The University of Pittsburgh
Department of Mathematics

Presents

The Edmund R. Michalik
Distinguished Lecture in the
Mathematical Sciences

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The University of Texas Austin

Foundations of Predictive Computational Science:
Selection and Validation of Models of Complex Systems in the Presence of Uncertainty

Interest in a subject some call predictive computational science has emerged in recent years, mainly because of dramatic advances in computers and computational science. These advances have pushed computer modeling from a qualitative endeavor to a quantitative science in which specific predictions are sought as a basis for important, sometimes life and death, decisions: climate change, predictive medicine, design of new materials, drug design, manufacturing processes, and many other subjects. What has fueled concerns about computer predictions, and led to the study of predictive computational science, is their reliability. What factors determine the reliability of computer predictions, particularly in the presence of inevitable uncertainties? How can one quantify the uncertainty in computer predictions when every phase of the prediction process faces often confounding uncertainties: in observational data, in model selection, in model parameters, and in targeted quantities of interest?

This lecture presents an introduction to mathematical, statistical, and philosophical issues underlying computer predictions in the presence of uncertainties. It is argued that a Bayesian approach provides the most logical setting for addressing these issues, complimented with tools from information theory. We describe OPAL—the Occam Plausibility Algorithm, as an adaptive approach to model selection and validation. The process of selection, calibration, validation, and implementation of models of tumor growth and effects of cancer treatments is described as a canonical example of an application of principles of predictive science.

Reception Immediately Following the Lecture

This public lecture is part of an annual series in honor of Professor Edmund R. Michalik, established through a gift from the Michalik family.

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