CMSC 435 Assignment 3

Fall 2020
(individual work; 10 pts total)

This assignment asks you to assemble, 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 provided 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 proteins 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 compute models with version 9.7 (or higher) of the RapidMiner Studio using four different algorithms. Three of these four algorithms must be the Logistic Regression, Decision Tree, and Support Vector Machine (SVM). You can choose any of the other predictive algorithms for the fourth selection. You should parametrize each of these algorithms (select the best possible combination of values of their parameters), to the best of your ability, in order to maximize predictive performance. Note that you will need to read, make an educated guess, and/or use trial-and-error approach to figure out which parameters make a difference and how to use them. **Do not use the "advanced parameters"**. Do not attempt to sample the dataset, i.e., do not perform feature or sample/object selection.

Evaluation and comparison of predictive models
You must evaluate the predictive performance using accuracy ("% of correctly classified instances"). 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 ("percentage split")
- using the 5 fold cross-validation

The 5-fold cross-validation divides the dataset at random into 5 equal-size subsets, where one subset is used to test the model and the remaining four to compute the prediction model. This is repeated 5 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 5.

Deliverables
1. **List and briefly describe** the methods that you used. One sentence per method that explains what type of model and how it produces. Provide a **list of the key parameters** for each method, i.e., parameters that allowed you to improve results when compared with the default parameter values. The key parameters could/should be a subset of all available parameters.
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 selected parameters. In total, you have 4*3*2 = 24 results to report. **List the best selected values of parameters** for each model and each test type.
3. **Briefly explain** which of the three types of the tests would be appropriate to provide the most reliable estimate of expected predictive performance, i.e., the performance that a user of your model should expect to observe **on new proteins that were not included in the provided dataset**.

4. Were you able to obtain 100% accuracy results? 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**?
5. **Discuss** whether trying multiple algorithms and adjusting their parameters helped you in developing a more accurate predictive model. If yes then **comment** on whether the corresponding amount of the improvement justifies the amount of effort. Make sure that you rely the **most appropriate test results** (see question 3) when answering this question.
6. **Give** "confusion matrix" for the most accurate result computed based on the cross-validation experiments (selected among the 8 corresponding experiments). 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.

NOTES

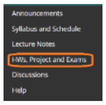
- Use a separate, **clearly marked paragraph** for each of the six deliverables.
- The report should be typed single-spaced, using 12-point font size (Times New Roman font would be a good choice) and with standard margins. Convert the file into the **pdf** format for submission.
- The table from the second deliverable must be in the following format; for your convenience this table is provided in the word docx format on the Blackboard. Example (fake) values are in green.

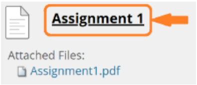
Reported information	Test type	Decision Tree	Logistic Regression	SVM	
Accuracy with default parameters	Entire dataset	12.34			
	50%	23.45			
	Cross-validation	34.56			
Accuracy with best parameters	Entire dataset	45.67			
	50%	56.78			
	Cross-validation	67.89			
List names of parameters		maximal depth apply pruning criterion			
List selected best values of parameters (in the same order as in the list of names)	Entire dataset	10 True gain_ratio			
	50%	13 True gain_ratio			
	Cross-validation	-1 False informaton_gain			

Due Date

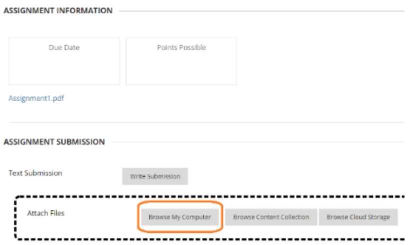
Your assignment must be received by 12:30pm Eastern Time (beginning of the lecture) on October 1 (Thursday), 2020. Submissions of the pdf file must be done via the class web page in Blackboard. 4-step instructions are included below.

1. Go to the section "HWs, Projects and Exams" and select Assignment 2 by clicking on the assignment title





2. Select your submission files by clicking on "Browse My Computer".



ASSIGNMENT INFORMATION

Due Date

Points Possible

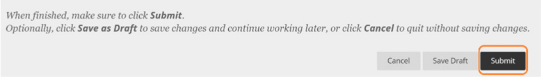
Assignment1.pdf

ASSIGNMENT SUBMISSION

Text Submission

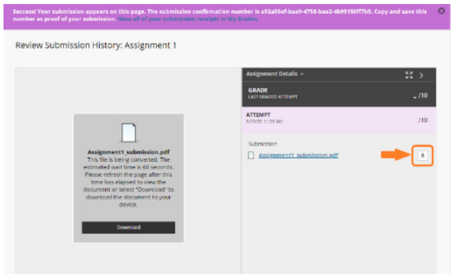
Attach Files

3. [Important!] Your file(s) will be submitted only after you click the submit button.



*When finished, make sure to click **Submit**.*
*Optionally, click **Save as Draft** to save changes and continue working later, or click **Cancel** to quit without saving changes.*

4. [Important!] Make sure you download your submission and double check if the correct files are sent.



Success! Your submission appears on this page. The submission confirmation number is a92a55ef-baa9-4758-baa2-4b99150ff7b5. Copy and save this number as proof of your submission. View all of your submission receipts in My Grades.

Review Submission History: Assignment 1

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Submission
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