CMSC 435 Assignment 3

Fall 2022
(individual work; 8 pts total)

This assignment asks you to design, evaluate and compare models for the prediction of proteins that interact with nucleic acids using a provided dataset.

Dataset
The dataset (*dataset_a3.csv* file) is in the text-based, comma-separated format where each protein is represented by 10 numeric features and 1 symbolic outcome. The outcome feature (called "Class") annotates each protein as *Yes* (interacting with nucleic acids) vs. *No* (non-interacting). The dataset includes 8795 proteins, with 936 labeled *Yes* and 7859 labeled *No*.

Development of predictive models
You are required to develop models with version 9.10 (or higher) of the RapidMiner Studio using four different algorithms. Two of these four algorithms must be the **Naïve Bayes and k-NN**, the algorithms from the list of the top 10 data mining methods. You can choose any of the other predictive algorithms for the other two selections, however, at **least one of these algorithms must have parameters that can be adjusted** (details below). You should parametrize each of these four algorithms (i.e., select the best possible combination of values of their parameters), to the best of your ability, in order to **maximize** predictive performance that you will quantify with accuracy ("% of correctly classified instances"). You will need to make an educated guess and/or use trial-and-error approach to figure out which **key parameters** make a difference and how to use them, i.e., you will use the key parameters to increase accuracy when compared with the accuracy generated using default parameter values. While you should consider all parameters, select **no more than 3 key parameters** from among all available parameters for a given algorithm. **Do not use the "advanced parameters"**, which means that you do not need to parametrize methods that do not have non-advanced parameters. Do not attempt to sample or modify the dataset, i.e., do not perform feature or sample/object selection.

Testing of predictive models
For each algorithm you must perform three types of tests:
- on the entire dataset ("use training dataset")
- on 50% of the dataset; you will use the other 50% to compute the model ("50% split")
- using the three-fold cross-validation

The 50% split can be implemented in RapidMiner with the "Split Data" operator. The three-fold cross-validation divides the dataset at random into three equal-size subsets, where one subset is used to test the model and the remaining two to compute the prediction model. This is repeated three times, each time using a different subset as the test set. Consequently, this results in predicting every protein in the dataset. This test type is implemented in the RapidMiner Studio with the "Cross Validation" operator where the number of folds is **set to three**.

Deliverables

1. The .rmp file that you created in RapidMiner to solve this assignment. You can create this file by selecting the "Export Process" option under the "File" in the top menu. The file **must be named** a3.rmp.
2. Answers to the following five questions:
   2.1. **List and briefly describe** the two algorithms that you selected. You should **name** the algorithms and briefly explain **why** you selected them and what **type of models** they produce.
   2.2. Using the table shown below, **report the accuracies** for the four algorithms and the three test types. The accuracy values must be reported with two digits after the decimal point, e.g., 91.05.

You must include the accuracies of the models that use the default parameters and the best values of the key parameters. In total, you have 4*3*2 = 24 results to report. **Name the key parameters and list their best selected values** for each model and each test type; leave this part of the table empty if there are no parameters. Use the provided template of the table and upload the answer to this question as .jpg, .png or .pdf file.

2.3. You should obtain 100% accuracy for at least one method and one type of test. Which type of test produced this accuracy value? Do you think 100% accuracy is a good result if we assume that data in this dataset, including the yes/no Class feature, is **noisy**?

2.4. **Provide** "confusion matrix" for the most accurate result computed based on the **three-fold cross-validation experiments** (selected among the 8 corresponding experiments). This is the matrix in the PerformanceVector view. Use this matrix to **explain** whether this predictor would be better suited to identify proteins that interact with nucleic acids (Class = *Yes*), proteins that do not interact with nucleic acids (Class = *No*), or both types of proteins. Upload the answer to this question as .jpg, .png or .pdf file

2.5. Using the results from the **three-fold cross-validation tests, briefly discuss** whether trying multiple algorithms and adjusting their parameters helped you in developing a more accurate predictive model compared to the results that rely on the simple Naïve Bayes method. Argue **whether or not** this amount of improvement over the Naïve Bayes is large – try your best to **justify your argument**. Consider the fact that it is trivial/easy to produce predictions that are 89.36% accurate if we simply predict all proteins with label "No".

Notes

- Late submissions will be subject to deductions: 15% in first 12 hours and 30% for between 12 and 48 hours. We will not accept submissions that are over 48 hours late.
- We will check for **plagiarism**. Develop your own rmp file and provide your own answers.
- The table for question 2.2 must be in the following format; for your convenience this table is provided in the word docx format in Canvas. Example **fake** values are in green font.

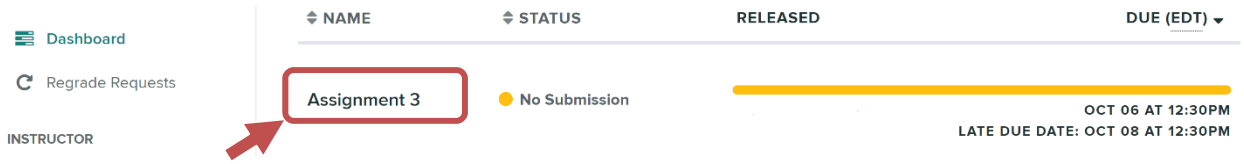
Reported information	Test type	k-NN	Naïve Bayes		
Accuracy with default parameters	Entire dataset	12.34%			
	50%	23.45%			
	Cross-validation	34.56%			
Accuracy with best parameters	Entire dataset	45.67%			
	50%	56.78%			
	Cross-validation	67.89%			
List names of parameters		k measure types			
List selected best values of parameters (in the same order as in the list of names)	Entire dataset	123 MixedMeasures			
	50%	456 NominalMeasures			
	Cross-validation	789 NumericalMeasures			

Due Date

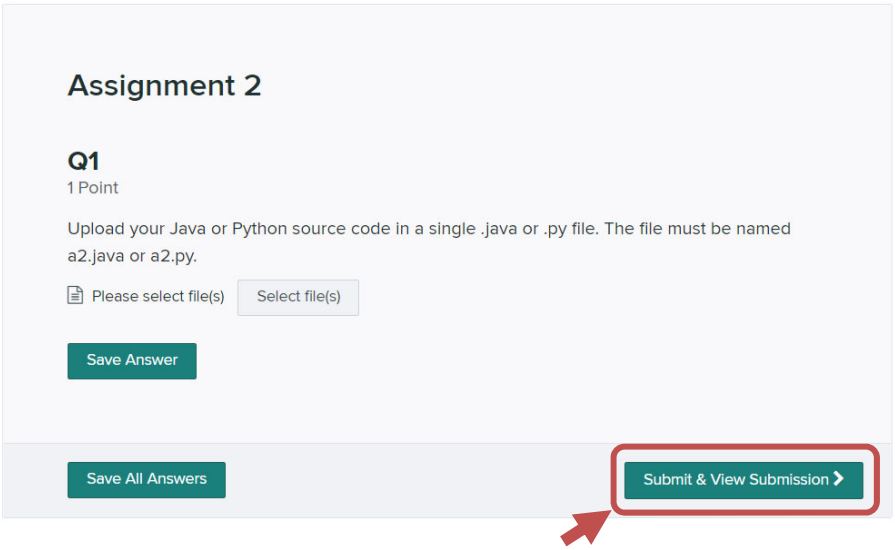
Your assignment must be received before 12:30 pm Eastern Time on October 6 (Thursday), 2022. Submissions must be done using Gradescope. Use the below instructions.

Submitting assignment

Once you accessed the course in Gradescope successfully, click on "Assignment 3" in the dashboard



For the questions for which **answers require a table (2.2 and 2.4)**, you should upload the answer as **.jpg, .png** or **.pdf** file in Gradescope.
After answering the questions, you must click on the "Submit and View" button, which is at the bottom of the page, before the deadline to submit your assignment on-time. The "Save answer" or "Save All Answers" buttons only save your answers and do not submit the assignment.



After clicking the submit you will be able to review your submission and double check that it is complete. You can submit multiple times and only your last submission will be graded.