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Random Walk Approximation for Irreversible Drift-Diffusion Process on Manifold: Ergodicity, Unconditional Stability and Convergence

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Abstract. Irreversible drift-diffusion processes are very common in biochemical reactions. They have a non-equilibrium stationary state (invariant measure) which does not satisfy detailed balance. For the corresponding Fokker-Planck equation on a closed manifold, using Voronoi tessellation, we propose two upwind finite volume schemes with or without the information of the invariant measure. Both schemes possess stochastic Q-matrix structures and can be decomposed as a gradient flow part and a Hamiltonian flow part, enabling us to prove unconditional stability, ergodicity and error estimates. Based on the two upwind schemes, several numerical examples – including sampling accelerated by a mixture flow, image transformations and simulations for stochastic model of chaotic system – are conducted. These two structure-preserving schemes also give a natural random walk approximation for a generic irreversible drift-diffusion process on a manifold. This makes them suitable for adapting to manifold-related computations that arise from high-dimensional molecular dynamics simulations.

AMS subject classifications: 60H30, 60H35, 65M75, 65M12

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1 Introduction

A general stationary (time-homogeneous) dynamical system with white noise, can be modeled by a stochastic differential equation for $\mathbf{y}_t \in \mathbb{R}^\ell$

$$\mathrm{d}\mathbf{y}_t = \boldsymbol{b}(\mathbf{y}_t)\,\mathrm{d}t + \sqrt{2}\sigma\,\mathrm{d}B_t, \tag{1.1}$$

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where σ is a noise matrix and B_t is an ℓ-dimensional Brownian motion. Denote $D := \sigma\sigma^T \in \mathbb{R}^{\ell\times\ell}$. For simplicity, we assume D is a constant positive semi-definite matrix. By Ito's formula, SDE (1.1) gives the following Fokker-Planck equation, which is the master equation for the time marginal density $\rho_t(\mathbf{y})$

$$\partial_t\rho = -\nabla\cdot(\boldsymbol{b}\rho)+\nabla\cdot(D\nabla\rho) =: \mathcal{L}^*\rho. \tag{1.2}$$

In some physical systems, the drift vector field $\boldsymbol{b} = -D\nabla\varphi$ for some potential φ representing the energy landscape. Then the Gibbs measure $\pi(\mathbf{y}) \propto e^{-\varphi(\mathbf{y})}$ is the invariant measure. The simplest example is the Ornstein-Uhlenbeck process with $\boldsymbol{b}(\mathbf{y}_t) = -\gamma\mathbf{y}_t$ and the diffusion coefficient $\sigma = \sqrt{\varepsilon\gamma}$. In this case, (1.1) is called Langevin dynamics, and the corresponding Fokker-Planck equation has a gradient flow structure; see (2.22). In this Langevin dynamics case, the Markov process defined by (1.1) is reversible[†], i.e., if we take π as the initial density, the time-reversed process has the same law as that of the forward process. Equivalently, the invariant measure satisfies the detailed balance condition

$$\text{steady flux } F^\pi := -\boldsymbol{b}\pi + D\nabla\pi = 0. \tag{1.3}$$

However, numerous dynamical systems in physics and biochemistry are described by irreversible Markov processes (without detailed balance), i.e., there does *not* exist a potential function such that the drift vector field $\boldsymbol{b} = -D\nabla\varphi$ in (1.1). For instance, the stochastic Lorenz system, the Belousov–Zhabotinsky reaction, or the Hodgkin–Huxley model describe the excitation and propagation of sodium and potassium ions in a neuron. The irreversibility in the nonequilibrium circulation balance is almost literally the primary characteristic of life activities [19]. In this case, the invariant measure π is still stationary in time, but there is a positive entropy production rate; see (3.12). Thus PRIGOGINE named such an invariant measure π as "stationary non-equilibrium states" or "non-equilibrium steady states" in [29, Chapter VI]. We will simply call it steady state or invariant measure. Later, Hill explains Prigogine's theory using Markov chain stochastic models for some simple biochemical reactions such as muscle contraction and clarifies the formula (3.12) for the entropy production rate [19, eq. (9.20)]. Another situation is that for a Markov process on manifold, which is induced via dimension reductions (such as diffusion map [7]) from a higher dimensional Markov process based on collected data, some classical schemes such as the Euler-Maruyama scheme will break the detailed balance property.

Therefore, in this paper we focus on designing numerical schemes to simulate a general irreversible Markov process on a closed manifold $\mathcal{N}$; see (1.4). In terms of the SDE, we will design a random walk approximation which enjoys ergodicity and accuracy. In terms of Fokker-Planck equation (1.2), we will design two upwind schemes with a Q-matrix[‡] structure so that they also enjoy ergodicity, unconditionally stability and accuracy.

[†]In some physics literature, it is referred as microscopic reversibility [28].
[‡]a.k.a. infinitesimal generator matrix for a Markov chain