

Chemical Engineering Dissertation Defense

Modern Data-Driven Approaches for Modeling and Control of Nonlinear Process Systems: Applications to Behavioral Medicine, Pandemic Preparedness, and Sustainability

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Abstract

This dissertation presents research aimed at addressing real-world challenges in healthcare, epidemiology, and sustainable industrial processes through judicious experiment design, principled data-driven dynamic modeling, and robust model predictive control. It is hypothesized and validated that, despite the complex, nonlinear, and uncertain nature of these systems, accessible yet powerful data-driven methods can be developed to meet rigorous performance and robustness criteria. With this aim, this dissertation develops a suite of approaches spanning three critical problems: designing input signals for informative, plant-friendly data generation, estimating meaningful predictive models, and formulating efficient closed-loop controllers robust to uncertainties and disturbances. Each method utilizes a priori system knowledge to balance judicious signal power allocation, model parsimony, simplified tuning, and is validated through experimental studies and realistic simulations across multiple applications.

Key contributions include stochastic search-based system identification and control tools that scale effectively to high-dimensional dynamics. Model-on-Demand (MoD)-based multivariable nonparametric frameworks are introduced for highly interacting nonlinear systems, eliminating reliance on global parametric models and shifting engineering effort from model selection to informative data collection, which underpins all modern data-driven approaches. These tools enable idiographic modeling of real-world behavioral data and support interventions that promote long-term, sustained improvements in physical activity.

The dissertation further develops control-relevant experiment design guidelines for identifying and controlling integrating processes, supported by experimental validation on a large-scale raceway photobioreactor in Almería, Spain. Constrained, plant-friendly excitation strategies suitable for safety-critical systems are also proposed, as demonstrated through benchmark epidemic models. Several advanced control algorithms are developed with an emphasis on intuitive tuning and constraint handling, including a three-degree-of-freedom (3DoF) Kalman filter-based MPC framework and a 3DoF-KF hybrid MPC that incorporates physical and societal constraints, enabling practically relevant epidemic control strategies.

Additionally, a 3DoF MoD-based MPC architecture integrating online estimation and control is proposed for highly nonlinear systems. A further key contribution is a Direct Weight Optimization (DWO)-based predictive control approach for operations under severe data limitations, including missingness, uncertainty, and sparsity, with significantly fewer user involvement compared to MoD-based methods. Collectively, these contributions bridge theoretical rigor and practical applicability, enabling sophisticated control strategies across diverse real-world systems.

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