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Analysis of Kolmogorov flow and Rayleigh–Bénard convection using persistent homology

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ABSTRACT

We use persistent homology to build a quantitative understanding of large complex systems that are driven far-from-equilibrium. In particular, we analyze image time series of flow field patterns from numerical simulations of two important problems in fluid dynamics: Kolmogorov flow and Rayleigh–Bénard convection. For each image we compute a persistence diagram to yield a reduced description of the flow field; by applying different metrics to the space of persistence diagrams, we relate characteristic features in persistence diagrams to the geometry of the corresponding flow patterns. We also examine the dynamics of the flow patterns by a second application of persistent homology to the time series of persistence diagrams. We demonstrate that persistent homology provides an effective method both for quotienting out symmetries in families of solutions and for identifying multiscale recurrent dynamics. Our approach is quite general and it is anticipated to be applicable to a broad range of open problems exhibiting complex spatio-temporal behavior.

1. Introduction

We introduce new mathematical techniques for analyzing complex spatiotemporal nonlinear dynamics and demonstrate their efficacy in problems from two different paradigms in hydrodynamics. Our approach employs methods from algebraic topology; earlier efforts have shown that computing the homology of topological spaces associated to scalar or vector fields generated by complex systems can provide new insights into dynamics [1–6]. We extend prior work by using a relatively new tool called persistent homology [7–9].

Complex spatiotemporal systems often exhibit complicated pattern evolution. The patterns are given by scalar or vector fields representing the state of the system under study. Persistent homology can be viewed as a map PD that assigns to every field a collection of points in $\mathbb{R}^2$, called a *persistence diagram*. For a given scalar field $f: D \to R$, the points in the persistence diagram $\mathsf{PD}(f) = \{\mathsf{PD}_k(f)\}_{k=0}^{\infty}$ encode geometric features of the sub-level sets $\mathsf{C}(f, \theta) = \{x \in D \mid f(x) \leq \theta\}$ for all values of θ. A feature encoded by the point $(\theta_b, \theta_d) \in \mathsf{PD}_k(f)$ represents a feature at the kth homology level that appears in $\mathsf{C}(f, \theta_b)$ for the first time and disappears in $\mathsf{C}(f, \theta_d)$. Therefore, θ_b and θ_d are called birth and death coordinates of this feature. The lifespan $\theta_d - \theta_b > 0$ indicates the prominence of the feature. In particular, features with long lifespans are considered important and features with short lifespans are often associated with noise. Thus, the persistence diagram is a highly simplified representation of the field generating the pattern.

The space of all persistence diagrams, Per, can be endowed with a variety of metrics under which PD is a Lipschitz function. This has several important implications that we exploit in this paper. First, the Lipschitz property implies that small changes in the field pattern, e.g. bounded errors associated with measurements or numerical approximations, lead to small changes in the persistence diagrams. Second, by using different metrics, we can vary our focus of interest between larger and smaller changes in the persistence diagrams. Moreover, by comparing different metrics, we can infer if the changes in a pattern affect geometric features

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with longer or shorter life spans. Finally, since, applying the map PD to a time series of patterns produces a time series in Per, the distance between the consecutive data points in Per can be used to quantify the average rate at which the geometry of the patterns is changing.

As mentioned above, the dynamics of spatiotemporal systems are characterized by the time-evolution of the patterns corresponding to the fields generated by the system. However, capturing these vector fields, either experimentally or numerically, results in multi-scale high dimensional data sets. In order to efficiently analyze these data sets, a dimension reduction must be performed. We use persistent homology to perform nonlinear dimension reduction from a time series of patterns to a time series of persistence diagrams. We show that this reduction can cope with redundancies introduced by symmetries (both discrete and continuous) present in the system. In particular, this approach directly quotients out symmetries and, thereby, permits easy identification of solutions that lie on a group orbit. Alternative approaches to nonlinear dimension and symmetry reduction include both the method of slices [10] and recent advances in identifying unstable exact solutions of nonlinear partial differential equations [11]. While a detailed comparison of these methods is beyond the scope of this paper, it is worth pointing out that the application of persistent homology does not rely on knowledge of the underlying governing equations.

Separately, we also apply persistent homology to extract information about dynamical structures in the reduced data. Characterizing dynamics in the space of persistence diagrams cannot be done using conventional methods (e.g., time delay embeddings), since choosing a coordinate system in Per is currently an open problem [12]. However, since Per is a metric space, the geometry of the point cloud X, generated by the time series of the reduced data, is encoded by a scalar field which assigns to each point in Per its distance to X. We show how persistent homology may be applied to describe dynamics by characterizing the geometry of X.

An outline of the paper is as follows. In Section 2 we present a brief overview of the two fluid flows examined in this paper: (1) Kolmogorov flow and (2) Rayleigh–Bénard convection. We note here, for emphasis, that while persistent homology can be applied to vector fields, it will be sufficient for this paper to focus on scalar fields drawn from these systems (specifically, one component of the vorticity field for Kolmogorov flow, and the temperature field for Rayleigh–Bénard convection).

In Section 3 we discuss key issues related to the application of persistent homology. By now, the mathematical theory of persistent homology is well developed. Therefore, our main emphasis is on the computational aspect of passing from the data to the persistence diagrams. Section 4 describes the correspondence between the geometric features of a scalar field and the points in its corresponding persistence diagram. Section 5 discusses the structure of the space Per and the properties of the associated metrics.

In Sections 6 and 7 we discuss how these metrics can be used to analyze dynamics. First, we interpret distance between the persistence diagrams representing the consecutive data points in the time series as a rate at which geometry of the corresponding scalar fields is changing. Second, we motivate and explain the procedure for extracting the geometric structure of the point cloud in Per.

We close the paper by applying the developed techniques to the following problems. In Section 8, we identify distinct classes of symmetry-related equilibria for Kolmogorov flow. In Section 9, we show that a relative periodic orbit for Kolmogorov flow collapses to a closed loop in Per. Finally, in Section 10, we deal with identifying recurrent dynamics that occur on different time scales in our study of Rayleigh–Bénard convection flow.

2. The systems to be studied

2.1. Kolmogorov flow

For the study of turbulence in two dimensions, Kolmogorov proposed a model flow where the evolution of a two-dimensional (2D) velocity field $\mathbf{u}(x, y, t)$ is given by

$$\frac{\partial \mathbf{u}}{\partial t} + \beta \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} - \alpha \mathbf{u} + \mathbf{f} \qquad (1)$$
$$\nabla \cdot \mathbf{u} = 0$$

(with $\beta = 1$ and $\alpha = 0$). In the above equation, $p(x, y)$ is the pressure field, ν is the kinematic viscosity, ρ is fluid density, and $\mathbf{f} = \chi \sin(\kappa y)\hat{\mathbf{x}}$ is the forcing that drives the flow [13]. Laboratory experiments in electromagnetically-driven shallow layers of electrolyte can exhibit flow dynamics that are well-described by Eqs. (1) with appropriate choices of β and α to capture three-dimensional effects, which are commonly present in experiments [14]. In this paper, we refer to all models described by Eqs. (1) (including experimentally-realistic versions) as Kolmogorov flows.

It is convenient to use the vorticity–stream function formulation [15] to study Kolmogorov flow analytically and numerically. Eqs. (1), written in terms of the z-component of the vorticity field $\omega = (\nabla \times \mathbf{u}) \cdot \hat{\mathbf{k}}$, a scalar field, take the form

$$\frac{\partial \omega}{\partial t} + \beta \mathbf{u} \cdot \nabla \omega = \nu \nabla^2 \omega - \alpha \omega + \chi \kappa \cos(\kappa y). \qquad (2)$$

For the current study, we choose $\beta = 0.83$, $\nu = 3.26 \times 10^{-6}$ m^2/s, $\alpha = 0.063$ s^{-1}, $\rho = 959$ kg/m^3, and $\lambda = 2\pi/\kappa = 0.0254$ m. We express the strength of the forcing in terms of a non-dimensional parameter, the Reynolds number $Re = \sqrt{\frac{\lambda^3 \chi}{8\nu^2}}$.

Eq. (2) is solved numerically by using a semi-discrete, pseudo-spectral method [16], assuming periodic boundary conditions in both x and y directions, i.e., $\omega(x, y) = \omega(x + L_x, y) = \omega(x, y + L_y)$, where $L_x = 0.085$ m and $L_y = 4\lambda = 0.1016$ m are the dimensions of the domain in the x and y directions, respectively. The vorticity field is discretized in the Fourier space using 128×128 modes, which corresponds to spatially resolving the domain on a 2D mesh with spacing $\Delta x = L_x/128$ and $\Delta y = L_y/128$ in the x and y directions, respectively. A time step of $dt = 1/32$ is chosen for the temporal discretization.

It is important to note that Eq. (2), with periodic boundary conditions, is invariant under any combination of three distinct coordinate transformations: (1) a translation along x: $\mathcal{T}_{\delta x}(x, y) = (x + \delta x, y)$, $\delta x \in [0, L_x]$; (2) a rotation by π: $\mathcal{R}(x, y) = (-x, -y)$; and (3) a reflection and a shift: $\mathcal{D}(x, y) = (-x, y + \lambda/2)$. Because of these symmetries, each particular solution to Eq. (2) generates a set of solutions which are dynamically equivalent. Physically, invariance under continuous translation leads to the existence of relative equilibria (REQ) and relative periodic orbit (RPO) solutions, in addition to equilibria (EQ) and periodic orbit (PO) solutions.

For $Re = 25.43$, the flow is characterized by a steady RPO; Fig. 1(a) shows a projection, plotted using the three dominant Fourier modes of this RPO. The RPO has a period 34.78 s and a drift speed 1.354×10^{-6} m/s. The tunnel-like structure is a result of the periodic motion superposed over the slow drift along the x-direction. For larger forcing ($Re = 26.43$), the flow becomes weakly turbulent, as can be seen from the Fourier projections in Fig. 1(b). The turbulent dynamics in this regime are of great interest as the flow explores a region of the state space which contains "weakly" unstable EQ, PO, REQ, and RPO solutions. Recent theoretical advances have shown that the identification of these solutions could aid the understanding of weakly turbulent dynamics [17].