Parameterised Quantum Circuits for High-dimensional Data

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1 Introduction

We are in an exciting era where quantum machine learning is on its advancement. The high dimensionality of Bloch sphere exibits quantum supremacy and might deliver solution to problems that are of quantum nature. The variational quantum classifier, takes advantages of both classical machine learning algorithms and quantum algorithms, is one of the hybrid quantum classical algorithms. It consists of quantum circuits which allow variations of parameters, which are otherwise fixed in traditional machine learning algorithms. Based on the quantum circuit, we can build a supervised learning model. Fig. 1 illustrates a supervised learning model using a parametrised quantum circuit (PQC).

PQCs often involve a series of gates, controlled gates such as controlled NOT gates and adjustable gates such as rotation gates. In HQC algorithms, the PQCs work as the interface between the quantum block and the classical block, where the former takes quantum data as inputs, and the latter tunes the parameters coming out of the quantum block. Based on a PQC we can build a supervised learning model.

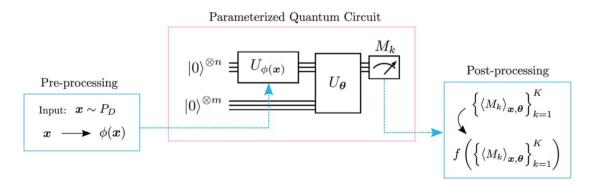


Figure 1: A supervised learning model implementing HQC algorithm. The model consists of three components: the classical pre/post processing blocks and the quantum block with PQC. Adapted from Fig. 2 by Benedetti et al. (2019).

In the pre-processing step, the classical data is embedded into quantum states. One way of doing this is by mapping the vector components of an input data into amplitudes of a quantum state. In addition, pre-processing methods such as standardising or Principal Component Analysis (PCA) also applies. The transformed data will subsequently be fed into the circuit with a sequence of gates, and the outcome will then be used to compute the loss.

2 Methods

2.1 PCA

Principal component analysis (PCA) is a statistical analysis algorithm which essentially transforms the features of observed data, which might be correlated, to a set of linearly uncorrelated variables,

these variables are known as "principal components". The rank of the principal components are determined according to their variances, i.e. the first principal component corresponds to that with the largest variance.

The original dataset consists of 569 entries, each with 30 features. There are two target groups: "0" for benign and "1" for malignant. Fig. 2 shows the distribution of the two target groups.

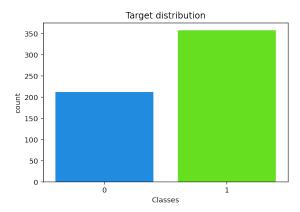


Figure 2: Distribution of the two target groups: "0" stands for benign and "1" for malignant.

There are 30 features in total, which is way beyond the scope of quantum circuits, thus we want to find a way to reduce the dimensionality of feature space. Since some of the features are correlated, and some appear to be self-independent, we want to quantitatively determine the degree of correlation between the features, for this we can take advantage of the correlation matrix, which calculates the correlation between any pair of features. Fig. 3 shows the correlation matrix of the 30 features (together with the target).

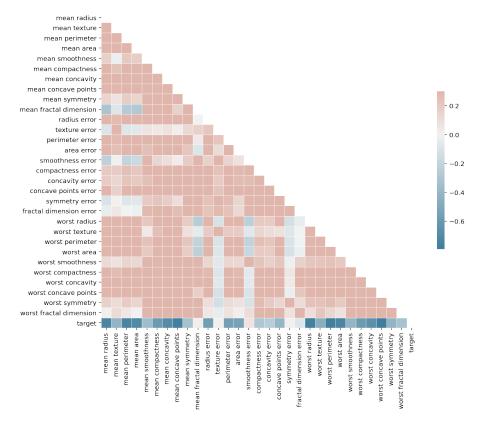


Figure 3: Correlation matrix showing the correlation between the features.

The colour(values) given by the correlation matrix measures the degree of correlation between two features, if it is close to 1, it means the two features are of positive correlation; if it is close to -1, then the two features are of negative correlation; if it is close to 0, then it means the two features are self-independent. The last row of the matrix gives the correlations between a feature and the target. To select features that are useful for successfully separating the two target groups, the following is done:

- In the last row of the correlation matrix, features that are of Pearson's correlation values greater than 0.75 are dropped.
- For the remaining rows, features with any value greater than 0.5 are dropped.

Fig. 4 shows the Pearson's correlation values between features and the target.

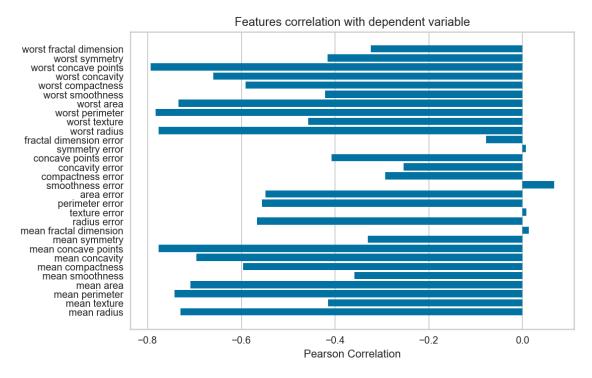


Figure 4: The Pearson correlation values between the features and the targets.

This leaves us 19 features in the end. Fig. 5 shows the distributions of the two target group over the selected feature space.

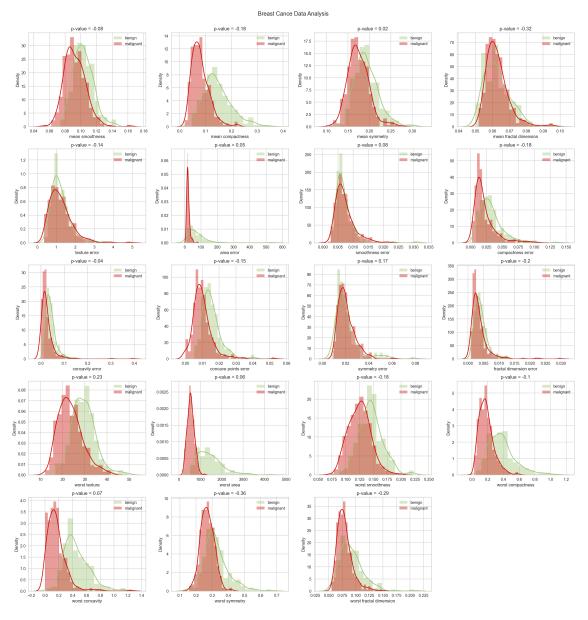


Figure 5: The distributions of the two target groups over different features.

With the selected 19 features, we can finally implement PCA algorithm. This is done by using sklearn.decomposition.PCA. With the parameter n_components specified as the number of qubits to use in the parametrised quantum circuit, we can reduce the dimensionality of the selected features to the number of qubits. Fig. 6 shows the scatter plot of the two target groups on principal component 1 and principal component 2, for the 2-qubit case.

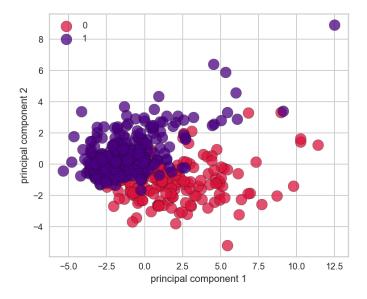


Figure 6: Scatter plot of the two target groups on the principal component space.

Now that the features have been prepared and ready for the quantum circuit, we need to build our quantum circuit to train the data. The quantum circuit consists of two part: a feature map, which maps classical data into quantum states. The other is the variational circuit, whose parameters are used to compute the cost function, and affects the results of training. From my experience of the previous Quantum Algorithms' project, the following feature map and variational circuit are chosen, which can be seen in Fig. 7 and Fig. 8, respectively.

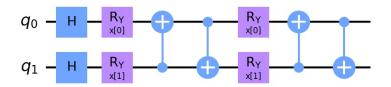


Figure 7: The feature map used in this project. The number of layers is set to be 2.

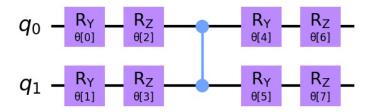


Figure 8: The variational circuit used in this project. The number of layers is set to be 3.

2.2 Cost function

Very much like a classifier, for the PQC we also need to specify a cost function. For this project, since the problem to solver is the classification between "0"s and "1"s, cross-entropy loss

is chosen as the cost function. The cost function is defined as (Zhang & Sabuncu, 2018)

$$H(\mathbf{p}, \mathbf{q}) = -\sum_{i=1}^{N} p_i \log q_i \tag{1}$$

where $\mathbf{p} \in [0,1]^N$ corresponds to the classification targets (labels), $\mathbf{q} \in [0,1]^N$ corresponds to the output predicted by the quantum classifier (predictions). One should notice that, in practice the cost function is normalised by a factor of N^{-1} .

2.3 Cross validation

Lastly, cross validation is implemented, so that we can make sure the model does not overfit. It works as follows. Firstly, the data set with reduced features are split into k folds with equal size, and we loop over the divided folds: the iterated fold will be used for training the network, and the remaining two folds are used only when the training is completed and as test set. We do that for all folds and in the end we have k number of estimations of the accuracy on the test set. Then by taking the average value we have the final estimated accuracy on the test set. Additionally, another validation set can be created in the beginning, and can be used for final validation of the model in the end of k-fold training. For all experiments in this project, 3-fold cross validation is implemented.

3 Results

There are a number of parameters that may influence on the performance of the quantum circuit: number of shots, layers of the feature map, layers of the variational circuit, circuit architecture... In this project, I will focus on the impact of the number of qubits.

3.1 2 qubits

Fig. 9 shows the cost functions for the 3 folds (on the training set), for a 2-qubit parametrised quantum circuit with above described 2-layer feature map and 3-layer variational circuit.

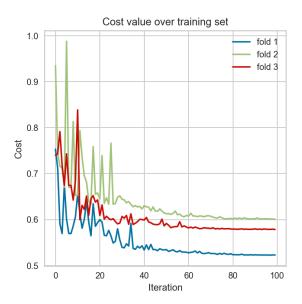


Figure 9: The cost functions for a 2-qubit parametrised quantum circuit, with 3-fold cross validation.

Fig. 9 shows the cost functions for the 3 folds, for a 3-qubit parametrised quantum circuit with above described 2-layer feature map and 3-layer variational circuit.

¹see the qiskit documentation for details.

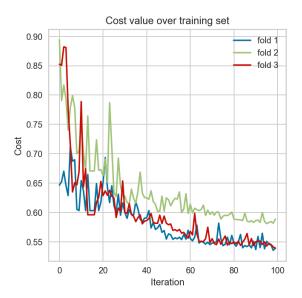


Figure 10: The cost functions for a 3-qubit parametrised quantum circuit, with 3-fold cross validation.

Fig. 9 shows the cost functions for the 3 folds, for a 4-qubit parametrised quantum circuit with above described 2-layer feature map and 3-layer variational circuit.

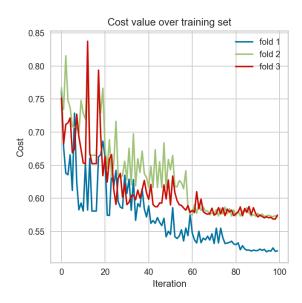


Figure 11: The cost functions for a 4-qubit parametrised quantum circuit, with 3-fold cross validation.

From Fig. 9- 11 it can be seen, for each case, the cost function reached convergence for all 3 folds, and did not escape from the local minimum. Now we can have a look at the accuracies on the test set.

Table 1: Test set accuracy for the 3 experiments.

Experiments	Fold 1	Fold 2	Fold 3	Avg.
2 qubit	0.60	0.73	0.72	0.68
3 qubit	0.68	0.65	0.69	0.67
4 qubit	0.61	0.63	0.79	0.68

From Table 1 it can be seen, with increasing number of qubits, the average accuracy on the test set over 3 folds does not improve significantly.

4 Conclusion

In this project, I implemented PQC to solve a classification problem with high-dimensional data. The BreastCancer data set initially consists of 569 entries, with 30 features. After feature selection based on their Pearson's correlation values, 19 features were left. These selected features were then standardised and reduced to the number of qubits for the following experiments, using PCA algorithm. It is found, with other parameters of the quantum circuits fixed: number of shots, circuit architecture, number of layers, etc., the accuracy on the test set stays almost invariant, with increasing number of qubits. From the cost functions we can learn that, the fluctuations grow with increasing number of qubits, making it harder and harder for the quantum circuit to be stablised. The fact that accuracy is almost invariant with increasing number of qubits, might be a result of increasing stochasticity. It can be learned that, if our goal is to increase the accuracy on the test set, a more promising solution might be to tune other parameters.

References

Benedetti, M., Lloyd, E., Sack, S., & Fiorentini, M. 2019, Quantum Science and Technology, 4, 043001

Zhang, Z., & Sabuncu, M. R. 2018, arXiv preprint arXiv:1805.07836

Appendix

```
#!/usr/bin/env python
    coding: utf-8
    In /1 :
  get_ipython().run_line_magic('config', "InlineBackend.figure_format = 'retina'")
  import time
  import numpy as np
10
  from sklearn.datasets import load_wine,load_breast_cancer
12
13
  # In[2]:
15
16
17
  data = load_breast_cancer()
18
19
20
  # In[3]:
21
22
23
  data.data.shape
25
26
  # In [4]:
28
29
  print(data['DESCR'])
31
32
  # In [5]:
33
34
  import matplotlib.pyplot as plt
```

```
37 import seaborn as sns
   fig = plt.figure()
38
   sns.countplot(x="target", data=data, palette="gist_rainbow_r")
   plt.xlabel("Classes")
   plt.title("Target distribution")
   plt.show()
43
44
   # In [9]:
46
47
48
   import seaborn as sns
49
   import pandas as pd
   \begin{array}{ll} d = pd.DataFrame(\,data.\,data\,,\,\,columns\!\!=\!\!data.\,feature\_names\,) \\ d\left[\,'target\,'\,\right] = \,data\left[\,'target\,'\,\right] \end{array}
51
52
   d.head()
   # Compute the correlation matrix
54
   corr = d.corr()
55
56
   \# Generate a mask for the upper triangle
57
   mask = np.triu(np.ones_like(corr, dtype=bool))
58
   # Set up the matplotlib figure
60
   f, ax = plt.subplots(figsize = (11, 9))
62
   \# Generate a custom diverging colormap
63
   cmap = sns.diverging_palette(230, 20, as_cmap=True)
64
   # Draw the heatmap with the mask and correct aspect ratio
   sns.heatmap(corr, mask=mask, cmap=cmap, vmax=.3, center=0,
67
                  square=True, linewidths=.5, cbar_kws={"shrink": .5})
68
69
70
   # In[10]:
71
72
73
   from yellowbrick.target import FeatureCorrelation
   from yellowbrick.target.feature_correlation import feature_correlation
76 X = data['data']
77 y = data['target']
   features = np.array(data['feature_names'])
   \#visualizer = Feature Correlation (labels = features)
79
   visualizer = feature_correlation(X, y, labels=features)
80
81
                                      \# Fit the data to the visualizer
82
   \#visualizer.fit(X, y)
   visualizer.show()
83
84
   # In[11]:
86
87
88
89
   # absolute for positive values
   abs_corr = abs(d.corr()["target"])
   \verb|abs_corr| = \verb|np.array| (\verb|np.abs| (\verb|abs_corr|))
92
   # random threshold for features to keep
   relevant_features = abs_corr < 0.75
94
95
96
   # In [13]:
97
98
99
   ind = np.arange(30)[relevant_features[:30]]
100
101
102
   # In[45]:
103
104
105
   \mathbf{def} \ \ \mathbf{select} \ \ 20 \ (\mathbf{x}, \mathbf{tol} = .9) :
106
        to_drop = []
107
        for i in range(x.shape[0]):
108
```

```
for j in range(i):
109
                                          if np.abs(x[i][j])>tol:
110
111
                                                     to_drop.append(j)
                    return np.unique(to_drop)
112
113
114
115
116
        # In [48]:
117
118
119
         col_{-} = select_{-}20 (np.array(corr)[:30,:30])
120
121
        col\_rem = np.delete(np.arange(30), col\_)
        ind = np.intersect1d(ind,col_rem)
        print(len(ind))
123
124
125
        # In [49]:
126
127
128
        from scipy.stats import pearsonr
129
        fig = plt.figure(figsize = (20, 25))
131
        j = 0
132
133
        for num, i in enumerate(ind):
                   ax = plt.subplot(6, 4, j+1)
134
135
                   j += 1
                   ax = sns.distplot(data.data[:,i][data.target==0], color='g', label = 'benign')
ax = sns.distplot(data.data[:,i][data.target==1], color='r', label =
136
137
                    'malignant')
                   p =
138
                   pearsonr\left(\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==0\,]\,[\,:40\,]\,,\\ data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,target\,==1\,]\,[\,:40\,]\,\right)\,\left[\,0\,\right]\,,\\ data\,.\,data\,\left[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i\,\,]\,[\,data\,.\,data\,[\,:\,,\,i
                   ax.set_title('p-value = '+str(round(p,2)))
139
                   ax.set_xlabel(data.feature_names[i])
140
141
                   ax.legend(loc='best')
         fig.suptitle('Breast Cance Data Analysis')
142
        fig.tight_layout()
143
        fig.subplots_adjust(top=0.95)
        plt.show()
145
146
147
        # In[12]:
148
149
150
        from sklearn.decomposition import PCA
151
        from sklearn.preprocessing import StandardScaler
153
154
155
        len_0 = len(data.target[data.target==0])
156
        len_1 = len(data.target[data.target==1])
157
        new_len = np.min([len_0, len_1])
158
159
        newtarget = np.hstack((data.target[:new_len],data.target[len_1:len_1+new_len]))
160
        pca = PCA(n\_components=2)
161
         scaler = StandardScaler()
162
         features = scaler.fit_transform(data.data[:,ind])
         features = pca.fit_transform(features)
164
        newdata = np.vstack((features[:new\_len], features[len\_1:len\_1+new\_len]))
165
        data0 = np.column_stack((newtarget.reshape(len(newtarget),1),newdata[:,:3]))
166
167
168
        # In [51]:
169
170
        plt. figure (figsize = (6,4))
172
173
        lbs = data0[:,0]
        i1 = np.where(lbs==0)[0]
        i2 = np. where(lbs==1)[0]
175
        plt. figure (figsize = (6,5))
176
        plt.scatter(data0[:,1][i1],data0[:,2][i1],edgecolors='k',alpha=0.75,s=150,color='crimson',label='0')
        plt.scatter(data0[:,1][i2],data0[:,2][i2],edgecolors='k',alpha=0.75,s=150,color='ind|go',label='1')
```

```
plt.xlabel('principal component 1')
    plt.ylabel ('principal component 2')
180
181
    plt.legend()
    plt.show()
182
183
184
    # In [6]:
185
186
187
188
    \textbf{from} \hspace{0.2cm} \textbf{qiskit} \hspace{0.2cm} \textbf{import} \hspace{0.2cm} \textbf{Aer} \hspace{0.2cm}, \textbf{BasicAer} \hspace{0.2cm}, \textbf{QuantumCircuit}
    from qiskit.aqua import QuantumInstance, aqua_globals
190
191
    from qiskit.aqua.algorithms import VQC
    from qiskit.aqua.components.optimizers import SPSA
    from qiskit.circuit import ParameterVector
193
    from qiskit.circuit.library import ZZFeatureMap, ZFeatureMap, PauliFeatureMap
194
    from qiskit.circuit.library import RealAmplitudes, EfficientSU2, TwoLocal,
195
         NLocal\,,\ PauliTwo Design\,, Real Amplitudes
    from qiskit.aqua.components.optimizers import ADAM, SPSA, COBYLA, AQGD, TNC,
         SLSQP, L_BFGS_B
197
198
    class DataSet(object):
199
200
         """Docstring for CrossValidation. """
201
202
203
         \label{eq:continuit_self} \textbf{def} \ \_\texttt{-init}\_\_(\, \textbf{self} \;, \; \; \text{data} \;, \; \; k\!\!=\!\! \textbf{None}, \; \; A\!\!=\!\!0, \; B\!\!=\!\!1) \colon
               """TODO: to be defined.
204
               self.data = data.copy()
205
               self.k = k
206
               self.A = A
207
              self.B = B
208
               \#self.C = C
209
               self.dataA = self.data[self.data[:,0] == self.A]
210
211
               self.dataB = self.data[self.data[:,0] = self.B]
              \#self.dataC = self.data[self.data[:,0] = self.C]
212
213
         def CV(self, data):
214
              k = self.k
215
               size = len(data)
216
               index = np.arange(size)
217
               np.random.shuffle(index)
218
              DATA_IND={}
219
               ind_split = np.array_split(index, k)
220
              for name in range(k):
221
                    sub = \{\}
222
                    train_split = []
223
                    \mathbf{for} \ \ \mathbf{i} \ \ \mathbf{in} \ \ \mathbf{range} \, (\, \mathbf{k} \, ) :
224
                         if i==name:
                              sub['test_ind'] = ind_split[i]
226
227
                         else:
                              train_split.append(ind_split[i])
228
                    sub\left[\begin{array}{cc} \texttt{`train\_ind'} \end{array}\right] \; = \; np \, . \; hstack \left(\begin{array}{cc} \texttt{train\_split} \end{array}\right)
229
                   DATA_IND.update({name: sub})
230
               return DATA_IND, index
231
232
         def data_gen(self):
233
              ind, = self.CV(self.dataA)
234
235
               for i in range(self.k):
                    tr_input = {
236
                          'A': self.dataA[ind[i]['train_ind']][:,1:]
237
                         'B': self.dataB[ind[i]['train_ind']][:,1:]}
238
239
                    te_input = {
                          'A': self.dataA[ind[i]['test_ind']][:,1:]
240
                    242
243
                    yield {
    'k': i,
244
245
                         'tr_input': tr_input,
246
                         'te_input': te_input,
247
                         'testing_input': np.concatenate((te_input['A'], te_input['B'])),
248
```

```
'testing_label': np.concatenate(te_label)
249
                         }
250
251
252
253
    class Main(object):
254
255
         """Docstring for CrossValidation. """
256
257
        def __init__(self, shots=2048, reps=2, num_qubits=3, fm_func=None,
258
        vc_func=None, seed=10598):
              """TODO: to be defined.
259
260
             self.shots = shots
             self.reps = reps
261
             self.num_qubits = num_qubits
262
             self.fm_func = fm_func(reps=self.reps,num_qubits=self.num_qubits)
263
             self.vc_func = vc_func(reps=self.reps+1,num_qubits=self.num_qubits)
264
             self.seed = seed
265
             self.counts =
266
             self.values = []
267
        self.backend = Aer.get_backend('qasm_simulator')
self.backend_options = {"method": "statevector", "max_parallel_threads":
0, "max_parallel_experiments": 2, "max_parallel_shots": 1}
268
269
270
271
        def drawfmap(self, fname):
             return self.fm_func.draw(output='mpl', filename=fname+'_fmap.jpg')
272
273
        def drawvmap(self, fname):
274
             return self.vc_func.draw(output='mpl', filename=fname+'_var_circ.jpg')
275
276
        def call_back_vqc(self, eval_count, var_params, eval_val, index):
277
278
             text = "index({}): current cross entropy cost: {}".format(eval_count,
        eval_val)
             self.counts.append(eval\_count)
279
280
             self.values.append(eval_val)
             #print(text)
281
282
        def optimization(self, training_input, test_input):
             self.quantum_instance = QuantumInstance(
284
285
                  self.backend,
                  shots = self.shots,
286
                  seed_simulator=self.seed,
287
288
                  seed_transpiler=self.seed,
                  backend_options=self.backend_options)
289
             self.vqc = VQC(optimizer=self.opt,
290
                feature_map=self.fm_func,
291
                var_form=self.vc_func,
292
293
                callback=self.call_back_vqc,
                {\tt training\_dataset}{=}{\tt training\_input}\ ,
294
                test_dataset=test_input)
295
296
        def train(self, training_input, test_input):
297
             {\bf self.optimization} \, (\, {\tt training\_input} \,\, , \,\, {\tt test\_input} \,)
298
             start = time.process_time()
299
300
             result = self.vqc.run(self.quantum\_instance)
301
             \#val\_prob, val\_labels = self.vqc.predict(val\_input)
302
303
             print("time taken: ")
304
             print(time.process_time() - start)
305
             print("testing success ratio: {}".format(result['testing_accuracy']))
return result['testing_accuracy']
306
307
308
309
310
311
312
313
   # In [7]:
314
315
316
317 np.__version__
```

```
318
319
   # In [8]:
320
321
322
   import qiskit
323
   qiskit . __version__
324
325
326
   # In [9]:
327
328
329
330
   def feature_map_expr1(reps=2, num_qubits=3):
331
        feature_map = QuantumCircuit(num_qubits)
332
        x = ParameterVector('x', length=num_qubits)
333
334
            _ in range(reps):
335
            for i in range(num_qubits):
336
                 feature\_map.ry(x[i], i)
337
                 feature\_map.rz(x[i], i)
338
            for i in range (num_qubits - 1, 0, -1):
339
                 feature_map.cx(i, i-1)
340
341
342
        return feature_map
343
344
   def feature_map_expr2(reps=2, num_qubits=3):
        feature_map = QuantumCircuit(num_qubits)
345
        x = ParameterVector('x', length=num_qubits)
346
347
            _ in range(reps):
348
            for i in range(num_qubits):
349
                 feature\_map.rx(x[i],\ i)
350
                 feature_map.rz(x[i], i)
351
352
            for i in range (num_qubits -1, 0, -1):
                 feature\_map.cx(i, i-1)
353
        return feature_map
354
355
356
   def feature_map_expr3(reps=2, num_qubits=3):
357
        feature_map = QuantumCircuit(num_qubits)
358
        x = ParameterVector('x', length=num_qubits)
359
360
            _ in range(reps):
361
            for i in range(num_qubits):
362
                 feature\_map.rx(x[i],\ i)
363
                 feature_map.rz(x[i], i)
364
            for i in range (num_qubits -1, 0, -1):
365
                 feature\_map.cz(i, i-1)
366
        return feature_map
367
368
   def feature_map_expr4(reps=2, num_qubits=3):
369
        feature_map = QuantumCircuit(num_qubits)
370
371
        x = ParameterVector('x', length=num_qubits)
372
373
        for
            in range (reps):
            for i in range(num_qubits):
374
                 feature\_map.rx(x[i], i)
375
376
                 feature\_map.rz(x[i], i)
            for control in range(num_qubits -1, -1, -1):
377
                 for target in range(num_qubits-1, -1, -1):
378
379
                     if control != target:
                          feature_map.rz(x[target], target)
380
                          feature_map.cx(control, target)
381
382
                          feature_map.rz(x[target], target)
        return feature_map
383
384
   def feature_map_expr5 (reps=2, num_qubits=3):
385
        feature_map = QuantumCircuit(num_qubits)
386
        x = ParameterVector('x', length=num_qubits)
387
388
        for _ in range(reps):
389
```

```
for i in range(num_qubits):
390
                 feature_map.rx(x[i], i)
391
392
                 feature_map.rz(x[i], i)
            feature_map.barrier()
393
            for control in range(num_qubits-1, 0, -1):
394
                 target = control - 1
395
                 feature_map.rx(x[target], target)
396
397
                 feature_map.cx(control, target)
                 feature_map.rx(x[target], target)
398
                 feature_map.barrier()
399
400
            for i in range(num_qubits):
                 feature\_map.rx(x[i], i)
401
402
                 feature\_map.rz(x[i], i)
            feature_map.barrier()
403
        return feature_map
404
405
406
   def feature_map_expr6(reps=2, num_qubits=3):
407
408
        feature_map = QuantumCircuit(num_qubits)
        x = ParameterVector('x', length=num_qubits)
409
410
        for _ in range(reps):
411
            for i in range(num_qubits):
412
413
                 feature\_map.ry(x[i], i)
                 feature_map.rz(x[i], i)
414
            for i in range(num_qubits - 1, 0, -1):
415
416
                 feature\_map.cz(i, i-1)
            feature\_map.ry(x[1], 1)
417
            feature\_map.rz(x[1], 1)
418
        return feature_map
419
420
421
   def feature_map_expr7(reps=2, num_qubits=3):
422
        feature_map = QuantumCircuit(num_qubits)
423
424
        x = ParameterVector('x', length=num_qubits)
425
        for _ in range(reps):
426
427
            \#for \ i \ in \ range(num\_qubits):
                  feature\_map.h(i)
428
429
            for i in range(num_qubits):
430
                 feature_map.ry(x[i], i)
            feature_map.cx(num_qubits-1, 0)
431
432
            for i in range (num_qubits-1):
                 feature\_map.cx(i, i+1)
433
            for i in range(num_qubits):
434
                 feature\_map.ry(x[i], i)
435
            feature_map.cx(num_qubits -1, num_qubits -2)
436
            \texttt{feature\_map.cx} \left( 0 \,, \ \texttt{num\_qubits} \, - \, 1 \right)
437
            for i in range (1, num\_qubits - 1):
438
                 feature\_map.cx(i, i-1)
439
        return feature_map
440
441
442
   def feature_map_expr8 (reps=2, num_qubits=3):
443
444
        return ZZFeatureMap(feature_dimension=num_qubits, reps=reps)
445
446
   def variational_circuit(reps=3, num_qubits=2):
447
448
        #var_circuit = EfficientSU2(num_qubits, entanglement='linear', reps=2,
449
        insert_-barriers = True)
        var_circuit = TwoLocal(num_qubits, ['ry', 'rz'], 'cz', reps=3)
# var_circuit = TwoLocal(num_qubits, ['ry', 'rz'], ['cx'],
450
451
        entanglement='linear', reps=4, insert_barriers=True)
452
        return var_circuit
453
454
   def variational_circuit1(reps=3, num_qubits=2):
455
456
        var_circuit = EfficientSU2(num_qubits, entanglement='linear', reps=3)
457
        #var_circuit = TwoLocal(num_qubits, ['ry', 'rz'], 'cz', reps=reps)
458
```

```
# var_circuit = TwoLocal(num_qubits, ['ry', 'rz'], ['cx'],
459
        entanglement='linear', reps=4, insert_barriers=True)
460
        return var_circuit
461
   def variational_circuit2(reps=3, num_qubits=2):
462
463
        \#var\_circuit = EfficientSU2(num\_qubits, entanglement='linear', reps=2,
464
        insert_-barriers = True)
        var_circuit = PauliTwoDesign(num_qubits, reps=reps)
465
          \# \ var\_circuit = TwoLocal(num\_qubits, \ ['ry', \ 'rz'], \ ['cx'], \\ entanglement='linear', \ reps=4, \ insert\_barriers=True) 
466
467
468
        return var_circuit
469
   def variational_circuit3(reps=3, num_qubits=2):
470
471
        #var_circuit = EfficientSU2(num_qubits, entanglement='linear', reps=2,
472
        insert_barriers=True)
473
        var_circuit = RealAmplitudes(num_qubits, reps=reps)
        \# \ var\_circuit = TwoLocal(num\_qubits, ['ry', 'rz'], ['cx'],
474
        entanglement='linear', reps=4, insert_barriers=True'
475
        return var_circuit
476
477
478
   # In[10]:
479
480
481
   def wrap(data, k=5, feature_map=None, opt_func=None, var_circuit=None,
482
        opt_params={}, maxiter=100, reps=2, num_qubits=3,shots=2048, callback=False):
        mds = DataSet(data, k=k, A=0, B=1)
483
        log = "nqubits({}), reps {}, feature_map {}, opt_func {}:".format(
484
            num_qubits,
485
486
            reps.
487
            feature_map.__name__,
            opt_func.__name__
488
489
        print ("="*80+"\n"+log)
490
        Accuracy = []
491
492
        plt.figure(figsize=(5,5))
        with open('result.log', 'a+') as fp:
493
            result_log = '\#' + log + ' \setminus n
494
495
            fp.writelines(result_log)
            for d in mds.data_gen():
496
                 print(log+" fold {}...".format(d['k']))
497
                 run = Main(shots=shots,
498
                              reps=reps, num_qubits=num_qubits, fm_func=feature_map,
499
        vc_func=var_circuit)
                 run.opt = opt_func(maxiter=maxiter, **opt_params)
500
                 acc = run.train(d['tr_input'], d['te_input'])
fp.writelines("{}, {}\n".format(d['k'], acc))
501
502
                 Accuracy.append(acc)
503
504
                 count = run.counts
505
                 vals = run.values
                 plt.plot(count, vals, label='fold '+str(d['k']+1))
506
        plt.title('Cost value over training set')
507
        plt.xlabel('Iteration')
508
        plt.ylabel('Cost')
509
510
        plt.legend()
511
        plt.show()
512
        return np. asarray (Accuracy)
513
            #run.drawfmap(log.replace('
514
          "").replace(",","").replace(":","").replace("(","").replace(")",""))
            #run.drawvmap(log.replace('
515
        ',"").replace(",",").replace(":","").replace("(","").replace(")",""))
516
517
518
   \# \# \# Qubits
519
520
521 # In [13]:
```

```
522
523
    len_0 = len(data.target[data.target==0])
524
    len_1 = len(data.target[data.target==1])
525
    new_len = np.min([len_0, len_1])
526
    newtarget = np.\,hstack \,(\,(\,data\,.\,target\,[\,:\,new\_len\,]\,,data\,.\,target\,[\,len\_1\,:\,len\_1 + new\_len\,]\,)\,)
528
    pca = PCA(n\_components=3)
529
    scaler = StandardScaler()
530
    features = pca.fit_transform(data.data[:,ind])
531
    features = scaler.fit_transform(features)
    newdata = np.vstack((features[:new_len],features[len_1:len_1+new_len]))
533
    data1 = np.column_stack((newtarget.reshape(len(newtarget),1),newdata[:,:3]))
534
535
536
    # In[14]:
537
538
539
    newtarget = np. hstack((data.target[:new_len],data.target[len_1:len_1+new_len]))
540
    pca = PCA(n\_components=4)
541
    scaler = StandardScaler()
542
    features = pca.fit_transform(data.data[:,ind])
    features = scaler.fit_transform(features)
544
    newdata = np.vstack((features[:new\_len], features[len\_1:len\_1+new\_len]))
545
546
    data2 = np.column_stack((newtarget.reshape(len(newtarget),1),newdata[:,:4]))
547
548
    # In [60]:
549
550
551
    fig, ax = plt.subplots(1,2,figsize=(12,4))
552
    lbs = data1[:,0]
553
    i1 = np.where(lbs==0)[0]
554
    i2 = np. where (lbs==1)[0]
555
    ax[0].scatter(data1[:,1][i1],data1[:,2][i1],edgecolors='k',alpha=0.75,s=150,color='crimson',label='0')
556
    ax[0].scatter(data1[:,1][i2],data1[:,2][i2],edgecolors='k',alpha=0.75,s=150,color='i\pi digo',label='1')
557
   ax[0].set_xlabel('feature 1')
ax[0].set_ylabel('feature 2')
558
559
    ax [0]. legend()
560
561
   ax[1]. scatter(data1[:,1][i1], data1[:,3][i1], edgecolors='k', alpha=0.75, s=150, color='crimson', label='0') ax[1]. scatter(data1[:,1][i2], data1[:,3][i2], edgecolors='k', alpha=0.75, s=150, color='indigo', label='1')
562
563
564
    ax[1].set_xlabel('feature 1')
    ax[1].set_ylabel('feature 3')
565
    ax [1]. legend()
566
    plt.show()
567
568
569
    # In [61]:
570
571
572
    data0.shape
573
574
575
    # In / /:
576
577
578
    qubits = [data0, data1, data2]
579
580
    acc_fmap = np.zeros((len(qubits),3))
    for i in range (2):
581
        params = {"k":3, "maxiter":100, "num_qubits":qubits[i].shape[1]-1, "reps":2}
582
        params ["var_circuit"] = variational_circuit
params ["feature_map"] = feature_map_expr7
params ["opt_func"] = COBYLA
583
584
585
        params["opt_params"] = {"disp":True, "tol":1e-6}
586
        acc_fmap[i] = wrap(qubits[i], **params)
587
588
589
    # In [69]:
590
591
592
   data2.shape
```

```
594
595
      # In[16]:
596
597
598
599
      qubits = [data0, data1, data2]
600
     params \, = \, \left\{\text{"k":3, "maxiter":200, "num_qubits":qubits[2].shape[1]-1, "reps":2}\right\}
601
     params ["var_circuit"] = variational_circuit
params ["feature_map"] = feature_map_expr7
602
603
     params["eature-map] = reature-maplexprr
params["opt_func"] = COBYLA
params["opt_params"] = {"disp":True, "tol":1e-6}
acc_fmap[i] = wrap(qubits[2], **params)
605
606
607
608
     # In[ ]:
609
610
611
     \texttt{acc\_fmap} \, = \, \texttt{np.array} \, ( \, [ \, 0.6018518518518518519 \, , 0.7314814814814815 \, , ] \, ) \, . \, \texttt{reshape} \, ( \, 3 \, , 3 ) \, ) \, . \, \\
612
613
614
     # In[100]:
615
616
617
618
     x = [2, 3, 4]
     y = np.mean(acc_fmap, axis=1)
619
     yerr = np.std(acc\_fmap,axis=1)
     plt.figure(figsize=(6,5))
plt. Figure (Figs12e = (0,3))
plt. errorbar (x,y,yerr=yerr,ls='none',marker='o')
plt. title ('Test set accuracy for different number of qubits')
plt.xlabel ('Number of qubits')
     plt.ylabel ('Test set accuracy')
     plt.show()
```

AQA_assignment1.py