Remarks on Monte Carlo method approximation evolution equations

E.V. Lezhnev

NSTU, Department of Applied Mathematics and Computer Science, Novosibirsk, Russia, Phone: +7-383-226-6879, E-mail: lionlev@ngs.ru

***Abstract.-* In this paper specifying scheme of random walking, which used in Monte Carlo method for approximation diffusion and telegraph equations.**

Keywords: Monte Carlo method, master-equation.

I. INTRODUCTION

In [2], [3] the master-equation method [1] was established conformably to Brownian motion type and wave type processes. A problem of these boundary evolutional processes embedding into a system of generalized type on the basis of generalized evolution process operator. An evolutional operator constructed in the paper includes both diffusion and wave operators. The operator creation is based on the master-equation method evolved in [2], [3]. This paper revises random walking scheme in Monte Carlo method of obtaining numerical solution of corresponding equation.

II. RANDOM WALKING AND IT'S PARAMETERS

Let us consider next random walking: time interval $[0,T]$, divided into intervals $\Delta t = t_k - t_{k-1} = = T/n$, particle each time interval Δt moves with constant speed v on distance $\Delta x = \mathrm{v}\Delta t$. Each time interval it changes direction with probability $a\Delta t$ and preserve direction with probability $1 - a\Delta t$.

Let us define random quantity $\varepsilon_k = \varepsilon(t_k)$, $k = 0,1,...,n$:

$$\varepsilon_k = \begin{cases} -1, \text{with a probability } a(\Delta t)\Delta t \\ 1, \text{with a probability } 1 - a(\Delta t)\Delta t \end{cases} \quad (1)$$

Meaning +1 of quantity (1) corresponds to trajectory direction preservation and meaning –1 corresponds to trajectory direction changing. We require that property of trajectory direction preservation or changing in the t_k time point doesn't depend on the property realization for all others t_i, $i \neq k$. Therefore for mean of distribution $\langle \varepsilon_k \rangle$ follows that:

$$\langle \varepsilon_1 \varepsilon_2 ... \varepsilon_n \rangle = \langle \varepsilon_1 \rangle \langle \varepsilon_2 \rangle ... \langle \varepsilon_n \rangle \quad (2)$$

Definition 1. Using (1) and definitions of parameters Δx, Δt, v and random quantity ε, we define random process $N^{\pm}(x,t_k)$: $R^1 \times [0,T] \to R^1$:

$$t_k \to N^{+}(x,t_k) = x + \Delta x(1 + \varepsilon_1 + ... + \varepsilon_1\varepsilon_2 ... \varepsilon_{k-1}) \quad (3a)$$

$$t_k \to N^{-}(x,t_k) = x - \Delta x(1 + \varepsilon_1 + ... + \varepsilon_1\varepsilon_2 ... \varepsilon_{k-1}) \quad (3b)$$

where $k = 1,2,...,n$, that is defined for $x \in R^1$, and for cases (a) and (b) it implements at the initial state on the interval (t_0, t_1) increasing or decreasing respectively.

Let consider random walking (3). First we find mean value by all ε_i:

$$\langle N^{+}(x,t_k) \rangle =$$
$$= \langle x + \Delta x(1 + \varepsilon_1 + .. + \varepsilon_1 ... \varepsilon_{k-1}) \rangle = \Delta x + a\Delta t \langle N^{-}(x,t_{k-1}) \rangle +$$
$$+ (1 - a\Delta t)\langle N^{+}(x,t_{k-1}) \rangle = x + \Delta x \frac{1 - (1 - 2a\Delta t)^{k-1}}{2a\Delta t}.$$

Dispersion of this walking is

$$\frac{n-1}{a\Delta t}(1 - a\Delta t) + \frac{4a\Delta t - 3 + 4(1 - a\Delta t)(1 - 2a\Delta t)^{n-1}}{4(a\Delta t)^2} +$$
$$\frac{+ (1 - 2a\Delta t)^{2n-2}}{4(a\Delta t)^2}.$$

Probability of right direction in time i is $\frac{1 - (1 - 2a\Delta t)^{i-1}}{2}$. Obviously, if $a\Delta t \neq 1/2$ then probability of right direction in time j is dependent from previous time i. So $N^{+}(x,t_k)$ is sum of dependant random quantities. Only in case $a\Delta t = 1/2$, $N^{+}(x,t_k)$ is sum of independent random quantities and we can prove convergence of this sums to Normal distribution.

III. RECURRENCE RELATIONS FOR RANDOM PROCESS

Let $t_k \to N^{\pm}(x,t_k)$ is random process (3) with parameters Δt, Δx, $a(\Delta t)$, $\mathrm{v}(\Delta t)$. Let us determine averaging for all ε_i ($i = 1,...,k$) for any smooth function $x \to \varphi(x) \in R^1$ bounded with all its derivatives $\forall x \in R^1$ as following [1]:

$$F_k^{\pm}(x) \equiv \langle \varphi(N^{\pm}(x,t_k)) \rangle \equiv$$

$$\equiv \left\langle \varphi\left(x \pm \Delta x\left(1+\varepsilon_1+\varepsilon_1\varepsilon_2+\ldots+\varepsilon_1\varepsilon_2\ldots\varepsilon_{k-1}\right)\right)\right\rangle \equiv$$

$$\equiv \sum_{\substack{\varepsilon_{i_1}=\ldots=\varepsilon_{i_\alpha}=1 \\ \varepsilon_{i_i}=\ldots=\varepsilon_{i_\beta}=-1 \\ \alpha+\beta=k-1}} \varphi\left(x \pm \Delta x\left(1+\varepsilon_1+\varepsilon_1\varepsilon_2+\ldots+\varepsilon_1\varepsilon_2\ldots\varepsilon_{k-1}\right)\right)\times$$

$$\times\left(1-a\Delta t\right)^{\alpha}\left(a\Delta t\right)^{\beta} \quad (4)$$

where summing up is making for all possible sets of ε_i, taking up meaning +1 or −1 with probability $(1-a\Delta t)$ and $a\Delta t$ respectively.

We obtain recurrence relations on $F_k^{\pm}(x)$ defined in (4) by following [3]:

$$\begin{cases} F_k^+(x) = a\Delta t F_{k-1}^-(x+\Delta x) + (1-a\Delta t)F_{k-1}^+(x+\Delta x), \\ F_k^-(x) = a\Delta t F_{k-1}^+(x-\Delta x) + (1-a\Delta t)F_{k-1}^-(x-\Delta x). \end{cases} \quad (5)$$

IV. THE MASTER-EQUATION FOR RANDOM PROCESS

We obtain following presentation for finite differences $\left(F_k^+(x)-F_{k-1}^+(x)\right)/\Delta t$, $\left(F_k^-(x)-F_{k-1}^-(x)\right)/\Delta t$ using (5):

$$\begin{cases} \dfrac{F_k^+(x)-F_{k-1}^+(x)}{\Delta t} = \mathrm{v}\dfrac{F_{k-1}^-(x+\Delta x)-F_{k-1}^-(x)}{\Delta x} + \\ a\left(F_{k-1}^-(x+\Delta x)-F_{k-1}^+(x+\Delta x)\right) \\ \dfrac{F_k^-(x)-F_{k-1}^-(x)}{\Delta t} = -\mathrm{v}\dfrac{F_{k-1}^+(x)-F_{k-1}^+(x-\Delta x)}{\Delta x} + \\ a\left(F_{k-1}^+(x-\Delta x)-F_{k-1}^-(x-\Delta x)\right). \end{cases} \quad (6)$$

Then denote following functions from (6) [1], [2], [3] as:

$$F_{\pm l}^k = F_k^+(x \pm l\Delta x) + F_k^-(x \pm l\Delta x),$$
$$G_{\pm l}^k = F_k^+(x \pm l\Delta x) - F_k^-(x \pm l\Delta x), \quad (7)$$

where index l corresponds to space step-interval on space variable x, and index k corresponds to time step-interval on time variable t. When index l is missed then it is assumed that it is equal to zero. Notice that if a dynamic process have an unlimited variation then actual range for x is whole number axis when $\Delta t \to 0$, $N \to \infty$.

Then we get $F_k^{\pm}(x)$ by means of $F_{\pm l}^k$ and $G_{\pm l}^k$ by using (11) and put obtained expressions into (10). After simplifications applying we obtained following system of equations:

$$\begin{cases} \dfrac{1}{\mathrm{v}}\dfrac{F^k - F^{k-1}}{\Delta t} = \dfrac{G_{+1}^{k-1} - G^{k-1}}{\Delta x} - \dfrac{a}{\mathrm{v}}\left(G_{+1}^{k-1} - G_{-1}^{k-1}\right) + \\ + \dfrac{\left(F_{+1}^{k-1} - G_{+1}^{k-1}\right) - 2\left(F^{k-1} - G^{k-1}\right) + \left(F_{-1}^{k-1} - G_{-1}^{k-1}\right)}{2\Delta x} \\ \dfrac{1}{\mathrm{v}}\dfrac{G^k - G^{k-1}}{\Delta t} = \dfrac{F_{+1}^{k-1} - F^{k-1}}{\Delta x} - \dfrac{a}{\mathrm{v}}\left(G_{+1}^{k-1} + G_{-1}^{k-1}\right) - \\ - \dfrac{\left(F_{+1}^{k-1} - G_{+1}^{k-1}\right) - 2\left(F^{k-1} - G^{k-1}\right) + \left(F_{-1}^{k-1} - G_{-1}^{k-1}\right)}{2\Delta x} \end{cases} \quad (8)$$

We call the master-equation the obtained relation (8). In [1] and [3] we proved that with $a\Delta t \to 1/2$ and $\mathrm{v}^2\Delta t \to D$ master-equation converges to diffusion equation

$$\frac{\partial F}{\partial t} = \frac{D}{2}\frac{\partial^2 F}{\partial x^2} \quad (9)$$

and with $a\Delta t \to 0$ and $\mathrm{v}(\Delta t) \to \mathrm{v}$, where v – finite constant, master-equation converges to telegraph equation:

$$\frac{\partial F}{\partial t} = \frac{2a}{\mathrm{v}^2}\frac{\partial^2 F}{\partial x^2} - \frac{\partial F}{\partial x} \quad (10)$$

This means we can use random process (3) to obtaining numerical solutions of equations (9) and (10) by Monte Carlo method.

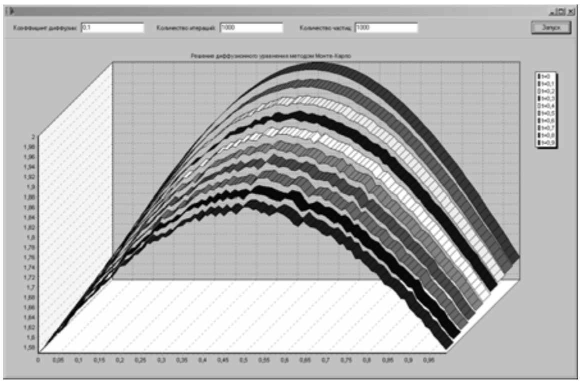
V. MONTE CARLO METHOD FOR DIFFUSION EQUATION

Let consider Monte Carlo method for diffusion equation. From (7) and (4) we obtaining that function F^k is represented in next way: F^k $\left\langle \varphi\left(N^+(x,t_k)\right)\right\rangle + \left\langle \varphi\left(N^-(x,t_k)\right)\right\rangle = F_k^+(x) + F_k^-(x) =$

Let's we have n trajectories. Consider averaging by all these trajectories: $\hat{N}^+ = \frac{1}{n}\sum_{i=1}^{n} N_i^+(x,t_k) = \hat{N}^+ =$

$$= \frac{1}{n}\sum_{i=1}^{n} N_i^+(x,t_k) = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{k}\Delta x\prod_{m=1}^{j-1}\varepsilon_m^i = \sum_{j=1}^{k}\frac{1}{n}\sum_{i=1}^{n}\Delta x\prod_{m=1}^{j-1}\varepsilon_m^i.$$

Since ε_i independent, $E\left(\hat{N}^+\right) = \left\langle \varphi\left(N^+(x,t_k)\right)\right\rangle$, so $\hat{N}^+$ converges to $\left\langle \varphi\left(N^+(x,t_k)\right)\right\rangle$ with $n \to \infty$. Hence we obtain Monte Carlo method for approximation of (4). In case $a\Delta t = 1/2$ and $\mathrm{v}^2\Delta t = D$ we obtain diffusion equation, [2], [3]. We realize this method in program. The work of this program presented in picture P.1.



P.1. Programm realizing Monte Carlo method for approximation of diffusion equation.

This method also may be applied for approximation telegraph equation. But in this case we must realizing event with probability $a\Delta t \to 0$. In [1] proposed using Poisson process in this case.

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