Structural Inference of Networked Dynamical Systems with Universal Differential Equations[1]

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Networked dynamical systems are common throughout science in engineering; e.g., biological networks, reaction networks, power systems, and the like. For many such systems, nonlinearity drives populations of identical (or near-identical) units to exhibit a wide range of nontrivial behaviors, such as the emergence of coherent structures (e.g., waves and patterns) or otherwise notable dynamics (e.g., synchrony and chaos). For many such systems, one can construct equation-based models - in the form of coupled ordinary differential equations (ODEs) - that can successfully mimic these diverse behaviors.

The Kuramoto family of coupled oscillators [2] are among the simplest nonlinear oscillators that exhibit many of these qualitative behaviors of networked physical systems. The generic Kuramoto oscillator possesses an assumed natural frequency and an all-to-all (meaning each node is coupled with each other node) sinusoidal coupling. The utility of the Kuramoto model is enshrined in its simplicity: basic modifications to the network topology (encoded through an adjacency matrix) and coupling term can produce simple, interpretable models for chaos, turbulence, chimeras, and bifurcations between behaviors on an application-by-application basis. We are motivated by the inverse problem: given observations of these rich dynamics for a particular system, we wish to recover a interpretable model analogous to these graph-coupled Kuramoto oscillators. Furthermore, if successful in obtaining an appropriate model, we wish to investigate the potential to infer properties of networked systems with respect to network topology and/or external perturbations. In other words, we wish to answer hypotheticals such as "what would happen if we remove this node?"

Thus, in this work, we seek to (i) model the intrinsic physics of a base unit of a population, (ii) identify the underlying graphical structure shared between units, and (iii) model the coupling physics of a given networked dynamical system given observations of nodal states. We draw upon the graph-coupled Kuramoto oscillators as an appropriate ODE *ansatz* for our modeling task; that is, a population of 'units' with some intrinsic physics (evolving according to a natural frequency for the standard Kuramoto oscillator), connections forming a graph or network, and coupling physics acting on these pairwise connections.

These tasks are formulated around the notion of the Universal Differential Equation [3, 4], whereby unknown dynamical systems can be approximated with neural networks, mathematical terms known a priori (albeit with unknown parameterizations), or combinations of the two. For this work, the prior knowledge that we include in our model construction is the networked ODE ansatz inspired by the Kuramoto family of models. Because the structure of the model ODE is fixed by construction, we seek to learn effective models specifically for the units' intrinsic physics and coupling physics (with simple feed-forward neural networks) and the underlying connectivity of the units (i.e. an adjacency matrix). Learning an adjacency matrix from data can be ill-posed in general - to circumvent this, we assume that the true connectivity is sparse. We seek a sparse adjacency matrix (i.e. penalize dense connectivities). During training, the tunable parameters of the model (weights and biases of the neural networks and the entries in the adjacency matrix) are guided towards appropriate values through backpropagating residuals (weighted sum of time series MSE and sparsity penalty) through the chosen ODE solver.

The effectiveness and utility of these methods is shown with their application to (i) canonical networked nonlinear coupled oscillators and (ii) graph-coupled resistance-capacitance (RC) networks. For the former, we demonstrate the value of these inference tasks by investigating not only future state predictions but also the inference of system behavior on unseen network topologies. This is a challenging problem in which one needs to elicit not only the intrinsic physics of individual nodes of the network, but also what nodes talk to whom and how that communication influences nodal behaviors. For the latter, we demonstrate how the inclusion of prior knowledge (RC-based physics) with the networked ODE ansatz can provide estimates of nodal time constants.

While successful in a variety of synthetic experiments, the presented methodology has several limitations. First, assumed is that observations from the complete population of coupled units are observable, which is rarely the case. Similarly, the population of units was assumed to be homogeneous. Ultimately, the appropriateness of these assumptions should be evaluated in the context of the particular application, but deviations from these assumptions make for an increasingly complex learning problem (e.g. attempting to model an unknown number of heterogeneous interacting agents). These questions warrant future investigations on the robustness and applicability of the presented methods.

References

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