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A new framework for extracting coarse-grained models from time series with multiscale structure

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ABSTRACT

In many applications it is desirable to infer coarse-grained models from observational data. The observed process often corresponds only to a few selected degrees of freedom of a high-dimensional dynamical system with multiple time scales. In this work we consider the inference problem of identifying an appropriate coarse-grained model from a single time series of a multiscale system. It is known that estimators such as the maximum likelihood estimator or the quadratic variation of the path estimator can be strongly biased in this setting. Here we present a novel parametric inference methodology for problems with linear parameter dependency that does not suffer from this drawback. Furthermore, we demonstrate through a wide spectrum of examples that our methodology can be used to derive appropriate coarse-grained models from time series of partial observations of a multiscale system in an effective and systematic fashion.

1. Introduction

Many natural phenomena and technological applications are characterized by the presence of processes occurring across different length and/or time scales. Examples range from biological systems [1] and problems in atmosphere and ocean sciences [2,3] to molecular dynamics [4], materials science [5] and fluid and solid mechanics [6–8], to name but a few. Studying the full dynamics of such systems is often a very intricate task due to the complex structure of the systems which also hampers the ability to obtain governing equations from first principles. However, it is often possible to exploit, e.g., scale separation in order to obtain a reduced (low-dimensional) model for a few selected degrees of freedom. The coefficients and/or parameters in the reduced model must be derived from the full dynamics through an appropriate coarse-graining procedure; see, e.g. [9–11] for recent works on various coarse-graining methods. As mentioned above, it is often not possible to obtain such a coarse-grained equation in explicit form and one must necessarily resort to observations [12,13]. It is thus desirable to appropriately fit a reduced stochastic coarse-grained model to the observations of the underlying complex process.

The general problem of obtaining a reduced coarse-grained model from the full system can be formulated as follows. Let the underlying system be given in terms of a dynamical system Z which evolves, symbolically written, according to the dynamics

$$\frac{dZ}{dt} = F(Z)\,, \tag{1}$$

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where the state space $\mathcal{Z}$ of Z is high (or even infinite) dimensional and F is a nonlinear function. For instance, the semilinear partial differential equation of the type $u_t = \mathcal{A}u + \psi(u, \nabla u, \nabla^2 u, \ldots)$ with periodic boundary conditions in an extended domain, often appearing in pattern formation dynamics of spatially extended systems, can be written as an infinite dimensional system of ordinary differential equations (ODEs) in Fourier space in the form of (1) in which case F depends on the operator $\mathcal{A}$ and the function ψ. As we are only interested in the evolution of a few selected degrees of freedom, i.e. only some components of the full dynamics Z solving (1), we assume that one can separate these resolved degrees of freedom (RDoF) in the dynamical system from the unresolved degrees of freedom (UDoF). The choice of RDoF and UDoF is a part of our modeling strategy. Standard examples include systems with well-separated time scales, e.g. the decomposition between climate and weather degrees of freedom in atmosphere–ocean science and the use of reaction coordinates in the study of chemical kinetics or in molecular dynamics. For such systems, one decomposes the state space into subspaces $\mathcal{X}$ and $\mathcal{Y}$ that contain the RDoF and UDoF, respectively:

$$\mathcal{Z} = \mathcal{X} \oplus \mathcal{Y} ,$$

with $\dim(\mathcal{X}) \ll \dim(\mathcal{Y})$ typically. We also introduce the projection operators onto these spaces $P : \mathcal{Z} \mapsto \mathcal{X}$ and $(I - P) : \mathcal{Z} \mapsto \mathcal{Y}$, respectively. Let now X be the projection of Z onto the space of $\mathcal{X}$, i.e. $X = PZ$. Then we postulate the existence of a reduced coarse-grained stochastic model describing the evolution of X alone. Here we assume that the stochastic model for X is given via a stochastic differential equation (SDE):

$$dX = f(X)\,dt + \sqrt{g(X)}\,dW_t , \tag{2}$$

where W denotes a standard Brownian motion of dimension equal to $\dim(\mathcal{X})$. Once the coarse-grained model (2) is identified, it can be a used to study the dynamic characteristic features of the full system (1). Indeed, its low-dimensionality and simplicity makes it particularly accessible for both rigorous and computational treatment; see [14–16] for examples. For many practically relevant cases however, and as we emphasized earlier, it is not possible to derive a coarse-grained model (2) analytically, because of the complexity of the underlying full system or simply because the full model (1) is not completely known. Consequently, the only way to obtain a coarse-grained model in such a situation is to use observations, e.g. experimental and/or simulation data, of the full dynamics projected onto the subspace $\mathcal{X}$, i.e. onto of RDoF. That is, it is desirable to identify the coarse-grained SDE model (2) in a data-driven fashion.

An important class of dynamical systems for which coarse-grained equations of the form (2) are known to exist, is when the dynamical system (1) is given as system of SDEs with two widely separated time scales. Such systems are a natural testbed for data-driven coarse-graining techniques, as one has explicit information about the coarse-grained model. Specifically, let us consider the following as a prototypical multiscale system

$$dX^\varepsilon = \left(\frac{1}{\varepsilon}a_0(X^\varepsilon, Y^\varepsilon) + a_1(X^\varepsilon, Y^\varepsilon)\right)dt + \alpha_0(X^\varepsilon, Y^\varepsilon)\,dU_t + \alpha_1(X^\varepsilon, Y^\varepsilon)\,dV_t , \tag{3a}$$

$$dY^\varepsilon = \left(\frac{1}{\varepsilon^2}b_0(X^\varepsilon, Y^\varepsilon) + \frac{1}{\varepsilon}b_1(X^\varepsilon, Y^\varepsilon)\right)dt + \frac{1}{\varepsilon}\beta(X^\varepsilon, Y^\varepsilon)\,dV_t , \tag{3b}$$

with $\varepsilon \ll 1$ controlling the time scale separation. That is, X^ε denotes the degrees of freedom we are interested in (i.e. the RDoF) and for which we would like to obtain a coarse-grained model describing the evolution of X^ε independent of Y^ε as $\varepsilon \ll 1$. Mathematically, the derivation of such coarse-grained models can be made rigorous in the limit of $\varepsilon \to 0$ using averaging and homogenization techniques; see e.g. [17] and the references therein for details. In particular, the slow process X^ε converges weakly in $C([0, T], \mathbb{R}^d)$ to X solving an SDE of the form (2):

$$dX = f(X)\,dt + \sqrt{g(X)}\,dW_t . \tag{4}$$

The drift and diffusion coefficients (i.e. the functions f and g) can be formally derived using standard results from homogenization theory. A data-driven coarse-graining strategy would then be to use available observations of the multiscale system, specifically of X^ε in (3), to identify the coarse-grained model (4) by inferring the functions f and g.

Often it is possible to justify proposing a coarse-grained equation with a particular structure based on theoretical arguments or previous experience with similar systems. In these cases the inference problem for f and g in Eq. (4) reduces to estimating unknown parameters in the SDE. There is a vast and rich literature on the parametric inference problem for SDEs; see [18–20] for instance. For a data-driven coarse-graining approach for Eq. (4) based on observations from Eq. (3) it turns out, however, that commonly used estimators can be biased due to small scale effects in the observations. In fact, estimators, such as the maximum likelihood estimator and the quadratic variation of the path estimator, are highly sensitive to the scale separation. While these estimators do converge (as $\varepsilon \to 0$) to the parameters in the coarse-grained model on the shorter advective time scale, they become biased on the longer diffusive time scale [12,21]. The systematic bias due to multiscale effects on the diffusive time scale can be reduced by subsampling the data at an appropriate rate. However, the idea of subsampling does not necessarily lead to an efficient algorithm that can be used by practitioners, because the optimal sampling rate is known only for very simple systems (see e.g. [22–24]) and since, furthermore, subsampling the data increases the variance of the estimator. A satisfactory algorithm for fitting a coarse-grained SDE to data based on the idea of subsampling at the optimal rate combined with an appropriate variance reduction step has been developed only for