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Variance-reduced multiscale simulation of slow–fast stochastic differential equations

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ABSTRACT

We study a variance reduction strategy based on control variables for simulating the averaged macroscopic behavior of a stochastic slow–fast system. We assume that this averaged behavior can be written in terms of a few slow degrees of freedom, and that the fast dynamics is ergodic for every fixed value of the slow variable. The time derivative for the averaged dynamics can then be approximated by a Markov chain Monte Carlo method. The variance-reduced scheme that is introduced here uses the previous time instant as a control variable. We analyze the variance and bias of the proposed estimator and illustrate its performance when applied to a linear and nonlinear model problem.

1. Introduction

Stochastic differential equations (SDEs) are ubiquitous in a multitude of real-life applications, appearing in different scientific domains such as climate and environmental sciences [1–3], molecular dynamics [4,5] and bacterial chemotaxis [6]. Many of these applications contain processes that inherently evolve over multiple time scales, leading to an excessive computational cost with standard time discretization methods. As a consequence, there is currently a large interest in developing dedicated numerical methods that circumvent, or even exploit, the presence of a time-scale separation in the problem at hand.

Clearly, the development of new numerical techniques needs to be supplemented by a detailed analysis of their efficiency and accuracy, and this for a set of model problems of which the multiscale nature is well understood. One prototypical example system that was proposed in [5] to analyze such convergence behavior is a singularly perturbed slow–fast system in which the slow variable is described deterministically, while the model for the fast variable contains stochastic effects. The specific form is as follows:

$$\begin{cases} dx(t) = f(x,y)dt, & x(0) = x_0 \in \mathbb{R} \\ dy(t) = \dfrac{1}{\varepsilon} g(x,y)dt + \dfrac{1}{\sqrt{\varepsilon}} \beta(x,y)dW(t), & y(0) = y_0 \in \mathbb{R}. \end{cases} \tag{1}$$

where the scalar quantities $x(t) : [0, T] \to \mathbb{R}$ and $y(t) : [0, T] \to \mathbb{R}$ represent the slow and fast evolving stochastic processes, respectively. The functions $f(x, y), g(x, y) \in \mathbb{R}$ are called the drift functions and $\beta(x, y) \in \mathbb{R}$ is termed the diffusion function. Furthermore, $W(t) \in \mathbb{R}$ denotes a standard Brownian motion. The parameter $\varepsilon \ll 1$ is a positive small-scale parameter that measures the time scale separation between the fast and slow variable in system (1). In addition, we assume that the fast dynamics is ergodic for every fixed state $X \in \mathbb{R}$ of the slow variable, implying the existence and uniqueness of an invariant measure [7]. We note that the differential form used in system (1) is purely formal, given that Brownian paths are continuous everywhere but nowhere differentiable. Consequently, system (1) should be understood in the integral form, where stochastic integrals are interpreted in the Itô-sense. In general, the SDE may be very high-dimensional (especially with many fast degrees of freedom), see, for instance, [5].

Often, one is only interested in the evolution of the slow variable of system (1) and not in the detailed evolution of the fast variable. However, the fast dynamics cannot be omitted, since the slow process explicitly depends on the fast variable. Due to the stiffness in system

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(1), explicit simulation techniques such as the Euler–Maruyama or higher-order Milstein schemes are computationally prohibitive. Also, implicit methods fail to capture the correct invariant measure, thus introducing a bias, see [8].

The difficulties related to direct simulation can be avoided by exploiting the time scale separation of system (1): for $\varepsilon \to 0$, the averaging principle yields a reduced description for the slow variable:

$$\frac{dX}{dt} = F(X), \qquad F(X) = \int_{\mathcal{Y}} f(X, y) d\mu_X^\infty(y), \tag{2}$$

in which $\mu_X^\infty(y)$ denotes the invariant measure induced by the fast dynamics of system (1) keeping $x = X$ fixed, see, for instance, [7] and references therein. Eq. (2) is known as the *averaged*, *macroscopic* or *reduced* equation for the slow variable.

Based on this averaged equation, a method for (1) was proposed in [9] and analyzed in [10]. It consists of a macroscopic solver, such as the forward Euler or a higher-order Runge–Kutta method, to simulate (2), combined with a procedure to estimate the time derivative $F(X)$ in Eq. (2). If the invariant measure $\mu_X^\infty(y)$ is known explicitly and can readily be sampled, the integral in (2) can be approximated by a direct Monte Carlo estimator (see, e.g., [11] and references therein). In general, however, the invariant measure is not known explicitly. Then, one may resort to a Markov chain Monte Carlo method, as is done in [9]. This method fits in the class of *heterogeneous multiscale methods* (HMM) that was introduced in [12] for a broad class of multiscale problems and provides a natural setting for numerical analysis, see also [13] for a recent review. Similar methods have been introduced based on the concept of *coarse projective integration* [14]. There, instead of performing one (or a few) long Markov chain Monte Carlo simulation of the fast equation, one initializes a *large ensemble* of realizations, which are simulated on a short time interval. This method falls in the class of *equation-free methods* [15,16], see also [17], and can also be used in a more general setting where one is unable to identify or constrain the slow degree of freedom.

Unfortunately, the statistical error of the above-described methods can be quite large, and decreases only as $M^{-1/2}$ when the number of samples M tends to infinity. In this work, which expands the results reported in [18], we therefore propose a variance-reduction technique based on control variables, see, for instance, [11,19]. The method can be applied both in the projective integration and the HMM setting, and bears some resemblance to the technique that was proposed in [20] for variance-reduced coarse projective integration of SDEs of the form (1). While we present the method and main analysis in the HMM framework, we will comment on coarse projective integration where appropriate. The control variable that we introduce is based on correlating estimations of the time derivative $F(X)$ in Eq. (2) on different time instants. The remainder of this paper is structured as follows. In Section 2, we introduce the stochastic slow–fast system that we intend to solve numerically. In Section 3, we describe the HMM framework to efficiently integrate these slow–fast systems. In that section, we also present the variance-reduced HMM method, and we comment on the applicability of this method for coarse projective integration. Next, in Section 4 we analyze the numerical properties of the proposed variance reduction method. Numerical results are reported in Section 5. We conclude in Section 6 with a brief discussion and ideas for future work.

2. Slow–fast system

The general form of slow–fast systems we consider in this work is given in Eq. (1). In what follows, we will always assume that the fast dynamics of system (1) is ergodic for all fixed values of the slow variable. This means that the fast equation produces a unique invariant measure for every fixed value X, denoted by $\mu_X^\infty(y)$. Ergodicity implies that the statistical properties of the ensemble of the stochastic process at a fixed time instant and those of one realization of the process over an infinite time interval are the same. Consequently, for an ergodic process, averaging a function with respect to the invariant measure yields the same result as averaging this function over one infinitely long time path of the process:

$$F(X) = \int_{\mathcal{Y}} f(X, y) d\mu_X^\infty(y) = \lim_{T\to\infty} \frac{1}{T} \int_0^T f(X, y(t+s)) ds. \tag{3}$$

Eq. (3) serves as a base for numerical methods avoiding explicit knowledge of the invariant measure $\mu_X^\infty(y)$. Additionally, we will always assume that the invariant measure possesses a density ρ_X^∞ with respect to the Lebesgue measure: $d\mu_X^\infty(y) = \rho_X^\infty(y)dy$.

Moreover, we assume that the function $F(X)$ in Eq. (2) is Lipschitz continuous with Lipschitz constant L_c, implying the following inequality:

$$|F(X_1) - F(X_2)| \le L_c |X_1 - X_2|, \qquad \forall X_1, X_2 \in \mathbb{R}, \tag{4}$$

and we assume that the functions f, g and β are sufficiently differentiable such that all derivatives exist that are required during the analysis.

In the following two paragraphs, we introduce the linear and nonlinear illustrative examples that will be used in the numerical experiments throughout the text.

Linear system. In the linear setting, system (1) takes on the following form:

$$\begin{cases} dx(t) = (\lambda x(t) + p y(t))dt, & x(0) = x_0 \in \mathbb{R} \\ dy(t) = \dfrac{1}{\varepsilon}(q x(t) - A y(t))dt + \dfrac{1}{\sqrt{\varepsilon}} dW(t), & y(0) = y_0 \in \mathbb{R}, \end{cases} \tag{5}$$

in which the parameters λ, p, q and A are all real scalars. In addition, to ensure that solutions decay exponentially with time, we require that $\lambda < 0$ and $A \in (pq/-\lambda, 2]$.

For this linear system, the fast equation corresponds to a linear Ornstein–Uhlenbeck equation with parameters q and A for which the invariant measure can be calculated analytically as [7]:

$$\mu_X^\infty(y) \sim \mathcal{N}(m_\infty, \sigma_\infty^2), \qquad m_\infty = \frac{q}{A} X, \qquad \sigma_\infty^2 = \frac{1}{2A}, \tag{6}$$

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