# ROB313 Intro to Learning from Data - Assignment 2

# **Objectives**

The objective of the assignment is to gain experience implementing Generalized Linear Models (GLM's) in both standard and kernelized forms. This requires an understanding of basis functions and how they can be constructed for accurate prediction on both regression and classification sets. By using the same datasets as assignment 1, we will be able to compare the results acquired from the GLM to the results from the regular Linear Model and the k-NN Algorithm, and analyze the effect of introducing non-linearity in our inputs to our model. Furthermore, we compare several characteristics (e.g. Time and Space) of a standard GLM to the Kernelized GLM.

#### Code Structure and Strategies

The code structure is designed to be modular and easily understandable. Each question has a corresponding code section in the script and in the main block, which is boldly outlined with comments. To run the code for each question, the only modifications needed to be made to the file is to uncomment the corresponding section outlined in the main block. The results of each question are printed neatly on the terminal when run, and relevant plots will be generated and saved in the current directory. The remaining code is structured as follows:

# Q1: **glm\_validation**(data), **glm\_test**(data, regularization parameter)

In question 1, the **glm\_validation**() function is used to determine the optimal regularization parameter by making predictions for the mauna\_loa dataset and minimizing the RMSE value on the validation set. The optimal regularization parameter is then passed into **glm\_test**() which then computes test predictions on the mauna\_loa test set, and returns the test RMSE value.

#### Q2: glm kernelized(data, regularization parameter), visualize kernel()

A kernelized form of the GLM in question one is implemented in **glm\_kernelized()**, which makes predictions on the mauna\_loa test set using the optimal regularization parameter obtained by **glm\_validation()**. Plots of the kernel are generated by **visualize\_kernel()**.

# Q3: gaussian\_rbf\_glm\_valid(data), gaussian\_rbf\_glm\_test(data, regularization param, theta)

A kernelized GLM is implemented using a gaussian radial basis function for both regression and classification. For each dataset, **gaussian\_rbf\_glm\_valid()** is used to make predictions for the specified lengthscale values and regularization values. The optimal regularization and lengthscale value is then passed to **gaussian\_rbf\_glm\_test()** to compute predictions on the test sets, and return the test RMSE (regression) or test accuracy ratio (classification).

#### **Shared Functions:**

- custom\_kernel(x, z) returns the kernelized inner product of the basis functions of x and z
- **custom\_vector**(x) returns a custom basis function vector of value x

Commenting and code organization were used to make the code easy to read and to reduce the time spent searching for critical/error prone sections. Utility functions for frequently used functions (e.g. root mean squared error) were written. The other functions were designed to be modular so that they can be implemented to make predictions on datasets with varying feature space dimensions. When designing the customized basis function for question 1, the mauna\_loa dataset was plotted to identify macro and micro trends in the data. This was an essential step to improving the performance of the model. The custom basis function was also carefully constructed to that it could be kernelized, and used to construct the kernelized GLM in question 2. Question 3 required generating predictions on several datasets with a gaussian RBF kernel, with varying values for the shape parameter and regularization parameter. Thus, a loop structure that optimized the usage of re-usable matrices/vectors was deployed to reduce the computational complexity of the predictions.

# Q1 – GLM with Customized Basis Function (Primal Approach)

A generalized linear model was implemented to make predictions on the one-dimensional mauna\_loa dataset. The optimal regularization ( $\lambda$ ) parameter was selected by looping over values  $\lambda \in [0, 30]$  and selecting the regularization parameter that minimized the RMSE error on the validation set. This regularization parameter was then used to compute the predictions on the test set, and the test RMSE was computed. The performance of the model is shown in Table 1.

Table 1 – Results of GLM on the mauna\_loa Dataset

Dataset	$\lambda_{optimal}$	Test RMSE	
Mauna Loa	14	0.103937949238	

The model was constructed using the basis function mapping the one-dimensional dataset to five-dimensional feature space:

$$\phi(x): \mathbb{R} \to \mathbb{R}^5, \phi(x) = \left[1, \sqrt{2}x, x^2, xsin(\omega x), xcos(\omega x)\right]^T$$

The angular frequency  $\omega = \frac{2\pi}{0.0565}$  was determined empirically by plotting the mauna\_loa training set and computing the period of oscillation of the macro trend. The basis function was designed to fit both the macro and micro trends of the mauna\_loa dataset. The macro trend of the dataset displayed characteristics of a linearly increasing sinusoid, with micro trends that could be approximated with linear and quadratic terms. The original basis function included an  $x^3$  term to approximate cubic micro trends, however, the associated reduction in error was not significant enough to justify its inclusion in the basis function. With the above basis function, the performance of the model was quite impressive with a Test RMSE at approximately 10% with a regularization parameter equal to 14 (i.e. significant improvement to regular Linear Model). The predictions on the test set are shown in Figure 1.

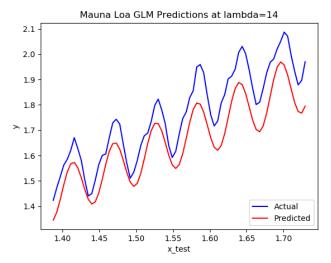


Figure 1 – GLM Predictions on Mauna Loa Test Set

# <u>Q2 – Kernelized GLM (Dual Perspective)</u>

A kernelized form the GLM from question one was constructed from the dual perspective. This process involved deriving a kernel function representing fast inner products of the basis function shown in question 1. The kernel was simplified to the following form:

$$k(x, z) = \phi(x)^{T} \phi(z) = (1 + x * z)^{2} + \cos(\omega(x - z))$$

The predictions to the mauna\_loa test set are shown in Figure 2, and the Test RMSE value with a regularization parameter of 14 in shown in Table 2. As expected, the results are identical to the primal GLM as the models are numerically equivalent, but expressed in different forms.

Table 2 – Results of Kernelized GLM on the mauna\_loa Dataset

Dataset	$\lambda_{optimal}$	Test RMSE	
Mauna Loa	14	0.103937949238	

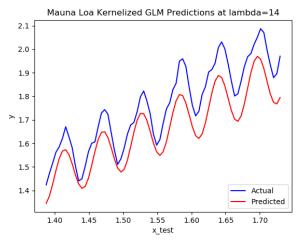
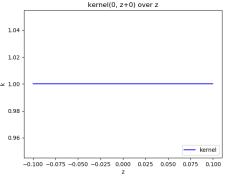
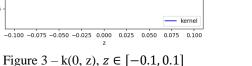


Figure 2 – Kernelized GLM Predictions on Mauna Loa Test Set

In this case, the kernelized GLM is actually worse in terms of both computational cost and memory requirements. The Gram matrix used in the kernelized GLM dominates the memory requirements for the model, making it  $O(N^2)$ . The standard GLM memory requirements is bounded by O(N \* M) which comes from storing the  $\Phi$  matrix which consists of the basis function for all training points. In terms to computational cost, the kernelized GLM is bounded  $O(N^3)$ , while the SVD used in the standard GLM dominates the computational cost with  $O(2N(M+1)^2+11N(M+1)^3)$ . In our case, M=5 but N is a significantly larger number. Since the computational cost of the kernelized model is proportional the  $N^3$ , while the standard GLM is only linearly proportional to N (i.e.  $(M+1)^3$  is almost negligible compared  $N^2$ ), it is evident that the standard GLM is computationally more efficient for the designed basis function.

The kernel was analyzed by developing two plots. Each graph plots the kernel at a specific value of x across a range of z values such that  $z \in [-0.1, 0.1]$ . The plots are shown in Figures 3-4.





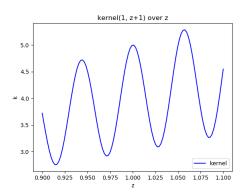


Figure  $4 - k(1, z+1), z \in [-0.1, 0.1]$ 

0.870967741935 | 1.0

Analyzing the above figures, it is evident that the kernel is not translationally invariant. The kernel is shown depend on more than just the numerical difference between datapoint x and points z. As we can see, adding a constant value of i = 1 to k(0 + i, z + i) provides a very different result in Figure 4 in comparison to Figure 3.

#### Q3 – Gaussian RBF Model for Regression and Classification

A GLM model using a gaussian RBF kernel was constructed to preform regression on both the mauna\_loa and rosenbrock datasets, and classification on the iris dataset. For each dataset, the regularization parameter and length scale pair that minimized validation RMSE (regression) or maximized the validation accuracy ratio (classification) was acquired and used to make predictions on the test sets. Table 3 summarizes the results for each dataset.

Dataset	Data Type	$\lambda_{optimal}$	$ heta_{optimal}$	Validation RMSE/Ratio	Test RMSE/Ratio
Mauna Loa	Regression	0.001	1	0.124478670316	0.14977338772
Rosenbrock	Regression	0.001	2	0.193239586974	0.14812442755

0.5

Table 3 – Gaussian RBF GLM Results on Regression and Classification Sets

Classification

Iris

# <u>Q4 – Tikhonov Regularization</u>

# Q5 – Weight Estimation comparison to the Dual Perspective

Objective function for under 
$$\{l(x, \alpha) = \sum_{i=1}^{N} \alpha_i : k(x, x^{(i)}) = k^T \alpha_i$$
 is given as  $\sum_{i=1}^{N} (y^{(i)} - l(x^{(i)}, \alpha))^2 + 2 \sum_{i=1}^{N} \alpha_i^2$  Vericles, functions  $\sum_{i=1}^{N} (y^{(i)} - l(x^{(i)}, \alpha))^2 + 2 \sum_{i=1}^{N} \alpha_i^2$  where  $\sum_{i=1}^{N} \alpha_i^2 = \sum_{i=1}^{N} \alpha_i^2$  where  $\sum_{i=1}^{N} \alpha_i^2 = \sum_{i=1}^{N} \alpha_i^2 = \sum_{i=1}^{N} \alpha_i^2$  where  $\sum_{i=1}^{N} \alpha_i^2 = \sum_{i=1}^{N} \alpha_i^2 = \sum_$ 

It is clear that this result is different than the expression derived in class. The previous expression, (1)  $\alpha = (K + \lambda I)^{-1}y$ , was derived by using the Matrix Inversion Lemma to transform  $\omega = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T y$  into a form that kernelized the model with fast inner products between basis functions. In this question, the box result was derived by minimizing the L2-loss of a pre-kernelized model. A proof below is presented to support this argument.

Proof: Let 
$$\underline{x}' = (\underline{K}^T\underline{K} + \lambda \underline{1})^T\underline{K}^T\underline{y}$$
 (result of minization of abjective fluction)

and  $\underline{\alpha} = (\underline{K} + \lambda \underline{1})^T\underline{Y}$  (dual perspective result)

Set  $\underline{A} = \underline{\alpha}' = \underline{\gamma}$  ( $\underline{K}^T\underline{K} + \lambda \underline{1})^T\underline{K}^T\underline{Y} = (\underline{K} + \lambda \underline{1})^T\underline{Y}$ 
 $\underline{K}^T(\underline{K} + \lambda \underline{1}) = \underline{K}^T\underline{K} + \lambda \underline{1}$ 
 $\lambda \underline{K}^T = \lambda \underline{1}$ 

Thus,  $\alpha = \alpha'$  implies that  $K^T = 1$ , which is not true. The im, jth clement in K is  $k(x^{(i)}, x^{(j)})$ .

O Need  $K(\underline{x}^{(i)},\underline{x}^{(j)}) = 0$  for  $i \neq j$  ? Necessary for  $\underline{K} = \underline{1}$ O and  $K(\underline{x}^{(i)},\underline{x}^{(j)}) = 0$  for i = j ?

However, anditions O and @ are not true for majority of basis functions and Herreto. Therefore, we have a conflict.

Therefore, a ≠ a'

```
1 import numpy as np
 2 import math
 3 from matplotlib import pyplot as plt
 4 from data_utils import load_dataset
 6
   __author__ = 'Christopher Agia (1003243509)'
 7
   __date__ = 'February 18, 2019'
 9
10
11 # Useful Utility Functions
12 def compute_rmse(y_test, y_estimates):
       return np.sqrt(np.average((y_test-y_estimates)**2))
13
14
15
16 def 12_norm(x1, x2):
       return np.linalg.norm([x1-x2], ord=2)
17
18
19
20 # Kernel Functions and Custom Vector Function
21 def custom kernel(x0, x1):
22
       # Customer kernel incorporates a polynomial expansion term and product of two sinusoidal terms
23
       return (1+x0*x1)**2 + x0*x1*math.cos(2*math.pi/0.0565*(x0-x1))
24
25
26 def custom_vector(x):
27
       freq = 2*math.pi/0.0565
      row = list()
28
29
      row.append(1)
30
       row.append(math.sqrt(2)*x)
31
       row.append(x**2)
32
       row.append(x * math.sin(freq * x))
33
       row.append(x * math.cos(freq * x))
34
       return np.array(row)
35
36
       ----- Question 1 -----
37 #
38
39 def glm_validation(x_train, x_valid, y_train, y_valid, l_vals=None):
40
41
       # Regularization Parameters ranging from 0-30
42
       if not l_vals:
           l_vals = list(range(0, 31))
43
44
45
       # Create and Populate the PHI Matrix
46
       shape = (len(x_train), 5)
47
       phi = np.empty(shape)
48
       for i in range(len(x_train)):
49
           phi[i, :] = custom_vector(x_train[i])
50
51
       # Create validation phi matrix
52
       shape = (len(x_valid), 5)
53
       phi_valid = np.empty(shape)
54
       for i in range(len(x_valid)):
55
           phi_valid[i, :] = custom_vector(x_valid[i])
56
57
       # Compute SVD
       U, S, Vh = np.linalg.svd(phi)
58
59
60
       # Invert Sigma
61
       sig = np.diag(S)
       filler = np.zeros([len(x_train) - len(S), len(S)])
62
63
       sig = np.vstack([sig, filler])
64
65
       # Compute weights and predictions with varying lambda values
66
       min_rmse = np.inf
       for l_val in l_vals:
67
68
           temp0 = np.dot(sig.T, sig)
69
           temp1 = np.linalg.inv(temp0 + l_val*np.eye(len(temp0)))
70
71
           w = np.dot(Vh.T, np.dot(temp1, np.dot(sig.T, np.dot(U.T, y_train))))
72
           predictions = np.dot(phi_valid, w)
```

```
2/28/2019
  74
              rmse_val = compute_rmse(y_valid, predictions)
  75
  76
              if rmse_val < min_rmse:</pre>
                  min_rmse = rmse_val
  77
  78
                  l_min = l_val
  79
          return 1 min
  80
  81
  82
  83 def glm test(x train, x valid, x test, y train, y valid, y test, l val):
  84
  85
          x_total = np.vstack([x_train, x_valid])
  86
         y_total = np.vstack([y_train, y_valid])
  87
          # Create and Populate the training PHI Matrix
  88
  89
          shape = (len(x_total), 5)
  90
          phi = np.empty(shape)
  91
          for i in range(len(x_total)):
  92
              phi[i, :] = custom_vector(x_total[i])
  93
  94
          # Create test PHI matrix
  95
          shape = (len(x_test), 5)
  96
          phi_test = np.empty(shape)
  97
          for i in range(len(x_test)):
  98
              phi_test[i, :] = custom_vector(x_test[i])
  99
 100
          # Compute SVD
 101
         U, S, Vh = np.linalg.svd(phi)
 102
 103
          # Invert Sigma
          sig = np.diag(S)
 104
 105
          filler = np.zeros([len(x_total) - len(S), len(S)])
 106
          sig = np.vstack([sig, filler])
 107
 108
          # Compute Test Predictions
 109
          temp0 = np.dot(sig.T, sig)
 110
          temp1 = np.linalg.inv(temp0 + l_val * np.eye(len(temp0)))
 111
          w = np.dot(Vh.T, np.dot(temp1, np.dot(sig.T, np.dot(U.T, y_total))))
 112
          predictions = np.dot(phi_test, w)
 113
 114
          test_error = compute_rmse(y_test, predictions)
 115
 116
          plt.figure(1)
         plt.plot(x_test, y_test, '-b', label='Actual')
plt.plot(x_test, predictions, '-r', label='Predicted')
 117
 118
          plt.title('Mauna Loa GLM Predictions at lambda=' + str(l_val))
 119
          plt.xlabel('x_test')
 120
 121
          plt.ylabel('y')
 122
          plt.legend(loc='lower right')
 123
          plt.savefig('mauna_loa_glm_estimates.png')
 124
 125
          return test_error
 126
 127
       ----- Question 2 -----
 128 #
 130 def glm_kernelized(x_train, x_valid, x_test, y_train, y_valid, y_test, l_val):
 131
 132
          x_total = np.vstack([x_train, x_valid])
 133
         y_total = np.vstack([y_train, y_valid])
 134
 135
          # Create and Populate the Gram Matrix (K)
 136
          shape = (len(x total), len(x total))
 137
          K = np.empty(shape)
 138
          prev_computed = {}
                                                        # Stores previously computed custom kernels
 139
          for i in range(len(x_total)):
 140
              for j in range(len(x_total)):
 141
                  a = x_total[i]
 142
                  b = x_total[j]
                  # Add to previously computed dictionary
 143
 144
                  if str((a, b)) not in prev_computed:
 145
                      prev_computed[str((a, b))] = custom_kernel(a, b)
 146
                      prev_computed[str((b, a))] = prev_computed[str((a, b))]
                  # Add kernel to K (Gram) Matrix
```

# Create and Populate the Gram Matrix (K) at the current theta value

# Gram Matrix

# Store previously computed gaussian kernel

K = np.empty(shape)

prev\_computed = {}

shape = (len(x\_train), len(x\_train))

for j in range(len(x\_train)):

for i in range(len(x\_train)):

215

216 217

218

219

220

```
2/28/2019
                        C:\Users\Christopher Agia\Desktop\Year 3\Term 2\ROB313 Intro to Learning from Data\Assignment 2\glm main.py
                      a = x_train[i]
 222
 223
                      b = x_train[j]
 224
                      if str((a, b)) not in prev_computed:
 225
                          prev_computed[str((a, b))] = gaussian_rbf(a, b, theta)
 226
                          prev_computed[str((b, a))] = prev_computed[str((a, b))]
 227
                      # Add kernel to K (Gram) Matrix
                      K[i, j] = prev_computed[str((a, b))]
 228
 229
 230
              # Only alpha changes with regularization value, thus calculate k vector (and extend to matrix form = kM)
 231
              kM = np.empty((len(x_valid), len(x_train)))
 232
              for i in range(len(x_valid)):
 233
                  # Create k vector, containing the kernel products of x_test and all x_training points
 234
                  k = list()
 235
                  vec = x_valid[i]
 236
                  for j in range(len(x_train)):
 237
                      k.append(gaussian_rbf(vec, x_train[j], theta))
 238
                  kM[i, :] = np.array(k)
 239
 240
              # K, kM matrix computed, compute test errors for each regularization value at current theta
 241
              for l_val in reg_vals:
 242
                  # Cholesky Factorization of K + lambda*1, here R is lower triangular
 243
                  R = np.linalg.cholesky((K + l_val * np.eye(len(K))))
 244
 245
                  # Find inverse, P = inv(R) makes it quicker to find matrix inverse
 246
                  P = np.linalg.inv(R)
 247
                  # Estimate dual-variables alpha
 248
                  alp = np.dot(np.dot(P.T, P), y_train)
 249
 250
                  # Compute Test RMSE for regresion datasets
 251
                  if dataset == 'mauna_loa' or dataset == 'rosenbrock':
 252
                      # Compute predictions
 253
                      predictions = np.dot(kM, alp)
 254
                      # Compute model validation error at current regularization-theta pair, and store in results
 255
                      results[(theta, l_val)] = compute_rmse(y_valid, predictions)
 256
                  # Compute Test Accuracy Ratio for classification datasets
 257
 258
                  else:
 259
                      # Compute predictions
                      predictions = np.argmax(np.dot(kM, alp), axis=1)
 260
 261
                      y valid0 = np.argmax(1 * y valid, axis=1)
                      # Compute model prediction accuracy at current regularization-theta pair, and store in results
 262
 263
                      results[(theta, l_val)] = (predictions == y_valid0).sum() / len(y_valid0)
 264
 265
          # Acquire the optimal theta and regularization values, return them to be used for test set
 266
          if dataset == 'mauna loa' or dataset == 'rosenbrock':
 267
              opt_res = np.inf
 268
              for theta, l_val in results:
 269
                  if results[(theta, l_val)] < opt_res:</pre>
 270
                      opt_res = results[(theta, l_val)]
 271
                      opt_theta = theta
 272
                      opt_reg = l_val
 273
          else:
 274
              opt_res = np.NINF
 275
              for theta, l_val in results:
 276
                  if results[(theta, 1 val)] > opt res:
 277
                      opt_res = results[(theta, l_val)]
 278
                      opt_theta = theta
 279
                      opt_reg = l_val
 280
 281
          return opt_theta, opt_reg, opt_res
 282
 283
 284 def gaussian_rbf_glm_test(x_train, x_valid, x_test, y_train, y_valid, y_test, l_val, theta, dataset):
 285
 286
         x_total = np.vstack([x_train, x_valid])
 287
         y_total = np.vstack([y_train, y_valid])
 288
 289
          # Create and Populate the Gram Matrix (K) at the current theta value
 290
          shape = (len(x_total), len(x_total))
 291
          K = np.empty(shape) # Gram Matrix
          prev_computed = {} # Store previously computed gaussian kernel
 292
 293
          for i in range(len(x_total)):
 294
              for j in range(len(x_total)):
                  a = x total[i]
```

```
370
371
        # visualize_kernel()
372
373
        # print('Test Root Mean-Squared Error: ' + str(test_rmse))
374
        # print('')
375
376
        # ------ Ouestion 3 -----
377
378
        # print('-----' Overall Results for Question 3 -----')
        # print('')
379
380
        #
        # x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset('mauna_loa')
381
         \begin{tabular}{ll} \# theta, reg, valid\_error = gaussian\_rbf\_glm\_valid(x\_train, x\_valid, y\_train, y\_valid, 'mauna\_loa') \end{tabular} 
382
        \#\ test\_rmse = gaussian\_rbf\_glm\_test(x\_train,\ x\_valid,\ x\_test,\ y\_train,\ y\_valid,\ y\_test,\ reg,\ theta,\ 'mauna\_loa')
383
        # print('--- Results for mauna_loa ---')
384
        # print('Optimal Lengthscale: ' + str(theta))
385
        # print('Optimal Regularizer: ' + str(reg))
386
387
        # print('Valid RMSE: ' + str(valid_error))
        # print('Test RMSE: ' + str(test_rmse))
388
389
        # print('')
390
         \# \ x\_train, \ x\_valid, \ x\_test, \ y\_train, \ y\_valid, \ y\_test = load\_dataset('rosenbrock', \ n\_train=1000, \ d=2) 
391
392
         \begin{tabular}{ll} \# theta, reg, valid\_error = gaussian\_rbf\_glm\_valid(x\_train, x\_valid, y\_train, y\_valid, 'rosenbrock') \end{tabular} 
393
        \# test_rmse = gaussian_rbf_glm_test(x_train, x_valid, x_test, y_train, y_valid, y_test, reg, theta, 'rosenbrock')
        # print('--- Results for rosenbrock ---')
394
395
        # print('Optimal Lengthscale: ' + str(theta))
        # print('Optimal Regularizer: ' + str(req))
396
        # print('Valid RMSE: ' + str(valid_error))
# print('Test RMSE: ' + str(test_rmse))
397
398
        # print('')
399
400
401
        # x train, x valid, x test, y train, y valid, y test = load_dataset('iris')
402
        # theta, reg, valid_ratio = gaussian_rbf_glm_valid(x_train, x_valid, y_train, y_valid, 'iris')
        # test_ratio = gaussian_rbf_glm_test(x_train, x_valid, x_test, y_train, y_valid, y_test, reg, theta, 'iris')
403
404
        # print('--- Results for iris ---')
        # print('Optimal Lengthscale: ' + str(theta))
405
        # print('Optimal Regularizer: ' + str(reg))
# print('Valid Accuracy Ratio: ' + str(valid_ratio))
406
407
        # print('Test Accuracy Ratio: ' + str(test_ratio))
408
409
        # print('')
410
411
412
        413
        # Done on paper
        # ------ Question 5 -----
414
415
        # Done on paper
```