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Parameter identification for chaotic dynamical systems via optimal transport

Parameter identification determines the essential system parameters required to build real-world dynamical systems by fusing crucial physical relationships and experimental data. However, the data-driven approach faces main difficulties, such as a lack of observational data, discontinuous or inconsistent time trajectories, and noisy measurements. The ill-posedness of the inverse problem comes from the chaotic divergence of the forward dynamics. Motivated by the challenges, we shift from the Lagrangian particle perspective to the state space flow field's Eulerian description. Instead of using pure time trajectories as the inference data, we treat statistics accumulated from the Direct Numerical Simulation (DNS) as the observable, whose continuous analog is the steady-state probability density function (PDF) of the corresponding Fokker–Planck equation (FPE). We reformulate the original parameter identification problem as a data-fitting, PDE-constrained optimization problem. An upwind scheme based on the finite-volume method that enforces mass conservation and positivity preserving is used to discretize the forward problem. We present theoretical regularity analysis for evaluating gradients of optimal transport costs and introduce three different formulations for efficient gradient calculation. Numerical results using the quadratic Wasserstein metric from optimal transport demonstrate this novel approach's robustness for chaotic dynamical system parameter identification.