

ANALYSIS OF THE NUMERICAL STOCHASTIC APPROXIMATION METHODS FOR NONSTATIONARY LINEAR DIFFUSION PROBLEM

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Abstract. Weak approximation methods for initial value problem for the parabolic equation are considered. We propose some simple tests to investigate the quality of RNG used in Monte-Carlo simulations. Numerical examples are given to illustrate the application of stochastic approximation methods.

Key words: parabolic differential equation, stochastic differential equation, weak approximation, pseudorandom number generators.

1. Introduction. Consider the following initial value problem for the parabolic equation

$$\begin{aligned} \frac{\partial u(t, x)}{\partial t} &= \frac{1}{2} \sigma^2(t, x) \frac{\partial^2 u(t, x)}{\partial x^2} + a(t, x) \frac{\partial u(t, x)}{\partial x}, \\ u(0, x) &= f(x), \quad x \in R. \end{aligned} \quad (1)$$

In the case of sufficiently smooth function f deterministic methods for solving this problem are well known (see Thomee, 1984, Samarskij, 1988). But this problem is much more complicated for “rough” initial data $f \in L_2$. The error estimates of order $O(\frac{\tau + h^2}{t})$ are proved by Bramble *et al.* (1977) and Luskin and Rannacher (1981). The negative influence of quotient $O(\frac{1}{t})$ is most important for small time t and this effect dissipates away for large times $t \gg 0$. However in many biological and chemical applications the small time behavior is important. The method of finite difference and the Galerkin method formally diverges as $t \rightarrow 0$, therefore the important problem is to study the suitability and performance of stochastic approximation methods.

Consider the Itô stochastic differential equation (SDE)

$$dX(t) = a(t, X(t))dt + \sigma(t, X(t))dw(t), \quad X(0) = x, \quad (2)$$

where $w(t)$ is the Wiener process. We will suppose that drift $a(t, x)$ and diffusion $\sigma(t, x)$ coefficients are Lipschitz continuous functions. We will also suppose that $E|X(0)|^2 < \infty$, so we have that a unique solution of (2) exists.

There is a simple connection between solutions of (1) and (2). We will prove it very briefly for the completeness of our paper (see Milstein, 1995).

Let denote $\tilde{X}(t)$ a solution of the following SDE

$$\begin{aligned} d\tilde{X}(s) &= a(s, \tilde{X}(s)) ds + \sigma(s, \tilde{X}(s)) dw(s), \\ \tilde{X}(t) &= x, \quad 0 \leq s \leq t. \end{aligned} \quad (3)$$

By Itô's formula we obtain for a sufficiently smooth function $u(t, x)$

$$u(t, x) - u(0, \tilde{X}(0)) = \int_0^t Lu(s, \tilde{X}(s)) ds + \int_0^t \Lambda u(s, \tilde{X}(s)) dw(s), \quad (4)$$

where

$$L = \frac{\partial}{\partial t} + a(t, x) \frac{\partial}{\partial x} + \frac{1}{2} \sigma^2(t, x) \frac{\partial^2}{\partial x^2}, \quad \Lambda = \sigma(t, x) \frac{\partial}{\partial x}.$$

Notice, that it is possible to get (2) from (3) by using the substitution $\tilde{s} = t - s$. Let us denote $X_{0,x}(t)$ the solution of (2) satisfying initial condition $X(0) = x$. Then from (4) we get

$$\begin{aligned} u(t, x) - u(0, X_{0,x}(t)) &= \int_0^t \Lambda u(s, X(s)) dw(s) \\ &+ \int_0^t \left(-\frac{\partial}{\partial s} + a(s, X_{0,x}) \frac{\partial}{\partial x} + \frac{1}{2} \sigma^2(s, X_{0,x}) \frac{\partial^2}{\partial x^2} \right) u(s, X(s)) ds. \end{aligned}$$

Let $u(t, x)$ be a solution of (1). Then the first integral is equal to zero and we obtain the equality

$$u(t, x) - f(X_{0,x}(t)) = \int_0^t \Lambda u(s, X(s)) dw(s). \quad (5)$$

By taking the average in (5) we arrive at a probabilistic representation of the solution (1)

$$u(t, x) = Ef(X_{0,x}(t)). \quad (6)$$

2. Solution algorithm. In this section we define numerical algorithms for the evaluation of the quantity

$$Ef(X_{0,x}(t))$$

and consider the errors introduced by the approximation schemes.

We will simulate the approximating processes $\bar{X}(t)$, which can be obtained from the stochastic Taylor expansion of the solution of (2) (see Kloeden and Platen, 1992)

$$\begin{aligned} X(t+h) = & X(t) + \sigma \int_t^{t+h} dw(s) + ah + \Lambda\sigma \int_t^{t+h} (w(s) - w(t))dw(s) \\ & + L\sigma \int_t^{t+h} (s-t)dw(s) + \Lambda a \int_t^{t+h} (w(s) - w(t))ds \\ & + \Lambda\Lambda\sigma \int_t^{t+h} \int_t^s (w(s_1) - w(t))dw(s_1)dw(s) + La\frac{h^2}{2} + \rho, \end{aligned}$$

where the remainder ρ has at least the second order of smallness. This expansion contains all terms of order of smallness up to $3/2$ and one term of the second order. For the last term it is characteristic that the integral in it does not involve Wiener processes, and so its mathematical expectation is not equal to zero.

DEFINITION (see Milstein, 1995). *If an approximation \bar{X} is such that*

$$|Ef(\bar{X}(t)) - Ef(X(t))| \leq Ch^p, \quad h = t/n$$

for f from a sufficiently large class of functions, then the order of weak convergence of the approximation \bar{X} is p .

In this paper we consider numerical integration methods, which have the first or the second order of accuracy.

A simple approximation method for solving (2) is the Euler method (see Milstein, 1995)

$$\bar{X}(t+h) = \bar{X}(t) + a(t, \bar{X}(t))h + \sigma(t, \bar{X}(t))\Delta_t w(h), \quad (7)$$

where $\Delta_t w(h) = w(t+h) - w(t)$.

The global error satisfies the inequality

$$|Ef(\bar{X}(t)) - Ef(X(t))| \leq Ch,$$

where C depends only on f .

A more simple method (see Milstein, 1995)

$$X_{k+1} = X_k + a_k h + \sigma_k \sqrt{h} \varepsilon_k \quad (8)$$

can be also used to approximate the exact solution $X(t)$, where

$$X_0 = x, \quad a_k = a(kh, X_k), \quad \sigma_k = \sigma(kh, X_k)$$

and ε_k are independent random variables taking the values $+1$ and -1 with probabilities $1/2$. This method also has the first order of accuracy in the sense of weak approximation.

The second source of the error arises when we use the Monte-Carlo method to approximate the mathematical expectation by the finite sum

$$Ef(\bar{X}(t)) \approx \frac{1}{N} \sum_{i=1}^N f(\bar{X}^{(i)}(t)),$$

where $\bar{X}^{(i)}(t)$, $i = 1, \dots, N$ are independent realizations of the process $\bar{X}(t)$.

The error of the method can be estimated as follows

$$P \left\{ \left| Ef(\bar{X}(t)) - \frac{1}{N} \sum_{i=1}^N f(\bar{X}^{(i)}(t)) \right| \leq j \sqrt{\frac{\text{Var} f(\bar{X}(t))}{N}} \right\} = \gamma_j,$$

where $\text{Var} f(\bar{X}(t))$ is variance and $\gamma_1 = 0.68$, $\gamma_2 = 0.95$, $\gamma_3 = 0.997$ are level of significance.

3. RNG testing. The key ingredient in the modelling of process $\bar{X}(t)$ and successful application of Monte-Carlo simulation methods lies in the quality of random numbers used, which are usually produced by deterministic pseudorandom number generator algorithms (RNG). Using of bad quality RNG can lead to inaccurate results. Hence we have the third source of errors in our method for solving SDE. The analysis of this error is not so obvious as of previous two errors. The bounds from above are proved for both of the former errors and

these errors can be made sufficiently small by taking appropriate parameters h and N .

We propose some simple tests to investigate the quality of RNG used in our experiments. On no account this examination does not claim on perfect all-round analysis of random number sequences. Our aim is to carry out minimal set of tests and fulfillment of these tests is a necessary condition for the convergence of algorithms used to solve the concrete problem.

In the Euler method (8) we must generate the sequence $\{\varepsilon_k\}$ of independent random variables taking the values $+1$ and -1 with probabilities $1/2$. In order to construct $\{\varepsilon_k\}$ we generate a random number sequence $\{\xi_k\}$, which is uniformly distributed on $[0, 1)$, then $\{\varepsilon_k\}$ is introduced by the following rule

$$\varepsilon_k = \begin{cases} -1, & \xi_k \in [0, \frac{1}{2}), \\ 1, & \xi_k \in [\frac{1}{2}, 1). \end{cases}$$

The algorithms RANDOM and URAND (see Forsythe *et al.*, 1977) were used for uniform random number generation.

Test 1. *Confidence interval estimate of the mean value of the Bernoulli process.*

Let outcome of number 1 of ε_k be referred as a success. If μ is the number of successes in a random sample of size m , according to the Central Limit Theorem the variable

$$\eta = \frac{\mu - m/2}{\frac{1}{2}\sqrt{m}}$$

approaches the standard normal distribution as m approaches infinity. We only construct confidence interval estimate of the mean value of η .

Let us denote u_α normal deviate value, that is a solution of the equation

$$\Phi(u_\alpha) = 1 - \alpha, \quad \Phi(u_\alpha) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u_\alpha} e^{-\frac{u^2}{2}} du.$$

For large samples inequality $|\eta| \leq u_{\frac{\alpha}{2}}$ is fulfilled with the probability $1 - \alpha$

$$P\{|\eta| \leq u_{\frac{\alpha}{2}}\} \approx 1 - \alpha,$$

where $1 - \alpha$ is called the *confidence coefficient*. Then we have

$$\frac{\mu}{m} - \frac{1}{2\sqrt{m}} u_{\frac{\alpha}{2}} \leq \frac{1}{2} \leq \frac{\mu}{m} + \frac{1}{2\sqrt{m}} u_{\frac{\alpha}{2}}.$$

Hence the confidence interval for μ/m can be written as

$$\frac{1}{2} \left(1 - \frac{1}{\sqrt{m}} u_{\frac{\alpha}{2}} \right) \leq \frac{\mu}{m} \leq \frac{1}{2} \left(1 + \frac{1}{\sqrt{m}} u_{\frac{\alpha}{2}} \right).$$

The results of numerical experiments obtained with the confidence coefficient $1 - \alpha = 0.8$ are given in Table 1.

Table 1. The confidence interval estimates

RNG	l	m	d	s
RANDOM	100	10^4	0.012900	79
	10	10^5	0.004079	7
	10	10^6	0.001290	8
URAND	100	10^4	0.012900	80
	10	10^5	0.004079	9
	10	10^6	0.001290	9

We have presented the number of testing samples l , the number of trials in one sample m , the length of the confidence interval d and the number of successful samples s , when the confidence interval actually contains the simulated value μ/m .

We see that the first test was successfully passed by both generators.

The first test is not very difficult and certainly it can not guarantee that some given sequence $\{\varepsilon_k\}$ defines random sequence. For example the deterministic sequence $\{1, -1, 1, -1, \dots\}$ also passes this test.

Test 2. *The Bernoulli scheme.*

The experimental sequences $\{\varepsilon_k\}$ were used in the Bernoulli scheme experiments with samples of small length m . We calculated experimental frequencies of all possible combinations. By the theory the frequency of such combinations can be calculated by formula C_m^i (combination of i out of m trials). We estimated the error introduced by RNG by using the following norm

$$\text{Err} = \sum_{i=0}^m \frac{C_m^i}{2^m} \left| \frac{C_m^i}{2^m} - \frac{r(i)}{n} \right|,$$

Table 2. The error of experimental frequencies in the Bernoulli scheme

RNG	n	$m = 6$	$m = 2$
RANDOM	1000	0.010070	0.010000
	2000	0.007500	0.001666
	4000	0.005142	0.009166
	8000	0.002964	0.005590
	16000	0.001232	0.001958
URAND	1000	0.008142	0.016670
	2000	0.004928	0.00760
	4000	0.002892	0.00500
	8000	0.002142	0.006250
	16000	0.001571	0.003083

where $r(i)$, $i = 1, \dots, m$ is an experimental frequency of one specific combination in the n simulations of experimental samples.

Test 3. Parabolic problem with smooth data.

Next we will solve problem (1) with smooth initial data. We are interested in the comparison of effectivity of deterministic numerical methods and the methods of stochastic approximation. In the case of smooth problem the advantage of application of deterministic methods is indisputable and stochastic modelling is used only as the RNG quality test.

Consider parabolic equation (see Kloeden *et al.*, 1995)

$$\begin{aligned} \frac{\partial u(t, x)}{\partial t} &= 0.005 \frac{\partial^2 u(t, x)}{\partial x^2} + 2x \frac{\partial u(t, x)}{\partial x}, \\ u(0, x) &\equiv f(x) = x. \end{aligned} \quad (9)$$

The corresponding SDE is defined as follows:

$$dX(t) = 2X(t)dt + 0.01dw(t), \quad X(0) = x.$$

We know that the exact value

$$Ef(X(t)) = EX(t) = xe^{2t}.$$

Approximation (8) generates the simplified Euler method

$$X_{k+1} = X_k + 2X_k h + 0,01\sqrt{h}\varepsilon_{k+1}, \quad X_0 = X(0).$$

We have solved numerically problem (9) on the interval $[0, t]$. The functional $Ef(X(t))$ is calculated by using N discrete processes $\bar{X}(t)$ which are obtained with step sizes $h = t/n$. The maximal and the minimal errors and the confidence intervals for the error

$$|Ef(\bar{X}(t)) - Ef(X(t))|,$$

and errors are given in Table 3 with $X(0) = 0.1$, $t = 1$, and the confidence $\gamma = 0.95$.

Table 3. Errors for problem (9) with smooth data

n	N	ε_{\min}	ε_{\max}	δ_{\min}	δ_{\max}
1	1000	0.001102	0.003737	0.001892	0.001894
1	4000	0.000564	0.003557	0.009454	0.009468
1	16000	0.001596	0.002820	0.000473	0.000473
1	64000	0.002097	0.002250	0.000236	0.000236
2	1000	0.000162	0.003728	0.001383	0.003535
2	4000	0.000007	0.001617	0.001719	0.001746
2	16000	0.000708	0.001660	0.000865	0.000873
2	64000	0.000768	0.001291	0.000433	0.000435

We have presented minimal and maximal global errors ε_{\min} and ε_{\max} and also minimum and maximum of the Monte-Carlo approximation error $\delta = 2\sqrt{\text{Var}f(\bar{X}(t))/N}$ for 10 samples.

Talay and Tubaro (1990) have proposed stochastic extrapolation methods for the numerical solution of SDE based on simulations of functionals of the stochastic Euler scheme with different step sizes. Extrapolation methods give good results only for N large enough, namely, in the case when

$$\frac{1}{Nh} \left[\sum_{i=1}^N f(\bar{X}^{h(i)}(t)) - \frac{1}{2} \sum_{i=1}^{2N} f(\bar{X}^{h/2(i)}(t)) \right]$$

is independent from N (see Talay and Tubaro, 1990).

We use the scheme (8) to obtain the second order extrapolation following Kloeden *at al.* 1995. At first we simulate the functional

$$Ef(X^h(t))$$

for step size h , then for step size $h/2$, and finally the two results are combined to yield the second-order extrapolation

$$2Ef(\overline{X}^{\frac{h}{2}}(t)) - Ef(\overline{X}^h(t)).$$

Errors of the Euler method and extrapolation errors are given in Table 4 with $X(0) = 0.1$, $t = 1$.

Table 4. Global errors of the Euler scheme and of the second order extrapolation for the problem with smooth data

n	N	ε_h	$\varepsilon_{h/2}$	$\varepsilon_{\text{extrap}}$
4	2000	0.2317	0.1427	0.0537
8	2000	0.1433	0.0806	0.0179
16	2000	0.0808	0.0426	0.0043
32	2000	0.0431	0.0220	0.0010

Test 4. Parabolic problem with discontinuos initial data.

Consider the heat equation with discontinuos initial data

$$\begin{aligned} \frac{\partial u(t, x)}{\partial t} &= \frac{1}{2} \frac{\partial^2 u(t, x)}{\partial x^2}, \\ u(0, x) = f(x) &= I_{(0,1/4]}(x) - I_{(1/4,1/2]}(x) \\ &+ I_{(1/2,3/4]}(x) - I_{(3/4,1]}(x). \end{aligned} \quad (10)$$

where

$$I_{(a,b]}(x) = \begin{cases} 1, & x \in (a, b], \\ -1, & x \notin (a, b]. \end{cases}$$

Then we obtain the exact solution (see Fix and Korzeniowski, 1989)

$$u(t, x) = -\Phi\left(\frac{-x}{\sqrt{t}}\right) + 2\Phi\left(\frac{-x + 1/4}{\sqrt{t}}\right) - 2\Phi\left(\frac{-x + 1/2}{\sqrt{t}}\right) \\ + 2\Phi\left(\frac{-x + 3/4}{\sqrt{t}}\right) - \Phi\left(\frac{-x + 1}{\sqrt{t}}\right).$$

Using stochastic Taylor formula we get for the approximation

$$X(t+h) = X(t) + \int_t^{t+h} dw(s).$$

Then we find numerical approximation of the solution by using the scheme

$$X_{k+1} = X_k + \sqrt{h}\varepsilon_{k+1}, \quad X_0 = x, \quad (11)$$

where ε_k are independent two-point distributed random variables with $P\{\varepsilon_k = \pm 1 = 1/2\}$. The second approximation scheme is defined as follows

$$X_{k+1} = X_k + \sqrt{h}U_{k+1}, \quad X_0 = x, \quad (12)$$

where U_k are independent $N(0, 1)$ distributed Gaussian random variables. Both schemes have the same first order of weak convergency. But scheme (11) is simpler in simulation.

Table 5. Errors for problem (10) with discontinuous data

n	N	ε_{\min}	ε_{\max}	δ_{\min}	δ_{\max}
for (11)					
2	1000	0.00092	0.02992	0.02169	0.02252
2	4000	0.00392	0.02454	0.01107	0.01121
2	16000	0.00954	0.01970	0.00555	0.00561
2	64000	0.01067	0.01397	0.00279	0.00280
for (12)					
2	1000	0.00073	0.02473	0.04171	0.04497
2	4000	0.00073	0.02352	0.02140	0.02197
2	16000	0.00034	0.00834	0.01072	0.01098
2	64000	0.00040	0.00424	0.00541	0.00544

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NESTACIONARAUS TIESINIO DIFUZIJOS UŽDAVINIO SKAITINIAI STOCHASTINIAI APROKSIMAVIMO METODAI

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Šiame darbe nagrinėjami parabolinės lygties pradinio uždavinio silpnos aproksimacijos metodai. Pateikti paprasti testai atsitiktinių skaičių generatorių kokybei tirti. Įvertinti pagrindiniai stochastinių paklaidų tipai ir atlikta jų analizė. Pateikti skaitinio eksperimento rezultatai, iliustruojantys teorines išvadas.