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Report Title

Final Report: Uncertainty Quantification for Unobserved Variables in Dynamical Systems and Optimal Experimental Design

ABSTRACT

Dynamical systems are frequently used to model biological systems. When these models are fit to data it is necessary to ascertain the uncertainty in the model fit. In our work, we present prediction deviation, a metric of uncertainty that determines the extent to which observed data have constrained the model's predictions. This is accomplished by solving an optimization problem that searches for a pair of models that each provide a good fit for the observed data, yet have maximally different predictions. We developed a method for estimating a priori the impact that additional experiments would have on the prediction deviation, allowing the experimenter to design a set of experiments that would most reduce uncertainty. We used prediction deviation to assess uncertainty in a model of interferon-alpha inhibition of HIV infection, and to select a sequence of experiments that reduces this uncertainty. Finally we proved a theoretical result which shows that prediction deviation provides bounds on the trajectories of the underlying true model. These results show that prediction deviation is a meaningful metric of uncertainty that can be used for optimal experimental design. (Joint work with Ben Letham, Portia Letham, and Edward P. Browne)

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received	Paper
01/16/2017	1 Benjamin Letham, Portia A. Letham, Cynthia Rudin, Edward P. Browne. Prediction uncertainty and optimal experimental design for learning dynamical systems, Chaos: An Interdisciplinary Journal of Nonlinear Science, (): 063110. doi:
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Patents Submitted

Patents Awarded

Awards

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Cynthia Rudin	0.00						
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Inventions (DD882)

Scientific Progress

Our Chaos paper contains methodological advances, theoretical advances, and practical experimental advances. This final report is for a small grant that funded work on part of this paper.

Technology Transfer

Interactions with DARPA - I'm on the faculty advisory board for DARPA. This project was published in a top journal - it's a really stellar paper. I plan to continue this line of research, hoping to provide a software package and more methodology.