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Cynthia Rudin

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Massachusetts Institute of Technology (MIT
77 Massachusetts Ave.
NE18-901
Cambridge, MA 02139 -4307

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14. 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

15. SUBJECT TERMS
dynamical systems, optimal experimental design, differential equations, uncertainty quantification

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Cynthia Rudin
UU	UU	UU	UU		19b. TELEPHONE NUMBER 609-273-2777

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:
TOTAL:	**1**	

Number of Papers published in peer-reviewed journals:

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

Received		Paper
TOTAL:		

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received	Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Ben Letham	0.10	
FTE Equivalent:	**0.10**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Cynthia Rudin	0.00	
FTE Equivalent:	**0.00**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Ben Letham (.1)
Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

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.