CS 468 / CS 568 / BME 568:
Computational Modeling for Bioengineering
Spring 2022
Syllabus

Matthew R. Lakin

January 11, 2022

COVID-19 syllabus language

UNM Administrative Mandate on Required Vaccinations

UNM requires COVID-19 vaccination and a booster for all students, faculty, and staff, or an approved exemption (see: UNM Administrative Mandate on Required Vaccinations). Proof of vaccination and booster, or a medical, religious, or online remote exemption, must be uploaded to the UNM vaccination verification site. Failure to provide this proof may result in a registration hold and/or disenrollment for students and disciplinary action for UNM employees.

Booster Requirement: Individuals who received their second dose of a Pfizer or Moderna vaccine on or before June 15, 2021, or their single dose of a Johnson & Johnson vaccine on or before October 15, 2021, *must provide documentation of receipt of a booster dose no later than January 17, 2022*.

Individuals who received their second dose of a Pfizer or Moderna vaccine after June 15, 2021 or who received their single dose of Johnson & Johnson after November 15, 2021 *must provide documentation of receipt of a booster within four weeks of eligibility*, according to the criteria provided by the FDA (6 months after completing an initial two-dose Moderna vaccine, 5 months after completing the Pfizer sequence, and 2 months after receiving a one-dose Johnson and Johnson vaccine).

International students: Consult with the Global Education Office.

Exemptions: Individuals who cannot yet obtain a booster due to illness should request a medical, religious, or online remote exemption (which may have an end date) and upload this to the vaccination verification site.

Medical and religious exemptions validated in Fall 2021 (see your email confirmation) are also valid for Spring 2022 *unless an end date was specified in the granting of a limited medical exemption*. Students must apply for a remote online exemption every semester.

UNM Requirement on Masking in Indoor Spaces

All students, staff, and instructors are required to wear face masks in indoor classes, labs, studios and meetings on UNM campuses, see the masking requirement. Students who do not wear a mask indoors on UNM campuses can expect to be asked to leave the classroom and to be dropped from a class if failure to wear a mask occurs more than once in that class. Students and employees who do not wear a mask in classrooms and other indoor public spaces on UNM campuses are subject to disciplinary actions. Medical/health grade masks are the best protection against the omicron variant and these masks should be used, rather than cloth.

COVID-19 Symptoms and Positive Test Results

Please do not come to a UNM campus if you are experiencing symptoms of illness, or have received a positive COVID-19 test (even if you have no symptoms). Contact your instructors and let them know that you should not come to class due to symptoms or diagnosis. Students who need support addressing a health or personal event or crisis can find it at the Lobo Respect Advocacy Center.

Course Information

Course title: Computational Modeling for Bioengineering.
Course numbers: CS468 / CS568 / BME568.
Course credits: 3.
Class meeting days: Tuesdays and Thursdays.
Class time: 3:30pm - 4:45pm.
Class room: Centennial Engineering Center room 1028.
Semester: Spring 2022.

Instructor

Name: Matthew Lakin.
Email: `mlakin@cs.unm.edu`
Office phone: (505) 277-3351.
Office hours: Mondays 2-4pm.
Office: Farris 3240.

Course delivery

This class will be offered via the "Face to Face" modality. Logistical details of midterm examinations will be decided closer to the time, but note that these will be required to be sat in person (excepting any accommodations administered by the ARC).

Course description

This course will cover the use of computational modeling as a tool for analyzing scientific data, making predictions based on that analysis, and rational design of engineered systems. The course and course examples will use the Python programming language. As such, the early part of the course will offer a brief overview of Python programming in general, and of the libraries used for the examples in the course.

The course will cover case studies of modeling applied to a range of scientific problems from the biological and chemical sciences and bioengineering. There will be a particular focus on modeling the kinetics of biomolecular interactions in various situations and at various levels of abstraction, including analysis of gene expression levels in genetic regulatory networks and predicting the behavior of engineered gene networks.

The course is intended for advanced undergraduate and graduate students in Computer Science and Biomedical Engineering. Prior experience with Python is helpful but not required. No knowledge of the specific scientific concepts used as examples will be assumed, but basic knowledge of scientific and mathematical fundamentals will be helpful.

The course will consist of lectures, occasional written, modeling, and programming assignments, and examinations.

Student learning outcomes

- Students can define the basic principles and concepts in scientific modeling.
- Students can select and apply appropriate tools to carry out scientific modeling tasks.
- Students can write and use Python scripts for scientific data analysis.
- Students can describe and apply basic principles of the case studies covered.

Textbook and course materials

The Python programming component of the course will broadly follow the textbook:

- "A Primer on Scientific Programming with Python (5th edition)" by Hans Petter Langtagen (ISBN: 978-3-662-49886-6).

This textbook can be downloaded for free in PDF format via the UNM network, from:

- https://link.springer.com/book/10.1007%2F978-3-662-49887-3

All lecture materials will be made available via UNM Learn.

The UNM Learn email list functionality will be used for administrative announcements.

Course requirements

You are expected to attend class regularly, read any assigned reading before class, and participate in class discussions.

Short written and/or programming homework assignments will be given to consolidate lecture material. In the early part of the course, these tasks will be drawn from the general domains of mathematics, science, and engineering, to practice programming skills; in the later part of the course the tasks will be drawn from the case studies covered in class.

There will be two in-class, closed book midterm exams.

Instead of a final exam there will be an individual final project, which will draw on the tools and techniques covered in the course to model and analyze the behavior of biological and chemical systems.

Grading

Final grades will be based on the sum of all possible course points. Grading option change requests will not be considered after the last class period. The contributions of homeworks, exams, and final projects to the overall course grade will be as follows:

- Homeworks: 30%
- Exams: 30% (15% for each midterm)
- Individual final project: 30%
- Quizzes: 10%

Course schedule

Broadly, the course will cover basic Python programming, theoretical preliminaries on chemical kinetics and chemical reaction networks, and case studies of computational modeling from the primary literature. Examples of case studies from the primary literature include:

- M. B. Elowitz and S. Leibler, "A synthetic oscillatory network of transcriptional regulators," Nature, vol. 403, pp. 335–338, 2000. DOI: 10.1038/35002125
- A. A. K. Nielsen, B. S. Der, J. Shin, P. Vaidyanathan, V. Paralanov, E. A. Strychalski, D. Ross, D. Densmore, and C. A. Voigt, "Genetic circuit design automation," Science, vol. 352, no. 6281, aac7341, 2016. DOI: 10.1126/science.aac7341
- M. W. Gander, J. D. Vrana, W. E. Voje, J. M. Carothers, and E. Klavins, "Digital logic circuits in yeast with CRISPR-dCas9 NOR gates," Nature Communications, vol. 8, p. 15 459, 2017. DOI: 10.1038/ncomms15459

- C. Y. Hu, M. K. Takahashi, Y. Zhang, and J. B. Lucks, "Engineering a functional small RNA negative autoregulation network with model-guided design," ACS Synthetic Biology, vol. 7, no. 6, pp. 1507–1518, 2018. DOI: 10.1021/acssynbio.7b00440

Credit-hour statement

This is a three credit-hour course. Class meets for two 75-minute sessions of direct instruction for fifteen weeks during the Fall 2021 semester. Students are expected to complete a minimum of six hours of out-of-class work (or homework, study, assignment completion, and class preparation) each week.

Academic integrity statement

Each student is expected to maintain the highest standards of honesty and integrity in academic and professional matters. The University reserves the right to take disciplinary action, up to and including dismissal, against any student who is found guilty of academic dishonesty or otherwise fails to meet the standards. Any student judged to have engaged in academic dishonesty in course work may receive a reduced or failing grade for the work in question and/or for the course.

Academic dishonesty includes, but is not limited to, dishonesty in quizzes, tests, or assignments; claiming credit for work not done or done by others; hindering the academic work of other students; misrepresenting academic or professional qualifications within or without the University; and nondisclosure or misrepresentation in filling out applications or other University records.

All students will be required to sign and submit a warning regarding issues of academic integrity and possible sanctions prior to any submissions being graded.

Accommodation statement

In accordance with University Policy 2310 and the Americans with Disabilities Act (ADA), academic accommodations may be made for any student who notifies the instructor of the need for an accommodation. It is imperative that you take the initiative to bring such needs to the instructors attention, as I am not legally permitted to inquire. Students who may require assistance in emergency evacuations should contact the instructor as to the most appropriate procedures to follow. Contact Accessibility Resource Center at 277-3506 or arcsrvs@unm.edu for additional information.

UNM is committed to providing courses that are inclusive and accessible for all participants. As your instructor, it is my objective to facilitate an accessible classroom setting, in which students have full access and opportunity. If you are experiencing physical or academic barriers, or concerns related to mental health, physical health and/or COVID-19, please consult with me after class, via email/phone or during office hours. You are also encouraged to contact Accessibility Resource Center at arcsrvs@unm.edu or by phone 277-3506.

Title IX statement

In an effort to meet obligations under Title IX, UNM faculty, Teaching Assistants, and Graduate Assistants are considered "responsible employees". This designation requires that any report of gender discrimination which includes sexual harassment, sexual misconduct and sexual violence made to a faculty member, TA, or GA must be reported to the Title IX Coordinator at the Office of Compliance, Ethics, and Equal Opportunity. For more information on the campus policy regarding sexual misconduct, see: `https://policy.unm.edu/university-policies/2000/2740.html`