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MODEL DISCRIMINATION BY RANDOM PATTERN DATA

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Mathematical models allow establishing a connection between a pattern observed on a macroscopic scale and a hypothetical underlying mechanism. But different mechanisms may result in a similar pattern. As a topical example, in developmental biology the de novo formation of periodic structures similar to purely chemical Turing patterns can also be obtained using mechano-chemical models with only one diffusing morphogen [1]. A computational approach allowing model calibration to a certain pattern will enable not only model identification based on experimental data but also comparison of different mechanisms. However, model parameter identification by pattern data only is challenging. Patterns obtained with fixed model parameter values but small random perturbations of the initial data will significantly differ in location and shape, while being of the "same" type. In this sense, for unknown initial values, each model parameter corresponds to a family of patterns rather than a fixed solution. This rules out the use of standard estimation methods such as least squares. Most typically, one has to resort to tedious and subjective hand-tuning. Here we present a solution for such problems. We consider classical Turing-type reaction-diffusion systems and one-dimensional mechano-chemical models of pattern formation with different coupling mechanisms between mechanical and chemical parts. The problem of parameter identification for these models is analogous to the identification of chaotic systems: in both cases slightly different initial values lead to different solutions which, however, can be considered to belong to the same family of solutions. So we modify a recently developed statistical approach for parameter studies of chaotic systems to the non-chaotic reaction-diffusion systems and mechano-chemical models. We demonstrate how the approach provides a cost function that enables a statistically sound identification of the model parameters by steady-state pattern data only, without known initial values or transient data. This is the situation often faced in experimental work. The accuracy of the cost function is verified by adaptive MCMC methods.

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