Assignment - 2
Classification of Peptides

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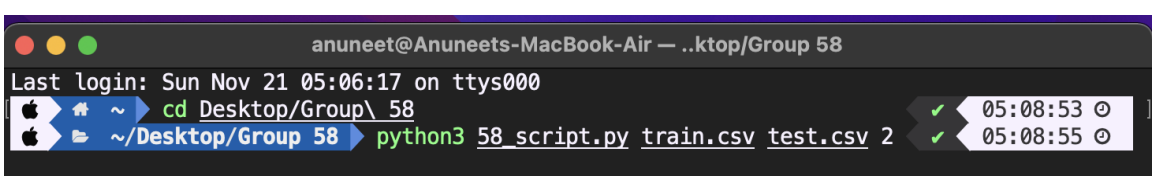
Files

- 58_script.py: Python code file with all the models.
- train.csv: Provided training dataset.
- test.csv: Provided test dataset.
- Submission_x.csv: 2 Files corresponding to 2 models with probabilities.
- Predictions_x.csv: 2 Files corresponding to 2 models with binary values.

Usage

- Requirements: scikit_learn, xgboost (Google Colab version), numpy, pandas
- The given script takes the training dataset, test dataset and model number of predefined models as arguments and accordingly generates the predictions as CSV files in the same directory.
- The train_data and test_data files should be present in the same directory.
- Valid values for the model are 1, 2 (corresponding to our 2 best models) and 0 to run all the models.
- We generate Submission_x.csv files for predicted probabilities (used on Kaggle) and also Prediction_x.csv files for predicted 0/1 values.
- We had to drop the last row of the training dataset as it had some unknown characters that couldn't be parsed.
- Note that Model 2 might generate different output based on XGBoost Version. Hence it should be run on Google Colab to reproduce the same file.

```
Usage: python3 58_script.py <train_data> <test_data> <model>
```



Feature Generation

- Amino Acid Composition was calculated by our own function.
- Dipeptide Composition was calculated by our own function.
- Mass and Charge was calculated using the pyteomics library.
- Isoelectric Point was calculated using the Bio.SeqUtils library.

Models

- **Model 1:** We used Amino Acid Composition, Dipeptide Composition, Mass, Charge and Isoelectric point of the given peptide sequences as features. The model consists of a BaggingClassifier (100 estimators) with RandomForest as a base estimator (100 trees). The predicted probabilities are stored in Submission_1.csv which has the same name on Kaggle.
  Public Score: 0.78620
  Private Score: 0.77318

- **Model 2:** We used Amino Acid Composition, Mass, Charge and Isoelectric point of the given peptide sequences as features. The model consists of a BaggingClassifier with a tuned XGBClassifier as a base estimator. There are 23 base estimators and they each have 100 estimators. The predicted probabilities are stored in Submission_2.csv which has the name submission11.csv on Kaggle.
  Public Score: 0.77427
  Private Score: 0.75699