Robustness of coherent sets computations

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Summary. The notion of coherence in time-dependent dynamical systems refers to mobile sets that do not freely mix with the surrounding regions in phase space. Coherent sets can be identified using set-oriented numerical methods involving transfer operators. Typically, such approach relies on the integration of a large number of particle trajectories computed from test points initialized in the elements of a fine partition of phase space. This can be prohibitively expensive in complex flows involving turbulence. Here, we systematically study the robustness of such computations in an example system. We demonstrate that the transfer operator based framework still gives reliable results even when both the number of partition elements and the number of test points are reduced significantly.

Introduction

Set-oriented numerical methods involving transfer operators have only recently been recognized as powerful tools for analyzing and quantifying transport processes in time-dependent flows. Central to this concept are coherent sets [1, 2, 3], mobile regions in phase space that move about with minimal dispersion. Coherent sets can be efficiently identified via Perron-Frobenius operators (or transfer operators). These linear Markov operators can be approximated within a set-oriented framework. Subdominant singular vectors of the resulting stochastic matrices are heuristically used to determine the structures of interest. However, a systematic analysis of the robustness of the results is still missing.
In this contribution, we will briefly review the transfer operator based framework for the description of coherent behavior and its numerical treatment within a set-oriented approach. We will discuss the different discretization steps required for the identification of coherent sets and systematically study the robustness of the results in an example system.

Coherent sets and transfer operators

We consider a flow map $\Phi(\cdot; t, \tau) : X \to X$, $X \subset \mathbb{R}^d$, where $\Phi(x; t, \tau)$ maps a point x initialized at time t to its position at time $t + \tau$. Following [1], coherent sets are defined as pairs $(A_t, A_{t+\tau})$, where A_t and $A_{t+\tau}$ are "regular" subsets of X at times t and $t + \tau$, respectively, such that

$$\rho(A_t, A_{t+\tau}) = \frac{\mu(A_t \cap \Phi(A_{t+\tau}; t + \tau, -\tau))}{\mu(A_t)}, \tag{1}$$

is maximized (subject to regularizing constraints). Here μ is a probability measure (e.g. normalized volume). This problem is NP-hard, but can be termed as an optimization problem involving transfer operators. The Perron-Frobenius operator $\mathcal{P}_{t,\tau} : L^1(X, m) \circlearrowleft$ related to the flow map $\Phi(\cdot; t, \tau)$ is defined by $\mathcal{P}_{t,\tau} f(x) = \frac{f(\Phi(x,t+\tau,-\tau))}{|\det D\Phi(\Phi(x,t+\tau,-\tau),t,\tau)|}$. So if $f(x)$ is a density at time t, $\mathcal{P}_{t,\tau} f(x)$ describes the density at time $t+\tau$ under the action of the flow map. As shown in [2, 3], the left and right singular vectors to the second largest singular value of a compact operator $\mathcal{L}_{t,\tau}$ similar to $\mathcal{P}_{t,\tau}$ serve as relaxed indicator functions of the sets of interest. To be more precise, $\mathcal{L}_{t,\tau} f := \mathcal{D}_\epsilon \mathcal{P}_{t,\tau} \mathcal{D}_\epsilon (f \cdot h_\mu)/(\mathcal{D}_\epsilon \mathcal{P}_{t,\tau} \mathcal{D}_\epsilon (h_\mu))$ where $\mathcal{D}_\epsilon$ is a diffusion operator and h_μ denotes the particle density (of the measure μ on X) [2, 3].

Set-oriented numerical approach

Using Ulam's method, a finite-rank approximation of $\mathcal{P}_{t,\tau}$ can be numerically constructed as the row-stochastic matrix

$$P_{ij} = \frac{vol(B_i \cap \Phi(B_j, t + \tau, -\tau))}{vol(B_i)}, \tag{2}$$

where $\{B_1, \ldots, B_n\}$ is a fine partition of X (e.g. obtained by taking a grid on X), $n \in \mathbb{N}$ and vol denotes the volume (Lebesgue) measure on X [4].
In practice, the entries P_{ij} of the transition matrix are estimated by the proportion of test points $x_{i,k}$, $k = 1, \ldots, N$, initialized in B_i that will be mapped to B_j under the action of the flow map. The corresponding matrix L is obtained by a similarity transformation of P. For this, the reference probability measure μ at time t is represented as a probability vector p with $p_i = \mu(B_i)$, $i = 1, \ldots, k$. The image probability vector at time $t + \tau$ is then simply computed as $q = pP$. Assuming only positive components in p, q, we form L via $L_{ij} = \frac{p_i P_{ij}}{q_j}$. Coherent sets are approximated via a line search on the second singular vectors of the resulting sparse stochastic matrix L [1, 2, 3], or more generally, by a k-clustering of the k leading singular vectors.
Obviously, the discretization of the transfer operator is determined (i) by the fineness of the partition $\{B_1, \ldots, B_n\}$ of X, and (ii) by the number N of test points initialized in each partition element. As the resulting computational effort depends crucially on the overall number of trajectories needed (i.e. $n \cdot N$), the question is: How robust are the results with respect to changes in (i) and (ii)? This will be systematically analyzed in the Bickley jet flow [5].

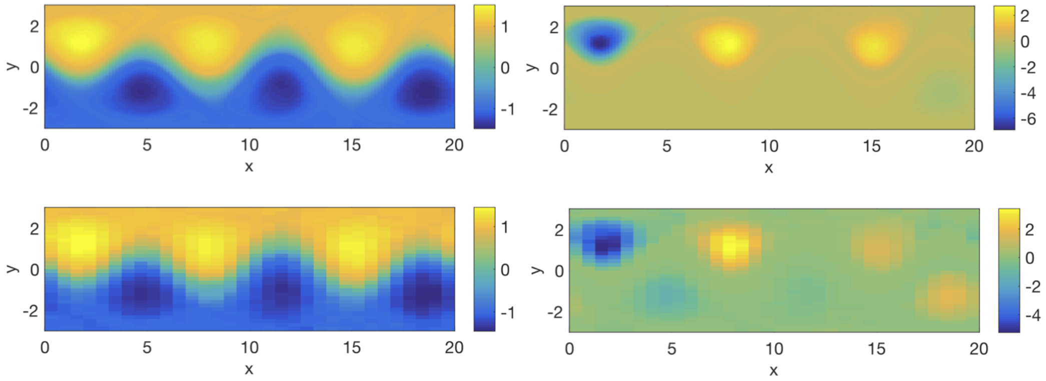

Figure 1: Leading singular vectors of the numerical transfer operator L are indicators of coherent sets: 2nd (left) and 3rd singular vectors (right) from a fine ($n = 2^{14}$, $N = 100$, top) and a coarse approximation ($n = 2^{10}$, $N = 16$, bottom) of the transfer operator.

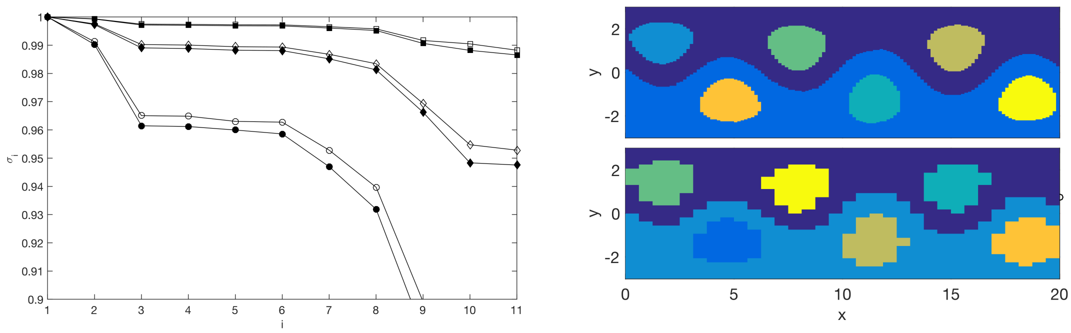

Figure 2: Left: Spectral gap after the eighth singular value of L (for different settings) indicates the existence of eight coherent sets. $\circ$: $n = 2^{10}$, $N = 100$ and $N = 16$ (filled), $\diamond$: $n = 2^{12}$, $N = 100$ and $N = 16$ (filled); $\square$: $n = 2^{14}$, $N = 100$ and $N = 16$ (filled). Right: Coherent sets extracted from the eight leading singular vectors of L ($n = 2^{14}$, $N = 100$ (top); $n = 2^{10}$, $N = 16$ (bottom)).

Robustness study and results

We consider the flow map of the Bickley jet with fixed initial and final times. The matrix P is constructed via (2) using $n = 2^{10}$, 2^{12}, and 2^{14} partition elements, then L is formed based on the uniform density. The number of test points initialized on a regular grid in each partition element is varied from 4 to 400. Figure 1 shows the second and third left singular vectors obtained from both a fine and coarse approximation of the transfer operator. These vectors appear to highlight the same structures. In addition, we demonstrate that the spectrum itself is very robust under changes in n and N, as shown in Figure 2 (left). All settings produce qualitatively similar results, in particular with a spectral gap after the eighth singular value. This indicates the existence of eight coherent sets, which we extract from the eight leading singular vectors by k-means clustering. Also here fine and coarse computations identify the same sets, see Figure 2 (right).
An outcome of our study is that the number of partition elements has a larger impact on the results than the number of test points (cf. Fig. 2 (left)). In our two-dimensional test case, even test points on a 3×3 or 4×4 grid gave meaningful results, which were very much comparable to those obtained by using a 20×20-grid. Such small numbers are in large contrast to those used in [1, 2, 3]. This observation also applies to the approximation of finite-time entropy [6], a transfer operator based stretching measure similar to FTLE (not shown here). Consequently, in computationally demanding settings, we propose to consider a sufficiently fine partition of phase space while keeping the number of test points low. These numerical findings will require further analytical investigations, which we are currently working on.

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