



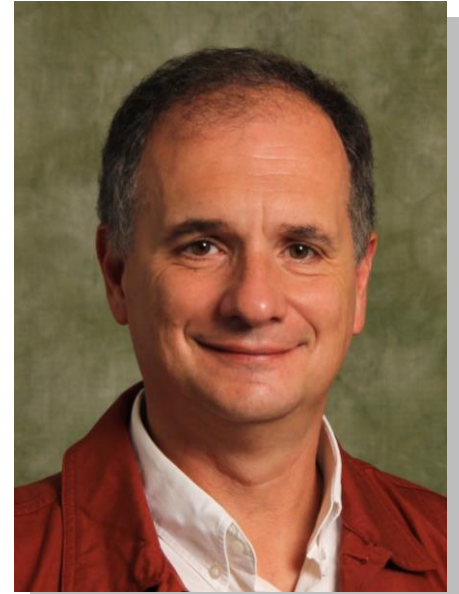
CoCo Seminar Series

Fall 2021

Towards Causal Explanation and Control of Complex (Biochemical) Systems

Dr. Luis Rocha
George J. Klir Professor of Systems Science
Binghamton University

Wednesday October 13, 2021 11:00am-12:00pm EDT
Hybrid (EB-T1 & Zoom; meeting link available on
<http://coco.binghamton.edu/>)



Inductive inference as used in most machine learning methods leads to biases and failures in predicting and controlling the multilevel complexity that defines humanity's most pressing problems. I will start by reviewing how systems science has dealt with this problem and led to the current complex systems methods that unite inductive and deductive strategies to design actionable models that can consider previously unseen scenarios. I will then present the contribution my research group has made to such (large team) pipelines with recent work on mapping causal interactions underlying genetic control and cellular signaling in complex biochemical networks. Our approach centers on identifying and removing redundancy present in the nonlinear interactions that define automata network models used in systems biology. Aggregating the necessary interactions results in the effective graph, a probabilistic but precise characterization of multivariate dynamics in a causal graph form. I will show that the effective graph provides an accurate explanation of how dynamical perturbation and control signals, such as those induced by cancer drug therapies, propagate in biochemical pathways. I will show, further, that it is possible to obtain a deterministic map that captures all possible roles that variables and interactions play in the logic of automata networks. To do so, a move is needed from simple weighted graphs to more complex multivariate relations such as hypergraphs or threshold networks with different types of nodes, such as the dynamics canalization map that I will also present. Both the effective graph and the dynamics canalization map can be computed for very large networks as the inference method scales linearly with number of nodes, though the former is more directly interpretable and amenable to the well-known graph-theoretical analysis and methods of network science. In either case, the methodology provides an analytical explanation of the causal relationships that arise from nonlinear network dynamics rather than from Monte Carlo simulations. I argue that such analysis leads to improved explainability, prediction, and control of complex dynamical systems in general and biochemical regulation in particular.

Dr. Luis Rocha is the George J. Klir Professor of Systems Science in the Department of Systems Science and Industrial Engineering at Binghamton University, State University of New York. He is also a Principal Investigator at the Instituto Gulbenkian da Ciencia in Portugal. His research interests include complex networks & systems, computational & systems biology, and computational intelligence. Dr. Rocha obtained his PhD in Systems Science at Binghamton University in 1997. He was a permanent staff scientist at the Los Alamos National Laboratory in 1998-2004 and then a professor of Informatics and director of the NSF-NRT Complex Networks and Systems graduate program at Indiana University, before joining Binghamton University in Fall 2021.

For more information, contact Hiroki Sayama (sayama@binghamton.edu).

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