Math 728 - Selected Topics in Applied Mathematics: Uncertainty Quantification in Physical and Biological Applications

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Office Hours: M 1:00-3:00PM,
Wed 10:00-11:00 AM, *and by appointment*
Class Hours: M/W/F 12:00-12:50PM
Office: LeConte 305 **Class Room**: LeConte 315

Course Description

Modeling and simulation provides an efficient way of understanding complex physical and biological problems, as well as making predictions for informed decision making. However, the underlying assumptions of the models and input parameters are subject to variability. This course will introduce the field of uncertainty quantification (UQ), including basic statistical methods, uncertainty propagation, inverse problem methodologies, surrogate modeling and emulation, and methods for handling model-form, parametric, and data induced uncertainty. The course will focus on the application of these methods to mathematical models in the physical and biological sciences.

Prerequisites

Students should have some background in MATLAB and/or Python programming. Some exposure to ordinary and partial differential equations (ODEs and PDEs) and their application to modeling and simulation is also recommended. Those with backgrounds in applied and computational mathematics, engineering, physical sciences, and statistics are strongly encouraged to take this course.

Required Materials

The course will follow the text *Uncertainty Quantification: Theory, Implementation, and Applications, Second Edition* by Ralph Smith (ISBN:978-1-61197-783-7). I will follow the content in the textbook, but will also provide my own notes where applicable. Those who are SIAM members can obtain a discount during purchase (those who are not SIAM members can join for relatively cheap). You can find the textbook here.

Course Objectives

Students taking this course will be encouraged to identify specific aspects of their research or future research and careers that will benefit from formal UQ methods. In particular, students enrolled in this course will

1. learn the basics behind common statistical distributions;
2. develop preliminary skills in computational modeling in physical and biological applications;
3. conduct model sensitivity analyses using local and global sensitivity analysis methods;
4. identify whether model parameters are identifiable given limited noisy data;
5. apply optimization and inference methodologies for model calibration;
6. contrast frequentest and Bayesian inference methods and results;
7. construct surrogate modeling (emulation) methods to speed up computational simulations;
8. explain uncertainty in both input (parameter) and output space for mathematical models, including in the presence of model discrepancy; and
9. implement algorithms from custom and open-source software packages to conduct UQ.

Students will be able to apply methods developed in this course to various modeling and simulation projects. These skills will be transferable to numerous careers, especially those in the geosciences, civil engineering, aerospace, mechanical engineering, epidemiological, and healthcare domains. In particular, students will become familiar with the following concepts:

- basic statistical distributions and their moments
- statistical characterizations of inverse problems
- numerical implementations to solve inverse problems
- local and global sensitivity analysis methods
- regularization for inverse problems
- uncertainty propgation
- Markov chain Monte Carlo (MCMC) methods
- Gaussian process emulation
- polynomial chaos expansions

- frequentist posterior uncertainty quantification
- Bayesian inference and Bayesian posterior uncertainty quantification
- model discrepancy

Tentative Course Schedule

While the course schedule will fluctuate, below the tentative schedule of content area and chapters from the textbook:

1. Applications and examples (0.5 weeks; chapters 2 and 3)
2. Fundamentals of probability, random processes, and statistics (1.5 weeks; chapters 4 and 6)
3. Representation of random inputs (1 week; chapter 5)
4. Parameter selection techniques, sensitivity analyses, active subspaces (3 weeks; chapters 7-10)
5. Frequentist and Bayesian model calibration (3 weeks; chapters 11-12)
6. Uncertainty propagation (2 weeks; chapter 13)
7. Model discrepancy (1 week; chapter 14)
8. Surrogate/reduced order modeling (2.5 weeks; chapters 15-19)
9. Sparse grids (0.5 weeks (if time allows) chapter 20)

Grading

Students will be assessed on weekly homework's (60% of the total grade) and a final project (40%). Students will be allowed to work in pairs on the homework, though an individual copy from each student will be required. Students will answer questions using both MATLAB/Python code and mathematical/statistical reasoning. Your attendance is paramount to success, and will ensure that the class collectively benefits all students. If you have an excused absence, please notify the instructor promptly and preferably 48 hours in advance. Grades will be assigned as:

A: 90-100

B+: 85-89, B: 80-84

C+: 75-79, C: 70-74

D+: 65-69, D: 60-64

F: 59 and below

Makeup Policy

Students missing homework deadlines will be given sufficient time to turn in homework late, **if the students notify the instructor at least 48 hours in advance of the due date.** Special situations will be considered. Please consult the Graduate Academic Regulations for full details.

Homework

Homework (60% of your grade) will be assigned throughout the semester, and may cover multiple sections of the textbook. A majority of the questions will be from the recommended text book. A hard copy of the homework is required. This can be typed (Word or LaTeX) or written, though MATLAB/Python figures will be necessary for some of the homework problems. You are more than welcome to work together on the homework, **but you must turn in your own individual copy in order to receive credit.** Disputes regarding homework grades should be brought to the instructors attention **no later than seven days after it is returned.** Partial credit will be provided when work is shown; however, solutions that do not have work or processes clearly laid out will not be able to receive partial credit. **Late homework will have 10% off per day it is late.**

Final Project

I will require each student to work on a final project, which will be turned in the last day of class. The final project should apply multiple methods discussed in the course to a specific problem they are interested in. This will require a mathematical model that is distinct from those used as examples in the class. I am more than happy to provide example models to any student who is unsure what to do. **Students will need to identify their final projects and discuss their tentative approach with the instructor by the halfway point in the course**. A final document will be required, as well as MATLAB/Python code that replicates the results of the final project.

Final Exam

There will be no exams or final exam. The final project will take the place of the final exam.

Academic Integrity Statement

Cheating and plagiarism will not be tolerated. While you are encouraged to discuss homework problems with others, it is expected that you provide your own homework solutions. Suspicions of alleged violations of Cheating –defined as “unauthorized assistance in connection with any academic work” and/or Falsification, which includes “Misrepresenting or misleading others with respect to academic work or misrepresenting facts for an academic advantage” – will be referred to the Office of Student Conduct and Academic Integrity. You are expected to practice the highest possible standards of academic integrity. Any deviation from this expectation will result in a minimum academic penalty of your failing the assignment and will result in additional disciplinary measures. The first tenet of the Carolinian Creed is, "I will practice personal and academic integrity." Students are expected to follow university guidelines: http://www.sc.edu/academicintegrity.

Disability Services

The Student Disability Resource Center (SDRC) empowers students to manage challenges and limitations imposed by disabilities. In order to receive reasonable accommodations from me, you must be registered with the Student Disability Resource Center (1705 College Street, Close-Hipp Suite 102, Columbia, SC 29208, 803-777-6142). Any student with a documented disability should contact the SDRC to make arrangements for appropriate accommodations. Once registered, students with disabilities are encouraged to contact me (within the first week of the semester) to discuss the logistics of any accommodations needed to fulfill course requirements.

Mental Health

If stress is impacting you or getting in the way of your ability to do your schoolwork, maintain relationships, eat, sleep, or enjoy yourself, then please reach out to any of USC's mental health resources. Most of these services are offered at no cost as they are covered by the Student Health Services tuition fee. For all available mental health resources, check the USC mental health website. The 24-hr Mental Health Support Line can be reached by phone at (833) 664-2854.