



Joint MUMS Program Transition - SPUQ Workshop
May 14-17, 2019
SPEAKER/ABSTRACT

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“Gaussian Process Model Assisted Active Learning of Physical Laws”

Abstract:

PDE and ODE are commonly used to describe a wide variety of physical phenomena such as sound, heat, diffusion, electrostatics, electrodynamics, fluid dynamics, elasticity, and quantum mechanics, etc. Discovering the governing equations from noisy data is an essential challenge in many areas of science and engineering, which is critical to understand the physical phenomena and predict the future behaviors of the dynamical system. However, in many cases, data are costly or time-consuming to obtain. Therefore, it is desirable to use the smallest possible amount of data to learn the PDE or ODE systems with a user-specified level of accuracy. To achieve this goal, this paper provides an active learning method to estimate the underlying PDE and ODE models. We propose an adaptive design criterion combining the D-optimality and the maximin space-filling criterion, with the weights automatically decided by the data. Different from the typical active learning methods for statistical models, the proposed design criterion involves both the function values and the different orders of derivatives, which are unobserved at the potential design points before data collection. Thus, we use the Gaussian process model to make predictions for these values at the potential design points. After the data collection, variable-selection-based regression methods are used to estimate the PDE or ODE models. The proposed active learning approach is entirely data-driven and requires no tuning parameters. Through three case studies of the commonly used PDE and ODE models, we show the proposed approach outperforms the current literature in terms of model accuracy and data economy.