Informatics Skunkworks Education Curriculum

Part 1: Curriculum Information

Instructor Information

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Curriculum Description

This curriculum provides students an introduction to using machine learning tools and the associated necessary background on machine learning methods and statistical analysis. Throughout the curriculum, students will focus on using two software tools (Citrination and MAST-ML) to generate machine learning models. They will learn key ideas for assessing model performance and decision making skills for how to improve or modify a model.

It is expected that between synchronous (and asynchronous) meetings, work groups, and completion of activities that students will spend ~9 hours of time on work related to their participation in the Skunkworks Education group each week. This corresponds to approximately a 3 credit hour course if receiving credit for an independent study course.

Learning Outcomes

By the end of the curriculum, students will be able to:

- Build machine learning models from existing data sets.
- Explain the array of output information needed to analyze models.
- Make decisions on how to modify models to improve model quality.
- Have skills to develop models with Citrination and MAST-ML tools.

Curriculum Materials

- A laptop or desktop computer
- An Internet connection

Prerequisite Knowledge

Students are not expected to have any prerequisite technical skills or knowledge, though familiarity with basic programming concepts and python

specifically may provide a smoother transition into using the software tools in this curriculum.

Grading

For students receiving course credit grading is primarily assessed via completion of activities associated with each module in the curriculum. Students will create a weekly slide deck which summarizes the results of each activity and these slide decks as well as a final end of semester slide deck will be used to assess completion. This will account for 90% of the grade. In addition attendance and participation in weekly meetings will account for 10% of the grade.

Curriculum Structure

The curriculum is divided up into modules. Each module takes approximately three - five hours to complete. Each module has two components. The first is information about a topic of machine learning which is delivered in a variety of mediums. The second component is a set of tasks for students to complete on their own. These tasks give students hands-on experience with the machine learning topic and seek to reinforce the ideas presented in the first section.

Part 2: Curriculum Outline

Note for Fall 2021: all links here are to the old google drive versions of activities. If you are working ahead of the schedule from meetings you will need to use these. For anyone following along with the pace of modules from meetings please use the links included in the meeting notes document here: https://docs.google.com/document/d/1Gh44Z7fcXKQTnMAp711Jd-lqP-WLK7c v5ut2A E-aRI/edit

• Module 0: Machine Learning Predictions Activity

- Learning Objectives
 - Students will familiarize themselves with a general overview of machine learning and how it can be used to make predictions.
- Activities
 - o Machine Learning Predictions video
 - o Review overview slides from Prof. Morgan

• Module 1: Basics of Machine Learning

- Learning Objectives
 - o Students are introduced to model types, key outputs, and metrics for assessing performance
 - o Students are introduced to effective practices for maintaining a useful record of research
 - o Students continue to learn about model types, key outputs, and metrics for assessing performance
 - Students continue discussing effective practices for maintaining a useful record of research

Activities

- o Video Introduction to Machine Learning
 - Powerpoint used in Video Introduction (to follow along)
- o Written Introduction to Machine Learning
 - Additional Resources
- Introduction to Machine Learning for Materials Science Lab Activity
 - <u>Video: Introduction to Machine Learning for Materials</u>
 Science Lab Activity
- Research Compact activity
- o Navigating Roadblocks and Obstacles

Module 1.5: Python Basics

- Learning Objectives
 - Students will learn some basics of programming in Python.
 - Students will learn how to import and export data for analysis.
 - Students will become familiarized with some of the structures and logic that computers use.
 - Students will learn how to execute code in a jupyter notebook through Google Colab.

Activities

o Python Basics

Module 2: Introduction to Citrination

- Learning Objectives
 - o Students will learn how Skunkworks is structured and how it will prepare them for undergraduate research projects
 - o Students will access the Citrination client, upload data, and create a random forest model.
 - o Students learn about how to establish group expectations, dynamics, communication
 - o Students will think critically about a dataset and identify good or bad data.
 - o Students discuss ways to address roadblocks and obstacles that frequently arise in research

Activities

- o Introduction to Citrination
- Ethical Data Cleaning

Module 3: Introduction to MAST-ML

- Learning Objectives
 - Students are introduced to the MAST-ML software and given a few sample workflows to run on their dataset. The models generated here can then be compared against those previously generated with Citrination.
 - Students explore various cross validation methods in MAST-ML

Activities

- MASTML Introduction
- Model Limitations

• Module 4: Modifying Workflows with MASTML

- Learning Objectives
 - Students learn how to modify workflows within MAST-ML to employ the software for various applications.
 - Students understand how MASTML can be used to recreate workflows from other machine learning software (like Citrination).

Activities

o Modifying Workflows in MASTML

Module 5: Hyperparameter Optimization

- Students learn about how model hyperparameters can affect performance and are introduced to some basic ideas on how these hyperparameters can be optimized.
- Students familiarize themselves with a hyperparameter optimization landscape and explore various methods of searching for a global minimum in model errors and avoiding getting trapped in a local minimum.
- Students familiarize themselves with neural networks, what they are, how to use them, and how to optimize them.
- Activities
 - Hyperparameter Optimization Presentation Slides
 - Hyperparameter Optimization activity

Part 3: Overview of Schedule

The education group will have 3 meetings a week, with students expected to attend one of the three options. (Mon/Tues/Thurs 4:00 PM - 5:15 PM central time) to introduce each activity, discuss new concepts and ideas, and review the results of the previous week's activity. The table below gives the outline of the structure for the semester.

Week	Machine Learning Activity	Professional Development Activities
0 - 9/27/2021	Introduction to Edu	optional: module 1.5

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	Group	basics of python
1 - 10/4/2021	Basics of Machine Learning	Group Compact
2 - 10/11/2021	Basics of Machine Learning (cont)	Navigating Roadblocks and Obstacles
3 - 10/18/2021	Intro to Citrination	
4 - 10/25/2021	Intro to Citrination (cont)	Ethical Data Cleaning
5 - 11/1/2021	Introduction to MAST-ML	Model Limitations
6 - 11/8/2021	Modifying MAST-ML Workflows	
7 - 11/15/2021	Hyperparameter Optimization	
8 - 11/22/2021	EoS project (Data Cleaning)	
9 - 11/29/2021	EoS project (Fit default model)	
10 - 12/6/2021	EoS project (Optimize Model)	

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