Data-Driven Flow-Map Models for Data-Efficient Discovery of Dynamics and Fast Uncertainty Quantification of Biological and Biochemical Systems

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Abstract

Computational models are increasingly used to investigate and predict the complex dynamics of biological and biochemical systems. Nevertheless, governing equations of a biochemical system may not be (fully) known, which would necessitate learning the system dynamics directly from, often limited and noisy, observed data. On the other hand, when expensive models are available, systematic and efficient quantification of the effects of model uncertainties on quantities of interest can be an arduous task. This paper leverages the notion of flow-map (de)compositions to present a framework that can address both of these challenges via learning data-driven models useful for capturing the dynamical behavior of biochemical systems. Data-driven flow-map models seek to directly learn the integration operators of the governing differential equations in a black-box manner, irrespective of structure of the underlying equations. As such, they can serve as a flexible approach for deriving fast-to-evaluate surrogates for expensive computational models of system dynamics, or, alternatively, for reconstructing the long-term system dynamics via experimental observations. We present a data-efficient approach to data-driven flow-map modeling based on polynomial chaos Kriging. The approach is demonstrated for discovery of the dynamics of various benchmark systems and a co-culture bioreactor subject to external forcing, as well as for uncertainty quantification of a microbial electrosynthesis reactor. Such data-driven models and analyses of dynamical systems can be paramount in the design and optimization of bioprocesses and integrated biomanufacturing systems.

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