

IQB Assignment 2

README

Along with predicting, this code also finds the Train & Test accuracy with K-Fold method and 5 folds.

Syntax Format:

```
python3 final.py -o <output File> -type {aminoacid | dipeptide | tripeptide} -model {SVC | RFC} { {-gamma | -n_estimators} <positive value> | -optimalParameters }
```

Understanding of Syntax:

- Type can only be 'aminoacid', 'dipeptide' or 'tripeptide'. These are the different ways of parsing the input peptide.
- Models:
 - SVC: Support Vector Classifier
 - RFC: Random Forest Classifier
- -gamma and -n_estimators are the parameters we pass into these models.
- -optimalParameters is a mode where it runs the model multiple times and plots the accuracy for the parameters. This way, we can find out the optimal gamma/n_estimators for a particular model.

Please Note:

- gamma can only be used if model is SVC.
- n_estimators can only be used if model is RFC.
- gamma & -n_estimators have to be positive values
- outputFile is preferred with .csv format
- In -optimalParameters, 3 inputs will be asked: start, end, step indexes for the parameters.
- If -optimalParameters mode is used, -gamma <val> cannot be used for obvious reasons.

Best Models (Acc to avg test accuracy):

1. Model: RFC

Type: Tripeptide

n_estimators: 700

CSV stored in: best1.csv

Code in: best1.py

python3 best1.py OR

python3 final.py -o best1.csv -type tripeptide -model RFC
-n_estimators 700

Output exported in best1.csv

Avg Train Accuracy: 1.0

Avg Test Accuracy: 0.8901960784313726

2. Model: SVC

Type: Tripeptide

Gamma: 15

CSV stored in: best2.csv

Code in: best2.py

python3 best2.py OR

python3 final.py -o best2.csv -type tripeptide -model SVC -gamma
15

Output exported in best2.csv

Avg Train Accuracy: 0.9859803921568627

Avg Test Accuracy: 0.8741176470588237

3. Model: SVC

Type: Dipeptide

Gamma: 91

CSV stored in: best2.csv

Code in: best2.py

python3 best3.py OR

python3 final.py -o best3.csv -type dipeptide -model SVC -gamma
91

Output exported in best3.csv

Avg Train Accuracy: 0.9981372549019607

Avg Test Accuracy: 0.8631372549019607

Example Syntax of optimalParameters:

```
python3 final.py -o a.csv -type aminoacid -model SVC  
-optimalParameters
```

```
Enter start parameter: 40  
Enter end parameter: 200  
Enter step parameter: 30  
Gamma : 40  
Avg Train Accuracy: 0.9235294117647058  
Avg Test Accuracy: 0.851764705882353  
Gamma : 70  
Avg Train Accuracy: 0.9575490196078432  
Avg Test Accuracy: 0.8623529411764705  
Gamma : 100  
Avg Train Accuracy: 0.9748039215686275  
Avg Test Accuracy: 0.8619607843137255  
Gamma : 130  
Avg Train Accuracy: 0.9858823529411765  
Avg Test Accuracy: 0.8564705882352941  
Gamma : 160  
Avg Train Accuracy: 0.9920588235294119  
Avg Test Accuracy: 0.8564705882352941  
Gamma : 190  
Avg Train Accuracy: 0.993921568627451  
Avg Test Accuracy: 0.8525490196078431
```

