Physics-Informed Neural Networks for Generalized Lotka-Volterra models: towards parameter estimation in microbial communities.

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We propose a Physics-Informed Neural Network (PINN) framework for parameter inference in Generalized Lotka-Volterra (GLV) models, motivated by the challenges of modeling microbial community dynamics under sparse, irregular, and noisy observational data. GLV systems are widely used to capture interaction patterns in microbial ecosystems, but their practical application is often hindered by the difficulty of accurately estimating interaction coefficients and growth rates from limited experimental data.

To address this, our approach embeds the GLV dynamics directly into the neural network's loss function as soft constraints, enabling the learning process to be guided not only by data fidelity but also by the underlying mechanistic structure. This dual supervision improves generalization, enhances robustness to noise and missing data, and promotes the identifiability of biologically meaningful parameters. Accurate inference of these parameters is essential for enabling systematic comparisons across experimental conditions, promoting data interoperability, and facilitating the integration of heterogeneous datasets collected under different protocols or time scales. Moreover, the method provides a flexible surrogate modeling tool that is both differentiable and scalable, allowing for its potential integration into broader digital twin frameworks for microbial ecosystems.

We demonstrate the efficacy of the approach using synthetic datasets designed to emulate experimentally realistic microbial dynamics, and evaluate its robustness under varying levels of measurement noise, uncertainty in initial conditions, and potential model misspecification. In addition to parameter recovery, we explore the interpretability and diagnostic potential of the trained PINN in uncovering structural features of the system and assessing model confidence.

This work, introduced in [1], positions PINNs as a powerful and generalizable framework for combining mechanistic modeling with modern machine learning techniques, offering a path forward for constructing interpretable, data-informed models in microbial ecology and beyond.

[1] P. J. Hossie, B. Laroche, T. Malou, L. Perrin, T. Saigre, L. Sala. *Surrogate modeling of interactions in microbial communities through physics-informed neural networks.*, 2025.

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