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Kinetic Models by Physics-Informed Statistical Learning Methods

Accelerated stability studies are a fundamental tool in the development of pharmaceutical and vaccine products, enabling the prediction of long-term stability from short-term experiments conducted under stressed conditions. In this context, kinetic models—such as the Šesták–Berggren formulation combined with Arrhenius-type temperature dependence—are widely used to describe degradation processes. However, reliably estimating such models from limited, noisy data remains a challenging problem.

This work proposes a physics-informed statistical learning framework that integrates mechanistic knowledge, expressed through ordinary differential equations (ODEs), with experimental observations. The approach is formulated as a regularised regression problem, where a data-fitting term is combined with a penalty enforcing consistency with a parametrized dynamical system. This formulation enables a flexible balance between data-driven modelling and adherence to physical laws, improving robustness in data-scarce settings.

To address the resulting estimation problem, we adopt a hierarchical strategy that separates the reconstruction of the system trajectory from the estimation of the kinetic parameters, allowing for efficient computation. The proposed estimator is a flexible tool that allows accurate estimation of ODE parameters when the ODE model is well-specified, while still guaranteeing good predictive performance in the case of a misspecified regularizing model.

The methodology is validated through simulation studies and applied to real data from accelerated stability experiments on vaccine antigenicity decay. Results demonstrate improved predictive performance and more reliable parameter estimation, highlighting the potential of physics-informed approaches for kinetic modelling in pharmaceutical applications.

Special/ Invited session

Classification

Both methodology and application

Keywords

physics-informed nonparametric regression, inverse problems, kinetic modeling

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