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Almost-invariant sets and invariant manifolds — Connecting probabilistic and geometric descriptions of coherent structures in flows

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ABSTRACT

We study the transport and mixing properties of flows in a variety of settings, connecting the classical geometrical approach via invariant manifolds with a probabilistic approach via transfer operators. For non-divergent fluid-like flows, we demonstrate that eigenvectors of numerical transfer operators efficiently decompose the domain into invariant regions. For dissipative chaotic flows such a decomposition into invariant regions does not exist; instead, the transfer operator approach detects *almost*-invariant sets. We demonstrate numerically that the boundaries of these almost-invariant regions are predominantly comprised of segments of co-dimension 1 invariant manifolds. For a mixing periodically driven fluid-like flow we show that while sets bounded by stable and unstable manifolds are almost-invariant, the transfer operator approach can identify almost-invariant sets with smaller mass leakage. Thus the transport mechanism of lobe dynamics need not correspond to minimal transport.

The transfer operator approach is purely probabilistic; it directly determines those regions that minimally mix with their surroundings. The almost-invariant regions are identified via eigenvectors of a transfer operator and are ranked by the corresponding eigenvalues in the order of the sets' invariance or "leakiness". While we demonstrate that the almost-invariant sets are often bounded by segments of invariant manifolds, without such a ranking it is not at all clear *which* intersections of invariant manifolds form the major barriers to mixing. Furthermore, in some cases invariant manifolds do not bound sets of minimal leakage.

Our transfer operator constructions are very simple and fast to implement; they require a sample of short trajectories, followed by eigenvector calculations of a sparse matrix.

1. Introduction

Transport and mixing processes play an important role in many natural phenomena and their mathematical analysis has received considerable interest in the last two decades. Areas of application include astrodynamics, molecular dynamics, fluid dynamics, and ocean dynamics; see e.g. [1–4] for discussions of transport phenomena. Analytical and numerical treatments of transport typically assume that the motion of a passive particle is completely determined by an underlying autonomous or nonautonomous velocity field. A variety of different concepts from dynamical systems theory may then be used to detect barriers to particle transport, to explain the transport mechanisms at work, and to quantify transport in terms of transition rates or probabilities. Two different families of approaches have been developed in the past for the analysis of transport and mixing processes in dynamical systems: (i) *geometric* methods which make use of invariant manifolds and related concepts and (ii) *probabilistic* techniques which attempt to approximate so-called almost-invariant sets. One of the main aims of this work is to demonstrate numerically in a number of case studies that there is a strong connection between the two approaches and that the combination of the two types of analyses leads to a richer understanding of the global dynamics.

The notion that geometrical structures such as invariant manifolds play a key role in dynamical transport and mixing for fluid-like flows has been around for almost two decades. In autonomous settings, invariant cylinders and tori form impenetrable dynamical barriers. This follows directly from the uniqueness of trajectories of the underlying ordinary differential equation (ODE). Slow mixing and transport in periodically driven maps and flows can sometimes be explained by lobe dynamics of invariant manifolds [5,6,3]. In non-periodic time-dependent settings, finite-time hyperbolic material lines [7] and surfaces [8] have been proposed as barriers to mixing. Both the theoretical and the numerical analysis of these Lagrangian coherent structures in mixing fluids in many different application areas has been the focus of considerable interest over the last decade and a half, see e.g. [7–13], and the references therein.

Unions of segments of invariant manifolds may form either complete or partial boundaries of regions that are completely or

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Probabilistic Description of Dynamics
Transfer Operator
Almost-invariant Sets

Identifies which geometric structures are the strongest barriers to global mixing $\downarrow$

$\uparrow$ Further informs the dynamics underlying almost-invariant sets

Geometric Description of Dynamics
Invariant Manifolds

Fig. 1. Connecting the probabilistic and the geometric approaches.

partially dynamically isolated. These dynamically isolated regions are either invariant sets or *almost-invariant* sets. One of the main aims of this work is to demonstrate numerically that the regions that are *maximally* almost-invariant often have boundaries comprised of segments of invariant manifolds.

Almost-invariant sets arose in the context of smooth maps and flows on subsets of $\mathbb{R}^d$ [14,15] about a decade ago. The main theoretical and computational tool is the Perron–Frobenius (or transfer) operator, and almost-invariant sets were estimated heuristically from eigenfunctions of the Perron–Frobenius operator. Further theoretical and computational extensions have since been constructed [16–18]. A parallel series of work specific to time-symmetric Markov processes and applied to identifying molecular conformations was developed in [19] and surveyed in [19,20]. The constructions of [20] are transfer operator based and the transfer operator is derived directly from ensemble simulation of the dynamics. Related ideas have also been developed for finite-state Markov chains [21,22], where the starting point is a Markov chain model of some physical system that is similar in spirit to a transfer operator.

Connections between eigenmodes of evolution operators and slow mixing in fluid flow have recently begun to appear. Liu and Haller [23] observe via simulation a transient "strange eigenmode" as predicted by classical Floquet theory. Pikovsky and Popovych [24,25] numerically integrated an advection–diffusion equation to simulate the evolution of a passive scalar, observing that it is the subdominant eigenmode of the corresponding transfer operator that describes the most persistent deviation from the unique steady state. The particular form of flow used in [24,25] admitted a convenient Fourier series representation that allowed calculation of leading eigenmodes. The numerical methods we describe in the present paper can be used to estimate eigenmodes for flows that are continuous in space and time and require only the calculation of many short trajectories.

Prior work related to connections between geometric and statistical objects include [26,27], where ergodic averages of observables have been used to identify *invariant* sets in autonomous and periodically driven fluid-like flows in two and three dimensions. Connections with finite-time invariant manifolds have been studied numerically in the aperiodically driven setting [28]. The approaches [26–28] have the disadvantages of (i) requiring possibly lengthy integration times and (ii) the ambiguity of selecting an observable to ergodically average. In contrast, our transfer operator approach employs relatively short integration times and directly constructs slow eigenmodes that carry information about invariant and almost-invariant sets. The first connection between almost-invariant sets and invariant manifolds appeared in [29], where graph algorithms were applied to analyse transport in astrodynamics. The present paper significantly extends the results of [29] by treating a wide variety of systems and framing the probabilistic approach in terms of eigenfunctions of transfer operators rather than graph partitioning. The spectral approach is more natural, especially under variation of initial flow times and flow durations and delivers significant benefits in terms of the transfer operator describing the global dynamics.

In this work via a number of case studies in two and three dimensions, for autonomous and time-periodic flows, and for fluid-like and dissipative flows, we compare the geometric, manifold based decomposition of the phase space with the decomposition provided by the transfer operator approach. We will show that the two approaches are largely compatible in the sense that the manifolds often form at least partial boundaries of the regions identified by the transfer operator approach. In such situations the methods are complementary: (see also Fig. 1)

- the probabilistic approach determines which regions are the most dynamically isolated and therefore which manifold intersections are the most important in defining the boundaries of such regions,
- recognising that the boundaries of the almost-invariant regions are pieces of invariant manifold allows a more detailed understanding of the dynamics near the boundaries of the sets and how transport occurs in and out of the almost-invariant regions.

An outline of this paper is as follows. In Section 2 we provide background definitions for invariant sets, invariant measures, and ergodic measures, and summarise the four dynamical settings we will investigate. In Section 3 we define almost-invariant sets and the Perron–Frobenius operator. We then describe our numerical method for producing a finite-rank approximation of the operator and detail an algorithm for using eigenvectors of this finite-rank operator to determine almost-invariant sets. In Section 4 we investigate the connection between the probabilistic description of coherent structures via almost-invariant sets and the geometric description using invariant manifolds. Sections 5–8 contain our four major case studies in which we demonstrate the efficiency of the transfer operator approach in determining and extracting the largest, most coherent structures. In each case study we additionally compute major geometrical structures and demonstrate a high degree of correlation between the geometric structures and the almost-invariant sets. We find one exception to this correlation in the second part of our final case study where we show that lobe related transport need not correspond to minimal leakage from a set.

2. Background: Flows, invariant sets, and invariant measures

Let $M \subset \mathbb{R}^d$ be compact and $F : M \times \mathbb{R} \to \mathbb{R}^d$ be a smooth vector field. Let m denote Lebesgue measure, normalised so that $m(M) = 1$. We consider the ODE

$$\dot{x} = F(x, t). \tag{1}$$

In the case where $F(x, t) = F(x)$, we will call the ODE *autonomous*, otherwise we call it *nonautonomous* or *time-dependent*. Let $\phi_\tau : M \times \mathbb{R} \to M$ be the flow, i.e. $\phi_\tau(x_0, t_0)$ is a solution to the ODE (1) with initial condition $x(t_0) = x_0$ and satisfies

$$\frac{\mathrm{d}\phi_\tau}{\mathrm{d}\tau}(x_0, t_0)|_{\tau=0} = F(x_0, t_0), \quad \text{for all } x_0 \in M, t_0 \in \mathbb{R}. \tag{2}$$