Spherical bacteria, re-identification of parameters in complex systems.

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Population dynamic models are valuable tools when combined with time series data of species abundances as they enable the inference of interactions. In the realm of microbiome research, comprehending microbial interactions is essential for achieving various objectives. These objectives include predicting population changes over time, assessing the impact of microbiome manipulations on dynamics, and designing synthetic microbiomes for specific tasks. Understanding the emergent behavior of complex systems, arising from the interactions among their constituent elements, presents a formidable yet crucial challenge in scientific exploration. Current model reduction techniques either have limited applicability or result in "black boxes" that lack a connection to the underlying microscopic physics.

In order to understand these models, parameter estimation from observational data is a typical problem, often approached through nonlinear least-squares minimization.

In this study, we examine a generalized Lotka-Volterra ecological model to assess the suitability of different approaches for parameter estimation. Firstly, synthetic data is generated using models with known parameters, and these parameters are then estimated using least square techniques to compare them with the original values. Additionally, a Bayesian model analysis is conducted. Although the model is structural identifiable[1], namely, all the parameters can be estimated *in principle*, we show that it is no practically identifiable (conditioned data) .

Furthermore, we perform a Model Reduction by Manifold Boundaries to identify parameter sets whose relationship makes re-identification impossible [2]. The parameter values of a model create a manifold within the space of data predictions. The goal of the minimization problem is to find the point on this manifold that best fits the experimental data. Using the model manifolds of Lotka-Volterra based models, we provide evidence that parameter inference in this type of models is not feasible, even in the case of 3 species. Moreover, it is important to note that the accurate capture of the sign of the interactions is generally impossible.
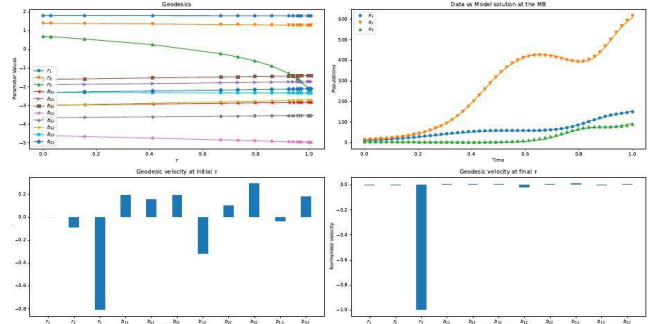

Fig. 1. In order to find the least relevant parameter combination, we identify the eigendirection of Fishers information matrix with smallest eigenvalue. We numerically construct a geodesic[4] from the initial parameters in this irrelevant direction until a boundary is identified. In the top left graph, we illustrate the evolution of geodesics for a 3-species LV model, which involves twelve parameters. By following a geodesic path towards the boundary of the manifold, it can be revealed a limiting behavior. Top right, the graph represents the data and the solution of the model. On the bottom, the geodesic velocity at the initial and final time is depicted.

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