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A trajectory-free framework for analysing multiscale systems☆

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HIGHLIGHTS

- A trajectory-free method to test for multiscale dynamics.
- Isolates the fast dynamics and determines the reduced slow dynamics.
- Based on the spectral properties of the transfer and Koopman operators.

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ABSTRACT

We develop algorithms built around properties of the transfer operator and Koopman operator which (1) test for possible multiscale dynamics in a given dynamical system, (2) estimate the magnitude of the time-scale separation, and finally (3) distill the reduced slow dynamics on a suitably designed subspace. By avoiding trajectory integration, the developed techniques are highly computationally efficient. We corroborate our findings with numerical simulations of a test problem.

1. Introduction

Effective numerical simulation of multiscale systems constitutes a formidable challenge. Consider a system which has slow dynamics on a time-scale of order one and fast dynamics on the scale of order $1/\epsilon$ for some parameter $\epsilon \ll 1$. To accurately simulate orbits numerically and to assure numerical stability, the time step of the integrator must be of the order of ϵ. To capture the relevant slow dynamics a total number of integration steps of the order of $1/\epsilon$ is required, making direct numerical simulations of orbits computationally impractical.

Numerical integrators are subject to two main sources of error. The first is truncation error, which is the inability of the numerical method (Runge–Kutta, Euler–Maruyama, etc.) to fully capture the actual dynamics of the system. The second is round-off error, due to implementing the numerical method on a computer with finite precision arithmetic. While truncation error decreases with a smaller time step, round-off error increases [1,2]. In a multiscale system, if the time-scale separation is large, it may be impossible to find a time step which is simultaneously small enough to avoid significant truncation error for the fast dynamics and sufficiently large to avoid detrimental accumulation of round-off error for the slow dynamics.

Even if orbits could be computed exactly, analysing a multiscale system using a time series extracted from a true orbit can still yield incorrect data about the diffusion process of the slow variables [3]. To avoid this problem, the time series must be sampled at a rate intermediate between the slow and fast variables and these rates might not be known in advance.

There exists a variety of numerical methods dealing with one or more aspects of these numerical difficulties (see [4] and references therein). These methods rely on producing trajectories of the dynamical system via some form of time-integration with some of the issues mentioned above remaining. In this paper, we

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develop algorithms which avoid trajectory integration altogether. Besides the advantages relating to the issues of time-integration mentioned above, the algorithm allows for a huge reduction in computational time. Our main objective is to develop numerical algorithms which, given a dynamical system,

1. test whether the system exhibits multiscale behaviour, and if so
2. determine the order of the time-scale separation, and then
3. construct effective reduced equations for the slow dynamics allowing for the application of large time steps.

The framework we adopt for this integration-free approach is based on the infinitesimal generator associated to the underlying continuous-time dynamical system.

The construction of effective reduced equations (point 3 above), requires the estimation of coordinates in which the fast and slow dynamics operate. In the situation where there is an attracting slow manifold, existing numerical methods to determine the slow manifold include [5–9] (see [10] for a recent review). Most of these methods rely on the existence of some *attracting* slow manifold towards which transient fast dynamics is approaching along fast fibres. Here we consider the situation of multiscale systems whose asymptotic behaviour does not necessarily occur on an *attracting* slow manifold. In contrast to methods which determine the fast fibres locally, we instead globally estimate the nonlinear foliation of fast fibres.

Once slow and fast coordinates are established, it is a further challenge to identify their dynamics. There are two approaches; either to devise an effective numerical method which allows for the reliable simulation of the slow coordinates or to construct closed equations for the slow coordinates. The first avenue has been successfully pursued by numerical methods such as the equation-free method [8] and the heterogeneous multiscale method [11,12] which employ short finely resolved bursts of the full dynamics to numerically estimate the averaged slow vector field which then subsequently may be propagated with a large time step. Here we tackle the second avenue of determining the slow dynamics explicitly without the need for temporally resolving the fast dynamics at each step. To compute reduced equations on the (in general, non-unique) slow coordinates, we nonlinearly project local computations along the fast fibres. Our approach does not rely on any temporal integration to estimate the reduced equations. Hence it does not suffer from possible sensitivity of these estimates to the choice of the length of the fast bursts. For example, in the case where the fast dynamics itself involves transitions between metastable states, a short temporal sampling of the full dynamics might not be sufficient to capture the fast invariant measure. This would then bias the averaged slow vector field.

In Section 2 we briefly review the notion of generators of transfer and Koopman operators. Section 3 introduces a trajectory-free test for multiscale behaviour. The degree of time-scale separation is estimated in algorithms described in Sections 4 and 5. A method to determine the reduced slow dynamics from a multiscale system without relying on statistics obtained from long time-integrations is given in Section 6. The algorithms are tested in numerical simulations in Section 7. We conclude with a discussion in Section 8.

2. Generators

We describe our methodology for Itō drift–diffusion processes, as these are a large and flexible class of dynamical systems, and the spectral properties of the corresponding transfer operators are relatively straightforward. Consider a drift–diffusion process

$$d\zeta_i = \mu_i\, dt + \sum_{k=1}^{\ell} \sigma_{ik}\, dW_k \quad \text{with } i = 1, \ldots, d \tag{1}$$

defined on a subset $\mathcal{Z}$ of $\mathbb{R}^d$ where $l \leq d$ and each W_k for $k = 1, \ldots, \ell$ represents an independent Wiener process. Given a probability density function at time $t = 0$, the density at future times is determined by the Fokker–Planck equation

$$\frac{\partial \rho}{\partial t} = \mathcal{L}\rho$$

where

$$\mathcal{L}\rho = -\sum_{i=1}^{N} \frac{\partial}{\partial z_i}\big[\mu_i\, \rho\big] + \frac{1}{2}\sum_{i,j=1}^{N} \frac{\partial^2}{\partial z_i\, \partial z_j}\big[D_{ij}\, \rho\big]. \tag{2}$$

The second order differential operator $\mathcal{L}$ is called the *Fokker–Planck operator*. At each point z in the phase space $\mathcal{Z}$, the vector $\mu(z) \in \mathbb{R}^d$ represents the drift of the process and the positive semi-definite matrix $D(z) = \sigma(z)\sigma(z)^\top \in \mathbb{R}^{d\times d}$ the diffusion. The operator $\mathcal{L}$ generates a family of operators $e^{t\mathcal{L}}$ for $t \geq 0$ such that $e^{s\mathcal{L}}e^{t\mathcal{L}} = e^{(s+t)\mathcal{L}}$ and $\lim_{t\to 0} \frac{1}{t}[e^{t\mathcal{L}} - Id] = \mathcal{L}$. If $\rho \in L^1(\mathcal{Z})$ is an initial probability density, then $e^{t\mathcal{L}}(\rho)$ is the density after time t. Thus, $e^{t\mathcal{L}}$ may be thought of as a transfer operator defined on $L^1(\mathcal{Z})$. Since the underlying system is a random dynamical system and $e^{t\mathcal{L}}$ represents an average over all possible random paths, it is an annealed transfer operator [13].

We now consider a setting where the Fokker–Planck operator has compact resolvent. Suppose the domain $\mathcal{Z}$ is a compact subset of $\mathbb{R}^d$ with piecewise smooth boundary. We also allow periodic boundary conditions, such as systems defined on the torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$, so long as the fundamental domain is compact with smooth boundary. Under such assumptions, the Lebesgue measure of $\mathcal{Z}$ is finite, and with respect to this measure, the Hilbert space $L^2(\mathcal{Z})$ is a subset of $L^1(\mathcal{Z})$. Further assume that the operator is *uniformly elliptic*, which holds if the matrix $D(z)$ is positive definite for every $z \in \mathcal{Z}$. Results in the theory of partial differential equations then imply that the Fokker–Planck operator defined on $L^2(\mathcal{Z})$ has compact resolvent. See [14, Chapter 7] for further details and proofs. The condition of uniform ellipticity can in some cases be replaced with the weaker condition of hypo-ellipticity; see [14–16].

Assuming the resolvent is compact, the spectrum of the operator then consists of a countable set of eigenvalues $\{\lambda_k\}_{k=0}^{\infty}$ which, when ordered by the convention

$$0 = \operatorname{Re}\lambda_0 \geq \operatorname{Re}\lambda_1 \geq \operatorname{Re}\lambda_2 \geq \cdots, \tag{3}$$

satisfy $\lim_{k\to\infty} \operatorname{Re}\lambda_k \to -\infty$. As a consequence, for each $t > 0$ the operator $e^{t\mathcal{L}}$ is compact with eigenvalues $e^{t\lambda_k}$ tending to zero as $k \to \infty$. The invariant density ρ_0 of the system is an eigenfunction of $\mathcal{L}$ associated to the eigenvalue $\lambda_0 = 0$.

The Kolmogorov backward equation is given by $\frac{\partial f}{\partial t} = \mathcal{L}^* f$ where the adjoint of the Fokker–Planck operator is given by

$$\mathcal{L}^* f = \sum_{i=1}^{N} \mu_i \frac{\partial f}{\partial z_i} + \frac{1}{2}\sum_{i,j=1}^{N} D_{ij} \frac{\partial^2 f}{\partial z_i\, \partial z_j}. \tag{4}$$

This adjoint operator generates a family of operators $K_t := e^{t\mathcal{L}^*} = (e^{t\mathcal{L}})^*$ for $t \geq 0$. If $f \in L^2(\mathcal{Z})$, then $K_t(f) \in L^2(\mathcal{Z})$ is given by $K_t(f)(z) = \mathbb{E}f(\zeta(t))$ where the expectation is over all paths $\zeta(t)$ in the drift–diffusion process which satisfy $\zeta(0) = z$. The operator K_t may therefore be regarded as an annealed Koopman or composition operator.

The operators $\mathcal{L}^*$ and $\mathcal{L}$ share the same eigenvalues λ_k. Consider the eigenfunction $\psi_k \in L^2(\mathcal{Z})$ of $\mathcal{L}^*$ associated to λ_k. This function ψ_k is an observable which evolves according to

$$K_t\psi_k = e^{t\lambda_k}\psi_k$$

and therefore decays to zero at the rate given by $|e^{t\lambda_k}|$ for $t > 0$. In general, the eigenfunctions of $\mathcal{L}^*$ associated to eigenvalues with real part closest to zero are the observables of the system which