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

S. Kalliadasis[a], S. Krumscheid[b,*], G. A. Pavliotis[b]

[a] *Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK*
[b] *Department of Mathematics, Imperial College London, London SW7 2AZ, UK*

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.

Keywords: parametric inference, stochastic differential equations, multiscale diffusion, chaotic dynamics, homogenization, coarse-graining

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, 7, 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, 10, 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

*Corresponding author

Email addresses: s.kalliadasis@imperial.ac.uk (S. Kalliadasis), s.krumscheid10@imperial.ac.uk (S. Krumscheid), g.pavliotis@imperial.ac.uk (G. A. Pavliotis)

Z which evolves, symbolically written, according to the dynamics

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

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 $u_t = \mathcal{A}u + \psi(u, \nabla u, \nabla^2 u, \dots)$ 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, 15, 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, 19, 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, 23, 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 some simple systems used in econometrics [22]. To our knowledge such a methodology has not been developed and implemented for problems arising in the natural sciences, such as in molecular dynamics or in statistical physics for example. In addition to the problem of typically not knowing the optimal subsampling rate, the numerical experiments in [12] moreover indicate that the optimal subsampling rate can vary between parameters in the same coarse-grained model. Related work that investigates the problem of parametric inference combined with subsampling techniques in various settings can be found e.g. in [25, 26, 27, 28], while parametric inference for multiscale problems with vanishing noise is, e.g., also [29]. Similar consistency questions arise also in fields other than parametric inference, including problems in stochastic filtering and stochastic control for SDEs with multiple scales [30, 31].

Related data-driven approaches have also been studied in the context of numerical methods for SDEs with multiple time scales, i.e. for systems of the form (3). We mention in particular the heterogeneous multiscale method [32, 33], which is based on the idea of evolving the solution of the reduced coarse-grained equation, when the coefficients in the coarse-grained equation are being evaluated "on the fly" by running short runs of the underlying fast dynamics. Similar ideas have been proposed in the framework of the equation-free methodology introduced by Kevrekidis and collaborators (see e.g. [34, 35, 36, 37]), where a coarse-grained model is evolved using appropriately initialized simulation on short time scales of the full multiscale system without

knowing the coarse-grained equation in closed form, making this methodology in principle also applicable for more general problems, such as kinetic equations. As such, these techniques can be viewed as a hybrid between numerical analysis and statistical inference.

To accurately infer coarse-grained models from observations of a multiscale system, one has to resort to alternative estimation methodologies, which are robust with respect to the multiscale effects of the dynamics. The present study is motivated by a recently introduced estimation methodology which demonstrated how to bypass the need to subsample data [13]. In the form as proposed in [13] this methodology is, however, only applicable for observations where an ensemble of short trajectories for multiple initial conditions is available; a design common in many computer-based simulations. In most real world experiments, such as in molecular dynamics simulations one typically has access only to a single long time series. The goal of the present work is therefore to generalize and appropriately extend the methodology developed in [13], so that it can be used for an observation design where only one long time series is available. Furthermore, we demonstrate by means of numerical experiments that the proposed inference methodology works well for various quite general dynamical systems of the form (1), for which a coarse-grained model of the form (2) is known to exist.

The rest of the paper is organized as follows. In Section 2 we follow the general procedure of [13] and present the necessary generalizations and extensions required for the case of the observational design of a single time series. Specifically, we will focus on problems where both the drift function f and the diffusion coefficient g depend linearly on an unknown parameter vector. This setting covers, for example, the cases where f and g can be expressed as an appropriate series (e.g. Taylor of Fourier) of known functions. Moreover, we believe that the ideas developed in this work for the case of linear parameter dependency can also be instrumental for the nonlinear case. To demonstrate the effectiveness of the developed methodology we apply it to a number of selected examples, which we discuss in Section 3. Specifically, we use the estimation methodology to identify coarse-grained models for Brownian motion in a two-scale potential (i.e. a stochastic multiscale systems), for a deterministic system exhibiting chaos, for a Kac–Zwanzig model, and for a deterministic model for Brownian motion. Finally, Section 4 offers a summary and discussion of our results.

2. Estimators for coarse-grained models

We outline here a general methodology that can be used to estimate parameters in SDEs based on a single trajectory of discrete time observations. For the sake of clarity, we first outline the derivation of the estimator for the case where no multiscale effects are present. To this end we derive an estimating equation in a continuous time setting, which will relate the unknown parameters to statistical properties of the solution to the SDE and discuss how to obtain parametric estimators from it. To obtain a functional relation between unknown parameters and statistical properties of the model, in Section 2.1 we follow the methodology outlined in [13] and generalize it appropriately. Most of the examples we are interested in are such that the coarse-grained model is one-dimensional, see Section 3, i.e. we focus on the case of a scalar diffusion process. It is, however, worthwhile to remark that the our derivation can be readily extended to the multidimensional case. Moreover, we discuss modifications and discretizations to the continuous time estimating equation to account for observations which are available in the from of a time series before discussing the coarse-graining scenario.

2.1. Estimating equation

Consider the scalar-valued Itô SDE

$$dX = f(X)\,dt + \sqrt{g(X)}\,dW_t\ , \quad X(0) = \xi\ , \tag{5}$$

on some finite time interval $[0, T]$, $T > 0$, with W denoting a standard one-dimensional Brownian motion. We assume that both the drift function f and the diffusion function g are such that Eq. (5) has a unique strong solution on $[0, T]$; details are given in [38, 39]. Let us denote by $X_\xi(t)$ the solution of Eq. (5) at time t started in ξ at time zero, i.e. $X_\xi(0) = \xi$. Moreover, denote by $\mathcal{L}$ the generator associated with (5), i.e. $\mathcal{L} := f\frac{d}{dx} + \frac{1}{2}g\frac{d^2}{dx^2}$. Then, Itô's formula together with the martingale property of the stochastic integral implies that

$$\mathbb{E}\Big(\phi\big(X_\xi(t)\big)\Big) - \phi(\xi) = \int_0^t \mathbb{E}\Big((\mathcal{L}\phi)\big(X_\xi(s)\big)\Big)\,ds\ , \tag{6}$$

for any $\phi \in C^2(\mathbb{R})$ and deterministic initial condition ξ. For the sake of completeness, we remark that other commonly used notations for $\mathbb{E}\big(\phi\big(X_\xi(t)\big)\big)$ are $\mathbb{E}\big(\phi\big(X(t)\big)\big|X(0) = \xi\big)$ or $\mathbb{E}_\xi\big(\phi\big(X(t)\big)\big)$, and that Eq. (6) is also known as Dynkin's formula [39, Ch. 7.4].

In this work we follow a semiparametric approach for the parametrization of Eq. (5). That is, we assume that both f and g depend on an unknown parameter vector $\theta \equiv (\theta_1, \ldots, \theta_n)^T \in \mathbb{R}^n$, $n \in \mathbb{N}$, which we wish to determine from observations. Specifically, we consider

$$f(x) \equiv f(x;\theta) := \sum_{j=1}^n \theta_j f_j(x) \quad \text{and} \quad g(x) \equiv g(x;\theta) := \sum_{j=1}^n \theta_j g_j(x)\ , \tag{7}$$

with some known functions f_j and g_j, $1 \le j \le n$. That is, both f and g can depend on the same parameter. If this not the case however, one can think of the first k, say, components of the vector θ parametrizing the drift function f while the remaining $n-k$ components the diffusion function g, and setting $f_j = 0$ for $k < j \le n$ as well as $g_j = 0$ for $1 \le j \le k$. For the numerical examples in Section 3 we will have that f and g are polynomials of some degree, so that f_j and g_j will be appropriate monomials, respectively. After substituting (7) into (6) and rearranging terms, we arrive at

$$\mathbb{E}\Big(\phi\big(X_\xi(t)\big)\Big) - \phi(\xi) = \sum_{j=1}^n \theta_j \int_0^t \mathbb{E}\Big((\mathcal{L}_j\phi)\big(X_\xi(s)\big)\Big)\,ds\ , \tag{8}$$

with $\mathcal{L}_j := f_j\frac{d}{dx} + \frac{1}{2}g_j\frac{d^2}{dx^2}$. To write this estimating equation (8) in a more compact manner, we define the following component functions for any fixed time $t \in [0, T]$ and any fixed function ϕ,

$$b_c(\xi) := \mathbb{E}\Big(\phi\big(X_\xi(t)\big)\Big) - \phi(\xi) \in \mathbb{R} \quad \text{and} \quad a_c(\xi) := \Big(\int_0^t \mathbb{E}\Big((\mathcal{L}_j\phi)\big(X_\xi(s)\big)\Big)\,ds\Big)_{1\le j\le n} \in \mathbb{R}^n\ ,$$

which highlight the dependency on ξ. Using these definitions, Eq. (8) reduces to

$$a_c(\xi)^T\theta = b_c(\xi)\ , \tag{9}$$

which is underdetermined for $n > 1$. To make this identity useful nonetheless, we exploit the fact that Eq. (9) is valid for any ξ; a technique that has already been used successfully in [13]. We now introduce the concept of *trial points*: as we work in an observation framework where only

one time series is available, we denote by ξ the trial point instead of initial condition to avoid confusion with the initial condition of the time series; see also Section 2.2.1. By considering a finite sequence of trial points $(\xi_i)_{1\leq i\leq m}$, we can assemble a system of linear equations, solved by the parameter vector θ:

$$A\theta = b\,, \tag{10}$$

where $A := \big(a_c(\xi_i)^T\big)_{1\leq i\leq m} \in \mathbb{R}^{m\times n}$ and right-hand side $b := \big(b_c(\xi_i)\big)_{1\leq i\leq m} \in \mathbb{R}^m$. Since this linear system does not have a unique solution in general, we define the estimator of θ based on A and b as the least squares solution of $A\theta = b$ with minimum norm:

$$\hat{\theta} := \operatorname*{arg\,min}_{x\in\mathcal{S}} \|x\|_2^2\,, \quad \mathcal{S} := \big\{x\in\mathbb{R}^n\colon\ \|Ax-b\|_2^2 = \min\big\}\,. \tag{11}$$

At this point, we can still exploit the degree of freedom for choosing ϕ in Eq. (8) freely. Motivated by [13] where approximations of the first and second moment provided very accurate estimates of θ, we use $\phi(x) := x + x^2$ throughout this work. In fact, the two-step estimation approach for θ presented in the aforementioned work can be recovered as a special case of the procedure outlined here. Indeed, using $\phi(x) = x$ causes Eq. (8) to degenerate to an equation not containing any parameters characterizing the diffusion function g. This then yields an estimator for the drift parameters only. After this first step, we substitute the obtained estimators into the parametrization of f. Repeating then the same steps with the function $\phi(x) = x^2$ gives an estimator of the remaining parameters determining g and the two-step scheme is completed. Finally, we mention that other choices for the function ϕ may work as well to construct the estimator (11). In view of the preceding discussion it is clear however, that ϕ cannot be chosen arbitrarily as it has to be such that Eq. (8) still depends on all unknown parameters that we want to estimate. The used function $\phi(x) = x + x^2$ thus appears to be the obvious candidate for various problems, while other choices of ϕ may be problem dependent. A more systematic study of how to choose ϕ in the context of the rigorous convergence analysis will be presented in [40].

2.2. Modifications due to discrete time observations

Recall that we seek to determine an approximation of the parameter vector θ in Eq. (5) with parametrization (7), based on a trajectory of discrete time observations. That is, we have access to N data $\mathbb{X}_N := \big(X(t_k)\big)_{1\leq k\leq N}$ with $t_k = (k-1)h$, where $h = T/(N-1)$. A constant sampling rate h is assumed here merely for simplicity and the proposed methodology can be readily extended to the case of non-constant sampling rates. To apply the methodology outlined above, we have to carry out two essential modifications to the purely continuous framework (8). Firstly, we have to estimate the conditional expectations of the form $\mathbb{E}\big(\varphi\big(X_\xi(\tau)\big)\big)$ based on $\mathbb{X}_N$. Secondly, we have to replace the temporal integrals with discrete versions. A detailed algorithmic description of the estimation procedure for discrete time observations based on these modifications is presented in Section 2.2.3.

2.2.1. Estimating the conditional expectation

Throughout the estimation procedure, we have to approximate conditional expectations of the form $\mathbb{E}\big(\varphi\big(X_\xi(\tau)\big)\big)$ for multiple values of the trial point ξ. The available time series $\mathbb{X}_N$ provides, however, only one initial condition which we cannot influence nor manipulate; thus the necessity to distinguish between trial point and initial condition. A way out of this predicament is possible when the time series (i.e. the discrete time process) is stationary and sufficiently mixing so that

$$\operatorname{Cov}\big(X(t), X(t+kh)\big) \leq C\rho^k\,,$$

for some finite $C > 0$ and $\rho \in [0, 1[$, which we will assume from now on; see e.g. [41, 42] for further details in the inference context and refer to e.g. [43, 44] and the references therein for a discussion of sufficient conditions on the drift function and the diffusion coefficient in SDE model (5). Related conditions on the covariance as a function of the lag k have also been used in other works on parametric inference for diffusion processes; see [24] for instance. Intuition in this case then suggests to sequentially search the time series $\mathbb{X}_N$ for the value of the trial point ξ and then to approximate the expectation by averaging over the events $\varphi(X)$ at τ time units after the occurrences of ξ in $\mathbb{X}_N$. A technique which makes this approximation idea precise is the class of so-called local polynomial kernel regression estimators [42]. Recall that the sampling time of the time series $\mathbb{X}_N$ is h. For a shift by $\tau > 0$ time units to be well-defined, we require that $\tau = lh$, for some $l \in \{1, 2, \ldots, N-1\}$ and for such a τ we set $N_\tau = N - \tau/h \in \mathbb{N}$. Then the simplest regression estimator (locally constant) yields the approximation

$$\mathbb{E}\Big(\varphi\big(X_\xi(\tau)\big)\Big)\Big|_{\tau=lh} \approx \frac{\sum_{k=1}^{N_\tau} \varphi\big(X(t_{k+l})\big) K\Big(\frac{X(t_k)-\xi}{\kappa_{N_\tau}}\Big)}{\sum_{k=1}^{N_\tau} K\Big(\frac{X(t_k)-\xi}{\kappa_{N_\tau}}\Big)}\,, \tag{12}$$

which is also known as the Nadaraya–Watson estimator [45, 46]. Here K is an appropriately chosen kernel, and $0 < \kappa_{N_\tau}$ denotes the bandwidth which decays to zero as $N_\tau \to 0$ at a rate depending on the sense of convergence in Eq. (12); details are given in [41]. Throughout this study we select the Gaussian kernel $K(x) := \exp(-x^2/2)/\sqrt{2\pi}$ for convenience, but we remark that other choices are possible.

Upon defining $w_{N_\tau,k}(\xi) := K\big((X(t_k)-\xi)/\kappa_{N_\tau}\big)/\sum_{k=1}^{N_\tau} K\big((X(t_k)-\xi)/\kappa_{N_\tau}\big)$, one can rewrite the regression estimator, i.e. the right-hand side in Eq. (12), as $\sum_{k=1}^{N_\tau} w_{N_\tau,i}(\xi)\varphi\big(X(t_{k+l})\big)$. That is, the regression estimator is given as a weighted average with non-identical weights $w_{N_\tau,k}(\xi)$. Let us finally note that if the trial point ξ is such that the denominator of the regression estimator in Eq. (12) is zero (roughly speaking this happens if ξ is not in the support of the stationary density of $\mathbb{X}_N$), then we set $w_{N_\tau,k}(\xi) = 1/N_\tau$ instead for well-posedness (see also Sect. 2.2.3 below). However, one should ensure that this event is avoided by selecting the trial points appropriately, otherwise the estimator's approximation accuracy would deteriorate due to incorporating unfeasible information. As the regression estimator in Eq. (12) essentially averages over the events $\varphi\big(X(t_{k+l})\big)$ for which $X(t_k) \approx \xi$, one should moreover try to ensure that the trial point ξ is located in a region where most of the observations are located in order to average over a sufficiently large sample; see Section 3 for a detailed description of how to chose the trial points in practice.

2.2.2. Temporal integrals

The integrands of the temporal integrals in Eq. (8) are precisely the conditional expectations discussed above. Let $u(\tau) := \mathbb{E}\big(\varphi\big(X_\xi(\tau)\big)\big)$ be such an expectation for a fixed trial point ξ and function φ. To replace the temporal integral of u over $[0, t]$ by a discrete version in (8), we use the composite trapezoidal rule with n_h equally spaced ($n_h = t/h$) subdivisions:

$$\int_0^t u(s)\,ds \approx \frac{h}{2}\left(u(0) + u(t) + 2\sum_{l=1}^{n_h-1} u(lh)\right). \tag{13}$$

The choice of an equally spaced subdivision of $[0, t]$ where the division length coincides with the sampling rate h of the available time series $\mathbb{X}_N$ is made for reasons of a consistent discretization. In fact, it ensures that the time points τ, say, at which the integrand u is evaluated, is an integer

Algorithm 1 Algorithmic description of the introduced estimation procedure.

Require: $0 < t$ such that $t/h \in \mathbb{N}$, $0 < h$, $\Xi \in \mathbb{R}^m$, and $\mathbb{X}_N \in \mathbb{R}^N$

1: $l \leftarrow \frac{t}{h}$
2: **for** $i = 1$ to m **do**
3: $\quad \xi \leftarrow \Xi_i$
4: $\quad$ **for** $j = 1$ to n **do**
5: $\quad\quad u_{j,0} \leftarrow f_j(\xi)(1 + 2\xi) + g_j(\xi)$
6: $\quad$ **end for**
7: $\quad$ **for** $k = 1$ to l **do**
8: $\quad\quad X \leftarrow \mathbb{X}_N(1 : N - k)$
9: $\quad\quad Y \leftarrow \mathbb{X}_N(1 + k : N)$
10: $\quad\quad$ **for** $j = 1$ to n **do**
11: $\quad\quad\quad u_{j,k} \leftarrow \texttt{nwe}\big(X, f_j(Y)(1 + 2Y) + g_j(Y), \xi\big)$
12: $\quad\quad$ **end for**
13: $\quad$ **end for**
14: $\quad X \leftarrow \mathbb{X}_N(1 : N - l)$
15: $\quad Y \leftarrow \mathbb{X}_N(1 + l : N)$
16: $\quad b_i \leftarrow \texttt{nwe}\big(X, Y + Y^2, \xi\big) - (\xi + \xi^2)$
17: $\quad$ **for** $j = 1$ to n **do**
18: $\quad\quad A_{i,j} \leftarrow \frac{h}{2}\big(u_{j,0} + u_{j,l} + 2\sum_{k=1}^{l-1} u_{j,k}\big)$
19: $\quad$ **end for**
20: **end for**
21: $\theta \leftarrow A^+ b$
22: **return** θ

multiple of h, so that the shifts by τ time units in the regression estimator (12) are well-defined. Other (possibly non-equally spaced) time discretizations, which are consistent in the sense that each trapezoidal node is an integer multiple of h, are of course possible. Finally, we mention that the use of trapezoidal rule (13) is motivated by the fact that the integrands u are replaced by the regression estimators (12) in practice, for which we cannot expect to provide sufficient smoothness. Under these conditions the trapezoidal rule is advantageous over higher order methods since higher order derivatives, as used in classical Taylor expansion based arguments, are not continuous [47].

2.2.3. An algorithmic description for discrete time observations

To illustrate how the combination of these approximations can be used to apply the developed methodology to discrete time observations, we present a detailed pseudocode in Algorithm 1. Here we assume that a parametrization for both drift function and diffusion function has been fixed by choosing f_j and g_j in Eq. (7), for $1 \leq j \leq n$. The input arguments of Algorithm 1 are the time series $\mathbb{X}_N$ of N discrete time observations corresponding to a constant sampling rate h, the m trial points Ξ, and the time t controlling the temporal integration in (8), which is assumed to be an integer multiple of h (cf. Section 2.2.1). We note that we use the colon notation [48, Ch. 1.1.8] in lines 8, 9 and 14, 15 to select several components of a vector at once, so that we can suppress additional iteration details. Similarly, the application of a function defined on $\mathbb{R}$ to a vector (such as in lines 11 and 16) is understood componentwise. We emphasize that the statement $\theta \leftarrow A^+ b$ in line 21 is merely meant as a formal notation for computing the least squares solution of $A\theta = b$ with minimum norm. In fact, in this work we use a

Algorithm 2 Pseudocode of the `nwe` procedure used in Algorithm 1 to approximate conditional expectations via the Nadaraya–Watson estimator.

Require: $X, Y \in \mathbb{R}^M$ and $\xi \in \mathbb{R}$

1: $\kappa \leftarrow \arg\min_{\delta>0}\Big(\frac{1}{\delta M^2\sqrt{2}}\sum_{i,j=1}^{M} K\big(\frac{X_i-X_j}{\delta\sqrt{2}}\big) - \frac{2}{M(M-1)}\sum_{i=1}^{M}\sum_{i\neq j} K\big(\frac{X_i-X_j}{\delta}\big)\Big)$

2: **if** $\sum_{i=1}^{M} K\big(\frac{X_i-\xi}{\kappa}\big) = 0$ **then**

3: $\quad u \leftarrow \frac{1}{M}\sum_{i=1}^{M} Y_i$

4: **else**

5: $\quad u \leftarrow \frac{\sum_{i=1}^{M} Y_i K\big(\frac{X_i-\xi}{\kappa}\big)}{\sum_{i=1}^{M} K\big(\frac{X_i-\xi}{\kappa}\big)}$

6: **end if**

7: **return** u

QR factorization with column pivoting to solve the least squares problem but other choices are possible, typically depending on the rank of A; see, e.g., [48, Ch. 5]. Furthermore, the procedure `nwe` (called in lines 11 and 16) implements the Nadaraya–Watson estimator (12) for the approximation of conditional expectations and its detailed pseudocode is given in Algorithm 2. Its input arguments are two lists X, Y of the same length as well as the trial point ξ and the algorithm returns an approximation of $\mathbb{E}(Y|X=\xi)$. In the pseudocode presented here, we use the least squares cross validation for a data-driven bandwidth selection (line 1). We mention, however, that this selection technique is used here merely for the sake of a compact notation and several other methods can be used alternatively [49, Ch. 8.5]. For the numerical examples discussed in Section 3 we tried different bandwidth selection methods (not shown) but did not observe any significant differences. We also note that there exist efficient computational strategies to evaluate the term in brackets in line 1 of Algorithm 2 via fast Fourier transform related approaches.

2.3. Estimators for coarse-grained models of multiscale systems

A central goal of this study is to identify a coarse-grained model based on observations of a multiscale system. Specifically, we consider the prototypical multiscale system (3), i.e.

$$dX^\varepsilon = \left(\frac{1}{\varepsilon}a_0(X^\varepsilon, Y^\varepsilon) + a_1(X^\varepsilon, Y^\varepsilon)\right)dt + \alpha_0(X^\varepsilon, Y^\varepsilon)\,dU_t + \alpha_1(X^\varepsilon, Y^\varepsilon)\,dV_t\,, \tag{14a}$$

$$dY^\varepsilon = \left(\frac{1}{\varepsilon^2}b_0(X^\varepsilon, Y^\varepsilon) + \frac{1}{\varepsilon}b_1(X^\varepsilon, Y^\varepsilon)\right)dt + \frac{1}{\varepsilon}\beta(X^\varepsilon, Y^\varepsilon)\,dV_t\,, \tag{14b}$$

equipped with appropriate initial conditions on the time interval $[0,T]$, where U and V denote independent Brownian motions, and $\varepsilon > 0$ is a small parameter controlling the scale separation. Here we assume that $1 = \dim(\mathcal{X})$, while $\dim(\mathcal{Y})$ is arbitrary, so that the coarse-grained model

$$dX = f(X)\,dt + \sqrt{g(X)}\,dW_t\,, \tag{15}$$

is also one-dimensional; W is a standard one-dimensional Brownian motion. In fact, using results from homogenization theory one can rigorously show that the process X^ε solving (14a) converges weakly in $C([0,T],\mathbb{R})$ to the process X solving (15) as $\varepsilon \to 0$, provided that the fast process Y^ε is ergodic and the centering condition is satisfied; see, e.g., [17] and the references therein.

Our data-driven coarse-graining strategy is to use the available observations of X^ε solving (14a) with $\varepsilon > 0$ and estimate both f and g in (15) using exactly the same estimation

methodology as presented in Section 2.1. We emphasize that we are facing a problem of model misspecification now: fitting model (15) to observation from (14a) which is not consistent with model (15). Parametric inference for misspecified models in the absence of multiscale effects has been studied, e.g. in [19, Ch. 2.6]. Here we expect that in the limit of infinite scale separation $\varepsilon \to 0$, the error due to the model misspecification vanishes [40]. Finally, our motivation to resort to the estimation methodology of Section 2.1 also for this setting stems from recent results in [13], where, as described in Section 1, a related scheme demonstrated to be able to accurately estimate the coarse-grained model from observations of the multiscale system. This favorable property agrees with our intuition that the estimated model should be close to the coarse-grained model if the model misspecification is small, i.e. if $\varepsilon \ll 1$. In fact, in view of the theoretical results presented in [40], it is expected that, in the absence of all other error contributions such as the finite sample size, the estimators converge in a probabilistic sense (in fact, the convergence is almost surely) to the parameters in the coarse-grained model in the limit $\varepsilon \to 0$.

Specifically, in this multiscale setting we have access to N discrete time observations of Eq. (14a), that is $\mathbb{X}_N^\varepsilon := \big(X^\varepsilon(t_k)\big)_{1\le k\le N}$ with $t_k = (k-1)h$, where $h = T/(N-1)$. Based on the semiparametric parametrization (7) of the drift and the diffusion coefficients in the the coarse-grained model (15), the multiscale time series $\mathbb{X}_N^\varepsilon$ is used to assemble the corresponding matrix A^ε and right-hand side b^ε in Eq. (10). The estimated parameter vector of the coarse-grained model based on the multiscale data $\mathbb{X}_N^\varepsilon$ is then given by the least squares solution of $A^\varepsilon\theta = b^\varepsilon$ with minimum norm. We denote the estimated parameter vector by $\hat{\theta}^\varepsilon$ to emphasize the dependency on the multiscale observations $\mathbb{X}_N^\varepsilon$. It is also worth mentioning that the estimation procedure is solely derived from the coarse-grained model (15). That is, the procedure does not incorporate any knowledge of the corresponding multiscale system (14). In addition, we are not assuming knowledge of the scale separation parameter ε. In other words, one can view the available time series $\mathbb{X}_N^\varepsilon$ as obtained purely from a "black box" model, which is close to the coarse-grained model (15) provided that $\varepsilon \ll 1$.

3. Numerical experiments

In this section we apply the proposed estimation procedure to several examples. We focus here on the inference problem for coarse-grained models based on multiscale observations, for which classical estimators are expected to fail. In Section 3.1 we first investigate a stochastic multiscale system, namely Brownian motion in a two-scale potential. The remaining examples are deterministic multiscale systems, for which we seek to identify a coarse-grained stochastic model from a single time series. Specifically, we estimate parameters in the coarse-grained model for a deterministic system exhibiting fast temporal chaos (Section 3.1), in a low-dimensional approximation of a large Hamiltonian system (Section 3.3), and in an Ornstein–Uhlenbeck process constructed in a purely deterministic setting (Section 3.4). To verify the accuracy of the estimated parameters in the coarse-grained models, we compare the obtained estimates with theoretically available ones. We will also address the question of selecting the time t controlling the temporal integrals in (8), in order to uniquely define the estimation procedure of Section 2. To emphasize the dependency of the estimated parameter vector based on multiscale data $\hat{\theta}^\varepsilon$ also on t, we use $\hat{\theta}^\varepsilon \equiv \hat{\theta}_t^\varepsilon$. To assemble the linear system (10) we use $m = 54$ trial point for all examples. As mentioned above already, these points ξ are selected a-priori for each example such that they cover most of the range of the time series $\mathbb{X}_N^\varepsilon$. One simple and ad hoc way is to identify the region for ξ by defining $a_N := (1-\nu)\min(\mathbb{X}_N^\varepsilon) + \nu\max(\mathbb{X}_N^\varepsilon)$ and $b_N := \nu\min(\mathbb{X}_N^\varepsilon) + (1-\nu)\max(\mathbb{X}_N^\varepsilon)$, for $0 < \nu < 1/2$. Furthermore, let $\eta_1, \eta_2, \ldots, \eta_m$ be

an independent and identically distributed sequence of random variables following a standard normal distribution. Then we set $l_m := \min_{1\leq i\leq m}(\eta_i)$ as well as $r_m := \max_{1\leq i\leq m}(\eta_i)$ and select the trial points by linearly mapping η_i to the region of interest $[a_N, b_N]$:

$$\xi_i := \frac{a_N - b_N}{l_m - r_m}\eta_i + \frac{l_m b_N - r_m a_N}{l_m - r_m} \ ,$$

for $1 \leq i \leq m$, which are then fixed throughout the numerical experiment. This rather naive procedure worked well for the examples that follow where we used $\nu = 0.2$, because the trial points ξ are located in regions where most of the observations are, so that estimates of the conditional expectations are expected to be accurate. We remark however, that other approaches are possible as well. In fact, a more systematic way to construct the trial points is via a resampling method, which exploits the shape of the empirical distribution function of $\mathbb{X}_N^\varepsilon$. In this case let $\eta_1, \eta_2, \ldots, \eta_m$ be an independent and identically distributed sequence of random variables following a uniform distribution on $[0, 1]$. Moreover, denote by $X_{1:N}^\varepsilon, X_{2:N}^\varepsilon, \ldots, X_{N:N}^\varepsilon$ the order statistic of $\mathbb{X}_N^\varepsilon$ so that $X_{1:N}^\varepsilon < X_{2:N}^\varepsilon < \cdots < X_{N:N}^\varepsilon$. Then the trail points may be constructed via

$$\xi_i := X_{k_i:N}^\varepsilon \ , \quad k_i := \min\left\{k \in \mathbb{N} \colon \eta_i N \leq k\right\} \ ,$$

for $1 \leq i \leq m$. Although we did not observe significant differences between these two trial point selection strategies for the examples considered here, the second systematic strategy may be advantageous in more general cases as it is purely data-driven. Finally, we note that we set the estimation procedure's defining parameters m, T, and h in such a way that their error contribution due to approximations are negligible compared to the scale separation ε. This is done to focus solely on the estimator's performance under the presence of multiscale effects in the observations, a scenario where other estimation techniques fail to be consistent.

3.1. Brownian particle in a two-scale potential

Let us begin with an example borrowed from [12], which was originally used to investigate the failure of classical parametric estimation techniques for multiscale diffusion processes. Specifically, we consider

$$dX^\varepsilon = -\frac{d}{dx}V\left(X^\varepsilon, \frac{X^\varepsilon}{\varepsilon}\right) dt + \sqrt{2\sigma}\, dW_t \ ,$$

which models the position of a Brownian particle moving in a two-scale potential V and being affected by thermal noise. Here W denotes a standard one-dimensional Brownian motion. We investigate the situation when the two-potential V is given by a large scale part V_α superimposed with a periodically fluctuating part p: $V(x, y) = V_\alpha(x) + p(y)$. Under this assumption, the multiscale SDE can be written as

$$dX^\varepsilon = -\left(V_\alpha'(X^\varepsilon) + \frac{1}{\varepsilon}p'\left(\frac{X^\varepsilon}{\varepsilon}\right)\right) dt + \sqrt{2\sigma}\, dW_t \ . \tag{16}$$

Notice that the SDE (16) can be rewritten as a fast/slow system of the form (14) by introducing the auxiliary variable $Y^\varepsilon := X^\varepsilon/\varepsilon$.

We consider the case where the fluctuating part p is a smooth periodic function with period L and the large scale part is a quadratic potential, i.e. $V_\alpha(x) = \alpha x^2/2$. Then, as $\varepsilon \to 0$, X^ε solving (16) converges weakly in $C([0, T], \mathbb{R})$ to the solution of the coarse-grained equation

$$dX = -AX\, dt + \sqrt{2\Sigma}\, dW_t \ , \tag{17}$$

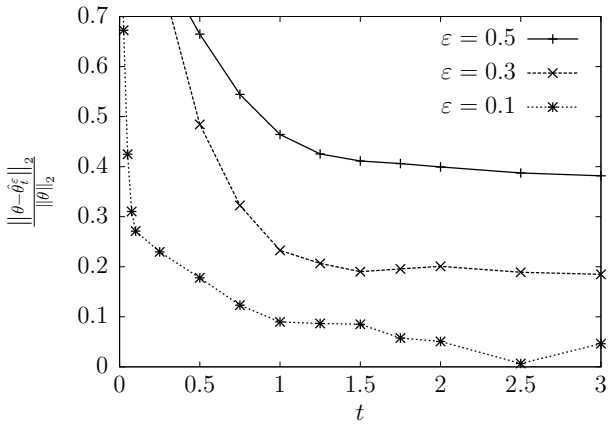


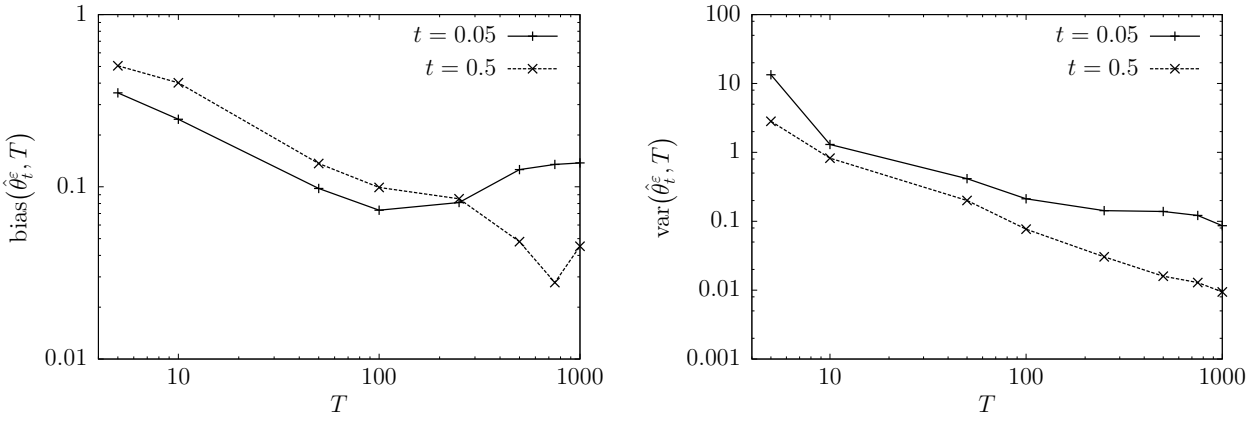
Figure 1: Relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ for (17) based on observations of (16) with $\alpha = 2$, $\sigma = 1$, and $\varepsilon \in \{0.1, 0.3, 0.5\}$.

where $A = \alpha L^2/(Z_+ Z_-)$ and $\Sigma = \sigma L^2/(Z_+ Z_-)$, with $Z_\pm = \int_0^L e^{\pm p(y)/\sigma}\, dy$; see [12] for details. We set the fluctuating part to be $p(y) = \cos(y)$. Then the constants $Z_\pm$ can be easily computed so that $A = \alpha/I_0(\sigma^{-1})^2$ and $\Sigma = \sigma/I_0(\sigma^{-1})^2$, where I_0 denotes the modified Bessel function of first kind. We note that both parameters in (17) depend non-trivially on σ.

To estimate the $n = 2$ parameters in (17), we choose the functions in the drift and diffusion parametrization (7) as $f_1(x) = x$, $f_2(x) = 0 = g_1(x)$, and $g_2(x) = 2$, with true parameter vector $\theta = (-A, \Sigma)^T$. The estimate of θ is then based on a time series on $[0, 1000]$ of the multiscale system (16) with $\alpha = 2$, $\sigma = 1$ for each $\varepsilon \in \{0.1, 0.3, 0.5\}$. The time series were obtained by numerically integrating (16) via the Euler–Maruyama method with step size $h = 0.001$ and initial condition $X^\varepsilon(0) = 0$. Fig. 1 shows the relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ as a function of t, for each value of ε respectively. For all three of them one observes that while very small values of t result in a large relative error, increasing t reduces the error significantly. In fact, for $t = 1$ and $\varepsilon = 0.1$ we find a relative error of 10% and for even larger values of t the relative error drops further significantly below 5%. For $t \geq 3$ (not shown here) the relative error starts fluctuating around 4% due to discretization errors but remains of the same order as the scale separation parameter ε, which is in agreement with the results presented in [40]. Consequently, it is possible to obtain very accurate estimates of the parameters in the coarse-grained model (17) based on observations of the multiscale system (16), once t is sufficiently large. In fact, by comparing the resulting relative errors for different values of ε, Fig. 1 suggests to choose t of $\mathcal{O}(1)$ for a relative error of $\mathcal{O}(\varepsilon)$.

We proceed by numerically studying the bias and the variance of the estimation procedure for a fixed time t as functions of the length of the time interval T. To this end we use M independent Brownian motions in Eq. (16) to generate an ensemble of independent trajectories $X_1^\varepsilon, X_2^\varepsilon, \ldots, X_M^\varepsilon$, each on the time interval $[0, T]$. Applying the estimation procedure to every such time series X_k^ε yields an estimated value, which we denote by $\hat{\theta}_t(X_k^\varepsilon, T)$ to emphasize the dependency on the k-th time series and on the final time T. Using these estimated values we approximate expectations by ensemble averages to define the bias and variance. Specifically, let $E_M^T(\hat{\theta}_t^\varepsilon) := \frac{1}{M}\sum_{k=1}^M \hat{\theta}_t(X_k^\varepsilon, T)$ be the average of these estimated values. Then we use

$$\text{bias}(\hat{\theta}_t^\varepsilon, T) := \left\| E_M^T(\hat{\theta}_t^\varepsilon) - \theta \right\|_2 \approx \left\| \mathbb{E}\big(\hat{\theta}_t(X^\varepsilon, T)\big) - \theta \right\|_2 ,$$



(A) bias (B) variance

Figure 2: Bias and variance of the estimation procedure as functions of T for $t \in \{0.05, 0.5\}$ and $\varepsilon = 0.1$. Expectations were approximated as described in the text.

to quantify the (absolute) bias and as a measure of the variance we use

$$\mathrm{Var}(\hat{\theta}_t^\varepsilon, T) := \frac{1}{M-1} \sum_{i=1}^{n} \sum_{k=1}^{M} \Big(e_i \cdot \big(\hat{\theta}_t(X_k^\varepsilon, T) - E_M^T(\hat{\theta}_t^\varepsilon) \big) \Big)^2 \approx \sum_{i=1}^{n} \mathrm{Var}\big(e_i \cdot \hat{\theta}_t(X^\varepsilon, T) \big) \ ,$$

with e_i, $1 \leq i \leq n$, denoting the canonical basis vectors of $\mathbb{R}^n$. In other words $\mathrm{Var}(\hat{\theta}_t^\varepsilon, T)$ is simply an approximation of the trace of the covariance matrix. Fig. 2 shows the behavior the estimation procedure's bias and variance as functions of T using $M = 100$ independent Brownian motions for $t \in \{0.05, 0.5\}$ and $\varepsilon = 0.1$. One observes that the variance $\mathrm{Var}(\hat{\theta}_t^\varepsilon, T)$ (Fig. 2(B)) decreases to zero as T increases, with slightly different rates for the different values of t. Conversely, the bias $\mathrm{bias}(\hat{\theta}_t^\varepsilon, T)$ (Fig. 2(A)) starts to decrease by increasing T for both values of t, however, after some value of T, the bias approaches a limiting value of approximately 0.15 for $t = 0.05$ and fluctuates around 0.04 for $t = 0.5$. This fluctuation persists even for $T > 1000$ (not shown here) and are mainly due to the error induced by approximating an expectation via an ensemble average of size $M = 100$, which becomes visible in this logarithmic scaling. The fact that the bias approaches a non-zero limiting value is not surprising (and in fact in agreement with the theoretical results), as one expects that the estimated value approaches the true value θ, as $T \to \infty$, plus an $\mathcal{O}(\varepsilon)$ error due to the multiscale effects in the data X^ε. Furthermore, we note that both values of t correspond to estimated values in Fig. 1 which have a considerable relative error, where the relative error for $t = 0.5$ is significantly smaller that the one for $t = 0.05$, hence explaining the different limiting values in Fig.2(A) as the constant of the $\mathcal{O}(\varepsilon)$ error is t dependent.

3.2. Fast deterministic chaos

We consider an ODE driven by the time rescaled Lorenz equations:

$$\frac{dX^\varepsilon}{dt} = \alpha\big(X^\varepsilon - (X^\varepsilon)^3\big) + \frac{\lambda}{\varepsilon}Y_2^\varepsilon \,, \tag{18a}$$

$$\frac{dY_1^\varepsilon}{dt} = \frac{10}{\varepsilon^2}(Y_2^\varepsilon - Y_1^\varepsilon) \,, \tag{18b}$$

$$\frac{dY_2^\varepsilon}{dt} = \frac{1}{\varepsilon^2}(28Y_1^\varepsilon - Y_2^\varepsilon - Y_1^\varepsilon Y_3^\varepsilon) \,, \tag{18c}$$

$$\frac{dY_3^\varepsilon}{dt} = \frac{1}{\varepsilon^2}\Big(Y_1^\varepsilon Y_2^\varepsilon - \frac{8}{3}Y_3^\varepsilon\Big) \,. \tag{18d}$$

Equations of this form have been used as a deterministic climate toy model, see [50] for instance. Our aim is to obtain a stochastic coarse-grained model from observations of (18). It is known that, as $\varepsilon \to 0$, the slow component X^ε of Eq. (18) converges weakly in $C([0,T],\mathbb{R})$ to the solution of the homogenized equation [51]

$$dX = A\big(X - X^3\big)\,dt + \sqrt{\sigma}\,dW_t \,. \tag{19}$$

In Eq. (19) the true parameter values are $A = \alpha$ and the diffusion coefficient σ is given in terms of the Green–Kubo formula [17]

$$\sigma = 2\lambda^2 \int_0^\infty \lim_{T\to\infty} \frac{1}{T} \int_0^T Y_2^{\varepsilon=1}(s) Y_2^{\varepsilon=1}(s+t)\,ds\,dt \,. \tag{20}$$

Obtaining a value for σ directly from Eq. (20) is computationally challenging so that the parametric estimation problem of σ from observations of Eq. (18a) arises naturally for this model, even without the connection to data-driven coarse-graining methodologies.

To estimate both the drift coefficient A and the diffusion coefficient σ (i.e. $n = 2$) in Eq. (19), a self-evident choice for the functions in Eq. (7) is $f_1(x) = x - x^3$, $f_2(x) = 0 = g_1(x)$, and $g_2(x) = 1$, where the true parameter vector is $\theta = (A, \sigma)^T$. To generate the time series we numerically integrate the multiscale system of ODEs (18) with $\alpha = 1/3$, $\lambda = 2/45$, and $\varepsilon = 0.1$ on $[0, 5000]$ with initial conditions $X^\varepsilon(0) = 1$, $Y^\varepsilon(0) = (1,1,1)^T$. For these parameter choices (mainly the value of ε) the ODE system (18) is only marginally stiff and we thus solve it using a fourth order Runge–Kutta scheme with step size $h = 0.001$. Since there is no exact value for σ in Eq. (19) available, we cannot compute the relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$. Instead Fig. 3 illustrates both estimated values $\hat{A}$ and $\hat{\sigma}$ as functions of t directly. One finds that the estimated drift parameter $\hat{A}$ is strongly biased for very small values of t. Increasing t reduces the bias significantly and the estimated value approaches the true value (dashed line), only with minor fluctuations. In fact, the relative error is smaller than 6% for $t \geq 0.5$. The estimated diffusion coefficient $\hat{\sigma}$ shows qualitatively the same behavior. Specifically, by increasing t the estimated value seems to approach a limiting value. In fact, averaging over the obtained estimated values for $t \geq 0.5$ (i.e. the region for which $\hat{A}$ is accurate), one finds $\hat{\sigma} \approx 0.113$ with minor fluctuations (standard deviation ≈ 0.002). This value of $\hat{\sigma}$ is in very good agreement with those reported in the literature [52, 13], albeit marginally smaller. In fact, the relative error between the obtained value here and the value reported in [13] is around 6%.

3.3. Large Hamiltonian systems: The Kac–Zwanzig model

Here we apply our methodology to the variant of the Kac–Zwanzig model studied in [53]. Specifically, we consider the case where one distinguished particle, with coordinate Q_M and

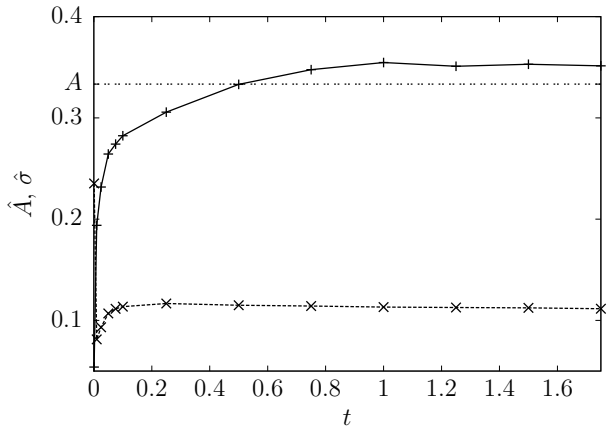


Figure 3: Parameter estimates $\hat{A}$ (+) and $\hat{\sigma}$ (×) for (19) based on observations X^ε of (18) with $\alpha = 1/3$, $\lambda = 2/45$, and $\varepsilon = 10^{-1}$.

momentum P_M, moves in an one-dimensional potential V and interacts with $M \in \mathbb{N}$ heat bath particles. Let the heat bath particles be described by coordinates $q \equiv (q_1, \dots, q_M)^T \in \mathbb{R}^M$ and momenta $p \equiv (p_1, \dots, p_M)^T \in \mathbb{R}^M$. Then we consider the Hamiltonian

$$H(P_M, Q_M, p, q) := \frac{1}{2}{P_M}^2 + V(Q_M) + \frac{1}{2}\sum_{j=1}^{M} \frac{{p_j}^2}{m_j} + \frac{1}{2}\sum_{j=1}^{M} k_j (q_j - Q_M)^2 \, .$$

That is, the j-th heat bath particle with mass m_j acts on the distinguished particle as a linear spring with stiffness constant k_j. The interaction with the bath is governed by the following $2(M+1)$-dimensional system of ODEs

$$\frac{dQ_M}{dt} = P_M \, , \qquad \frac{dP_M}{dt} = \sum_{j=1}^{M} k_j (q_j - Q_M) - V'(Q_M) \, , \tag{21a}$$

$$\frac{dq_j}{dt} = \frac{p_j}{m_j} \, , \qquad \frac{dp_j}{dt} = -k_j (q_j - Q_M) \, , \quad j = 1, \dots, M \, . \tag{21b}$$

The initial condition for this system are $Q_M(0) = Q_0$, $P_M(0) = P_0$, $q_j(0) = q_{j,0}$, and $p_j(0) = p_{j,0}$. We assume that the initial conditions for the heat bath particles are in equilibrium. That is, we assume that the $2M$-dimensional vector of initial conditions for the particles in the heat bath (positions and momenta) is randomly distributed according to a Gibbs distribution with density proportional to $\exp(-\beta H)$, conditioned on (Q_0, P_0). Here $\beta > 0$ denotes the inverse temperature. Under these conditions it is possible to derive a coarse-grained model for the distinguished particle; see e.g. [53, 54] and the references therein for details.

The precise form of the coarse-grained model depends mainly on the chosen values for the spring constants k_j and the particles' mass m_j, $1 \le j \le M$. Here we borrow Example 7.3 from [52]. Let $\alpha \in (0, 1)$ and define $\omega_j = M^\alpha \eta_j$, where $(\eta_j)_{1 \le j \le M}$ is an identically and independently distributed sequence of random variables with $\eta_1 \sim \mathcal{U}(0, 1)$. Moreover, we set $k_j = 2\alpha M^\alpha / \big(\pi(\alpha^2 + {\omega_j}^2)M\big)$ and $m_j = k_j / {\omega_j}^2$. Then, as $M \to \infty$, the process Q_M solving the full model (21) converges weakly in $C^2([0, T]; \mathbb{R})$ to the process Q which is the solution of the stochastic integro-differential equation

$$\ddot{Q}(t) + V'\big(Q(t)\big) + \int_0^t e^{-\alpha|t-s|} \dot{Q}(s) \, ds = Z(t) \, ,$$

where Z denotes the Ornstein–Uhlenbeck process solving $dZ = -\alpha Z\,dt + \sqrt{2\alpha/\beta}\,dW$. By introducing an auxiliary variable, it is possible to convert the integro-differential equation with nonlocal memory into a Markov process. Specifically, the limiting process Q is equivalently given as the solution of the augmented system of SDEs

$$\frac{dQ}{dt} = P\ , \tag{22a}$$

$$\frac{dP}{dt} = S - V'(Q)\ , \tag{22b}$$

$$dS = (\mu S - P)\,dt + \sqrt{2\sigma}\,dW\ , \tag{22c}$$

where the auxiliary variable S embodies the memory effects due to the heat bath interactions. Consequently, the coarse-grained model associated to the $2(M+1)$-dimensional Hamiltonian system (21) is given in form of a 3-dimensional stochastic system. The limiting parameters in the coarse-grained model (22) are given by $\mu = -\alpha$ and $\sigma = \alpha/\beta$, where we recall that β is the inverse temperature.

The goal now is to estimate μ and σ in (22c) from observations in form of a single time series of (Q_M, P_M). Although the coarse-grained model (22) is three-dimensional, we can use a slightly modified procedure of the one derived in Section 2 for one-dimensional models, since we are concerned with identifying parameters in only one of the equations in (22), namely in (22c). Using Itô's formula for (22) with the function $\phi(s) = s + s^2$, which only depends on s, we find

$$\mathbb{E}\Big(\phi\big(S_\xi(t)\big)\Big) - \phi(\xi) + \int_0^t \mathbb{E}\Big(P_{P_0}(\tau)\phi'\big(S_\xi(\tau)\big)\Big)\,d\tau = \int_0^t \mathbb{E}\Big((\mathcal{L}_0\phi)\big(S_\xi(\tau)\big)\Big)\,d\tau\ ,$$

with $(\mathcal{L}_0\varphi)(s) := \mu s\frac{d}{ds}\varphi(s) + \sigma\frac{d^2}{ds^2}\varphi(s)$. This is an estimating equation like (8) and we thus only have to modify the definition of the term b_c in (9) to account for the dependency of (22c) on the process P (the integral term on the left-hand side above). The rest of the procedure follows as in Section 2. In fact, we select the functions in parametrization (7) with $n = 2$ as $f_1(x) = x$, $f_2(x) = 0 = g_1(x)$, and $g_2(x) = 2$, where the true parameter vector is $\theta = (\mu, \sigma)^T$.

It is important to stress that we wish to estimate μ and σ in (22c), but that we do not observe the process S directly: unlike for Q and P where we observe Q_M and P_M which converge to Q and P, respectively, we do not have access to such a process for S. We only have observations of (Q_M, P_M) from the full Hamiltonian system (21) with sampling time h. In the absence of model misspecification (i.e., when observing Q, P directly and not just Q_M, P_M instead), this problem is typically associated to hidden Markov model techniques as S is unobserved (i.e. hidden); see e.g. [55]. Here we consider a simple approximation to reconstruct the unobserved process S, which we will need in the estimation procedure. To this end we use the observations we have in (22b) with a first order finite difference approximation:

$$S_M(t) := \frac{P_M(t+h) - P_M(t)}{h} + V'\big(Q_M(t)\big)\ .$$

We remark that, in principle, we can apply our methodology even if only Q_M is observed but not P_M. In that case one has to use both Eq. (22a) and Eq. (22b) with finite difference approximations to obtain suitable approximations of P and S. These finite difference approximation ideas have also been used in [54] within a customized maximum likelihood framework for the Kac–Zwanzig model. However, in their study the authors had to chose h sufficiently large as

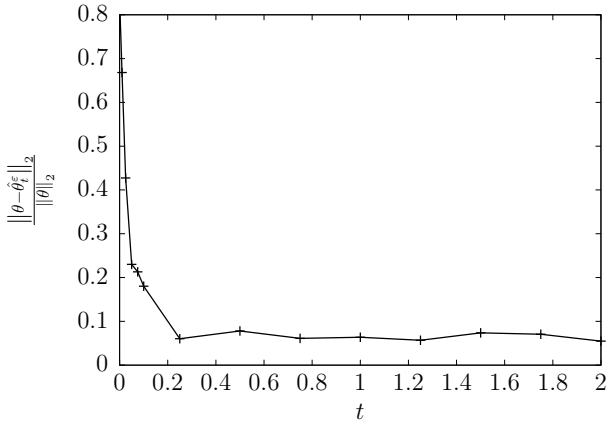


Figure 4: Relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ for (22c) based on observations (Q_M, P_M) of (21) with $\alpha = 1/22$, $\beta = 1$, and $M \equiv \varepsilon^{-1} = 5000$.

otherwise the parameter estimation performed poorly due to the presence of multiscale effects. Here we are not restricted by the multiscale structure of the problem.

For the numerical example we consider the case where the distinguished particle moves in a quartic potential, i.e. $V(x) = -x^2/2 + x^4/4$. Moreover, we use $M = 5000$ heat bath particles and set $\alpha = 1/2$ and $\beta = 1$. To obtain a time series for (Q_M, P_M) of the full Hamiltonian system (21) on $[0, 1000]$, we approximate it via a semi-implicit Euler scheme with time step $h = 10^{-3}$ started at $Q_0 = 1$, $P_0 = 0$. Fig. 4 depicts the relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ as a function of t, with the understanding that $\varepsilon \equiv M^{-1}$. Similar to the previous examples, one also observes here that it is possible to obtain accurate estimates once the value of t is sufficiently large. The relative error fluctuates closely around 6% for $t \geq 0.2$ and can be reduced even further by increasing M (not shown). To asses the obtained accuracy of 6%, we mention that in [54], as noted above, a specifically customized maximum likelihood method has been used to estimate parameters in a related problem and the authors report relative errors of 5–15%.

3.4. Deterministic Brownian motion

In [56] an Ornstein–Uhlenbeck process is constructed within a completely deterministic framework as an appropriate limit process of a chaotic dynamical system. Specifically, consider the position X^ε and the velocity V^ε of the dynamical system

$$\frac{dX^\varepsilon}{dt} = V^\varepsilon \,, \tag{23a}$$

$$\frac{dV^\varepsilon}{dt} = -\gamma V^\varepsilon + \eta_\varepsilon \,, \tag{23b}$$

with a deterministic perturbation $\eta_\varepsilon \equiv \eta_\varepsilon(t)$ in the velocity variable. Here we use

$$\eta_\varepsilon(t) = \sqrt{\varepsilon} \sum_{l=0}^{\infty} \zeta(t_l)\delta(t - t_l) \,, \tag{24}$$

so that the derivative of the velocity variable V^ε experiences small "kicks" at times $t_0, t_1, \ldots$, where $t_l = l\varepsilon$. Here ζ is a discrete time dynamical system of the form $\zeta(t_{l+1}) = \Phi(\zeta(t_l))$ and the function Φ is chosen such that the dynamical system ζ exhibits a strongly chaotic behavior. In our numerical example we used $\Phi(y) := \cos(3 \arccos(y))$. Based on this dynamical system ζ

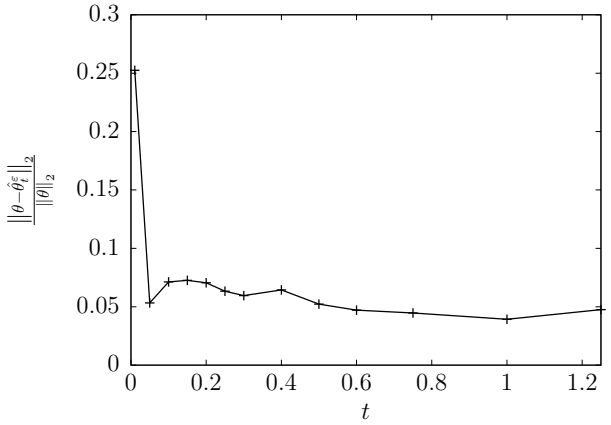


Figure 5: Relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ for (25b) based on observations X^ε of (23) with $\gamma = 1$ and $\varepsilon = 0.1$.

the perturbation η_ε in Eq. (24) is fixed and it follows from the results in [56] that the solution $(X^\varepsilon, V^\varepsilon)$ of the chaotic deterministic system (23) converges weakly in $C([0,T],\mathbb{R})$, as $\varepsilon \to 0$, to an Ornstein–Uhlenbeck process (X, V), which solves

$$dX = V\,dt\,, \tag{25a}$$

$$dV = -\gamma V\,dt + \sqrt{\sigma}\,dW_t\,, \tag{25b}$$

where the diffusion coefficient is $\sigma = 1/2$.

We now aim for estimating both γ and σ in (25b) based only on one long trajectory of observations of the position variable X^ε solving (23a). That is, we do not observe V^ε solving (23b) directly. Instead we will, as in Section 3.3, compute an approximation $\tilde{V}^\varepsilon$ based on a finite difference approximation in (25a) first, i.e. we set $\tilde{V}^\varepsilon(t_l) := (X^\varepsilon(t_{l+1}) - X^\varepsilon(t_l))/\varepsilon$, recalling that $t_{l+1} - t_l = \varepsilon$. Based on this approximate trajectory we can then directly apply the procedure introduced in Section 2 to estimate both γ and σ in (25b), since the velocity SDE is independent of the position. Therefore $(n = 2)$ and we select the functions $f_1(x) = x$, $f_2(x) = 0 = g_1(x)$, and $g_2(x) = 1$ in (7), corresponding to the true parameter vector $\theta = (-\gamma, \sigma)^T$. A time series of X^ε on $[0, 1000]$ with sampling rate $h = 0.01$ is obtained by solving the perturbed system (23) with $X^\varepsilon(0) = -0.15$, $V^\varepsilon(0) = -0.53$, $\gamma = 1$ and $\varepsilon = 0.1$. Fig. 5 shows the relative error of the estimated parameter vector $\hat{\theta}_t^\varepsilon$ as a function of t. Increasing t yields very accurate estimates with the relative error fluctuating around 5% for $t \geq 0.5$.

4. Conclusion

In this paper we have introduced a novel numerical/statistical procedure which allows us to estimate parameters in coarse-grained models based on partial observations of a corresponding multiscale system. For such systems commonly used estimators, such as the maximum likelihood estimator, are known to be biased. Our approach is based on our previous study in [13] where it was assumed that an ensemble of short trajectories for multiple initial conditions is available. Here we generalize and appropriately extend the work presented in [13] to the practically relevant setting where only one (long) time series is available. In fact, the examples presented demonstrate that the developed inference method yields accurate approximations of the parameters in coarse-grained models based on a time series of the "slow" component of a multiscale system. The examples range from coarse-grained models where the associated multiscale system is stochastic to coarse-grained models for fully deterministic multiscale systems.

We believe that this selection of examples highlights the broad occurrence of data-driven coarse-graining problems and thus the necessity for appropriate inference techniques which are robust against multiscale effects in the observation, as the one introduced here.

The illustrated robustness of an inference technique against multiscale effects (i.e. against perturbations that are small the weak sense) appears to be novel but also has important implications in practice. Specifically, it significantly widens the range of applications to problems where the observed process is not necessarily a diffusion process. For instance, it covers the case of non-Markovian processes that can be approximated by a Markov process in an augmented state space (see, e.g., [57, Ch. 8.2]) and the concept of diffusion approximation (see, e.g., [58, Ch. 7]), both allowing for non-negligible deviations of the observation process from the assumed SDE model.

The focus of our study was on demonstrating that the introduced methodology can accurately infer parameters in coarse-grained models from a time series, either stochastic or chaotic, of a multiscale system. Clearly there are still many challenges that remain to be addressed. One of them is the rigorous analysis of the algorithm to understand its asymptotic properties, but also to explore its limitations. Some first results concerning the convergence properties of the methodology have already been obtained and will be presented in [40]. A closely related and important avenue of future efforts is the study of the asymptotic distribution of the estimators, which in turn can be used to guide the construction of asymptotic confidence intervals for the estimated values. Another interesting topic, which is relevant in many applications, is the study of additional observation error. That is, one only observes a contaminated version $\tilde{X}^\varepsilon$ of X^ε:

$$\tilde{X}^\varepsilon(t_k) = X^\varepsilon(t_k) + \eta(t_k) \ ,$$

for any $k \geq 0$, where η denotes the observation error. To allow for this additional contamination, our methodology would have to be combined with appropriate filtering techniques, a very appealing prospect. The first results on combining filtering ideas with parametric inference techniques have been studied in [25] for a particular multiscale problem. See also [59] for more recent work on combining the MLE with filtering techniques for a class of multiscale problems. But also conceptually different approaches to the problem of data-driven coarse-graining appear worthwhile investigating. As, for example, most work on data-driven coarse-graining is based on a frequentist inference approach, investigating similar questions in a Bayesian approach poses a natural and interesting perspective as well; see [60] for related work in the context of inverse problems with a multiscale structure. We shall examine these and related questions in future studies.

Acknowledgements

We are grateful to the anonymous referees for their insightful comments and suggestions. We acknowledge financial support from the Engineering and Physical Sciences Research Council of the UK through Grants No. EP/H034587, EP/J009636, and EP/L020564 and from the European Research Council via Advanced Grant No. 247031.

[1] A. Chauvière, L. Preziosi, C. Verdier (Eds.), Cell Mechanics: From Single Scale-Based Models to Multiscale Modeling, Mathematical & Computational Biology Series, Chapman & Hall/CRC, 2010.

[2] A. J. Majda, C. Franzke, B. Khouider, An applied mathematics perspective on stochastic modelling for climate, Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. 366 (1875) (2008) 2429–2455. doi:10.1098/rsta.2008.0012.

[3] J. Culina, S. Kravtsov, A. H. Monahan, Stochastic parameterization schemes for use in realistic climate models, J. Atmospheric Sci. 68 (2) (2010) 284–299. doi:10.1175/2010JAS3509.1.

[4] M. Griebel, S. Knapek, G. W. Zumbusch, Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications, Texts in Computational Science and Engineering, Springer, 2007.

[5] J. Fish, Multiscale Methods: Bridging the Scales in Science and Engineering, Oxford University Press, 2009.

[6] P. Huerre, M.Rossi, Hydrodynamic instabilities in open flows, in: C. Godrèche, P. Manneville (Eds.), Hydrodynamic and Nonlinear Instabilities, Cambridge University Press, 1998, pp. 81–294.

[7] M. F. Horstemeyer, Multiscale modeling: A review, in: J. Leszczynski, M. K. Shukla (Eds.), Practical Aspects of Computational Chemistry, Springer, 2010, pp. 87–135. doi:10.1007/978-90-481-2687-3.

[8] N. Savva, S. Kalliadasis, G. A. Pavliotis, Two-dimensional droplet spreading over random topographical substrates, Phys. Rev. Lett. 104 (8) (2010) 084501. doi:10.1103/PhysRevLett.104.084501.

[9] A. J. Chorin, O. H. Hald, R. Kupferman, Optimal prediction and the Mori-Zwanzig representation of irreversible processes, Proc. Natl. Acad. Sci. USA 97 (7) (2000) 2968–2973. doi:10.1073/pnas.97.7.2968.

[10] B. Turkington, An optimization principle for deriving nonequilibrium statistical models of Hamiltonian dynamics, J. Stat. Phys. 152 (3) (2013) 569–597. doi:10.1007/s10955-013-0778-9.

[11] D. Venturi, G. E. Karniadakis, Convolutionless Nakajima–Zwanzig equations for stochastic analysis in nonlinear dynamical systems, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. 470 (2166) (2014) 20130754, 20. doi:10.1098/rspa.2013.0754.

[12] G. A. Pavliotis, A. M. Stuart, Parameter estimation for multiscale diffusions, J. Stat. Phys. 127 (4) (2007) 741–781. doi:10.1007/s10955-007-9300-6.

[13] S. Krumscheid, G. A. Pavliotis, S. Kalliadasis, Semiparametric drift and diffusion estimation for multiscale diffusions, Multiscale Model. Simul. 11 (2) (2013) 442–473. doi:10.1137/110854485.

[14] M. Pradas, D. Tseluiko, S. Kalliadasis, D. T. Papageorgiou, G. A. Pavliotis, Noise induced state transitions, intermittency, and universality in the noisy Kuramoto-Sivashinksy equation, Phys. Rev. Lett. 106 (6) (2011) 060602. doi:10.1103/PhysRevLett.106.060602.

[15] M. Pradas, G. A. Pavliotis, S. Kalliadasis, D. T. Papageorgiou, D. Tseluiko, Additive noise effects in active nonlinear spatially extended systems, European J. Appl. Math. 23 (5) (2012) 563–591. doi:10.1017/S0956792512000125.

[16] M. Schmuck, M. Pradas, S. Kalliadasis, G. A. Pavliotis, New stochastic mode reduction strategy for dissipative systems, Phys. Rev. Lett. 110 (24) (2013) 244101. doi:10.1103/PhysRevLett.110.244101.

[17] G. A. Pavliotis, A. M. Stuart, Multiscale Methods: Averaging and Homogenization, Springer, 2008.

[18] B. L. S. Prakasa Rao, Statistical Inference for Diffusion Type Processes, Vol. 8 of Kendall's Library of Statistics, Arnold, 1999.

[19] Y. A. Kutoyants, Statistical Inference for Ergodic Diffusion Processes, Springer, 2004. doi:10.1007/978-1-4471-3866-2.

[20] R. S. Liptser, A. N. Shiryaev, Statistics of Random Processes: I. General Theory, 2nd Edition, Stochastic Modelling and Applied Probability Series, Springer, 2010, translated by A. B. Aries.

[21] A. Papavasiliou, G. A. Pavliotis, A. M. Stuart, Maximum likelihood drift estimation for multiscale diffusions, Stochastic Process. Appl. 119 (2009) 3173–3210. doi:10.1016/j.spa.2009.05.003.

[22] L. Zhang, P. A. Mykland, Y. Aït-Sahalia, A tale of two time scales: determining integrated volatility with noisy high-frequency data, J. Amer. Statist. Assoc. 100 (472) (2005) 1394–1411. doi:10.1198/016214505000000169.

[23] R. Azencott, A. Beri, I. Timofeyev, Adaptive sub-sampling for parametric estimation of gaussian diffusions, J. Stat. Phys. 139 (6) (2010) 1066–1089. doi:10.1007/s10955-010-9975-y.

[24] R. Azencott, A. Beri, I. Timofeyev, Parametric estimation of stationary stochastic processes under indirect observability, J. Stat. Phys. 144 (1) (2011) 150–170. doi:10.1007/s10955-011-0253-4.

[25] C. J. Cotter, G. A. Pavliotis, Estimating eddy diffusivities from noisy Lagrangian observations, Commun. Math. Sci. 7 (4) (2009) 805–838.
URL `http://projecteuclid.org/euclid.cms/1264434134`

[26] S. C. Olhede, A. M. Sykulski, G. A. Pavliotis, Frequency domain estimation of integrated volatility for Itô processes in the presence of market-microstructure noise, Multiscale Model. Simul. 8 (2) (2009) 393–427. doi:10.1137/090756363.

[27] D. T. Crommelin, E. Vanden-Eijnden, Diffusion estimation from multiscale data by operator eigenpairs, Multiscale Model. Simul. 9 (4) (2011) 1588–1623. doi:10.1137/100795917.

[28] D. Crommelin, Estimation of space-dependent diffusions and potential landscapes from non-equilibrium data, J. Stat. Phys. 149 (2) (2012) 220–233. doi:10.1007/s10955-012-0597-4.

[29] K. Spiliopoulos, A. Chronopoulou, Maximum likelihood estimation for small noise multiscale diffusions, Stat. Inference Stoch. Process. 16 (3) (2013) 237–266. doi:10.1007/s11203-013-9088-8.

[30] P. Imkeller, N. Sri Namachchivaya, N. Perkowski, H. C. Yeong, Dimensional reduction in nonlinear filtering: A homogenization approach, Ann. Appl. Probab. 23 (6) (2013) 2290–2326. doi:10.1214/12-AAP901.

[31] W. Zhang, J. C. Latorre, G. A. Pavliotis, C. Hartmann, Optimal control of multiscale systems using reduced-order models, J. Computational Dynamics 1 (2) (2014) 279–306. doi:10.3934/jcd.2014.1.279.

[32] E. Vanden-Eijnden, Numerical techniques for multi-scale dynamical systems with stochastic effects, Commun. Math. Sci. 1 (2) (2003) 385–391.
URL http://projecteuclid.org/euclid.cms/1118152078

[33] W. E, D. Liu, E. Vanden-Eijnden, Analysis of multiscale methods for stochastic differential equations, Comm. Pure Appl. Math. 58 (11) (2005) 1544–1585. doi:http://dx.doi.org/10.1002/cpa.20088.

[34] C. Theodoropoulos, Y.-H. Qian, I. G. Kevrekidis, "coarse" stability and bifurcation analysis using time-steppers: A reaction-diffusion example, Proc. Natl. Acad. Sci. USA 97 (18) (2000) 9840–9843.
URL http://www.jstor.org/stable/123274

[35] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg, C. Theodoropoulos, Equation-free, coarse-grained multiscale computation: enabling microscopic simulators to perform system-level analysis, Commun. Math. Sci. 1 (4) (2003) 715–762.
URL http://projecteuclid.org/getRecord?id=euclid.cms/1119655353

[36] I. G. Kevrekidis, C. W. Gear, G. Hummer, Equation-free: The computer-aided analysis of complex multiscale systems, AIChE J. 50 (7) (2004) 1346–1355. doi:10.1002/aic.10106.

[37] I. G. Kevrekidis, G. Samaey, Equation-free multiscale computation: Algorithms and applications, Annu. Rev. Phys. Chem. 60 (1) (2009) 321–344. doi:10.1146/annurev.physchem.59.032607.093610.

[38] I. Karatzas, S. E. Shreve, Brownian Motion and Stochastic Calculus, 2nd Edition, Springer, 1991. doi:10.1007/978-1-4612-0949-2.

[39] B. K. Øksendal, Stochastic Differential Equations: An Introduction with Applications, Springer, 2003. doi:10.1007/978-3-642-14394-6.

[40] S. Krumscheid, Perturbation-based inference for diffusion processes: Obtaining coarse-grained models from multiscale data, submitted (2014).

[41] D. Bosq, Nonparametric Statistics for Stochastic Processes: Estimation and Prediction, 2nd Edition, Vol. 110 of Lecture Notes in Statistics, Springer, 1998. doi:10.1007/978-1-4612-1718-3.

[42] J. Fan, Q. Yao, Nonlinear Time Series: Nonparametric and Parametric Methods, Springer Series in Statistics, Springer, 2003. doi:10.1007/b97702.

[43] P. Doukhan, Mixing: Properties and Examples, Springer, 1994. doi:10.1007/978-1-4612-2642-0.

[44] X. Chen, L. P. Hansen, M. Carrasco, Nonlinearity and temporal dependence, J. Econometrics 155 (2) (2010) 155–169. doi:10.1016/j.jeconom.2009.10.001.

[45] E. A. Nadaraya, On estimating regression, Theory Probab. Appl. 9 (1) (1964) 141–142. doi:10.1137/1109020.

[46] G. S. Watson, Smooth regression analysis, Sankhyā Ser. A 26 (4) (1964) 359–372.
URL http://www.jstor.org/stable/25049340

[47] D. Cruz-Uribe, C. J. Neugebauer, Sharp error bounds for the trapezoidal rule and Simpson's rule, JIPAM. J. Inequal. Pure Appl. Math. 3 (4) (2002) Article 49, 22.
URL http://www.emis.de/journals/JIPAM/article201.html?sid=201

[48] G. H. Golub, C. F. van Loan, Matrix Computations, 3rd Edition, Johns Hopkins Studies in the Mathematical Sciences, Johns Hopkins University Press, 1996.

[49] D. P. Kroese, T. Taimre, Z. I. Botev, Handbook of Monte Carlo Methods, Wiley Series in Probability and Statistics, John Wiley and Sons, 2011.

[50] L. Mitchell, G. A. Gottwald, Data assimilation in slow-fast systems using homogenized climate models, J. Atmospheric Sci. 69 (4) (2012) 1359–1377. doi:10.1175/JAS-D-11-0145.1.

[51] I. Melbourne, A.M.Stuart, A note on diffusion limits of chaotic skew-product flows, Nonlinearity 24 (4) (2011) 1361–1367. doi:10.1088/0951-7715/24/4/018.

[52] D. Givon, R. Kupferman, A. M. Stuart, Extracting macroscopic dynamics: model problems and algorithms, Nonlinearity 17 (6) (2004) 55–127. doi:10.1088/0951-7715/17/6/R01.

[53] R. Kupferman, A. M. Stuart, J. R. Terry, P. F. Tupper, Long-term behaviour of large mechanical systems with random initial data, Stoch. Dyn. 2 (4) (2002) 533–562. doi:10.1142/S0219493702000571.

[54] R. Kupferman, A. M. Stuart, Fitting SDE models to nonlinear Kac-Zwanzig heat bath models, Phys. D 199 (3-4) (2004) 279–316. doi:10.1016/j.physd.2004.04.011.

[55] O. Cappé, E. Moulines, T. Rydén, Inference in Hidden Markov Models, Springer Series in Statistics, Springer, 2005.

[56] M. C. Mackey, M. Tyran-Kamińska, Deterministic Brownian motion: the effects of perturbing a dynamical system by a chaotic semi-dynamical system, Phys. Rep. 422 (5) (2006) 167–222. doi:10.1016/j.physrep.2005.09.002.

[57] G. A. Pavliotis, Stochastic Processes and Applications: Diffusion Processes, the Fokker-Planck and Langevin Equations, Springer, 2014.

[58] S. N. Ethier, T. G. Kurtz, Markov Processes: Characterization and Convergence, Wiley Series in Probability and Mathematical Statistics, John Wiley & Sons, Inc., 1986. doi:10.1002/9780470316658.

[59] A. Papanicolaou, K. Spiliopoulos, Filtering the maximum likelihood for multiscale problems, Multiscale Model. Simul. 12 (3) (2014) 1193–1229. doi:10.1137/140952648.

[60] J. Nolen, G. A. Pavliotis, A. M. Stuart, Multiscale modelling and inverse problems, in: O. L. I.G. Graham, T.Y. Hou, R. Scheichl (Eds.), Numerical Analysis of Multiscale Problems, Vol. 83, Springer, 2012, pp. 1–34. doi:10.1007/978-3-642-22061-6.