A new algorithm for numerical simulation of Langevin equations
H.Nakajima a and S.Furui b

a Department of Information Science, Utsunomiya University, Utsunomiya 321, Japan
E-mail address: nakajima@infor.utsunomiya-u.ac.jp

b School of Science and Engineering, Teikyo University, Utsunomiya 320, Japan
E-mail address: furui@dream.ics.teikyo-u.ac.jp

Formulated is a new systematic method for obtaining higher order corrections in numerical simulation of stochastic differential equations (SDEs), i.e., Langevin equations. Random walk step algorithms within a given order of finite $\Delta t$, are obtained so as to reproduce within that order a corresponding transition density of the Fokker-Planck equations, in the weak Taylor approximation scheme [1]. A great advantage of our method is its straightforwardness such that direct perturbative calculations produce the algorithm as an end result, so that the procedure is tractable by computer. Examples in general form for curved space cases as well as flat space cases are given in some order of approximations. Simulations are performed for specific examples of U(1) system and SU(2) systems, respectively.

1. Introduction
We propose a new systematic algorithm for obtaining higher order corrections in numerical simulation of SDEs, i.e., Langevin equations in either flat or curved space.

The problem is how to realize random walk step algorithms for $\Delta t$, so as to reproduce proper corrections within a given order $O(\Delta t^n)$ of corresponding transition density which evolves according to the Fokker-Planck equation.

Our systematic algorithm consists of all direct perturbative calculations within some order $O(\Delta t^n)$ such as normal ordering of the time evolution operator, exponentiation of polynomials, completing squares of polynomials, and inversion of polynomials. These direct perturbative calculations produce the random walk step algorithm as an end result without any matching equations, so that the procedure is tractable by computer.

It is to be noted that Drummond et al. [2] assumed linear step algorithms with respect to random variates, but we do not. In their scheme, equations becomes overconstrained and will have no solution in higher orders, since otherwise the obtained algorithm generates Gaussian distribution for the transition density, which is, however, generally impossible in higher orders.

2. Formalism
The Langevin equation in d dimensional curved space with an initial condition $x = x_0$ at $t = t_0$, reads as

$$\partial_t x^i = u^i(x) + e^i_\alpha(x) \eta^\alpha(t) \quad (i, \alpha = 1, 2, \cdots, d),$$

$$< \eta^\alpha(t) \eta^\beta(t') >= 2\sigma^{\alpha\beta} \delta(t - t'),$$

and

$$< \eta^\alpha(t) > = 0,$$

where (1) is understood as Ito’s SDE. Then we can derive the corresponding Fokker-Planck equation for the transition density in the curved space with an initial condition $P(t_0, x; t_0, x_0) = \delta(x - x_0)$ as

$$\partial_t P(t, x; t_0, x_0) = KP(t, x; t_0, x_0),$$

where

$$K = \partial_i(\partial_j g^{ij}(x) - u^i(x)),$$

and

$$g^{ij} = e^i_\alpha e^j_\beta \delta^{\alpha\beta}.$$
Given a $u^i(x)$, we are to find a random walk step algorithm $\Delta x^i$, a function of random variates $\eta^a$, so as to satisfy within a given order $O(\Delta^n)$, 

$$P(t_0 + \Delta t, x; t_0, x_0) = <\delta(x - (x_0 + \Delta x)) >$$

where

$$<\eta^a, \eta^b >= 2\delta^{ab}\Delta t,$$

and

$$<\eta^a > = 0.$$  \hfill (9)

2.1. A new systematic algorithm for higher order random walk step algorithms

First we write a truncated exponential operator of the $O(\Delta^n)$ formal solution

$$e^{\Delta t K} \delta(x - x_0)$$

in normal order, i.e., differential operators in the leftmost position, and then all velocity and metric fields and their derivatives may be evaluated at the position $x_0$ and become commutable with differential operators. Then we insert

$$e^{-\Delta t g^{ij}(x_0)\partial_i \delta(x - x_0)}$$

between $e^{\Delta t K}$ and $\delta$, and make use of

$$e^{\Delta t g^{ij}(x_0)\partial_i \delta(x - x_0)} = \frac{1}{\sqrt{(4\pi\Delta t)^d}g_0} e^{-\frac{1}{4}\n g_j(x_0)z^jz^i},$$

where $z^i = (x^i - x_0^i)/\sqrt{\Delta t}$, $g_0 = det(g^{ij}(x_0))$, and $\partial_i = \partial_i/\sqrt{\Delta t}$ to obtain the transition density in a form as

$$P(t_0 + \Delta t, x; t_0, x_0) = F(\sqrt{\Delta t}, z, \cdots)$$

$$\times \frac{N}{\sqrt{(4\pi\Delta t)^d}g_0} e^{-\frac{1}{4}\n g_j(x_0)z^jz^i}.$$  \hfill (14)

We use a singular coordinate $z^i = (x^i - x_0^i)/\sqrt{\Delta t}$ due to a singular nature of the perturbation expansion.

Within the given order, we exponentiate the polynomial factor $F(\sqrt{\Delta t}, z, \cdots)$, and proceed perturbatively order by order so as to eliminate the leading order corrections in the exponent polynomial by finding proper transformation, that is, by completing squares, to obtain

$$P(t_0 + \Delta t, x; t_0, x_0) = \frac{N}{\sqrt{(4\pi\Delta t)^d}g_0} e^{-\frac{1}{4}\n g_j(x_0)z^jz^i},$$

where $\delta^i$ is a polynomial of $z^i$, $\delta^i = \delta^i(\sqrt{t}, z)$ such that $z^i = z^i + c^i + \cdots$, and $N$ is a normalization constant independent of $z$. Using the $\delta-$function, we can write (15) as

$$P(t_0 + \Delta t, x; t_0, x_0) = \frac{N}{\sqrt{(4\pi\Delta t)^d}}$$

$$\times \int d\eta e^{-\frac{1}{4}\n \delta^i(\delta^i - \theta^i)},$$

where $\theta^i = \sqrt{g^{ij}(x_0)}\eta^j$, and inverting the argument of the $\delta-$function with respect to $z^i$, we rewrite the $\delta-$function as

$$\delta^i(\delta^i - \theta^i) = det(dz/d\theta)\delta^i(z^i - z^i(\theta))$$

to obtain

$$P(t_0 + \Delta t, x; t_0, x_0) = \frac{N}{\sqrt{(4\pi)^d}} \int d\eta e^{-\frac{1}{4}\n \delta^i(\delta^i - \theta^i)},$$

where $\Delta x^i = \sqrt{\Delta t z^i(\theta)}$. The final part of our procedure to reach the goal in the form

$$P(t_0 + \Delta t, x; t_0, x_0) = \frac{N}{\sqrt{(4\pi)^d}} \int d\eta e^{-\frac{1}{2}\n \delta^i(\delta^i - \theta^i)},$$

is to find a transformation $\eta^i = \eta^i(\eta)$ such that

$$\frac{N}{\sqrt{(4\pi)^d}} d\eta e^{-\frac{1}{4}\n \delta^i(\delta^i - \theta^i)} = \frac{1}{\sqrt{(4\pi)^d}} d\eta e^{-\frac{1}{2}\n \delta^i(\delta^i - \theta^i)}$$

which we prove to be always possible as follows.

Algorithm to find the transformation from $\eta^i$ to $\eta^i$: Noting that

$$det(dz/d\theta) = 1 + \cdots,$$  \hfill (20)

we exponentiate the determinant factor, and consider its exponent in a form of polynomial of $\eta$ as $-1/4(\eta^2 + \cdots)$. We assume that constant terms are absent since they can be factored out as normalization constant, and also that either linear or quadratic terms with respect to $\eta$ in the lowest leading order correction terms are absent since they can be eliminated by some linear transformation which only effects a constant Jacobian factor. Let us suppose that the least power terms in the leading order corrections may be of a $n$th
power of \(\eta\), then we can eliminate it by a suitable transformation, i.e., by completing square, which simply produces a \((n-2)\)th power term in the exponent when the corresponding Jacobian factor is exponentiated. This shows that the leading order terms can be transformed away by finite steps to give the r.h.s. of (20), and completes our systematic approach.

For the sake of practical validity of the method, we applied, in use of suitable computer softwares, the above algorithm to cases in the flat space and in the curved space within some orders \(O(\Delta t^m)\), respectively. The results are new as far as we know.

2.2. Flat space local order 3 algorithm

In flat spaces i.e. \(g_{\mu\nu} = \delta_{\mu\nu}\) the Langevin step algorithms that reproduce the transition density of the Fokker-Planck equations up to order \(\Delta t^3\) are obtained in the Taylor scheme and in the Runge-Kutta-like scheme, respectively. In the latter the higher order derivatives are absent.

Our final result in the Taylor scheme is

\[
\Delta x^i(s, \eta, x_0) = s\eta^i + s^2u^i + \frac{1}{2}s^3\eta^i\partial_j u^j \\
+ s^4\left(\frac{1}{6}\eta^i\eta^k\partial_j\partial_k u^j + \frac{1}{2}u^j\partial_j u^i + \frac{1}{6}\partial^2 u^i\right) \\
+ s^5\left(\frac{1}{3}\eta^i\eta^j\eta^k\partial_l\partial_k\partial_l u^j + \frac{1}{6}\eta^i\partial_j\partial_k u^j + \frac{1}{6}\partial^2\eta^i\partial^2 u^i\right) \\
+ \frac{1}{24}s^6\left(\frac{1}{3}\partial_j u^k\partial_j\partial_k u^j + \frac{1}{6}u^j\partial^2 u^i\partial_j u^j + \frac{1}{6}\partial^2 u^j\partial_j u^i\right) \\
+ \frac{1}{6}u^j\partial_j u^k\partial_k u^i + \frac{1}{3}u^j\partial_j\partial^2 u^i + \frac{1}{6}\partial^2\partial^2 u^i\right) \\
\]

(22)

Here \(s = \sqrt{\Delta t}\) and \(\eta^i\)'s are the Gaussian random variables which satisfy

\[
<\eta^i, \eta^j> = 2\delta^{ij} \quad (23)
\]

Remark that there are terms non-linear in \(\eta^i\).

We also derived the \(O(\Delta t^3)\) Runge-Kutta-like scheme which contains two sets of the Gaussian random variables \(\eta^i\) and \(\eta^{ij}\).

\[\text{Transcription of (22) to the pure Runge-Kutta scheme is impossible due to contraction structure of } \eta^i \text{ and } u^i \text{ in (22).}\]

2.3. Curved space local order 2 algorithm

In general positive metric curved spaces, the Langevin step algorithm that reproduces the transition density of the Fokker-Planck equation up to order \(\Delta t^2\) is obtained in the Taylor scheme.

Our final result is

\[
\Delta x^i(s, \eta, y_0) = s\theta^i \\
+ s^2\left(\frac{1}{4}\theta^i\theta^j\partial_j u^i + \frac{1}{4}\theta^i\eta^k\eta^j\partial_j\partial_k u^i + \frac{1}{2}\theta^i\eta^j\partial_j u^i + \frac{1}{6}\theta^i\partial^2 u^i\right) \\
+ s^3\left[\frac{1}{2}\theta^i\partial_j u^i + \frac{1}{4}\theta^i\eta^k\eta^j\partial_j\partial_k u^i + \frac{1}{4}\theta^i\eta^j\partial_j u^i + \frac{1}{6}\theta^i\partial^2 u^i\right] \\
+ s^4\left(\frac{1}{2}\theta^i\partial_j u^i + \frac{1}{2}\theta^j\eta^i\eta^j\partial_j u^i + \frac{1}{6}\theta^i\partial^2 u^i\right) \\
+ s^5\left(\frac{1}{3}\theta^i\theta^j\theta^k\partial_l\partial_k\partial_l u^j + \frac{1}{6}\theta^i\partial_j\partial_k u^j + \frac{1}{6}\theta^i\partial^2 u^j\partial_j u^i\right) \\
+ \frac{1}{6}\theta^i\partial_j u^k\partial_k u^i + \frac{1}{3}\theta^i\partial_j\partial^2 u^i + \frac{1}{6}\theta^i\partial^2\partial^2 u^i\right) \\
\]

(24)

Here all \(\theta^{ij}\)'s, \(u^i\)'s and their higher derivatives are evaluated at \(x_0\), and \(\theta^i\)'s are given by

\[
\theta^i = \sqrt{g^{ij}(x_0)\eta_j} \\
\]

(25)

and \(\eta^i\)'s are the Gaussian random variates as in (23).

As an example, we transcribe the above algorithm to the standard SU(2) algorithm on \(S^3\) manifold. The \(S^3\) manifold can be patched by two hemispheres and points \(x\) on the northern hemisphere are projected stereographically at \(y\) on the tangential plane at the north pole and points on the southern hemisphere are projected on the tangential plane at the south pole.

The \(x_4\)-component of a point on the northern hemisphere is parametrized as \(x_4 = \cos\theta\) and \(y = 2\tan\frac{\theta}{2}\frac{x}{|x|}\). Similar parametrization is done for the southern hemisphere.

Using 3 dimensional Gaussian random variates \(\eta^i\) of variance 1, the \(\Delta y^i\) can be written as

\[
\Delta y^i(s, \eta, y_0) = s\sqrt{2f}\eta^i \\
+ s^2[-(4\beta + f)\eta^i + \eta^i f(y^k\eta^k)/2] \\
+ s^3[\eta^i(-12\beta f + 8\beta + \frac{1}{2}(f^2 + f))] \\
- \frac{3}{8} f(y^k\eta^k\eta^i)/\sqrt{2} \\
+ s^4\left(16\beta^2 + 4(2f - 1)\beta - \frac{1}{2}(f^2 + f)\right) \\
\]

(26)

where \(f = 1 + y^2/4\).
The expectation value of $x_4$ is

$$< x_4 > = \frac{1}{N} \sum_{i=1}^{N} y_i^2 - 4 y_i^2 + 4.$$  \hspace{1cm} (27)

3. Numerical examples

We consider the standard probability distribution

$$p(x) \propto \exp(\beta S(x))$$  \hspace{1cm} (28)

where $x = \theta$ and $S = \cos \theta$ in U(1) case, and $S = 4x_4$ with a four-vector $x_i$ satisfying $x_i^2 = 1$ in SU(2) case, respectively.

3.1. U(1) on $S^1$

The numerical simulation of the expectation values $< \sin^2 \theta >$ is performed, and its data are shown in Fig.1. The data are taken from successive 2000 Langevin steps each of which are the average of 100,000 runs.

3.2. SU(2) on $S^3$

We performed numerical simulation of the expectation values $< x_4 >$ for $\beta = 1$, results of which are shown in Fig.2. Data are taken from successive Langevin times from $t = 2$ to $t = 12$ each of which are the average of 100,000 runs.

Figure 1. The results of simulation of $< \sin^2 \theta >$ in U(1) system. $\beta = 5$, standard method in the Taylor scheme.

Figure 2. The results of simulation of $< x_4 >$ of SU(2) in $S^3$. $\beta = 1$

4. Conclusion and Outlook

General algorithm for obtaining higher order corrections to the Langevin step algorithms with respect to $\Delta t$ was formulated. The method is straightforward without matching equations and is tractable by computer.

A local third order algorithm for simulating general flat space Langevin equations and a local second order algorithm for simulating general curved space Langevin equations were obtained.

This method is based on Gaussian distribution in use of noncompact coordinates, as its lowest leading order approximation to transition density. Even in case of compact curved spaces as $S^n$, however, patching algorithm in use of stereographic projection on two noncompact tangential planes turned out to be successful and fast on computer. Similar method is applicable in principle to simulation of imaginary time evolution of wave functions in quantum mechanics.

REFERENCES

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