MSSC 6000 – Scientific Computing
Spring 2023

My Contact Information

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Lectures:	MWF, 11:00am - 11:50am Cudahy Hall 208
Office Hours:	Mondays, 1:00pm - 2:00pm (in person, Cudahy 307) Wednesdays, 2:30pm - 3:30pm (virtual, on Teams) **and by appointment** (just email me!)

Bulletin Description

Foundational methods and techniques of scientific computing in the mathematical and statistical sciences. This course will cover fundamental computational algorithms aimed toward applications in science and engineering. Students will implement algorithms, and visualize and validate their outcomes. Further, students will be introduced to and implement best programming practices. Prereq: MATH 2450 or equiv. or consent of instructor; MATH 1700 or equiv. introductory statistics course or consent of instructor, and programming competency in a high-level language.

Course Content

This course is designed to prepare students to be scientists, whether in industry or academia, who solve problems with computers and analyze data. We will cover computational problem solving paradigms, technical skills, and programming best practices.

The precise topics covered will be decided on-the-fly depending on the audience and how the course is progressing, but the list below gives a rough idea of topics that might be covered. (If you have suggestions for additional topics, I would love to hear them!)

- ◇ brief review of programming basics and introduction to Python
- ◇ unix command line
- ◇ algorithmic paradigms for problem solving (brute force, greedy algorithms, backtracking, binary search, divide-and-conquer)
- ◇ classic problem solving models (traveling salesman, knapsack, etc.)
- ◇ version control with git/github
- ◇ code coverage and unit testing

- ◇ metaheuristic optimization (hill climbing, simulated annealing, tabu search, particle swarm optimization, ant colony systems, genetic / evolutionary algorithms)
- ◇ graph algorithms (community detection, centrality, network flow)
- ◇ linear programming and mixed-integer programming

All of the problem solving techniques will be taught in a domain-agnostic manner, with the goal of understanding the essence of each method, so that students will later be able to apply them to problems from many different scientific fields. We will study the computational efficiency of each of the methods, as well as their strengths and weaknesses.

Textbook

There is no single textbook covering all of these topics, and so we do not have a required textbook. I will be using many textbooks and other resources to build the course, and I may occasionally recommend those resources for students who are interested in going deeper into the material.

Programming Language

This course will use *Python* extensively. Python is a free, easy-to-learn, flexible programming language that is among the most widely used in the world and in all kinds of industries, from banking to data science to Silicon Valley start-ups.

Students are expected to come into this course with proficiency in a high-level language (e.g., Java, C, C++, C#, Julia, Matlab, R), but not necessarily Python. *This is not a programming course*, and students are expected to have a solid understanding of programming basics (control flow, including 'if' statements and 'for' and 'while' loops), functions/methods, data types). We will use some object-oriented programming, so knowledge of this is a plus, but it is not required.

Course Structure

Assessments and Grading Scale

Grades will be based on homework assignments (50%), a midterm exam (25%), and a final exam (25%). Depending on how the course progresses, one homework assignment near the end of the course may be to read a research paper that involves a computational method we cover and present it to the class.

Late work may be accepted with penalty at my discretion.

The letter grade scale is as follows:

A:	$[90, \infty)\%$
A-:	$[86, 90)\%$
B+:	$[82, 86)\%$
B:	$[78, 82)\%$
B-:	$[74, 78)\%$
C+:	$[70, 74)\%$
C:	$[60, 70)\%$
F:	$[0, 60)\%$

Homework Collaboration Policy

Discussing course material with your classmates is a very important part of the learning process, and collaborative learning is highly encouraged. However, in a class like this where most assessment will be based on code that you have written, there is a fine line between productive discussion, and cheating. Discussing and brainstorming *together* is good, one person telling another person how to solve a problem is bad – collaboration should be on equal footing. To help us stay on the right side of this fine line, I have decided that *all coding* should be done independently. Do not share your code with any classmates before an assignment is due. (After an assignment is grading, comparing code for the purpose of learning from each other is a great idea.)

Another fine line is using other resources (e.g., online) for help. It is *completely fine* to use online resources for generic coding and Python questions (for example, "How do I sort a list in Python?"). It is fine to use external resources to learn more about a particular topic (for example, "What are some possible cooling schedules for simulated annealing?"). It is not okay to search for anything that directly answers the questions you have been assigned. For instance, if your assignment is to write code to apply the simulated annealing algorithm to the traveling salesman problem, it is considered cheating to search for anything like "Python code for simulated annealing" or "Python code for traveling salesman".

You are required to list all external resources used to complete your assignment. This includes names of any classmates you worked with. Failure to do so may be considered plagiarism.

If you are ever in doubt about what is allowed, please just ask me!

Attendance

You are expected to arrive in class on time, having completed any assigned readings and problems, ready to engage in class, ask questions, and discuss. If a session is missed, you are responsible for obtaining notes from a classmate.

Office Hours

Office hours are scheduled times that I will be available to help you with course material, including topics from lecture, homework questions, revisions, etc. You are *strongly encouraged* to come to office hours frequently! You don't need an appointment, you can come in and out at any time, and often office hours are empty so they are essentially free one-on-one help. Please watch this instructional and informative video about office hours: https://vimeo.com/270014784.

Grading Disputes

If you believe that I have made an error in scoring an assignment, you must bring it to my attention within one week of the graded paper being returned. I will carefully reread, and if necessary rescore, the assignment.

Classroom Conduct

The classroom is an interactive learning environment in which everyone should feel valued and comfortable. I strongly encourage you to ask questions and give answers throughout the term, even if (particularly if!) you're not sure that your answers are correct. This is an important part of the learning process.

Returned Papers

You must retain all returned papers in case of any discrepancy with the recorded grades on D2L. I cannot correct any mistakes in grading or recording of scores without the original document. All concerns regarding grades on assignments must be brought to me within one week of the return of the paper.

Accommodations and Special Needs

If you have a disability and require accommodations, please contact your instructor during the first week of class so that your learning needs may be appropriately met. You will need to provide documentation of your disability to the Office of Disability Services. If you are unsure of what you need to qualify for services, visit the Office of Disability Services' website at http://www.marquette.edu/disability-services or contact their office by phone at (414) 288-1645.

Excused Absences

Students with absences due to legal obligations, religious observances, or participation in Division 1 athletics and other university sanctioned events will be given an opportunity to make up examinations or other graded assignments, if a request is made to the instructor prior to the absence. After all absences, excused or unexcused, you are responsible for contacting your classmates to obtain lecture note and any other missed materials.