2110581 BIOINFORMATIC I

Progress Report 4

non-coding RNA Classification

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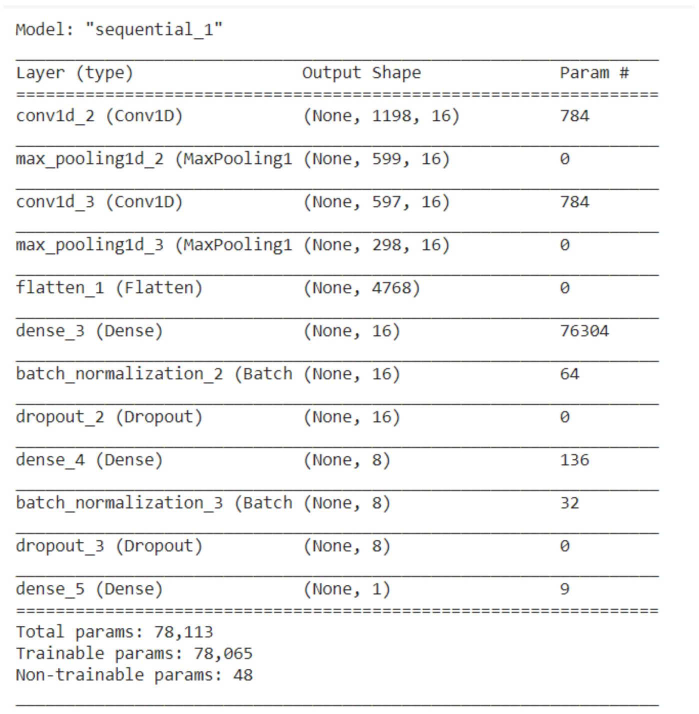
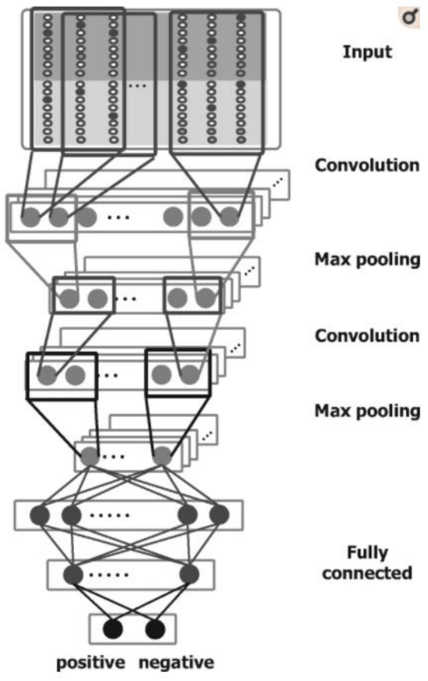
Report

Our code written in Python consists of 3 parts. First part is to convert data from input FASTA file format to ncRNA matrix. Second part is to generate ncRNApair data and ncRNApair label from ncRNA matrix from part one. The last part is to use the ncRNA data along with its label to train the neural network to recognize the pattern of data.

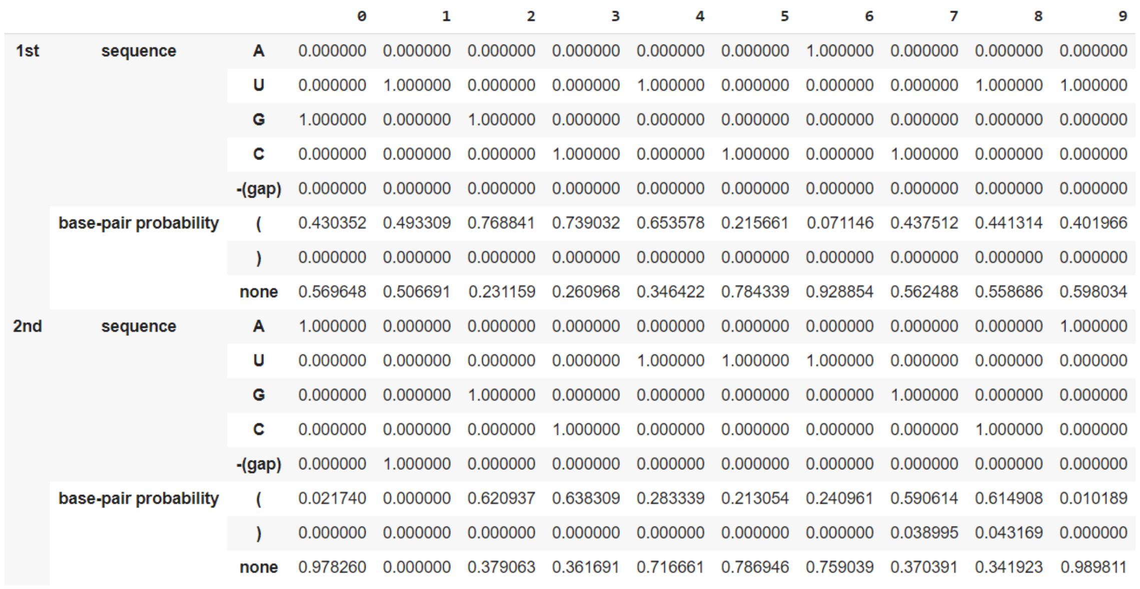
In the third part of deep learning, we deploy TensorFlow library to build our convolutional neural network. Our network applies a one-dimensional CNN to accurate clustering of ncRNA sequences, we developed a new CNN-based method for classification of pairwise alignments of ncRNA sequences. The architecture of model is described as the following.



```
Model: "sequential_1"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv1d_2 (Conv1D)            (None, 1198, 16)          784
_________________________________________________________________
max_pooling1d_2 (MaxPooling1 (None, 599, 16)           0
_________________________________________________________________
conv1d_3 (Conv1D)            (None, 597, 16)           784
_________________________________________________________________
max_pooling1d_3 (MaxPooling1 (None, 298, 16)           0
_________________________________________________________________
flatten_1 (Flatten)          (None, 4768)              0
_________________________________________________________________
dense_3 (Dense)              (None, 16)                76304
_________________________________________________________________
batch_normalization_2 (Batch (None, 16)                64
_________________________________________________________________
dropout_2 (Dropout)          (None, 16)                0
_________________________________________________________________
dense_4 (Dense)              (None, 8)                 136
_________________________________________________________________
batch_normalization_3 (Batch (None, 8)                 32
_________________________________________________________________
dropout_3 (Dropout)          (None, 8)                 0
_________________________________________________________________
dense_5 (Dense)              (None, 1)                 9
=================================================================
Total params: 78,113
Trainable params: 78,065
Non-trainable params: 48
_________________________________________________________________
```

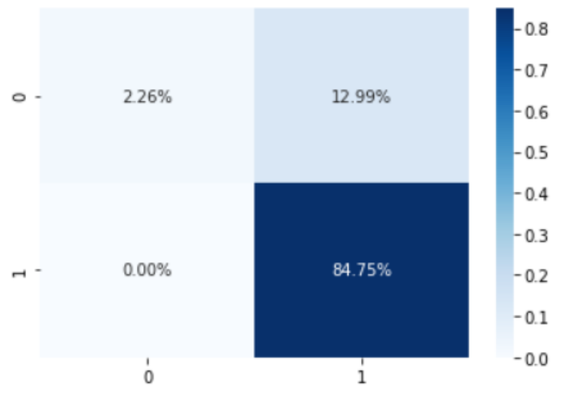


This is the sample of the input for the CNN obtained by One-hot encoding the pair of sequence ncRNA and concatenating the three-dimensional vector for representing secondary-structure information in column *i* consists of left-side base-pairing probability p^{left}_i, right-side base-pairing probability P^{right}_i and unpaired probability $p^{unpaired}_i$.

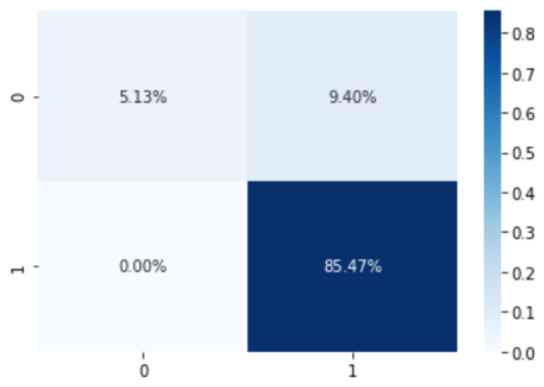


			0	1	2	3	4	5	6	7	8	9
1st	sequence	A	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000
		U	0.000000	1.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	1.000000	1.000000
		G	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
		C	0.000000	0.000000	0.000000	1.000000	0.000000	1.000000	0.000000	1.000000	0.000000	0.000000
		-(gap)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	base-pair probability	(	0.430352	0.493309	0.768841	0.739032	0.653578	0.215661	0.071146	0.437512	0.441314	0.401966
		)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
		none	0.569648	0.506691	0.231159	0.260968	0.346422	0.784339	0.928854	0.562488	0.558686	0.598034
2nd	sequence	A	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000
		U	0.000000	0.000000	0.000000	0.000000	1.000000	1.000000	1.000000	0.000000	0.000000	0.000000
		G	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	1.000000	0.000000	0.000000
		C	0.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	1.000000	0.000000
		-(gap)	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	base-pair probability	(	0.021740	0.000000	0.620937	0.638309	0.283339	0.213054	0.240961	0.590614	0.614908	0.010189
		)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.038995	0.043169	0.000000
		none	0.978260	0.000000	0.379063	0.361691	0.716661	0.786946	0.759039	0.370391	0.341923	0.989811

Then, we compile our model using 'Adam' optimizer and 'Accuracy' for a metrics. We the train the model with 10 epochs and get the final accuracy on training around 90%. We also deploy confusion_matrix and accuracy_score module from sklearn.metrics to evaluate the model's performance.



Confusion matrix for predicting training set



Confusion matrix for predicting test set

The performance of each method was evaluated as follows. For classification accuracy, given the prediction of one-dimensional CNN for a pair of ncRNA sequences in the test data, the prediction is defined as true positive (TP) if the pair is labeled as the positive class and the prediction is positive. In the same manner, false positives (FPs), true negatives (TNs) and false negatives (FNs) are defined if the pair is labeled as the negative class, but the prediction is positive, the pair is labeled as the negative class and the prediction is negative, or the pair is labeled as the positive class but the prediction is negative, respectively.

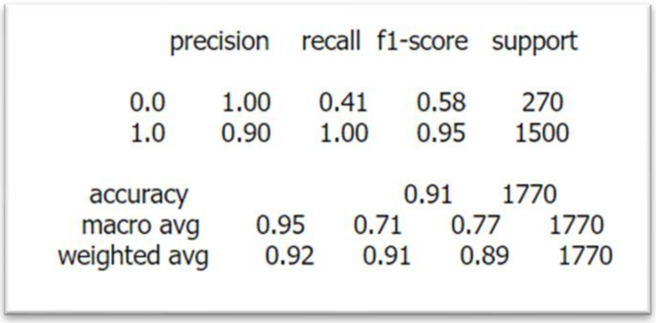
$$\text{Accuracy} = \frac{\#\text{TP} + \#\text{TN}}{\#\text{TP} + \#\text{FP} + \#\text{TN} + \#\text{FN}}$$

$$\text{Precision} = \frac{\#\#\text{TP}}{\#\text{TP} + \#\#\text{FP}}$$

$$\text{Recall} = \frac{\#\#\text{TP}}{\#\#\text{TP} + \#\#\text{FN}}$$

$$F - \text{value} = \frac{2\text{Recall} * \text{Precision}}{\text{Recall} + \text{Precision}}$$

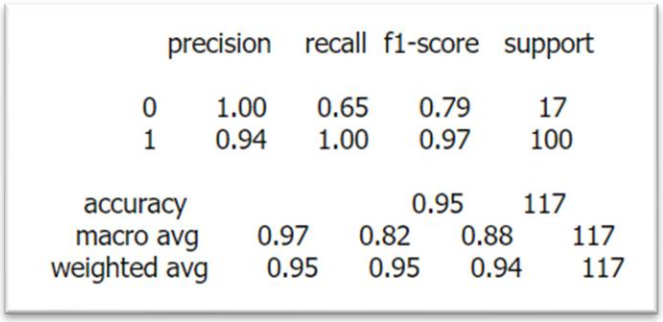
We calculated those measurement using sklearn.metrics.classification_report and this is the result of training set and test set respectively.



```
              precision    recall  f1-score   support

         0.0       1.00      0.41      0.58       270
         1.0       0.90      1.00      0.95      1500

    accuracy                           0.91      1770
   macro avg       0.95      0.71      0.77      1770
weighted avg       0.92      0.91      0.89      1770
```

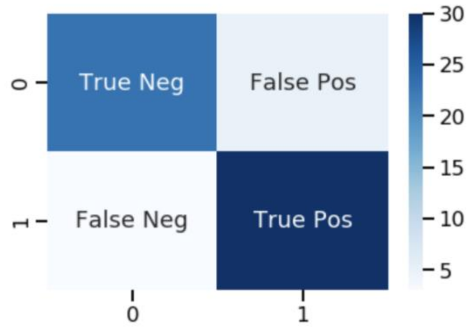


```
              precision    recall  f1-score   support

           0       1.00      0.65      0.79        17
           1       0.94      1.00      0.97       100

    accuracy                           0.95       117
   macro avg       0.97      0.82      0.88       117
weighted avg       0.95      0.95      0.94       117
```

Source code available on Github :
https://github.com/pakkaponwattanawaha/Bioinfomatics_TermProject



The confusion matrix used in this report is represented in this format.