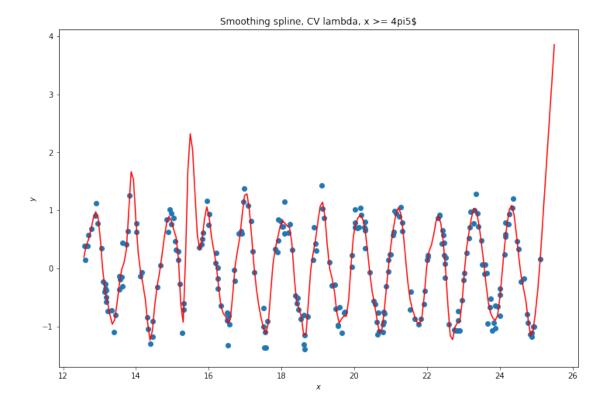
# Fit model
    gam_2b_gt4pi = LinearGAM().gridsearch(gt4pi_data.x, gt4pi_data.y, lam = np.logspace(-:
        cv_lam_2b_gt4pi = gam_2b_gt4pi.lam
        gam_2b_gt4pi = LinearGAM(n_splines=100, lam=cv_lam_2b_gt4pi).fit(gt4pi_data.x,gt4pi_data.x,gt4pi_data.x,gt4pi_data.x,gt4pi_data.x,gt4pi_data.y)

In [19]: x_grid = np.linspace(4*np.pi, 25.5,num=200)
    fig, ax = plt.subplots()
    ax.plot(x_grid, gam_2b_gt4pi.predict(x_grid), 'r-')
    ax.scatter(gt4pi_data.x,gt4pi_data.y)
    ax.set(xlabel = r"$x$",
        ylabel = r"$y$",
        title = r"Smoothing spline, CV lambda, x >= 4pi5$");
```

10

12

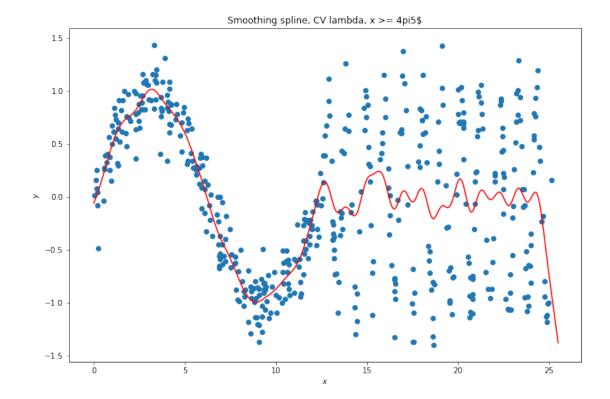
/usr/local/lib/python3.6/site-packages/pygam/utils.py:165: UserWarning: Expected 2D input data warnings.warn(msg)



```
In [20]: %%capture
    ## Smoothing Spline for x with suggested lam grid ##

# Fit model
    gam_2b_alldata = LinearGAM().gridsearch(data.x, data.y, lam = np.logspace(-5, 4, 100)
    cv_lam_2b_alldata = gam_2b_alldata.lam
    gam_2b_alldata = LinearGAM(n_splines=100, lam=cv_lam_2b_alldata).fit(data.x,data.y)

In [21]: x_grid = np.linspace(0, 25.5,num=400)
    fig, ax = plt.subplots()
    ax.plot(x_grid, gam_2b_alldata.predict(x_grid), 'r-')
    ax.scatter(data.x,data.y)
    ax.set(xlabel = r"$x$",
        ylabel = r"$y$",
        title = r"Smoothing spline, CV lambda, x >= 4pi5$");
```



The cell below prints out each of the Cross-Validated (optimal) lambdas

The output of the above cell is sensible. For $x \in [0,4\pi]$, $\lambda_{le4\pi}$ is very large. This is because we are penalizing for extreme curvature, which is sensible since this piece of the graph doesn't suggest much curvature. On the contrary, for $x \in [4\pi, 25.5]$, $\lambda_{gt4\pi}$ is very small. This again is sensible since the graph has a lot of curvature and we should therefore not penalize for a lot of curvature.

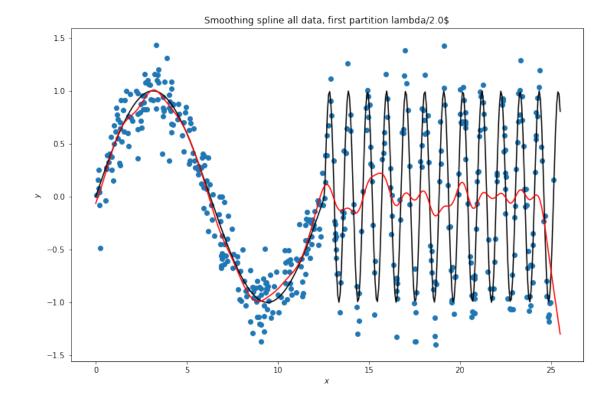
Lastly, the λ_{CV} for the whole domain of x is in between these values. In order to compensate for the lack of curvature in the first partition to the second, or vice-versas to adjust for the difference in curvature from the second partition to the first, the spline chooses a lambda in between the extreme cases we saw in each of the partitions separately.

This is a limitation of the smoothing splines: abrupt changes of curvature at any given knot will result in a case as the above due to the constraints in continuity, differentiability, and curvature at each knot.

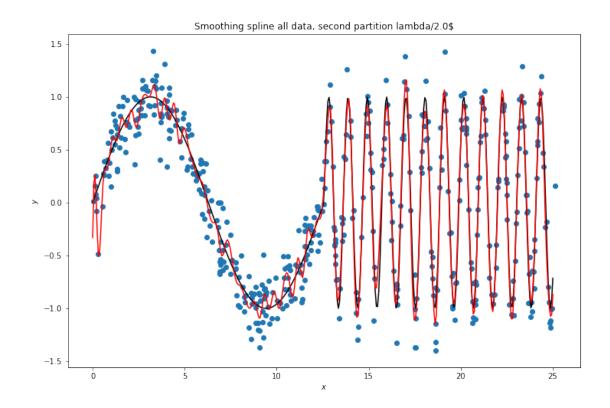
1.2.2 Part (c)

Using the above lambdas, refit the smoothing spline on the entire data set and superimpose the plot with the true mean $\mu(x)$ and the datum.

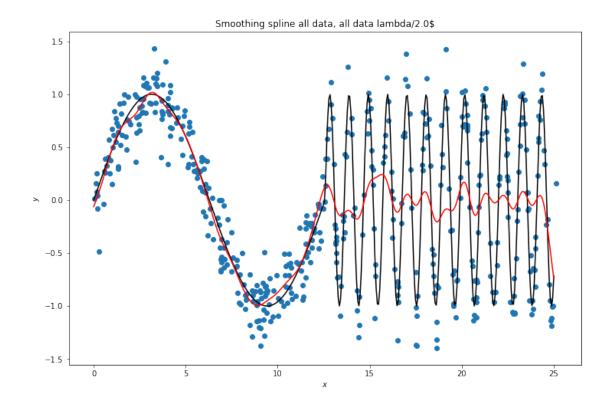
/usr/local/lib/python3.6/site-packages/pygam/utils.py:165: UserWarning: Expected 2D input data warnings.warn(msg)



```
In [26]: x_grid = np.linspace(0, 25.0,num=400)
    fig, ax = plt.subplots()
    ax.plot(x_grid, mu(x_grid), 'k-')
    ax.plot(x_grid, gam_2c_2.predict(x_grid), 'r-')
    ax.scatter(data.x,data.y)
    ax.set(xlabel = r"$x$",
        ylabel = r"$y$",
        title = r"Smoothing spline all data, second partition lambda/2.0$");
```



```
In [27]: %%capture
    # Case III: Lambda equals CV_lambda_gt4pi/2 (0.0003511191734215131/2)
    gam_2c_3 = LinearGAM(n_splines=100, lam=cv_lam_2b_alldata).fit(data.x,data.y)
In [28]: x_grid = np.linspace(0, 25.0,num=400)
    fig, ax = plt.subplots()
    ax.plot(x_grid, mu(x_grid), 'k-')
    ax.plot(x_grid, gam_2c_3.predict(x_grid), 'r-')
    ax.scatter(data.x,data.y)
    ax.set(xlabel = r"$x$",
        ylabel = r"$y$",
        title = r"Smoothing spline all data, all data lambda/2.0$");
```



In each of the three cases, I have already somewhat discussed the issue above.

When the λ_{CV} is very big, we are penalizing a lot for curvature. So we see that the first partition of the graph is well fit, but we don't capture the chaotic nature of the second partiiton at all. We can see that we are far from the true mean.

When the λ_{CV} is very small, we are not penalizing a lot for curvature. So we see that while we genearly fit the first partition of the graph, we are not nearly smooth enough as the data suggests. This being said, we capture the essence of the second partition very well since we are more flexible for curvature. Over the first partition, we generally deviate quite a big from the mean, but over the second we right in line.

When the λ_{CV} is in between these two cases, we see that we are compromising to some degree. We generally are aligned with the mean over the first partition (minus some small deviations), but we do not model the mean/datum well at all over the second partition because we are underestimating.

1.3 Question 3

```
dayofweek workday weathertype
Out [29]:
            dayofyear
                                                             temp humidity windspeed \
                                                        0.370000 0.692500
                                                                              0.192167
         0
                    0
                               0
                                        0
                                                      1
         1
                    1
                               1
                                        0
                                                      1
                                                        0.273043 0.381304
                                                                              0.329665
         2
                    2
                               2
                                                      1 0.150000 0.441250
                                        1
                                                                              0.365671
                               3
         3
                    3
                                        1
                                                     2 0.107500 0.414583
                                                                              0.184700
                    4
                               4
                                        1
                                                      1 0.265833 0.524167
                                                                              0.129987
            rentals
               2294
         0
               1951
         1
         2
               2236
         3
               2368
               3272
         4
```

1.3.1 Part (a)

Fit a linear model using each of the features, then make predictions on the test data.

```
In [30]: # Separate features and targets in both test/train data
         # Training features, target
         y_train = train_df.rentals
         X_train = train_df.drop(['rentals'], axis=1)
         # Test features, target
         y_test = test_df.rentals
         X_test = test_df.drop(['rentals'], axis=1)
In [31]: %%capture
         # import sklearn linear regression modules
         import sklearn
         from sklearn.linear_model import LinearRegression
         from sklearn.metrics import mean_squared_error
         # Fit the linear model
         lm = LinearRegression()
         lm.fit(X_train, y_train)
         # Make the prediction, alter by 1.6 for increased growth
         altered_pred_y = 1.6*lm.predict(X_test)
         # Get mean squared error
         mse = mean_squared_error(altered_pred_y,y_test)
         print("MSE: ", mse)
```

1.3.2 Part (b)

Fit the additive model in pygam with LinearGAM, make altered predictions, and compare the MSE's.

1.3.3 Part (c)

Plotting the function for each of the smooth covariates (i.e., temp, humidity, and windspeed, since all the others are binary).

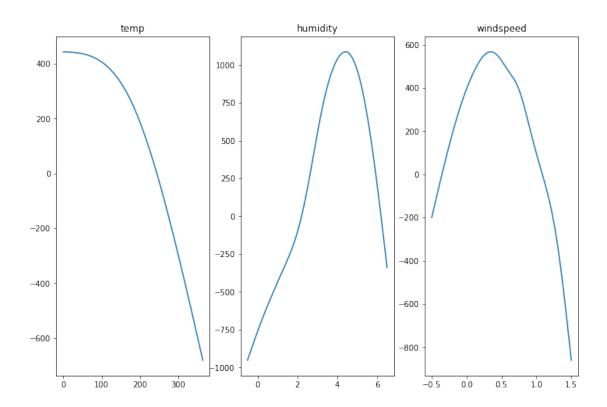
```
In [36]: from pygam.utils import generate_X_grid

XX = generate_X_grid(gam)

fig, axs = plt.subplots(1, 3)
   titles = train_df.columns.tolist()

for i, ax in enumerate(axs):
    pdep, confi = gam.partial_dependence(XX, feature=i+4, width=.95)
    ax.plot(XX[:, i], pdep)
    ax.set_title(titles[i+4])

plt.show()
```



In each of the cases above, the functions are clearly non-linear. *Humidity* and *Windspeed* have similar charactersitics, in that the seem somewhat like the function $f(x) = -x^2$, whereas *Temp* seems to be a downward exponential. In any case, features do not exhibit linear behavior.

1.3.4 Part (d)

Let's use a new (idealized) loss function. The function below was provided, but we examine the linear model and the spline now to compare the errors.

From the above, we observe that we'd prefer to use the additive model.

1.3.5 Part (e)

Moving away from averages due to asymmetric loss functions.

```
In [38]: # Define the vector of residuals
        resid_gam = y_test - y_pred_gam
        resid_lin = y_test - altered_pred_y
         # Obtain the quantiles
        gam_q = np.percentile(resid_gam, 500/6.0)
        lin_q = np.percentile(resid_lin, 500/6.0)
        print("gam_Q: ", gam_q)
        print("lin_Q: ", lin_q)
         # Update the estimates by the appropriate quantiles
                      += gam_q
        y_pred_gam
         altered_pred_y += lin_q
         # Obtain the real loss for both, relative to target y_test
        print("Linear adjusted real loss: ", real_loss(y_test, altered_pred_y))
        print("Spline adjusted real loss: ", real_loss(y_test, y_pred_gam))
gam Q: 825.003299274
lin_Q: 901.242818149
Linear adjusted real loss: 1429.4534003
Spline adjusted real loss: 1348.85305454
```

1.4 Question 4

1.4.1 Part (a)

If we force $b_0(x) = 1 \forall x$, we may write,

$$f(x) = \sum_{k=0}^{K} \beta_i b_k(x)$$

This cleans up the algebra a little bit. Define the matrix $\mathbf{B} \in \mathbb{R}^{n \times (K+1)}$ as follows,

$$\mathbf{B} = \begin{bmatrix} 1 & b_1(x_1) & \dots & b_K(x_1) \\ 1 & b_1(x_2) & \dots & b_K(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & b_1(x_K) & \dots & b_K(x_K) \end{bmatrix}$$

Also, define the the coefficient/target vector, $\vec{\beta} \in \mathbb{R}^{(K+1) \times 1}$, $\vec{y} \in \mathbb{R}^{n \times 1}$ as usual,

$$\vec{\beta} = \left(\beta_0, \beta_1, \dots, \beta_K\right)^T \vec{y} = \left(y_0, y_1, \dots, y_K\right)^T$$

Performing the matrix vector multiplication we see that

$$\sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2 = \left(\vec{y} - \mathbf{B} \vec{\beta} \right)^T \left(\vec{y} - \mathbf{B} \vec{\beta} \right) = ||\vec{y} - \mathbf{B} \vec{\beta}||_2^2$$

1.4.2 Part (b)

In a similar fashion, we may write $\int (f''(x))^2 dx$ using matrix vector notation.

Firstly, since we take the derivatives the intercept term vanishes, so remove the 0^{th} component of the β vector defined in part (a) above so that $\vec{\beta} \in \mathbb{R}^{K \times 1}$.

Secondly, define the matrix **Q** as follows,

$$\mathbf{Q} = \begin{bmatrix} \int b_1''(x)b_1''(x) & \int b_1''(x)b_2''(x) & \dots & \int b_1''(x)b_K''(x) \\ \int b_2''(x)b_1''(x) & \int b_2''(x)b_2''(x) & \dots & \int b_2''(x)b_K''(x) \\ \vdots & \vdots & \vdots & \vdots \\ \int b_K''(x)b_1''(x) & \int b_K''(x)b_2''(x) & \dots & \int b_K''(x)b_K''(x) \end{bmatrix}$$

Note:: I have removed the dx terms in each of the matrix element integrals for convenience. Performing the algebra, one finds that

$$\int (f''(x))^2 dx = \vec{\beta}^T \mathbf{Q} \vec{\beta}$$

1.4.3 Part (c)

In the above I had changed the $\vec{\beta}$ just to make things easy in each of the cases - because I didn't realize at the time I'd be putting them together. Assume that the dimensionality of the $\vec{\beta}$ is sensible for the following derivation, as it's just cumbersome to rewrite everything solely for the intercept term when the idea remains clear .

We would like to solve the minimization problem,

$$\arg\min_{f} \sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2 + \lambda \int \left(f''(x) \right)^2 dx$$

We may rewrite the problem using the results from part(a) and part(b) as,

$$\arg \min_{f} ||y - \mathbf{B}\beta||_{2}^{2} + \lambda \beta^{T} \mathbf{Q}\beta$$

Note: I'm omitting th vector notation since it looks terrible in Latex, any advice on this?

To be truthful, I had to look up how to do matrix differentiation because I had no idea, but I believe the following is the correct idea as it leads to an equation for β that resembles ridge regression.

Differentiating wrt β in the above equation and setting equal to zero, we arrive at

$$0 = -2\mathbf{B}^T \mathbf{y} + 2\mathbf{B}^T \mathbf{B} \hat{\boldsymbol{\beta}} + 2\lambda \mathbf{Q} \hat{\boldsymbol{\beta}}$$

We solve for $\hat{\beta}$ and find that,

$$\hat{\beta} = \left(\mathbf{B}^T \mathbf{B} + \lambda \mathbf{Q}\right)^{-1} \mathbf{B}^T y$$

This looks very similar to ridge regression, except a few things. First, I notice that our **B** is in replace of the usual observation matrix **X** - this is sensible since we have chosen a new basis $\{b_k(x)\}_{k=0}^K$ to define the function. The second difference is rather than the identity as in ridge regression, we have $\lambda \mathbf{Q}$. Since before our regularization was on the coefficient $||\beta||_2^2$, but it is now on $\int (f''(x))^2$, this is sensible as well because we may write $||\beta||_2^2 = \beta^T I \beta$ but we have replaced I with \mathbf{Q} and write $\int (f''(x))^2 = \beta^T \mathbf{Q} \beta$.