Applied Mathematics and Computation 274 (2016) 237–246

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Maximum likelihood estimation of McKean–Vlasov stochastic differential equation and its application

Jianghui Wen [a,c,*], Xiangjun Wang [b], Shuhua Mao [a], Xinping Xiao [a]

[a] School of Science, Wuhan University of Technology, Wuhan 430070, PR China
[b] School of Mathematics and Statistics, Huazhong University of Science and Technology, Wuhan 430074, P R China
[c] Intelligent Transport Systems, Wuhan University of Technology, Wuhan 430063, PR China

ARTICLE INFO

Keywords:
McKean–Vlasov stochastic differential equation
Maximum likelihood estimation
Ion diffusion
Numerical simulation

ABSTRACT

McKean–Vlasov stochastic differential equation is a class of complicated and special equation since the drift term is a function of stochastic process and its distribution. This paper discusses the maximum likelihood estimation of parameters in the drift term through transforming McKean–Vlasov stochastic process into homogeneous one and estimates parameters of the latter to discuss that of McKean–Vlasov equation. Then we build a McKean–Vlasov stochastic model for ion diffusion since ions moved by liquid viscous force and also by coulomb interaction related with ion charged distribution, and simulate the changing trajectory of the ion motion through numerical calculation. Results manifest that the ion motion shows strong random property and has the same tendency for different time intervals, however, the smaller of time lag, the more distinct of wave trajectory observed.

1. Introduction

With the development of science and technology, physical system has been designed to be smaller and smaller, even to nanometer and nanosecond scale. A kind of special system, that is, two large containers filled with electrolyte solution and a nanoscale hole connecting containers has important applications in molecular biology, such as a biological membrane is usually punctured by transport proteins so that the ions flow in and out of the cell and then continue some biological processes, including hormonal secrete, muscle coordination, information transmission and the control of the nervous system.

In order to describe the ion movement process, Schuss et al. [1] considered that it satisfied a kind of Poisson–Nernst–Planck equation, and generalized the statistical mechanism of equilibrium in ideal liquid to stationary nonequilibrium stature. As well-known that, pressure, concentration, flow rate and the number of ions in fluctuation are not constant and change over time, which is caused by the random movement of charged ions, the deterministic feedback mechanism, random time delay and measure error. However, Schuss and Eisenberg [2] still assumed that they ignored these fluctuations, which was against common practice. For solving this problem, some researchers proposed stochastic models of the ion motion, such as Nadler et al. [3] constructed Langevin equation with two state variables (location and motion rates) to describe ion tangency in state space, and characterized interaction among ions with power function; Singer et al. [4] and Hyon et al. [5] simulated diffusion system of ions by Brownian motion.

* Corresponding author. Tel.: +8613377885512.
E-mail address: jhwen86@gmail.com (J. Wen).

http://dx.doi.org/10.1016/j.amc.2015.11.019
0096-3003/

Since there are many positive and negative charged ions in electrolyte solution, they not only are affected by viscous force of liquid, but also coulomb force because of the coulomb interaction between each other in the ion movement process. Therefore, these ions' movements depend on their specific nanoscale geometry shapes and charge distribution of their and nearby areas, and McKean–Vlasov stochastic differential equation can exactly describe this phenomenon, rather than Brownian motion.

Let $(\Omega, \mathcal{F}, \mathcal{P}, \mathfrak{F})$ be a probability space, for functions $b : \mathbb{R}_+ \times \mathbb{R}^d \times M(\mathbb{R}) \to \mathbb{R}$ and $s : \mathbb{R}_+ \times \mathbb{R}^d \times M(\mathbb{R}) \to \mathbb{R}$, McKean–Vlasov stochastic differential equation [6–8] is

$$\begin{cases} dX_t = b(t, X_t, \mu(t))dt + s(t, X_t, \mu(t))dW_t \\ X_0 = \xi \end{cases}, \tag{1.1}$$

where $\mu(t)$ is probability distribution of X_t, $W_t^{(N)} = (W_t^1, \ldots, W_t^N)$ is a N dimensional Wiener process. Under lipschitz and linear growth condition of coefficients b and s, Eq. (1.1) exists signal strong solution X_t, as following

$$\begin{cases} X_t = X_0 + \int_0^t \int_{\mathbb{R}} b(X_\theta, y)\mu_\theta(dy)d\theta + \int_0^t \int_{\mathbb{R}} s(X_\theta, y)\mu_\theta(dy)dW_\theta \\ \mu_t, \qquad t \geq 0 \end{cases}. \tag{1.2}$$

And assume that distribution function of probability measure μ_t is $V(t, x)$, which satisfies

$$\begin{cases} \dfrac{\partial V(t,x)}{\partial t} = \dfrac{1}{2}\dfrac{\partial}{\partial x}\left[\int_{\mathbb{R}} s(x,y)\dfrac{\partial V(t,y)}{\partial x}dy\right]^2 \dfrac{\partial V(t,x)}{\partial x} - \left[\int_{\mathbb{R}} b(x,y)\dfrac{\partial V(t,y)}{\partial x}dy\right]\dfrac{\partial V(t,x)}{\partial x} \\ V(0,x) = V_0(x) \end{cases}. \tag{1.3}$$

Meanwhile, $\mu(t, x)$ is transform probability density function satisfying nonlinear Fokker–Planck equation:

$$\begin{cases} \dfrac{\partial \mu £t,x)}{\partial t} = \dfrac{1}{2}\dfrac{\partial^2}{\partial x^2}\left[\mu(t,x)\left(\int_{\mathbb{R}} s(x,y)\mu(t,y)dy\right)^2\right] - \dfrac{\partial}{\partial x}\left[\mu(t,x)\left(\int_{\mathbb{R}} b(x,y)\mu(t,y)dy\right)\right] \\ \mu(0,x) = \mu_0(x) \end{cases}. \tag{1.4}$$

Eq. (1.1) illustrates that the drift term not only depends on the stochastic process $\{X_t, t \geq 0\}$ at time t, but also on its distribution. Thus discussing its properties is more difficult, especially for parameter estimation. Many researchers had been studied statistic inference of the diffusion process, parameter estimation of diffusion had been researched from 1962 [9], and lots of articles focused on estimation of the drift parameter under continuous observation including linear homogeneous differential equation, nonlinear homogeneous differential equation and nonlinear nonhomogeneous differential equation, estimation methods include maximum likelihood estimation, bayesian estimation, moment estimation etc. [10–13]. Infinite dimensional models were more difficult to estimate parameters, and Bishwal [13] considered estimation of infinite generator for the drift parameter in strongly continuous semigroup of real separable Hilbert space. Under discrete observation case, Dorogovcev [14] used condition least square method; Ait–Sahalia [15] studied approximate maximum likelihood estimation of transform density by Hermite function whereas Pedersen [16] by Gaussian iteration, and Bibby [18] proposed a martingale function estimating equations method for ergodic diffusion. In recent years, nonparametric methods became a hot research field in parameter estimation of diffusion process. Ait–Sahalia [17] gave a linear form of the drift term and the diffusion term through Kolmogorov equation, and then did nonparametric estimation combined both forms under discrete observation. Other researches also carried out different nonparametric estimation methods for different diffusion processes [19,20].

However, parametric estimation of McKean–Vlasov stochastic differential equation can not use these estimation methods directly because of the distribution of stochastic process in the drift term. In Section 2, we transform this nonhomogeneous Markov process into homogeneous one and estimate parameters of the latter to discuss the parametric estimation problem of McKean–Vlasov stochastic differential equation, and obtain maximum likelihood estimation of parameters in the drift term. Then McKean-Vlasov stochastic differential equation is introduced in considering the ion motion process and we deduce its Fokker–Planck equation in the next section. Section 4 simulates the changing trajectory of ion motion through numerical calculation and Section 5 gives conclusions.

2. Parameter estimation of McKean–Vlasov stochastic differential equation

Define $\beta : [0, T] \times \mathbb{R} \to \mathbb{R}$, expressed as

$$\beta(\theta, t, x) := \int_{\mathbb{R}} b(\theta, x, y)\mu_t(dy), \tag{2.1}$$

and $\sigma : [0, T] \times \mathbb{R} \to \mathbb{R}$,

$$\sigma(\vartheta, t, x) := \int_{\mathbb{R}} s(\vartheta, x, y)\mu_t(dy). \tag{2.2}$$