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“Bayesian Parameter Estimation for Mathematical Models of Self-Organization and Biological Pattern Formation“

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ABSTRACT

This project is devoted to the development of a novel mathematical approach for data assimilation in mechanistic modeling of self-organization and biological pattern formation. We address questions of model selection and model calibration that are the main difficulty in mathematical modelling of spatio-temporal dynamics. In the project, we will develop a Bayesian methodology to estimate the parameters of the complex mathematical models based on information derived from the final pattern. A specific aim is to detect differences between two alternative biophysical mechanisms that have been so far indistinguishable given the experimentally observed pattern. It is a challenging problem, since patterns with fixed model parameters can significantly differ in location and shape due to small fluctuations of initial values, while being of the ''same'' type, thus requiring the comparison of families of patterns. This excludes standard estimation methods such as least squares.
Moreover, it is difficult to distinguish relative sensitivity to parameter change and to initial values, or to create a reliable cost function for parameter estimation. Currently this relies on tedious and subjective hand-tuning, while the goal of this project is to develop a statistically sound computational solution to the problem. Our approach employs dimension concepts of mathematical physics, which characterise the space-filling properties of the trajectory of a dynamical system. Instead of dimensions as such, we characterise the distance between point clouds by a summary statistic. Based on the empirical CDF of pairwise distances of observations from two attractors in phase space, the statistic is sensitive to changes in the underlying structure of the data. It provides a mapping from the original data to a Gaussian feature vector and allows for parameter estimation via adaptive MCMC. The method has been successfully applied to chaotic dynamical systems and has recently been modified for parameter estimation of Turing models on fixed domains by our collaborators. For genuine mechano-chemical models of self-organization, we will significantly improve the computational efficiency of the Bayesian methods via novel multilevel sampling strategies and surrogates for high-dimensional parametric PDEs.

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