Validation and Uncertainty Quantification in Computational Models
CSCI 6166
Spring 2025

Instructor:

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Class details:

Class meetings: T-Th 12:30 - 1:45, KITT Central S161
Office hours: W 1:30 - 2:30 and by appointment

Materials:

Lecture notes (R. Morrison, R. Moser, and T. Portone)
Various papers and book chapters, all available on Canvas

References

[1] T. M. Cover and J. A. Thomas. *Elements of Information Theory.* Wiley-Interscience, 2nd edition, 2006.

[2] D. Gillies. *Philosophical Theories of Probability.* Routledge, 2000.

[3] C. Howson and P. Urbach. *Scientific Reasoning: The Bayesian Approach.* Open Court, 2005.

[4] E. T. Jaynes. *Probability Theory: The Logic of Science.* Cambridge University Press, 2003.

[5] G. J. Klir. *Uncertainty and Information: Foundations of Generalized Information Theory.* Wiley-IEEE Press, 2005.

[6] S. B. McGrayne. *The Theory That Would Not Die: How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines, and Emerged Triumphant from Two Centuries of Controversy.* Yale University Press, 2012.

[7] D. S. Sivia and J. Skilling. *Data Analysis: A Bayesian Tutorial.* Oxford University Press, 2006.

[8] R. C. Smith. *Uncertainty Quantification: Theory, Implementation, and Applications.* SIAM, 2014.

Course description

This is a course on assessing the reliability of computational models. Computational models are used to describe physical and engineering systems in nearly every aspect of our lives, from the way an airplane wing interacts with turbulent air to how the human heart pumps blood. We consider the (common) setting in which the system of interest is described by a mathematical model, which in turn is implemented and solved by the computational model. There are three major reasons model results might not be reliable: (1) The mathematical model may not be a good representation of the system of interest; (2) The inputs to the mathematical model (e.g., parameters, initial and boundary conditions) may be uncertain; and (3) The computation may yield results that are not consistent with the solution of the mathematical model. The first two are assessed through validation and uncertainty quantification, respectively. The third is the domain of verification and, while important, it is not considered here. In this course, we will learn to formulate and analyze representations of uncertainty and validation tests for computational models.

Course objectives

In this course, students will learn how to:

- Analyze mathematical models and identify potential sources of uncertainty
- Use and interpret probabilistic representations of uncertainty
- Apply Bayes' theorem in various settings
- Express incomplete information using the principle of maximum entropy
- Characterize the uncertainties in observational data
- Formulate representations of model inadequacy
- Perform model calibration and model selection using Bayesian inference
- Formulate and apply probabilistic validation criteria
- Assess the reliability of extrapolative predictions
- Communicate, via scientific writing, the (sometimes complex or nuanced) concepts we have reviewed in class

Course work and grading

To review and solidify the basic concepts of the course, students will solve a series of exercises as homework. There will also be some small "projects" to apply the concepts of the course to example problems, to be done in small groups (2 to 3 people). We will conclude the semester with final projects, in which students will apply the course concepts to an example of their choice. Selecting an area that is relevant to the student's research is encouraged.

Grades will be determined based on the following: homework (25%), group projects (25%), and final project (50%).

Tentative outline*

Week	Days	Textbook	Tuesday	Thursday	Notes
1	1/14, 16	Ch 1	Intros, do Hw0	Assign Hw1	
2	1/21, 23	Ch 1, 2		Assign Hw2, Hw1 due	
3	1/28, 30	Ch 2			
4	2/4, 6	Ch 2		Assign Hw3, Hw2 due	
5	2/11, 13	Ch 3			
6	2/18, 20	Ch 3		Assign P1, Hw3 due	
7	2/25, 27	Ch 3, 4			
8	3/4, 6	Ch 4		Assign P2, P1 due	
9	3/11, 13	Ch 4		Assign final project	
10	3/18, 20	Ch 4, 6		FPs0 due (discuss in class), P2 due	
11	3/25, 27	—	Spring Break		
12	4/1, 3	Ch 6	Assign P3		FPs1 – 3
13	4/8, 10	Ch 6		Assign P4, P3 due	FPs4 – 6
14	4/15, 17	Ch 6			FPs7 – 8
15	4/22, 24	—	FP days or guest lectures	P4 due	FP write-up
16	4/29, 5/1	—	Final presentations		

* Hw = homework, P = project, FP = final project, FPs1 = final project step 1 (and so on)