ASSIGNMENT

CS5691 Pattern Recognition and Machine Learning

CS5691 Assignment 1 - Code

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1 Task **1**

1.1 Main Code

The code for Question 1 is as follows:

```
2 # ## CS5691 PRML Assignment 1
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10 # Install required Packages
11 # Uncomment if you are running for the first time
12 # !pip install -r requirements.txt
13 # try:
14 #
      !mkdir images/q1
15 # except:
16 #
       pass
19 import numpy as np
20 np.random.seed(0)
21 import pandas as pd
23 import warnings
24 warnings.filterwarnings("ignore")
25 import matplotlib.pyplot as plt
26 plt.style.use('science')
27 plt.rcParams['font.size'] = 18
28 plt.rcParams['axes.grid'] = True
29 plt.rcParams["grid.linestyle"] = (5,9)
30 plt.rcParams['figure.figsize'] = 8,6
32 from regression import PolynomialRegression
33 from gridsearch import GridSearch
35 df = pd.read_csv("../datasets/function1.csv", index_col=0)
36 df.sort_values(by=["x"], inplace=True)
37 df.head()
40 lmbda list = [0, 0.5, 1, 2, 10, 50, 100]
41 degrees allowed = [2, 3, 6, 9]
42 datasizes_considered = [10, 200]
43 complete_dataset_size = df.shape[0]
45 X = df["x"].to_numpy().reshape(-1,1)
y = df["y"].to_numpy().reshape(-1,1)
48 results_df_list = []
49 correspondance_list = []
50 for sample_size in datasizes_considered:
     gridsearch = GridSearch()
     df_result, correspondance = gridsearch.get_result(df, sample_size=...
        \verb|sample_size|, degrees_allowed=degrees_allowed|, lmbda_list=lmbda_list...
```

```
results_df_list.append(df_result)
      correspondance_list.append(correspondance)
55
      print("\nFor Sample Size of ", sample_size, " - GridSearch Results:")
56
      print(df_result)
57
      print("="*70)
      gridsearch.get_plots(X, y, correspondance, sample_size, show=True)
  61
 # From the resuts obtained, we see that degree=6, lambda=0.0
 # best fits the model.
63
64
67 best_degree = int(df_result.iloc[0]["degree"])
68 best_lmbda = df_result.iloc[0]["lambda"]
70 df_train = df.sample(frac=0.7, random_state=42)
71 df_test = df[~df.index.isin(df_train.index)]
72
73 X_train = df_train["x"].to_numpy().reshape(-1,1)
74 X_test = df_test["x"].to_numpy().reshape(-1,1)
75 y_train = df_train["y"].to_numpy().reshape(-1,1)
76 y_test = df_test["y"].to_numpy().reshape(-1,1)
78 regressor = PolynomialRegression()
79 X_train_poly = regressor.fit(X_train, y_train, degree=best_degree, lmbda=...
     best_lmbda)
80 y_train_pred = regressor.transform(X_train)
81 y test pred = regressor.transform(X test)
82 train_error = regressor.error(y_train, y_train_pred)
83 test_error = regressor.error(y_test, y_test_pred)
85 print("Training Error:", train_error)
 print("Testing Error:", test_error)
```

1.2 Polynomial Regression Code

The helper class used to perform PolynomialRegression is as follows:

```
import numpy as np
  class PolynomialRegression():
       def __init__(self):
4
           pass
5
6
       def fit(self, X, y, degree=2, lmbda=0):
7
           self.degree = degree
8
           self.lmbda = lmbda
10
           X_poly = self.get_polynomial_features(X)
11
           self.get_weights(X_poly, y)
12
           return X_poly
13
14
       def transform(self, X_val):
15
           X_poly = self.get_polynomial_features(X_val)
           y_val = X_poly @ self.W
           return y_val
18
19
```

```
def fit_transform(self, X, y, degree=2, lmbda=0):
20
           self.fit(X, y, degree, lmbda)
21
           return self.transform(X)
22
23
       def get_polynomial_features(self, X):
24
           X_new = np.ones(X.shape)
26
           for i in range(1, self.degree+1):
               X_new = np.append(X_new, X**i, axis=1)
27
           return X_new
28
       def get_weights(self, X_poly, y):
30
           d = X_poly.shape[1]
31
           self.W = ((np.linalg.inv(X_poly.T @ X_poly + self.lmbda*np.identity...
32
               (d))) @ X_poly.T) @ y
33
       def error(self, y_true, y_pred):
34
           rmse = np.linalg.norm(y_pred-y_true)/(y_true.size)**0.5
35
36
           return rmse
```

1.3 Grid Search Code

The helper class used to perform Grid Search are as follows:

```
import numpy as np
2 import pandas as pd
3 import matplotlib.pyplot as plt
4 from regression import PolynomialRegression
  class GridSearch():
       def __init__(self):
           pass
8
9
       def get_result(self, df, sample_size, degrees_allowed, lmbda_list):
10
           df_sample = df.sample(n=sample_size, random_state=42)
11
12
           df_train = df_sample.sample(frac=0.9, random_state=42)
13
           df_val = df_sample[~df_sample.index.isin(df_train.index)]
15
           X_train = df_train["x"].to_numpy().reshape(-1, 1)
16
           X_{val} = df_{val}["x"].to_{numpy}().reshape(-1, 1)
17
           y train = df train["y"].to numpy().reshape(-1, 1)
19
           y_val = df_val["y"].to_numpy().reshape(-1, 1)
20
21
           self.result = []
           self.correspondance = {}
23
24
25
           for degree in degrees_allowed:
               for lmbda in lmbda_list:
                   regressor = PolynomialRegression()
27
                   regressor.fit(X_train, y_train, degree=degree, lmbda=lmbda)
28
                   y_train_pred = regressor.transform(X_train)
29
                   y_val_pred = regressor.transform(X_val)
30
31
                   train_error = regressor.error(y_train, y_train_pred)
32
                   val_error = regressor.error(y_val, y_val_pred)
33
                   self.result.append([degree, lmbda, train_error, val_error])
35
```

```
self.correspondance[(degree, lmbda)] = {"df_sample":...
36
                       df_sample, "regressor":regressor}
37
           df_results = pd.DataFrame(self.result, columns=["degree", "lambda",...
38
                "Train error", "Validation error"])
           df_results["Sum Error"] = df_results["Train error"] + df_results["...
              Validation error"]
           df_results.sort_values(by="Sum Error", inplace=True)
40
           return df_results, self.correspondance
41
       def get_plots(self, X, y, correspondance, sample_size, show):
43
           for key in correspondance:
44
               df_sample = correspondance[key]["df_sample"]
45
               df_sample.sort_values(by=["x"], inplace=True)
46
               X_sample = df_sample["x"].to_numpy().reshape(-1,1)
47
               y_sample = df_sample["y"].to_numpy().reshape(-1,1)
48
49
50
               regressor = correspondance[key]["regressor"]
               y_pred_sample = regressor.transform(X_sample)
51
52
               title = "Curve Fitting - Degree: "+str(regressor.degree)\
               +"; Sample Size: "+str(sample_size)+"; $\lambda$: "\
54
               +str(regressor.lmbda)
55
               fname = "d_"+str(regressor.degree)+"_size_"+str(sample_size)+"...
56
                   _l_"+str(regressor.lmbda)+".png"
               plt.figure()
58
               plt.plot(X, y, label="True Value")
59
               if y_sample.size >= 100:
                   plt.plot(X_sample, y_sample, 'r.', alpha=0.5, label="...
61
                       Sampled points")
               else:
62
63
                   plt.plot(X_sample, y_sample, 'ro', alpha=0.75, label="...
                       Sampled points")
               plt.plot(X_sample, y_pred_sample, label="Predicted Value")
64
               if title:
                   plt.title(title)
               plt.xlabel("X-values")
67
               plt.ylabel("Y-values")
68
               plt.legend()
69
               plt.savefig("images/"+fname)
70
               if show:
71
                   plt.show()
72
```

2 Task 2

The code for Question 2 is as follows:

```
# # Task 2
13
func2d=pd.read_csv("function1_2d.csv",index_col = 0)
17
 18
 # ## 2.1 Generating the polynomial basis functions of degrees 2, 3 and 6: (...
19
     Sp to dataset 2)
20
 ### Creating the polynomial basis functions of degree M and number of ...
    examples = n:
23
 def create_phi(M,n,x1,x2):
24
    d=2
25
26
    D = int(ma.factorial(d+M)/(ma.factorial(d)*ma.factorial(M)))
    phi = np.zeros((n,D))
27
28
    if M == 2:
29
       exp_ar = [[0,0],[1,0],[0,1],[2,0],[0,2],[1,1]]
30
    if M == 3:
31
32
       exp_ar = ...
          [[0,0],[1,0],[0,1],[2,0],[0,2],[1,1],[2,1],[1,2],[3,0],[0,3]]
33
       exp_ar = [[0,0],[1,0],[0,1],[2,0],[0,2],[1,1],[2,1],[1,2],
34
               [3,0], [0,3], [3,1], [1,3], [2,2], [4,0], [0,4], [4,1],
35
               [1,4], [2,3], [3,2], [5,0], [0,5], [5,1], [1,5], [2,4],
               [4,2],[3,3],[6,0],[0,6]]
37
38
    for i in range(D):
39
       phi[:,i] = (x1**(exp_ar[i][0]))*(x2**(exp_ar[i][1]))
40
41
    return(phi)
42
 # ## 2.2 Solving for optimal parameters using regularization, lambda=0
                                                      for...
     unregularized: (versatile)
 # ### The function regularized_pseudo_inv(lamb,X) returns:
 # $$(\lambda I+X^TX)^{-1}X^T$$
48
 #
49
 # Where lambda is the hyperparameter in the quadratic regularization
 def regularized_pseudo_inv(lamb,phi):
53
    return(np.matmul(np.linalg.inv(lamb*np.identity(phi.shape[1])+np.matmul...
54
       (np.transpose(phi),phi)),np.transpose(phi)))
55
# ### The function opt_regularized_param(lamb,phi,y) returns an array of ...
    optimal parameter values calculated using regularized cost function for...
     an input design matrix phi, hyperparameter lambda and output values y.
 def opt_regularized_param(lamb,phi,y):
60
    return(np.matmul(regularized_pseudo_inv(lamb,phi),y))
61
```

```
# ## 2.3 The function y_pred(X,w) returns predicted function values for ...
     input matrix X and set of chosen parameter values w a: (versatile)
  # $$v=Xw$$
65
66
def y_pred(phi,w):
      return(np.matmul(phi,w))
69
70
  # ## 2.4 Splitting the data into train, cross-validation and test and ...
     helper function for surface plot: (versatile)
73
  def create_datasets(data,train_size,cv_size):
      data.sample(frac=1).reset index(drop=True)
76
      data_train=data[0:train_size]
77
      data_cv=data[train_size:train_size+cv_size]
78
      data_test=data[cv_size+train_size:]
     return(data_train,data_cv,data_test)
80
81
82
  def split_cols(data_train,data_cv,data_test):
85
      #x1_train,x2_train,y_train,x1_cv,x2_cv,y_cv,x1_test,x2_test,y_test
      x1_train=np.array(data_train)[:,0]
      x2_train=np.array(data_train)[:,1]
88
      y_train=np.array(data_train)[:,2]
89
      x1 cv=np.array(data cv)[:,0]
      x2 cv=np.array(data cv)[:,1]
      y cv=np.array(data cv)[:,2]
92
     x1_test=np.array(data_test)[:,0]
93
      x2_test=np.array(data_test)[:,1]
     y_test=np.array(data_test)[:,2]
95
96
97
      return(x1_train,x2_train,y_train,x1_cv,x2_cv,y_cv,x1_test,x2_test,...
        y_test)
98
99
  ### Function to calculate RMSE:
102
103
  def RMSE(y_pred, t):
104
      n = len(y_pred)
      return(np.sqrt(np.sum((y_pred - t)**2)/n))
106
107
  110 #plot the approximated function
111
112
  def plot_approxY(M,w,y_train,y_pred,train_size,l,a,b):
113
114
      # M is the degree of the complexity
115
      # w is the array of parameters
116
      # y is the actual value of y
117
      # l is the value of lambda
118
     x1 = np.arange(-16, 16, 0.5)
119
      x2 = np.arange(-16, 16, 0.5)
```

```
x1, x2 = np.meshgrid(x1,x2)
121
      Y = np.zeros((64,64))
122
      for i in range (64):
123
         for j in range(64):
124
             Y[i,j] = np.sum(np.matmul(create_phi(M,1,x2[i,j],x1[i,j]),w))
125
      fig = plt.figure(figsize=(15,8))
126
127
      ax=fig.gca(projection="3d")
      ax.plot wireframe(x1,x2,Y,label="Approximated function")
128
      x = b
129
130
131
      z = y_train
      ax.scatter(x,y,z,color='red',label="Original train data points")
132
      ax.set_ylabel("x1")
133
      ax.set_xlabel("x2")
135
      ax.set zlabel("y")
      ax.view_init(0,45)
136
      plt.legend(loc=4)
137
138
      plt.title("Surface plot with degree of complexity = %i, Train data size...
          = %i and regularization parameter, lambda = %.1f"%(M,train_size,1)...
      plt.show()
139
140
  141
  # ## 2.5 Predicting for degree 2, train size 50:
142
  data2_train50,data2_cv50,data2_test50=create_datasets(func2d,50,30)
145
146
147
  148
  x12_train50,x22_train50,y2_train50,x12_cv50,x22_cv50,y2_cv50,x12_test50,...
149
     x22_test50, y2_test50=split_cols(data2_train50,data2_cv50,data2_test50)
150
151
153 ### design matrix:
154 phi2_train50=create_phi(2,len(y2_train50),x12_train50,x22_train50)
phi2_cv50=create_phi(2,len(y2_cv50),x12_cv50,x22_cv50)
  phi2_test50=create_phi(2,len(y2_test50),x12_test50,x22_test50)
157
158
  159
160 y2_testpred50={}
161 y2_trainpred50={}
162 y2_cvpred50={}
lambda_list=[0,0.5,1,2,10,50,100]
164 rmse2_train50=[]
165 rmse2_test50=[]
  rmse2_cv50=[]
166
167
168
  170
  for 1 in lambda list:
      w_2_50=opt_regularized_param(1,phi2_train50,y2_train50);
171
      y2_trainpred50[1]=y_pred(phi2_train50,w_2_50)
172
      y2_testpred50[1] = y_pred(phi2_test50, w_2_50);
173
      y2_cvpred50[1]=y_pred(phi2_cv50,w_2_50);
174
      rmse2_train50.append(RMSE(y2_trainpred50[1],y2_train50))
175
      rmse2_test50.append(RMSE(y2_testpred50[1],y2_test50))
176
177
      rmse2_cv50.append(RMSE(y2_cvpred50[1],y2_cv50))
```

```
178
179
180
181
  182
  data2_50=pd.DataFrame(list(zip(lambda_list,rmse2_train50,rmse2_cv50,...
183
    rmse2_test50)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
184
185
  data2 50
187
188
189
191 plt.figure()
plt.plot(data2_50["Lambda"],data2_50["RMSE Train"],label="RMSE Train")
plt.plot(data2_50["Lambda"],data2_50["RMSE CV"],label="RMSE CV")
  plt.plot(data2_50["Lambda"],data2_50["RMSE test"],label="RMSE test")
195 plt.xlabel("Lambda->")
196 plt.ylabel("RMSE")
197 plt.legend()
 plt.title("RMSE vs lambda for train size = 50 and degree of complexity = 2"...
  plt.savefig("d2_50.png")
200
  plt.show()
201
 202
203 # ### Surface plots for various values of lambda:
204
 205
  for l in lambda list:
206
     plot_approxY(2, w_2_50,y2_train50,y2_trainpred50[1],50,1,x12_train50,...
207
       x22 train50)
     plt.savefig("surfaceplotsd2.png")
208
209
 210
211 # ## 2.6 Predicting for degree of complexity = 2 and train data size = 200
212
  213
  data2_train200,data2_cv200,data2_test200=create_datasets(func2d,200,90)
214
215
216
 217
  x12_test200,x22_test200,y2_test200=split_cols(data2_train200,...
    data2_cv200,data2_test200)
219
220
222 ### design matrix:
phi2_train200=create_phi(2,len(y2_train200),x12_train200,x22_train200)
phi2_cv200=create_phi(2,len(y2_cv200),x12_cv200,x22_cv200)
phi2_test200=create_phi(2,len(y2_test200),x12_test200,x22_test200)
226
227
229 y2_testpred200={}
230 y2_trainpred200={}
231 y2_cvpred200={}
232 lambda_list=[0,0.5,1,2,10,50,100]
```

```
233 rmse2_train200=[]
234 rmse2_test200=[]
235
  rmse2_cv200=[]
236
237
  238
239
  for l in lambda_list:
     w_2_200=opt_regularized_param(1,phi2_train200,y2_train200);
240
     y2_trainpred200[1]=y_pred(phi2_train200,w_2_200)
241
     y2_testpred200[1]=y_pred(phi2_test200,w_2_200);
242
     y2_cvpred200[1]=y_pred(phi2_cv200,w_2_200);
243
     rmse2_train200.append(RMSE(y2_trainpred200[1],y2_train200))
244
245
     rmse2_test200.append(RMSE(y2_testpred200[1],y2_test200))
     rmse2_cv200.append(RMSE(y2_cvpred200[1],y2_cv200))
246
247
248
249
  data2 200=pd.DataFrame(list(zip(lambda_list,rmse2_train200,rmse2_cv200,...
251
     rmse2_test200)),columns=["Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
252
253
  254
  data2_200
255
256
257
  258
  data2_200.to_csv("RMSE-lambda for complexity = 2 and train size = 200")
259
260
261
263 plt.figure()
264 plt.plot(data2_200["Lambda"],data2_200["RMSE Train"],label="RMSE Train")
265 plt.plot(data2_200["Lambda"],data2_200["RMSE CV"],label="RMSE CV")
266 plt.plot(data2_200["Lambda"],data2_200["RMSE test"],label="RMSE test")
267 plt.xlabel("Lambda->")
268 plt.ylabel("RMSE")
269 plt.legend()
270 plt.title("RMSE vs lambda for train size = 200 and degree of complexity = 2...
     ")
plt.savefig("d2_200.png")
  plt.show()
272
273
  274
275 # ### Surface plots for various values of lambda:
276
  277
  for l in lambda_list:
278
     plot_approxY(2, w_2_200,y2_train200,y2_trainpred200[1],200,1,...
279
        x12_train200,x22_train200)
280
282 # ## 2.7 Predicting for degree of complexity = 2 and train data size = 500
283
284
  data2_train500,data2_cv500,data2_test500=create_datasets(func2d,500,200)
  x12_train500,x22_train500,y2_train500,x12_cv500,x22_cv500,y2_cv500,...
     x12_test500,x22_test500,y2_test500=split_cols(data2_train500,...
     data2_cv500,data2_test500)
287
```

```
288 ### design matrix:
  phi2_train500=create_phi(2,len(y2_train500),x12_train500,x22_train500)
  phi2_cv500=create_phi(2,len(y2_cv500),x12_cv500,x22_cv500)
291 phi2_test500=create_phi(2,len(y2_test500),x12_test500,x22_test500)
292
293 y2_testpred500={}
y2_trainpred500={}
295 y2_cvpred500={}
296 lambda_list=[0,0.5,1,2,10,50,100]
297 rmse2 train500=[]
  rmse2 test500=[]
298
  rmse2_cv500=[]
299
300
  for l in lambda_list:
301
      w_2_500=opt_regularized_param(1,phi2_train500,y2_train500);
302
      y2_trainpred500[1]=y_pred(phi2_train500,w_2_500)
303
      y2_testpred500[1] = y_pred(phi2_test500, w_2_500);
304
305
      y2_cvpred500[1]=y_pred(phi2_cv500,w_2_500);
      rmse2_train500.append(RMSE(y2_trainpred500[1],y2_train500))
306
      rmse2_test500.append(RMSE(y2_testpred500[1],y2_test500))
307
      rmse2_cv500.append(RMSE(y2_cvpred500[1],y2_cv500))
308
309
310
311
  data2_500=pd.DataFrame(list(zip(lambda_list,rmse2_train500,rmse2_cv500,...
     rmse2_test500)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
314
315
  316
  data2 500
317
318
  320
  data2_500.to_csv("RMSE-lambda for complexity =2 train size =500")
321
322
323
  324
325 plt.figure()
326 plt.plot(data2_500["Lambda"],data2_500["RMSE Train"],label="RMSE Train")
  plt.plot(data2_500["Lambda"],data2_500["RMSE CV"],label="RMSE CV")
328 plt.plot(data2_500["Lambda"],data2_500["RMSE test"],label="RMSE test")
329 plt.xlabel("Lambda->")
330 plt.ylabel("RMSE")
331 plt.legend()
332 plt.title("RMSE vs lambda for train size = 500 and degree of complexity = 2...
  plt.savefig("d2_500.png")
  plt.show()
334
335
337 # ### Surface plots for various values of lambda:
338
  339
  for 1 in lambda_list:
340
      plot_approxY(2, w_2_500,y2_train500,y2_trainpred500[1],500,1,...
        x12_train500,x22_train500)
342
# ## 2.8 For train size =50 and degree of complexity = 3
```

```
345
  data3_train50,data3_cv50,data3_test50=create_datasets(func2d,50,30)
347
  x13_train50,x23_train50,y3_train50,x13_cv50,x23_cv50,y3_cv50,x13_test50,...
     x23_test50,y3_test50=split_cols(data3_train50,data3_cv50,data3_test50)
349
350
  ### design matrix:
phi3_train50=create_phi(3,len(y3_train50),x13_train50,x23_train50)
  phi3_cv50=create_phi(3,len(y3_cv50),x13_cv50,x23_cv50)
  phi3_test50=create_phi(3,len(y3_test50),x13_test50,x23_test50)
354
355 y3_testpred50={}
356 y3_trainpred50={}
357 y3_cvpred50={}
358 lambda_list=[0,0.5,1,2,10,50,100]
359 rmse3_train50=[]
360 rmse3_test50=[]
361
  rmse3_cv50=[]
362
  for l in lambda_list:
363
      w_3_50=opt_regularized_param(1,phi3_train50,y3_train50);
364
365
      y3_trainpred50[1]=y_pred(phi3_train50,w_3_50)
      y3_testpred50[1]=y_pred(phi3_test50,w_3_50);
366
      y3_cvpred50[1]=y_pred(phi3_cv50,w_3_50);
367
      rmse3_train50.append(RMSE(y3_trainpred50[1],y3_train50))
      rmse3_test50.append(RMSE(y3_testpred50[1],y3_test50))
369
      rmse3_cv50.append(RMSE(y3_cvpred50[1],y3_cv50))
370
371
372
373
  374
  data3_50=pd.DataFrame(list(zip(lambda_list,rmse3_train50,rmse3_cv50,...
375
     rmse3_test50)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
376
377
  378
  data3_50.to_csv("rmse lambda for complexity = 3 train sie =50")
379
380
381
  382
  plt.figure()
384 plt.plot(data3_50["Lambda"],data3_50["RMSE Train"],label="RMSE Train")
385 plt.plot(data3_50["Lambda"],data3_50["RMSE CV"],label="RMSE CV")
386 plt.plot(data3_50["Lambda"],data3_50["RMSE test"],label="RMSE test")
387 plt.xlabel("Lambda->")
388 plt.ylabel("RMSE")
389 plt.legend()
  plt.title("RMSE vs lambda for train size = 50 and degree of complexity = 3"...
  plt.savefig("d3_50.png")
391
392 plt.show()
393
  394
  # ### Surface plots for various values of lambda
395
  for 1 in lambda_list:
398
      plot_approxY(3, w_3_50,y3_train50,y3_trainpred50[1],50,1,x13_train50,...
399
         x23_train50)
400
```

```
402 # ## 2.9 For train size = 200 and degree of complexity = 3:
403
405 data3_train200,data3_cv200,data3_test200=create_datasets(func2d,200,90)
  x13_train200,x23_train200,y3_train200,x13_cv200,x23_cv200,y3_cv200,...
     x13_test200,x23_test200,y3_test200=split_cols(data3_train200,...
     data3 cv200, data3 test200)
407
  ### design matrix:
  phi3_train200=create_phi(3,len(y3_train200),x13_train200,x23_train200)
409
410 phi3_cv200=create_phi(3,len(y3_cv200),x13_cv200,x23_cv200)
  phi3_test200=create_phi(3,len(y3_test200),x13_test200,x23_test200)
413 y3_testpred200={}
414 y3_trainpred200={}
415 y3_cvpred200={}
416 lambda_list=[0,0.5,1,2,10,50,100]
417 rmse3_train200=[]
418 rmse3_test200=[]
419 rmse3_cv200=[]
420
  for l in lambda_list:
421
      w_3_200=opt_regularized_param(1,phi3_train200,y3_train200);
422
423
      y3_trainpred200[1]=y_pred(phi3_train200,w_3_200)
424
      y3_testpred200[1]=y_pred(phi3_test200,w_3_200);
      y3_cvpred200[1]=y_pred(phi3_cv200,w_3_200);
425
      rmse3_train200.append(RMSE(y3_trainpred200[1],y3_train200))
426
      rmse3_test200.append(RMSE(y3_testpred200[1],y3_test200))
427
      rmse3_cv200.append(RMSE(y3_cvpred200[1],y3_cv200))
428
429
430
  432
  data3_200=pd.DataFrame(list(zip(lambda_list,rmse3_train200,rmse3_cv200,...
     rmse3_test200)),columns=["Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
434
435
  436
  data3_200.to_csv("rmse lambda for complexity = 3, train size = 200")
437
438
439
441 plt.figure()
442 plt.plot(data3_200["Lambda"],data3_200["RMSE Train"],label="RMSE Train")
443 plt.plot(data3_200["Lambda"],data3_200["RMSE CV"],label="RMSE CV")
444 plt.plot(data3_200["Lambda"],data3_200["RMSE test"],label="RMSE test")
445 plt.xlabel("Lambda->")
446 plt.ylabel("RMSE")
447 plt.legend()
448 plt.title("RMSE vs lambda for train size = 200 and degree of complexity = 3...
plt.savefig("d3_200.png")
450 plt.show()
451
  # ### Surface Plots fror various values of lambda:
453
454
456 for l in lambda_list:
```

```
plot_approxY(3, w_3_200,y3_train200,y3_trainpred200[1],200,1,...
457
         x13_train200,x23_train200)
458
  459
  # ## 2.10 For train data size = 500 and degree of complexity = 3
460
461
  462
  data3_train500,data3_cv500,data3_test500=create_datasets(func2d,500,200)
  x13_train500,x23_train500,y3_train500,x13_cv500,x23_cv500,y3_cv500,...
     x13_test500,x23_test500,y3_test500=split_cols(data3_train500,...
     data3 cv500, data3 test500)
465
  ### design matrix:
467 phi3_train500=create_phi(3,len(y3_train500),x13_train500,x23_train500)
468 phi3_cv500=create_phi(3,len(y3_cv500),x13_cv500,x23_cv500)
  phi3_test500=create_phi(3,len(y3_test500),x13_test500,x23_test500)
469
470
471 y3_testpred500={}
472 y3_trainpred500={}
473 y3_cvpred500={}
474 lambda_list=[0,0.5,1,2,10,50,100]
475 rmse3_train500=[]
476 rmse3_test500=[]
  rmse3_cv500=[]
477
478
479
  for l in lambda_list:
      w_3_500=opt_regularized_param(1,phi3_train500,y3_train500);
480
      y3_trainpred500[1]=y_pred(phi3_train500,w_3_500)
481
      y3_testpred500[1]=y_pred(phi3_test500,w_3_500);
482
      y3_cvpred500[1]=y_pred(phi3_cv500,w_3_500);
483
      rmse3_train500.append(RMSE(y3_trainpred500[1],y3_train500))
484
      rmse3_test500.append(RMSE(y3_testpred500[1],y3_test500))
485
486
      rmse3_cv500.append(RMSE(y3_cvpred500[1],y3_cv500))
487
488
489
  data3_500=pd.DataFrame(list(zip(lambda_list,rmse3_train500,rmse3_cv500,...
491
     rmse3_test500)),columns=["Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
492
493
  494
  data3_500.to_csv("rmse lambda for complexity = 3 train size = 500")
495
496
499 plt.figure()
500 plt.plot(data3_500["Lambda"],data3_500["RMSE Train"],label="RMSE Train")
501 plt.plot(data3_500["Lambda"],data3_500["RMSE CV"],label="RMSE CV")
502 plt.plot(data3_500["Lambda"],data3_500["RMSE test"],label="RMSE test")
503 plt.xlabel("Lambda->")
504 plt.ylabel("RMSE")
505 plt.legend()
506 plt.title("RMSE vs lambda for train size = 500 and degree of complexity = 3...
  plt.savefig("d3_500.png")
  plt.show()
508
509
  # ### Surface Plots for various values of lambda:
```

```
512
  for 1 in lambda_list:
514
      plot_approxY(3, w_3_500,y3_train500,y3_trainpred500[1],500,1,...
515
         x13_train500,x23_train500)
516
  517
  # ## 2.11 Degree of complexity = 6 and train data size = 50
518
519
  data6 train50, data6 cv50, data6 test50=create datasets(func2d,50,30)
  x16_{train50}, x26_{train50}, y6_{train50}, x16_{cv50}, x26_{cv50}, y6_{cv50}, x16_{test50}, \dots
     x26_test50,y6_test50=split_cols(data6_train50,data6_cv50,data6_test50)
523
  ### design matrix:
524
phi6_train50=create_phi(6,len(y6_train50),x16_train50,x26_train50)
  phi6_cv50=create_phi(6,len(y6_cv50),x16_cv50,x26_cv50)
  phi6_test50=create_phi(6,len(y6_test50),x16_test50,x26_test50)
528
529 y6_testpred50={}
530 y6_trainpred50={}
531 y6_cvpred50={}
saz lambda_list=[0,0.5,1,2,10,50,100]
533 rmse6_train50=[]
  rmse6_test50=[]
535
  rmse6_cv50=[]
536
  for l in lambda_list:
537
      w_6_50=opt_regularized_param(1,phi6_train50,y6_train50);
538
      y6_trainpred50[1]=y_pred(phi6_train50,w_6_50)
539
      y6_testpred50[1]=y_pred(phi6_test50,w_6_50);
540
      y6_cvpred50[1]=y_pred(phi6_cv50,w_6_50);
541
542
      rmse6_train50.append(RMSE(y6_trainpred50[1],y6_train50))
      rmse6_test50.append(RMSE(y6_testpred50[1],y6_test50))
543
      rmse6_cv50.append(RMSE(y6_cvpred50[1],y6_cv50))
544
545
546
547
  data6_50=pd.DataFrame(list(zip(lambda_list,rmse6_train50,rmse6_cv50,...
549
     rmse6_test50)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
550
551
  data6_50.to_csv("rmse lambda complexity= 6, train = 50")
553
554
555
557 plt.figure()
558 plt.plot(data6_50["Lambda"],data6_50["RMSE Train"],label="RMSE Train")
plt.plot(data6_50["Lambda"],data6_50["RMSE CV"],label="RMSE CV")
560 plt.plot(data6_50["Lambda"],data6_50["RMSE test"],label="RMSE test")
561 plt.xlabel("Lambda->")
562 plt.ylabel("RMSE")
563 plt.legend()
  plt.title("RMSE vs lambda for train size = 50 and degree of complexity = 6"...
565 plt.savefig("d6_50.png")
  plt.show()
566
567
```

```
# ### Surface plots for various values of lambda:
570
  571
  for l in lambda_list:
572
      plot_approxY(6, w_6_50,y6_train50,y6_trainpred50[1],50,1,x16_train50,...
573
        x26_train50)
574
  # ## 2.12 For degree of complexity = 6 and train data size = 200
577
  578
  data6_train200,data6_cv200,data6_test200=create_datasets(func2d,200,90)
  x16_train200,x26_train200,y6_train200,x16_cv200,x26_cv200,y6_cv200,...
     x16_test200,x26_test200,y6_test200=split_cols(data6_train200,...
     data6_cv200,data6_test200)
581
582
  ### design matrix:
  phi6_train200=create_phi(6,len(y6_train200),x16_train200,x26_train200)
583
  phi6_cv200=create_phi(6,len(y6_cv200),x16_cv200,x26_cv200)
584
  phi6_test200=create_phi(6,len(y6_test200),x16_test200,x26_test200)
586
  y6_testpred200={}
587
588 y6_trainpred200={}
  y6_cvpred200={}
  lambda_list=[0,0.5,1,2,10,50,100]
591 rmse6_train200=[]
  rmse6_test200=[]
592
  rmse6_cv200=[]
593
594
  for l in lambda_list:
595
      w_6_200=opt_regularized_param(1,phi6_train200,y6_train200);
596
597
      y6_trainpred200[1]=y_pred(phi6_train200,w_6_200)
      y6_testpred200[1]=y_pred(phi6_test200,w_6_200);
598
      y6_cvpred200[1]=y_pred(phi6_cv200,w_6_200);
599
      rmse6_train200.append(RMSE(y6_trainpred200[1],y6_train200))
600
      rmse6_test200.append(RMSE(y6_testpred200[1],y6_test200))
601
      rmse6_cv200.append(RMSE(y6_cvpred200[1],y6_cv200))
602
603
604
605
  606
  data6_200=pd.DataFrame(list(zip(lambda_list,rmse6_train200,rmse6_cv200,...
607
     rmse6_test200)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
608
609
  610
  data6_200.to_csv("rmse lambda complexity = 6 train = 200")
611
612
613
615 plt.figure()
616 plt.plot(data6_200["Lambda"],data6_200["RMSE Train"],label="RMSE Train")
617 plt.plot(data6_200["Lambda"],data6_200["RMSE CV"],label="RMSE CV")
618 plt.plot(data6_200["Lambda"],data6_200["RMSE test"],label="RMSE test")
619 plt.xlabel("Lambda->")
620 plt.ylabel("RMSE")
621 plt.legend()
622 plt.title("RMSE vs lambda for train size = 200 and degree of complexity = 6...
     ")
```

```
623 plt.savefig("d6_200.png")
  plt.show()
625
  626
  # ### Surface plots for various values of lambda:
627
628
  629
  for l in lambda list:
630
      plot_approxY(6, w_6_200,y6_train200,y6_trainpred200[1],200,1,...
631
         x16_train200,x26_train200)
632
  633
  # ## 2.13 For degree of complexity = 6 and train data size = 500
634
635
  636
data6_train500,data6_cv500,data6_test500=create_datasets(func2d,500,200)
  x16_train500,x26_train500,y6_train500,x16_cv500,x26_cv500,y6_cv500,...
     x16_test500,x26_test500,y6_test500=split_cols(data6_train500,...
     data6_cv500,data6_test500)
639
  ### design matrix:
641
  phi6_train500=create_phi(6,len(y6_train500),x16_train500,x26_train500)
642 phi6_cv500=create_phi(6,len(y6_cv500),x16_cv500,x26_cv500)
  phi6_test500=create_phi(6,len(y6_test500),x16_test500,x26_test500)
643
645 y6_testpred500={}
646 y6_trainpred500={}
647 y6_cvpred500={}
lambda list=[0,0.5,1,2,10,50,100]
649 rmse6 train500=[]
650 rmse6 test500=[]
651 rmse6_cv500=[]
  for l in lambda list:
653
      w_6_500=opt_regularized_param(1,phi6_train500,y6_train500);
654
655
      y6_trainpred500[1]=y_pred(phi6_train500,w_6_500)
      y6_testpred500[1]=y_pred(phi6_test500,w_6_500);
656
      y6_cvpred500[1]=y_pred(phi6_cv500,w_6_500);
657
      rmse6_train500.append(RMSE(y6_trainpred500[1],y6_train500))
658
      rmse6_test500.append(RMSE(y6_testpred500[1],y6_test500))
659
      rmse6_cv500.append(RMSE(y6_cvpred500[1],y6_cv500))
660
661
662
  data6_500=pd.DataFrame(list(zip(lambda_list,rmse6_train500,rmse6_cv500,...
665
     rmse6_test500)),columns=["Lambda", "RMSE Train","RMSE CV","RMSE test"])
666
667
  data6_500.to_csv("rmse lambda complexity = 6 train = 500")
669
670
671
673 plt.figure()
674 plt.plot(data6_500["Lambda"],data6_500["RMSE Train"],label="RMSE Train")
675 plt.plot(data6_500["Lambda"],data6_500["RMSE CV"],label="RMSE CV")
676 plt.plot(data6_500["Lambda"],data6_500["RMSE test"],label="RMSE test")
677 plt.xlabel("Lambda->")
678 plt.ylabel("RMSE")
```

```
679 plt.legend()
680 plt.title("RMSE vs lambda for train size = 500 and degree of complexity = 6.
plt.savefig("d6_500.png")
  plt.show()
682
683
684
  685
  data6 500
686
  688
  # ### Surface plots for various values of lambda:
689
690
 691
692 for l in lambda list:
     plot_approxY(6, w_6_500,y6_train500,y6_trainpred500[1],500,1,...
693
        x16_train500,x26_train500)
694
  695
696 # # Conclusion:
697
  # The model with best RMSE values over all three datasets: train, cross-...
698
     validation and test is with degree of complexity 6, train data size = ...
     500 and regularization parameter lambda = 0
699
701 plt.figure()
702 plt.scatter(y6_train500,y6_trainpred500[0],label="predicted y")
703 plt.legend()
704 plt.xlabel("Actual y")
705 plt.ylabel("Predicted y")
706 plt.title("Predicted output vs actual output for train data set")
707 plt.savefig("predgoodtrain.png")
708 plt.show()
709
710
712 plt.figure()
plt.scatter(y6_cv500,y6_cvpred500[0],label="predicted y")
714 plt.legend()
715 plt.xlabel("Actual y")
716 plt.ylabel("Predicted y")
717 plt.title("Predicted output vs actual output for cross-validation data set"...
718 plt.savefig("predcv.png")
719 plt.show()
720
721
723 plt.figure()
724 plt.scatter(y6_test500,y6_testpred500[0],label="predicted y")
725 plt.legend()
726 plt.xlabel("Actual y")
727 plt.ylabel("Predicted y")
728 plt.title("Predicted output vs actual output for test data set")
  plt.savefig("predtest.png")
  plt.show()
730
731
732
```

```
734 ### rmse train:
735 rmse6_train500[0]
736
737
739 ### rmse cross validation:
740 rmse6_cv500[0]
741
742
744 ### rmse test data:
745 rmse6_test500[0]
746
747
749 plt.figure()
750 plt.scatter(x16_train500,y6_train500)
752
754 plt.figure()
755 plt.scatter(x26_train500,y6_train500)
756
757
759 plt.figure()
760 plt.scatter(y6_trainpred500[0]-y6_train500)
761
762
```

3 Task 3

3.1 No Regularization, L2 Regularization

The code for Question 3, No Regularization and L2 Regularization is as follows:

```
2 # ## CS5691 PRML Assignment 1
3 # **Team 1**
4 # **Team Members:**
5 # N Sowmya Manojna
               BE17B007
6 # Thakkar Riya Anandbhai PH17B010
7 # Chaithanya Krishna Moorthy PH17B011
10 # Install required Packages
11 # Uncomment if you are running for the first time
12 # !pip install -r requirements.txt
13 # try:
     !mkdir images/q3
14 #
15 # except:
16
     pass
19 import os
20 import missingno
21 import numpy as np
```

```
22 import pandas as pd
23 import seaborn as sns
24 import matplotlib.pyplot as plt
25 from preprocess import PreProcess
26 from gaussianbasis import GaussianBasis
27 from sklearn.cluster import KMeans
28 from mpl_toolkits.mplot3d import Axes3D
29 from statsmodels.stats.outliers_influence import variance_inflation_factor
32 print("Reading Dataset... ", end="")
33 df = pd.read_csv("../datasets/1_bias_clean.csv")
34 print("Done!")
36 print("Starting Preprocessing... ")
37 preprocess = PreProcess()
38 preprocess.clean(df, verbose=True)
39 print("="*60)
40 print("="*60)
41 print("Preprocessing Done!!")
43 df_save = pd.read_csv("../datasets/processed.csv", index_col=0)
44 df_new = df_save.copy()
45 df_new = df_new.drop(["Next_Tmax", "Next_Tmin"], axis=1)
47 num_clusters = [1]
48 num_clusters.extend(range(2,10))
49 num_clusters.extend(range(15, 31, 5))
50 num_clusters.extend(range(40, 101, 10))
52 print("Starting Regularization... ", end="")
53 lmbda_list = [0, 0.5, 1, 2, 10, 50, 100]
54 regressor = GaussianBasis()
55 output = regressor.fit_grid(df_new, df_save, num_clusters, regularization="...
      L2", lmbda_list=lmbda_list, verbose=True, show=False)
56 df_result, sse_dict, num_clusters = output
59 df_result["Sum Error"] = df_result["Error 1"] + df_result["Error 2"]
60 df_result.sort_values(by=["Sum Error"], inplace=True)
61 print(df_result)
62
63 sse_list = [sse_dict[i] for i in sse_dict]
64 plt.figure(figsize=[12,8])
65 plt.plot(num_clusters,sse_list )
66 plt.xlabel("Number of Clusters")
67 plt.ylabel("SSE")
68 plt.title("Knee Plot for determining the number of clusters")
69 plt.grid()
70 plt.show()
72 plt.figure(figsize=[12,8])
73 plt.plot(num_clusters[:5], sse_list[:5])
74 plt.xlabel("Number of Clusters")
75 plt.ylabel("SSE")
76 plt.title("Knee Plot for determining the number of clusters")
77 plt.grid()
78 plt.show()
```

3.1.1 Pre-Processing

The helper class used to perform PreProcessing is as follows:

```
1 import missingno
2 import numpy as np
_{\rm 3} import pandas as pd
4 import seaborn as sns
5 import matplotlib.pyplot as plt
6 from mpl_toolkits.mplot3d import Axes3D
7 from sklearn.cluster import KMeans
8 from statsmodels.stats.outliers_influence import variance_inflation_factor
  10
11 class PreProcess():
      def __init__(self):
12
13
          pass
14
      def clean(self, df, verbose=False):
15
          if verbose==True:
16
              print("="*60)
17
18
          if verbose==True:
              print("Sample of Dataset")
19
          if verbose==True:
20
              print(df.head())
22
          if verbose==True:
23
              print("="*60)
          if verbose==True:
               print("Information of Dataset")
26
          df.info()
27
28
          if verbose==True:
              print("="*60)
30
          if verbose==True:
31
              print("'Nan'
                             Distribution:")
          if verbose==True:
33
              print(df.isnull().sum())
34
35
          if verbose==True:
              print("="*60)
          if verbose==True:
38
              print("Description of the dataset:")
39
          if verbose==True:
               print(df.describe())
41
42
          plt.figure()
43
          missingno.matrix(df)
          plt.title("Missing Values Visualization")
45
          plt.show()
46
47
          if verbose==True:
48
               print("Removing the Rows with NaNs")
49
          df_clean = df.dropna(axis=0)
50
          plt.figure()
          missingno.matrix(df_clean)
          plt.title("Missing Values Visualization - After NaN removal")
54
          df = df_clean
55
56
          desc = df.describe()
          sum(desc.loc["std"] == 0)
57
```

```
58
            # sns.pairplot(df)
60
           plt.figure(figsize=[15,15])
61
            sns.heatmap(df.corr().round(2), linewidths=.5, annot=True)
           plt.title("Heatmap of the data")
           plt.show()
65
           if verbose==True:
66
                print("="*60)
            if verbose==True:
68
                print("Identifying highly correlated features... ")
69
           # Use the upper triangle to mask the correlation matrix
70
           df_new = df.copy()
           df_new = df_new.drop(["Next_Tmin", "Next_Tmax"], axis=1)
72
           upper_triangle = np.triu(np.ones(df_new.corr().shape)).astype(bool)
73
74
75
            # Get the correlation pairs
           correlation_pairs = df_new.corr().mask(upper_triangle).abs()....
76
               unstack().sort_values(ascending=False)
            correlation_pairs = pd.DataFrame(correlation_pairs)
            if verbose==True:
78
                print("Correlation between Features")
79
            if verbose==True:
80
                print(correlation_pairs.head(25))
            if verbose==True:
                print("="*50)
83
84
           # if verbose==True:
               print the highly correlated features
           highly_correlated = correlation_pairs[correlation_pairs[0]>0.75]
87
           if verbose==True:
88
                print("Highly Correlated Features")
            if verbose==True:
90
                print(highly_correlated)
91
92
            if verbose==True:
                print("="*50)
           # Remove each of the highly correlated features and check
95
           highly_correlated.reset_index(inplace=True)
           hc_features = highly_correlated["level_0"]
98
           df_new.head()
99
            if verbose==True:
100
                print("Done!")
102
           # Remove highly correlated features
103
           for feature in hc_features:
104
                if verbose==True:
105
                    print("Removing:", feature, "...")
106
                df_new = df_new.drop([feature], axis=1)
107
                upper_triangle = np.triu(np.ones(df_new.corr().shape)).astype(...
                c = df_new.corr().mask(upper_triangle).abs().unstack()....
109
                    sort_values(ascending=False)
                c = pd.DataFrame(c)
110
                if verbose==True:
111
                    print(c[c[0]>0.75])
112
                if verbose==True:
113
114
                    print("="*50, "\n")
```

```
if c[c[0]>0.75].size == 0:
115
116
                     if verbose==True:
                         print("The number of highly correlated fetaures has ...
117
                             become zero!")
                     if verbose==True:
118
                         print("Preventing all further removals :)")
119
120
                     break
121
            df_new.head()
122
123
            if verbose==True:
124
                print("="*60)
125
            if verbose==True:
126
                print("Checking for Variance Inflation Factor... ")
127
128
            # Variance Inflation Factor - directly correlated
            X_df = df_new.copy()
129
130
            vif = pd.DataFrame()
            vif["Features"] = X_df.columns
132
            vif["VIF Factor"]=[variance_inflation_factor(X_df.values, i) for i ...
133
                in range(X_df.shape[1])]
            vif.sort_values(by=["VIF Factor"], ascending=False, inplace=True)
134
135
            max_col = vif[vif["VIF Factor"]>1000]
136
            for feature in max_col["Features"]:
137
138
                max_col = vif[vif["VIF Factor"]>1000]
                if verbose==True:
139
                     print("Features with high VIF:")
140
                if verbose==True:
141
                     print(max col)
142
                if verbose==True:
143
                     print("Dropping", feature, "...")
144
                X_df.drop([feature], axis=1, inplace=True)
145
146
                vif = pd.DataFrame()
147
                vif["Features"] = X_df.columns
148
                vif["VIF Factor"]=[variance_inflation_factor(X_df.values, i) ...
149
                    for i in range(X_df.shape[1])]
                vif.sort_values(by=["VIF Factor"], ascending=False, inplace=...
150
                    True)
151
                if vif[vif["VIF Factor"]>1000].size==0:
152
                     if verbose==True:
153
                         print("The number of fetaures that have high VIF has ...
154
                             become zero!")
                     if verbose==True:
155
                         print("Preventing all further removals :)")
156
157
                     break
            if verbose==True:
158
                print("Done!")
159
160
            df new = X df
161
            df new.head()
162
163
            df_save = df_new.copy()
164
            df_save["Next_Tmin"] = df["Next_Tmin"]
165
            df_save["Next_Tmax"] = df["Next_Tmax"]
166
            df_save.to_csv("../datasets/processed.csv")
167
            # df_save.to_csv("processed.csv")
168
169
            if verbose==True:
```

```
print("Saved the data as processed.csv")
return 1
```

3.1.2 Gaussian Basis

The helper class used to perform GaussianBasis are as follows:

```
1 import os
2 import missingno
3 import numpy as np
4 import pandas as pd
5 import seaborn as sns
6 from tqdm import tqdm
7 import matplotlib.pyplot as plt
8 from preprocess import PreProcess
9 from sklearn.cluster import KMeans
10 from mpl_toolkits.mplot3d import Axes3D
  from statsmodels.stats.outliers_influence import variance_inflation_factor
12 from sklearn.cluster import KMeans
13
  class GaussianBasis():
14
       def __init__(self):
15
           pass
16
17
       def fit_grid(self, df_new, df_save, num_clusters, regularization=None, ...
18
          lmbda_list=[0], verbose=False, show=False):
           n_clu_hist = []
19
           lmbda_hist = []
20
           error1_hist = []
21
           error2_hist = []
           sse_dict = {}
23
24
           if regularization == None or regularization=="L2":
               print("Running K-Means...", end="")
26
               for n_clu in tqdm(num_clusters):
27
                   kmeans = KMeans(n_clusters=n_clu, random_state=42).fit(...
28
                       df_new.to_numpy())
                   sse_dict[n_clu] = kmeans.inertia_
29
30
                   mean_centers = kmeans.cluster_centers_
31
                   corresponding_center = mean_centers[kmeans.labels_,:]
33
                   X = df_new.to_numpy()
34
                   distance = np.linalg.norm(X-corresponding_center, axis=1)
35
                   var = np.var(distance)*distance.size
                   phi = np.ones((X.shape[0], 1))
38
                   for i in range(n_clu):
39
                        phi = np.append(phi, np.exp(-np.linalg.norm(X-...
40
                           mean_centers[i,:], axis=1)**2/var).reshape(-1,1), ...
                           axis=1)
                   for lmbda in lmbda_list:
                        n_clu_hist.append(n_clu)
43
                        lmbda_hist.append(lmbda)
44
45
                        W1 = (np.linalg.inv(phi.T @ phi + lmbda*np.identity(phi..
46
                           .shape[1])) @ phi.T) @ df_save["Next_Tmin"]
```

```
W2 = (np.linalg.inv(phi.T @ phi + lmbda*np.identity(phi...
47
                            .shape[1])) @ phi.T) @ df_save["Next_Tmax"]
                        W1 = W1.reshape(-1,1)
48
                        W1 = W2.reshape(-1,1)
49
                        pred1 = phi @ W1
50
                        pred2 = phi @ W2
52
                        plt.figure(figsize=[16,9])
53
                        plt.title("Clusters: "+str(n_clu))
54
                        plt.subplot(1, 2, 1)
                        plt.hist(pred1, alpha=0.5)
56
                        plt.hist(df_save["Next_Tmin"], alpha=0.5)
57
                        plt.title("Next_Tmin; Clusters: "+str(n_clu))
58
                        plt.grid()
                        plt.subplot(1, 2, 2)
60
                        plt.plot(df_save["Next_Tmin"], pred1, ".")
61
                        plt.plot(df_save["Next_Tmin"], df_save["Next_Tmin"], '....
62
                        plt.title("Next_Tmin; Clusters: "+str(n_clu))
63
                        plt.grid()
64
                        if show:
                             plt.show()
66
                        \label{eq:fname} \texttt{fname} \ = \ \texttt{"fit\_1\_k\_"+str(n\_clu)+"\_lmbda\_"+str(lmbda)+"} \dots
67
                        plt.savefig("images/q3/"+fname)
68
69
                        plt.figure(figsize=[16,9])
70
                        plt.title("Clusters: "+str(n_clu))
71
                        plt.subplot(1, 2, 1)
72
                        plt.hist(pred2, alpha=0.5, label="Predicted")
73
                        plt.hist(df_save["Next_Tmax"], alpha=0.5, label="True")
74
                        plt.title("Next_Tmax; Clusters: "+str(n_clu))
75
76
                        plt.grid()
                        plt.subplot(1, 2, 2)
77
                        plt.plot(df_save["Next_Tmax"], pred2, ".")
78
                        plt.plot(df_save["Next_Tmax"], df_save["Next_Tmax"], '....
79
                             ')
                        plt.title("Clusters: "+str(n_clu))
80
                        plt.grid()
81
                        if show:
82
                             plt.show()
83
                        fname = "fit_2_k_"+str(num_clusters)+"_lmbda_"+str(...
84
                            lmbda) + ".png"
                        plt.savefig("images/q3/"+fname)
                        error1 = np.linalg.norm(df_save["Next_Tmin"].to_numpy()...
87
                             .reshape(-1,1)-pred1)
                        error2 = np.linalg.norm(df_save["Next_Tmin"].to_numpy()...
88
                            .reshape(-1,1)-pred2)
89
                        error1_hist.append(error1)
90
                         error2_hist.append(error2)
                    print("Done!")
92
93
           df_result = pd.DataFrame()
94
           df_result["Cluster"] = n_clu_hist
           df_result["Lambda"] = lmbda_hist
96
           df_result["Error 1"] = error1_hist
97
           df_result["Error 2"] = error2_hist
98
           df_result.to_csv("../datasets/q3_gridsearch.csv")
```

```
100
101 return df_result, sse_dict
```

3.2 Tikhonov Regularization

The code for Question 3, Tikhonov Regularization is as follows:

```
2 from IPython import get_ipython
3 import numpy as np
4 import pandas as pd
5 import matplotlib.pyplot as plt
6 from mpl_toolkits.mplot3d import Axes3D
7 from sklearn.cluster import KMeans
8 import seaborn as sns
 get_ipython().run_line_magic('matplotlib', 'inline')
10
dataset2 = pd.read_csv('function1_2d.csv',index_col = 0)
14
dataset2['v']
17
18
21 num_clusters = [1]
22 num_clusters.extend(range(2,100,10))
  #num_clusters.extend(range(15, 31, 5))
24 #num_clusters.extend(range(40, 101, 10))
25
26 sse_list = []
27 label_list = []
28 cluster_centers_list = []
 error_list = []
  for n_clu in num_clusters:
32
     kmeans = KMeans(n_clusters=n_clu, random_state=42).fit(dataset2....
        to_numpy())
     sse_list.append(kmeans.inertia_)
33
     label list.append(kmeans.labels )
     cluster_centers_list.append(kmeans.cluster_centers_)
35
36
     mean_centers = cluster_centers_list[-1]
37
   # print("Mean shape:", mean_centers.shape)
38
     corresponding_center = mean_centers[label_list[-1],:]
39
40
     X = dataset2.to_numpy()
     distance = np.linalg.norm(X-corresponding_center, axis=1)
42
     var = np.var(distance)*distance.size
43
44
     phi = np.ones((X.shape[0], 1))
45
     for i in range(n_clu):
46
        A = X-mean_centers[i,:]
47
     # print("A shape:", A.shape)
        A = np.exp(-np.linalg.norm(X-mean_centers[i,:], axis=1)**2/var)
     # print("A shape:", A.shape)
50
```

```
phi = np.append(phi, np.exp(-np.linalg.norm(X-mean_centers[i,:], ...
51
             axis=1)**2/var).reshape(-1,1), axis=1)
52
      lmbda = 0
53
      W1 = (np.linalg.inv(phi.T @ phi + lmbda*np.identity(phi.shape[1])) @ ...
54
         phi.T) @ dataset2["y"]
      W1 = W1.reshape(-1,1)
55
      pred = phi @ W1
56
57
      plt.figure(figsize=[12,8])
      plt.title("Clusters: "+str(n clu))
59
      plt.subplot(1, 2, 1)
60
      plt.hist(pred, alpha=0.5)
      plt.hist(dataset2["y"], alpha=0.5)
      plt.title("Clusters: "+str(n_clu))
63
      plt.grid()
64
      plt.subplot(1, 2, 2)
65
      plt.plot(dataset2["y"], pred, ".")
66
      plt.plot(dataset2["y"], dataset2["y"], '.')
67
      plt.title("Clusters: "+str(n_clu))
68
      plt.grid()
      plt.savefig('')
70
      plt.show()
71
      error = np.linalg.norm(dataset2["y"].to_numpy().reshape(-1,1)-pred)
72
      error_list.append(error)
75
77 plt.figure(figsize=[12,8])
78 plt.subplot(1,2,1)
79 plt.plot(num_clusters, sse_list)
80 plt.xlabel("Number of Clusters")
81 plt.ylabel("SSE")
82 plt.title("Knee Plot for determining the number of clusters")
83 plt.grid()
84 plt.subplot(1,2,2)
85 plt.plot(num_clusters, error_list)
86 plt.xlabel("Number of Clusters")
87 plt.ylabel("SSE")
88 plt.title(("L2 Error for fit"))
89 plt.grid()
90 plt.show()
91
94 error_list = np.array(error_list)
95 df_error = pd.DataFrame({"Clusters":num_clusters, "Error":error_list})
96 df_error.sort_values(by=["Error"], ascending=True, inplace=True)
  df_error
98
99
  def create datasets(data,train size,cv size):
101
      data.sample(frac=1).reset_index(drop=True)
102
      data_train=data[0:train_size]
103
      data_cv=data[train_size:train_size+cv_size]
104
      data_test=data[cv_size+train_size:]
105
      return(data_train,data_cv,data_test)
106
107
```

```
109
  lambda_list = [0.01, 0.1, 1, 5, 10, 50, 100]
111
  trDS2, cvDS2, tDS2 = create_datasets(dataset2,1400,400)
113
114
  115
  def f(ds,1,n clu):
116
      sse_list = []
117
      label_list = []
118
      cluster centers list = []
119
120
      kmeans = KMeans(n_clusters=n_clu, random_state=42).fit(ds.to_numpy())
121
      sse_list.append(kmeans.inertia_)
122
123
      label_list.append(kmeans.labels_)
      cluster_centers_list.append(kmeans.cluster_centers_)
124
125
126
      mean_centers = cluster_centers_list[-1]
    # print("Mean shape:", mean_centers.shape)
127
      corresponding_center = mean_centers[label_list[-1],:]
128
129
      X = ds.to_numpy()
130
      distance = np.linalg.norm(X-corresponding_center, axis=1)
131
      var = np.var(distance)*distance.size
132
133
134
      phi = np.ones((X.shape[0], 1))
      for i in range(n_clu):
135
         A = X-mean_centers[i,:]
136
      # print("A shape:", A.shape)
137
         A = np.exp(-np.linalg.norm(X-mean_centers[i,:], axis=1)**2/var)
138
      # print("A shape:", A.shape)
139
         phi = np.append(phi, np.exp(-np.linalg.norm(X-mean_centers[i,:], ...
140
            axis=1)**2/var).reshape(-1,1), axis=1)
      #lmbda =
141
      return(phi,mean_centers,var)
142
143
  W1 = (np.linalg.inv(phi.T @ phi + 1*np.identity(phi.shape[1])) @ phi....
145
     T) @ dataset2["y"]
        W1 = W1.reshape(-1,1)
146
        pred = phi @ W1
147
148
  #
        return(W1,)
        error = np.linalg.norm(dataset2["y"].to_numpy().reshape(-1,1)-pred)
149
        error_list.append(error)
150
151
  152
  optClds2 = 10
153
154
155
157 error tr = []
  error cv = []
158
  error_t = []
  for l in range(len(lambda_list)):
160
      phi_tr = f(trDS2,1,optClds2)[0]
      phi_cv = f(cvDS2,1,optClds2)[0]
162
      phi_t = f(tDS2,1,optClds2)[0]
163
      w = (np.linalg.inv(phi_tr.T @ phi_tr + l*np.identity(phi_tr.shape[1]))
164
         @ phi_tr.T) @ trDS2["y"]
```

```
pred_cv = phi_cv @ w
165
     pred_t = phi_t @ w
     pred_tr = phi_tr @ w
167
     error_cv.append(np.linalg.norm(cvDS2["y"].to_numpy().reshape(-1,1)-...
168
       pred_cv))
     error_t.append(np.linalg.norm(tDS2["y"].to_numpy().reshape(-1,1)-pred_t...
169
     error_tr.append(np.linalg.norm(trDS2["y"].to_numpy().reshape(-1,1)-...
170
       pred tr))
171
172
pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
    Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
175
176
  177
178
  plt.plot(lambda_list,error_cv)
179
180
phi_tr = f(trDS2,1,optClds2)[0]
phi_t = f(tDS2,1,optClds2)[0]
  w = (np.linalg.inv(phi_tr.T @ phi_tr + 0.01*np.identity(phi_tr.shape[1])) @...
     phi_tr.T) @ trDS2["y"]
  pred_t = phi_t @ w
 pred_tr = phi_tr @ w
186
187
188
190 plt.scatter(trDS2.iloc[:,2],pred_tr)
191 plt.xlabel("Target output, training data")
192 plt.ylabel("Model output")
193 plt.title("Scatter plot of target vs model output for linear regression in ...
    gaussian basis and quadratic regularization")
  plt.savefig("scatter_ds2quad.png")
  plt.show()
196
197
  198
  plt.scatter(cvDS2.iloc[:,2],pred_cv)
200
201
203 plt.scatter(tDS2.iloc[:,2],pred_t)
204 plt.xlabel("Target output, test data")
205 plt.ylabel("Model output")
206 plt.title("Scatter plot of target vs model output for linear regression in ...
    gaussian basis and quadratic regularization")
  plt.savefig("scatter_ds2quadtest.png")
207
  plt.show()
208
209
210
212
213
214
 215
  def tikhanov_reg(phi,mu,sigma,l):
216
217
     K = len(mu)
```

```
phiT = np.zeros((K+1,K+1))
218
      phiT[0,0] = 1
219
      for i in range(1,K+1):
220
         for j in range(1,K+1):
221
             phiT[i,j] = np.exp(-(np.linalg.norm(mu[i-1]-mu[j-1])**2)/sigma...
222
      #1 = 300
223
224
      #print(phiT.shape)
      pinv = np.linalg.inv(phi.T @ phi+l*phiT) @ phi.T
225
      return(pinv)
226
227
228
  229
  lambda_list = [0,0.01,0.1,1,5]#,10,50,100]
230
231
232
234 error_tr = []
235 error_cv = []
236 error_t = []
237 for l in range(len(lambda_list)):
  #for 1 in [1]:
238
      phi_tr,mu_list,sig = f(trDS2,1,optClds2)
239
      phi_cv = f(cvDS2,1,optClds2)[0]
240
241
      phi_t = f(tDS2,1,optClds2)[0]
242
      #print(phi_tr.shape)
      #print(mu_list.shape)
243
      tikh = tikhanov_reg(phi_tr,mu_list,sig,l)
244
      #print("tikh shape ", tikh.shape)
245
      #print("phi_tr shape ", phi_tr.shape)
246
      #print("trDS2_y shape ", trDS2["y"].shape)
247
248
      w = tikh @ trDS2["v"]
      pred_cv = phi_cv @ w
250
      pred_t = phi_t @ w
251
252
      pred_tr = phi_tr @ w
      error_cv.append(np.linalg.norm(cvDS2["y"].to_numpy().reshape(-1,1)-...
253
      error_t.append(np.linalg.norm(tDS2["y"].to_numpy().reshape(-1,1)-pred_t...
254
      error_tr.append(np.linalg.norm(trDS2["y"].to_numpy().reshape(-1,1)-...
255
         pred_tr))
256
257
  pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
259
     Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
260
261
263 plt.plot(lambda_list,error_cv)
264 plt.title('Erms on cross-validation data vs regularization factor')
265 plt.xlabel('lambda')
266 plt.ylabel('rmse error')
267
  269
270 plt.hist(pred_tr, alpha=0.5)
  plt.hist(trDS2["y"], alpha=0.5)
271
272
```

```
273
275 error_list = np.array(error_list)
276 df_error = pd.DataFrame({"lambda":lambda_list, "Error":error_cv})
277 df_error.sort_values(by=["Error"], ascending=True, inplace=True)
278 df_error
279
280
282 \quad 1 = 0.01
283 phi tr = f(trDS2,1,optClds2)[0]
284 phi_t = f(tDS2,1,optClds2)[0]
tikh = tikhanov_reg(phi_tr,mu_list,sig,0.01)
w = tikh @ trDS2["y"]
w = (np.linalg.inv(phi_tr.T @ phi_tr + 0.1*np.identity(phi_tr.shape[1])) @ ...
    phi_tr.T) @ trDS2["y"]
288 pred_t = phi_t @ w
 pred_tr = phi_tr @ w
290
291
293 plt.scatter(trDS2.iloc[:,2],pred_tr)
294 plt.xlabel("Target output, training data")
295 plt.ylabel("Model output")
 plt.title("Scatter plot of target vs model output for linear regression in ...
    gaussian basis and Tikhonov regularization")
297 plt.savefig("scatter_ds2tikhtr.png")
298 plt.show()
299
300
302 plt.scatter(tDS2.iloc[:,2],pred_t)
303 plt.xlabel("Target output, test data")
304 plt.ylabel("Model output")
305 plt.title("Scatter plot of target vs model output for linear regression in ...
    gaussian basis and Tikhonov regularization")
306 plt.savefig("scatter_ds2tikhtest.png")
307 plt.show()
308
309
 311
312
313
315 df_new = pd.read_csv("processed_biasclean.csv",index_col = 0)
316
317
319 df new.head()
320
321
trDS3, cvDS3, tDS3 = create datasets(df new,1400,400)
324
325
327 num_clusters = [1]
num_clusters.extend(range(2,10))
329 num_clusters.extend(range(15, 31, 5))
```

```
330 num_clusters.extend(range(40, 101, 10))
331
332 sse_list = []
333 label_list = []
334 cluster_centers_list = []
   error_list = []
335
336
   for n_clu in num_clusters:
337
       kmeans = KMeans(n_clusters=n_clu, random_state=42).fit(df_new.to_numpy...
338
       sse list.append(kmeans.inertia )
339
       label_list.append(kmeans.labels_)
340
       cluster_centers_list.append(kmeans.cluster_centers_)
341
342
343
       mean_centers = cluster_centers_list[-1]
     # print("Mean shape:", mean_centers.shape)
344
       corresponding_center = mean_centers[label_list[-1],:]
345
346
       X = df_new.to_numpy()
347
       distance = np.linalg.norm(X-corresponding_center, axis=1)
348
       var = np.var(distance)*distance.size
349
350
       phi = np.ones((X.shape[0], 1))
351
       for i in range(n_clu):
352
           A = X-mean_centers[i,:]
354
       # print("A shape:", A.shape)
           A = np.exp(-np.linalg.norm(X-mean_centers[i,:], axis=1)**2/var)
355
       # print("A shape:", A.shape)
356
           phi = np.append(phi, np.exp(-np.linalg.norm(X-mean_centers[i,:], ...
357
               axis=1)**2/var).reshape(-1,1), axis=1)
358
       lmbda = 0
359
360
       W1 = (np.linalg.inv(phi.T @ phi + lmbda*np.identity(phi.shape[1])) @ ...
          phi.T) @ df_new["Next_Tmin"]
       W1 = W1.reshape(-1,1)
361
       pred = phi @ W1
362
363
       plt.figure(figsize=[12,8])
364
       plt.title("Clusters: "+str(n_clu))
365
       plt.subplot(1, 2, 1)
366
       plt.hist(pred, alpha=0.5)
367
       plt.hist(df_new["Next_Tmin"], alpha=0.5)
368
       plt.title("Clusters: "+str(n_clu))
369
       plt.grid()
370
       plt.subplot(1, 2, 2)
371
       plt.plot(df_new["Next_Tmin"], pred, ".")
372
       plt.plot(df_new["Next_Tmin"], df_new["Next_Tmin"], '.')
373
       plt.title("Clusters: "+str(n_clu))
374
       plt.grid()
375
       plt.show()
376
       error = np.linalg.norm(df_new["Next_Tmin"].to_numpy().reshape(-1,1)-...
377
           pred)
378
       error_list.append(error)
379
380
   382 plt.figure(figsize=[12,8])
383 plt.subplot(1,2,1)
384 plt.plot(num_clusters, sse_list)
385 plt.xlabel("Number of Clusters")
```

```
386 plt.ylabel("SSE")
387 plt.title("Knee Plot for determining the number of clusters")
388 plt.grid()
389 plt.subplot(1,2,2)
390 plt.plot(num_clusters, error_list)
391 plt.xlabel("Number of Clusters")
392 plt.ylabel("SSE")
393 plt.title(("L2 Error for fit"))
394 plt.grid()
  plt.show()
396
397
399 error_list = np.array(error_list)
400 df_error = pd.DataFrame({"Clusters":num_clusters, "Error":error_list})
401 df_error.sort_values(by=["Error"], ascending=True, inplace=True)
402 df_error
403
404
  405
  optClds3 = 9
407
408
  409
  lambda_list = [0.01, 0.1, 1, 5, 10]
410
411
412
414 error tr = []
415 error cv = []
416 error t = []
417 for l in range(len(lambda_list)):
418
     phi_tr = f(trDS3,1,optClds3)[0]
     phi_cv = f(cvDS3,1,optClds3)[0]
419
     phi_t = f(tDS3,1,optClds3)[0]
420
     w = (np.linalg.inv(phi_tr.T @ phi_tr + 1*np.identity(phi_tr.shape[1])) ...
421
        @ phi_tr.T) @ trDS3['Next_Tmin']
     pred_cv = phi_cv @ w
422
     pred_t = phi_t @ w
423
     pred_tr = phi_tr @ w
424
     error_cv.append(np.linalg.norm(cvDS3['Next_Tmin'].to_numpy().reshape...
425
        (-1,1)-pred_cv))
     error_t.append(np.linalg.norm(tDS3['Next_Tmin'].to_numpy().reshape...
426
        (-1,1)-pred_t)
     error_tr.append(np.linalg.norm(trDS3['Next_Tmin'].to_numpy().reshape...
        (-1,1)-pred_tr))
428
  430
  pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
     Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
432
433
435 plt.plot(lambda_list,error_cv)
436 plt.title('Error on cross-validation data vs regularization factor, ...
     Quadratic regularization')
437 plt.xlabel('lambda')
  plt.ylabel('rmse error')
```

```
440
442 error_list = np.array(error_list)
443 df_error = pd.DataFrame({"lambda":lambda_list, "Error":error_cv})
444 df_error.sort_values(by=["Error"], ascending=True, inplace=True)
446
447
450 phi_tr = f(trDS3,1,optClds3)[0]
451 phi_t = f(tDS3,1,optClds3)[0]
452 w = (np.linalg.inv(phi_tr.T @ phi_tr + l*np.identity(phi_tr.shape[1])) @ ...
     phi_tr.T) @ trDS3['Next_Tmin']
453 pred_t = phi_t @ w
454 pred_tr = phi_tr @ w
455
  457
458 plt.scatter(trDS3.iloc[:,17],pred_tr)
459 plt.xlabel("Target output, train data")
460 plt.ylabel("Model output")
461 plt.title("Scatter plot of target vs model with quadratic regularization, ...
     for Next_Tmin")
  plt.savefig("scatter_ds3quadtrainT_min.png")
  plt.show()
464
465
467 plt.scatter(tDS3.iloc[:,17],pred t)
468 plt.xlabel("Target output, test data")
469 plt.ylabel("Model output")
  plt.title("Scatter plot of target vs model output with quadratic ...
     regularization, for Next_Tmin")
471 plt.savefig("scatter_ds3quadtestT_min.png")
472 plt.show()
473
474
476 error_tr = []
  error_cv = []
477
  error_t = []
478
  for l in range(len(lambda_list)):
479
     phi_tr = f(trDS3,1,optClds3)[0]
480
     phi_cv = f(cvDS3,1,optClds3)[0]
481
     phi_t = f(tDS3,1,optClds3)[0]
482
     w = (np.linalg.inv(phi_tr.T @ phi_tr + 1*np.identity(phi_tr.shape[1])) ...
483
        @ phi_tr.T) @ trDS3['Next_Tmax']
     pred_cv = phi_cv @ w
484
     pred_t = phi_t @ w
485
     pred_tr = phi_tr @ w
486
     error_cv.append(np.linalg.norm(cvDS3['Next_Tmax'].to_numpy().reshape...
487
        (-1,1)-pred cv))
     error_t.append(np.linalg.norm(tDS3['Next_Tmax'].to_numpy().reshape...
488
        (-1,1)-pred_t)
     error_tr.append(np.linalg.norm(trDS3['Next_Tmax'].to_numpy().reshape...
489
        (-1,1)-pred_tr))
490
491
```

```
493 pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
     Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
494
495
497 plt.plot(lambda_list,error_cv)
498 plt.title('Error on cross-validation data vs regularization factor, ...
     Quadratic regularization')
499 plt.xlabel('lambda')
  plt.ylabel('rmse error')
501
502
504 error_list = np.array(error_list)
505 df_error = pd.DataFrame({"lambda":lambda_list, "Error":error_cv})
506 df_error.sort_values(by=["Error"], ascending=True, inplace=True)
507 df_error
508
509
511 1 = 1
512 phi_tr = f(trDS3,1,optClds3)[0]
phi_t = f(tDS3,1,optClds3)[0]
514 w = (np.linalg.inv(phi_tr.T @ phi_tr + l*np.identity(phi_tr.shape[1])) @ ...
     phi_tr.T) @ trDS3['Next_Tmax']
515 pred_t = phi_t @ w
516 pred_tr = phi_tr @ w
517
518
520 plt.scatter(trDS3.iloc[:,18],pred_tr)
521 plt.xlabel("Target output, train data")
522 plt.ylabel("Model output")
523 plt.title("Scatter plot of target vs model with quadratic regularization, ...
     for Next_Tmax")
524 plt.savefig("scatter_ds3quadtrainT_max.png")
525 plt.show()
526
527
529 plt.scatter(tDS3.iloc[:,18],pred_t)
530 plt.xlabel("Target output, test data")
531 plt.ylabel("Model output")
532 plt.title("Scatter plot of target vs model with quadratic regularization, ...
     for Next_Tmax")
533 plt.savefig("scatter_ds3quadtestT_max.png")
534 plt.show()
535
536
538 #Tikhonov reg for "Next_Tmin"
539
540 error tr = []
541 error cv = []
542 error_t = []
543 for l in range(len(lambda_list)):
544 #for l in [1]:
     phi_tr,mu_list,sig = f(trDS3,1,optClds3)
545
     phi_cv = f(cvDS2,1,optClds3)[0]
546
547
     phi_t = f(tDS2,1,optClds3)[0]
```

```
#print(phi_tr.shape)
548
      #print(mu_list.shape)
549
      tikh = tikhanov_reg(phi_tr,mu_list,sig,l)
550
      #print("tikh shape ", tikh.shape)
551
      #print("phi_tr shape ", phi_tr.shape)
552
      #print("trDS2_y shape ", trDS2["y"].shape)
553
554
555
      w = tikh @ trDS3['Next Tmin']
      pred_cv = phi_cv @ w
556
      pred_t = phi_t @ w
557
      pred tr = phi tr @ w
558
      error_cv.append(np.linalg.norm(cvDS3['Next_Tmin'].to_numpy().reshape...
559
         (-1,1)-pred_cv))
      error_t.append(np.linalg.norm(tDS3['Next_Tmin'].to_numpy().reshape...
560
        (-1,1)-pred_t)
      error_tr.append(np.linalg.norm(trDS3['Next_Tmin'].to_numpy().reshape...
561
         (-1,1)-pred_tr))
562
563
  564
  pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
     Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
566
567
  569 plt.plot(lambda_list,error_cv)
570 plt.title('Error on cross-validation data vs regularization factor, ...
     tikhonov regularization for Dataset 3')
571 plt.xlabel('lambda')
572 plt.ylabel('rmse error')
573
574
576 plt.hist(pred tr, alpha=0.5)
  plt.hist(trDS3["Next_Tmin"], alpha=0.5)
577
578
579
  580
581 error_list = np.array(error_list)
582 df_error = pd.DataFrame({"lambda":lambda_list, "Error":error_cv})
  df_error.sort_values(by=["Error"], ascending=True, inplace=True)
  df error
584
585
588 1 = .1
589 phi_tr = f(trDS3,1,optClds3)[0]
phi_t = f(tDS3,1,optClds3)[0]
  tikh = tikhanov_reg(phi_tr,mu_list,sig,0.01)
592 w = tikh @ trDS3["Next_Tmin"]
593 w = (np.linalg.inv(phi_tr.T @ phi_tr + 0.1*np.identity(phi_tr.shape[1])) @ ...
     phi tr.T) @ trDS3["Next Tmin"]
594 pred_t = phi_t @ w
595 pred_tr = phi_tr @ w
596
597
599 plt.scatter(trDS3.iloc[:,17],pred_tr)
600 plt.xlabel("Target output, train data")
601 plt.ylabel("Model output")
```

```
602 plt.title("Scatter plot of target vs model with Tikhonov regularization, ...
     for Next_Tmin")
  plt.savefig("scatter_ds3tikhtrainT_min.png")
  plt.show()
605
606
608 plt.scatter(tDS3.iloc[:,17],pred t)
609 plt.xlabel("Target output, test data")
610 plt.ylabel("Model output")
611 plt.title("Scatter plot of target vs model with Tikhonov regularization, ...
     for Next Tmin")
612 plt.savefig("scatter_ds3tikhtrainT_min.png")
613 plt.show()
614
615
617 #Tikhonov reg for "Next_Tmax"
618 error tr = []
619 error_cv = []
620 error_t = []
621 for l in range(len(lambda_list)):
  #for 1 in [1]:
622
      phi_tr,mu_list,sig = f(trDS3,1,optClds3)
623
      phi_cv = f(cvDS2,1,optClds3)[0]
625
      phi_t = f(tDS2,1,optClds3)[0]
      #print(phi_tr.shape)
626
      #print(mu_list.shape)
627
      n = len(trDS3)
628
      tikh = tikhanov_reg(phi_tr,mu_list,sig,l)
629
      #print("tikh shape ", tikh.shape)
630
      #print("phi_tr shape ", phi_tr.shape)
631
      #print("trDS2_y shape ", trDS2["y"].shape)
632
633
      w = tikh @ trDS3['Next_Tmax']
634
635
      pred_cv = phi_cv @ w
      pred_t = phi_t @ w
636
      pred_tr = phi_tr @ w
637
      error_cv.append(np.linalg.norm(cvDS3['Next_Tmax'].to_numpy().reshape...
638
         (-1,1)-pred_cv))
      error_t.append(np.linalg.norm(tDS3['Next_Tmax'].to_numpy().reshape...
639
         (-1,1)-pred_t)
      error_tr.append(np.linalg.norm(trDS3['Next_Tmax'].to_numpy().reshape...
640
         (-1,1)-pred_tr))
641
642
  643
  pd.DataFrame(list(zip(lambda_list,error_tr,error_cv,error_t)),columns=["...
     Lambda", "RMSE Train", "RMSE CV", "RMSE test"])
645
646
648 plt.plot(lambda list,error cv)
649 plt.title('Error on cross-validation data vs regularization factor, ...
     tikhonov regularization for Dataset 3, for T_max')
  plt.xlabel('lambda')
651
  plt.ylabel('rmse error')
652
653
```

```
655 plt.hist(pred_tr, alpha=0.5)
656 plt.hist(trDS3["Next_Tmax"], alpha=0.5)
657
658
660 error_list = np.array(error_list)
661 df_error = pd.DataFrame({"lambda":lambda_list, "Error":error_cv})
662 df error.sort values(by=["Error"], ascending=True, inplace=True)
663 df error
664
665
667 1 = .01
668 phi_tr = f(trDS3,1,optClds3)[0]
669 phi_t = f(tDS3,1,optClds3)[0]
670 tikh = tikhanov_reg(phi_tr,mu_list,sig,0.01)
671 w = tikh @ trDS3["Next_Tmax"]
672 w = (np.linalg.inv(phi_tr.T @ phi_tr + 0.1*np.identity(phi_tr.shape[1])) @ ...
     phi_tr.T) @ trDS3["Next_Tmax"]
673 pred_t = phi_t @ w
674 pred_tr = phi_tr @ w
675
676
678 plt.scatter(trDS3.iloc[:,18],pred_tr)
679 plt.xlabel("Target output, train data")
680 plt.ylabel("Model output")
681 plt.title("Scatter plot of target vs model output with Tikhonov ...
     regularization, for Next_Tmax")
682 plt.savefig("scatter ds3tikhtrainT max.png")
683 plt.show()
684
687 plt.scatter(trDS3.iloc[:,18],pred_tr)
688 plt.xlabel("Target output, test data")
689 plt.ylabel("Model output")
690 plt.title("Scatter plot of target vs model with Tikhonov regularization, ...
     for Next_Tmax")
691 plt.savefig("scatter_ds3tikhtestT_min.png")
  plt.show()
692
693
694
```