DOCTORAL THESIS

Machine Learning for Characterizing the Dynamics of Complex Systems: Methods and Applications

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Abstract

Complex systems are composed of multiple interconnected, interacting, and interdependent components and subsystems, and are often encountered in real-world scenarios. Modeling and understanding the dynamics of complex systems is a scientific challenge and a practical opportunity for professionals, such as scientists, engineers, and practitioners. This is because such efforts enable professionals to gain insights into how systems dynamical behavior evolves over time and thereby inform their strategies and decisions.

Model-based methods (i.e., simulations) are commonly adopted to represent certain behavioral features of complex systems based on predefined governing rules and/or parameterized equations. However, these methods can be very sensitive to model settings because of the high dependence of complex systems dynamical behavior on its initial conditions and parameters. Furthermore, the governing rules or parameters of a complex system are too complex to be unambiguously specified in reality.

Consequently, data-driven approaches, especially machine learning, have been recently introduced as an alternative to model-based methods. Instead of predefining models, data-driven methods learn models from data; that is, they understand the underlying relationships within complex systems by analyzing observations of their input and output (e.g., from historical data of systems behavior). Nevertheless, characterizing the behavior of complex systems using machine learning remains fundamentally challenging due to three key problems, which are defined in the research questions below.

1. How can we quantitatively model the interactions and interdependencies of multiple components of complex systems?
2. How can we appropriately represent and capture the dynamics of complex systems when we have only partial observations of the systems behavior?
3. How can we accurately characterize the aperiodic, irregular, or even chaotic behavior of complex systems?

In the work described in this thesis, we answer these three research questions in a systematic way by developing, analyzing, and demonstrating three innovative machine learning methods in the contexts of epidemiology and climatology, which are two fields of study that contain complex systems.

1. To answer the first question, we devise a physics-integrated learning method for an epidemiological scenario. This method quantifies the interdependencies of various components of complex systems by using human mobility data from different locations to construct a dynamical network between components/subsystems (i.e., metapopulations). We verify the effectiveness of the method by applying it to healthcare resource allocation.
2. To answer the second question, we devise a deep transfer learning method for an epidemiological scenario. This method learns epidemic dynamics in data-limited regions (i.e., target domains) by transferring useful information from a data-rich region (i.e., source domain). We theoretically demonstrate the adaptability of the method and empirically demonstrate its effectiveness in predicting infectious disease risk in data-limited regions.

3. To answer the third question, we devise a method denoted *Information-Tracking* for learning a climatological scenario. This method tracks and adapts to chaotic changes in a system's behavior by utilizing a probabilistic feedback mechanism to the forecast error of the next time step based on the current forecast. We provide a comprehensive theoretical analysis to guarantee the capability of the method to characterize the chaotic behavior of complex systems and illustrate its effectiveness in processing synthetic datasets and performing the challenging real-world task of decadal temperature prediction.

We conclude our thesis by summarizing its contributions and suggesting future research directions.

Keywords: Data-Driven Methods, Machine Learning, Complex Systems Dynamics, Subsystems Interactions, Partial Observations, Chaotic Behavior, Epidemiology, Climatology