Monte Carlo Method to Solve Diffusion Equation and Error Analysis

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Abstract: *Three different mathematical approaches for the evolution of diffusion equation are presented. The evolution process of the diffusion equation is explained by principle of conservation law, probability distribution procedure, and finally though stochastic differential equation (SDE) driven by Brownian motion. The Monte Carlo method is discussed to solve the diffusion equation by generating the normally distributed random numbers and the root mean square error is derived for the Monte Carlo method. The numerical solutions are computed for 1-dimensional diffusion equation and results are compared with exact solution. Finally, theoretical root mean square error is compared with the maximum error and the L_2-error by increasing the number of simulated points.*

Keywords: Diffusion equation, Monte Carlo method, Root mean square error, Brownian motion

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1 Introduction

Diffusion is the process by which matter is transported from one part of a system to another as a result of random molecular motion [2]. Due to the random molecular motion, the matter is always transported from higher to the low concentration. Many well-known phenomena in various fields in science, engineering, finance and many other problems are expressed by using the well-known evolution equations known as diffusion equation. Diffusion can be understood as Brownian motion of the particles in a medium where particles diffuse in a medium due to random collision by medium molecules. It is widely accepted that the Brownian motion is a general term of investigating subjects in various science fields relevant to the Markov process, such as material science, information science, life science, and social science [8].

In physics, the diffusion equation can be understood in accordance with the Gauss divergence theorem. The divergence theorem is applied to the diffusion problem for a material under the consideration of no sink and source of the material, it is found that the material conservation law is valid for the diffusion of particles, regardless of a thermodynamic state of material. The diffusion equation is also called the continuous equation and is extremely fundamental one in physics. In the history, the heat conduction equation, which is mathematically equivalent to the diffusion equation, was proposed by Fourier, regardless of the Markov process and the divergence theorem [8].

In this paper, three different mathematical procedures are discussed to develop the diffusion equation. Firstly, the conservation principle is used in which the rate of change of substance from a elementary region is equated to the substance in flow or out flow through the boundary of the region. Then, the diffusion equation is derived by applying the Fick's law [1]. Einstein also studied and derived the 1-dimensional diffusion equation from the concept of Brownian phenomenon of pollen grains suspended in a clean water [5]. The generalized version of the Einstein's work in higher dimensional space is presented and diffusion equation is derived. The random motion of the particles suspended in a medium (liquid or gas) can be explained by stochastic differential equation where the random motion of the particles is due to molecular collision of the medium, so the random motion of the particles is driven by Brownian motion [3, 9, 11]. Finally, the diffusion equation is derived from the stochastic differential equation using the Fokker-Plank equation [3, 9]. The Monte Carlo simulation is discussed to approximate the solution of the diffusion equation and the error due to the Monte Carlo method is derived. Finally, the Monte Carlo method is

implemented and 1-dimensional diffusion equation is solved numerically. The numerical solutions of the diffusion equation are presented graphically and compared with the exact solutions at different values of t. Finally, root mean square error is compared with the maximum error $\|\epsilon\|_\infty$ and L_2-error $\|\epsilon\|_2$ for different number of particles that diffuse in the medium and presented graphically .

2 Derivation of Diffusion Equation

There different approaches are discussed to derive the diffusion equation.

2.1 Using conservation principle

Let $\rho = \rho(t, \mathbf{x})$ denotes the concentration of a substance in a domain $\Omega \subset \mathbb{R}^d, d = 1, 2, 3$. Let $\Omega_t \subset \Omega$ be an infinitesimal element of Ω at a time instant t. By the principle of conservation law, the time rate of change of the amount the substance in the element Ω_t is equal to the flow of the substance in or out through the boundary $\partial\Omega_t$ of Ω_t. Mathematically [1],

$$\frac{d}{dt}\int_{\Omega_t} \rho(t, \mathbf{x}) d\mathbf{x} = -\int_{\partial\Omega_t} \mathbf{q} \cdot \mathbf{n}\, dA, \tag{1}$$

where $\mathbf{n}$ denotes the unit normal to the boundary Ω_t pointing outward and $\mathbf{q}$ denotes the flux through the boundary Ω_t. By Fick's law [1], the flux $\mathbf{q}$ is given by

$$\mathbf{q} = -D\ \nabla\rho, \tag{2}$$

where D denotes the diffusion coefficient. Using equation (2) in the equation (1) to get

$$\frac{d}{dt}\int_{\Omega_t} \rho(t, \mathbf{x}) d\mathbf{x} = \int_{\partial\Omega_t} \big(D\ \nabla\rho\big) \cdot \mathbf{n}\, dA, \tag{3}$$

Applying Renold's transport theorem and Gauss divergence theorem in the equation (3) to get

$$\int_{\Omega_t} \Big[\frac{\partial\rho}{\partial t} + \nabla \cdot (\mathbf{u}\rho)\Big] d\mathbf{x} = \int_{\partial\Omega_t} \nabla \cdot \big(D\ \nabla\rho\big) d\mathbf{x}$$

$$\implies \int_{\Omega_t} \Big[\frac{\partial\rho}{\partial t} + \nabla \cdot (\mathbf{u}\rho) - \nabla \cdot \big(D\ \nabla\rho\big)\Big] d\mathbf{x} = 0. \tag{4}$$

The relation (4) is true for every choice of $\Omega_t \subset \Omega$. Hence, by applying variational lemma to get

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\mathbf{u}\rho) = \nabla \cdot \big(D\ \nabla\rho\big) \tag{5}$$

Equation (5) is known as advection-diffusion equation. If there is no flow in the fluid, that means, $\mathbf{u} = 0$, then the pure diffusion equation is obtained

$$\frac{\partial\rho}{\partial t} = \nabla \cdot \big(D\ \nabla\rho\big) \tag{6}$$

2.2 Using statistical description

R. Brown in 1827 observed the irregular motion of pollen particles suspended in water [3]. It has been observed that

- the path of a given particle is very irregular, having a tangent at no point, and
- the motion of two particles appear to be independent.

Einstein in 1905 studied the one dimensional Brownian phenomenon [3, 5] and that is generalized in the higher dimensions in the following way :
Consider a cuboid box filled with clear water, into which a unit amount of ink at time $t = 0$ is injected at the position $\mathbf{x} = \mathbf{0}$. Let $\rho(t, \mathbf{x})$ denotes the density of the ink particles at the position $\mathbf{x} \in \mathbb{R}^d, d = 1, 2, 3$ at time $t \geq 0$.
At small time interval τ, the ink particles move from $\mathbf{x}$ to $\mathbf{x} + \mathbf{y}$ location and its probability density be $f(\tau, \mathbf{y})$. Then, the density at $\mathbf{x}$ in the time $t + \tau$ is given by

$$\rho(t + \tau, \mathbf{x}) = \int_{\mathbb{R}^d} \rho(t, \mathbf{x} + \mathbf{y}) f(\tau, \mathbf{y}) d\mathbf{y} \tag{7}$$

Applying Taylor's series expansion of the expression in LHS of the equation (7) to get

$$\rho(t + \tau, \mathbf{x}) = \rho(t, \mathbf{x}) + \tau \frac{\partial}{\partial t} \rho(t, \mathbf{x}) + O(\tau^2), \tag{8}$$

and applying Taylor's series expansion in the RHS of (7) to get

$$\int_{\mathbb{R}^d} \rho(t, \mathbf{x} + \mathbf{y}) f(\tau, \mathbf{y}) d\mathbf{y} = \int_{\mathbb{R}^d} \Big[\rho(t, \mathbf{x}) + \sum_{i=1}^{d} \frac{\partial}{\partial x_i} \rho(t, \mathbf{x}) y_i + \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial^2}{\partial x_i x_j} \rho(t, \mathbf{x}) y_i y_j + O(\|\mathbf{y}\|^3) \Big] f(\tau, \mathbf{y}) d\mathbf{y} \tag{9}$$

Now, assuming the symmetry of density function f, i.e., $f(\tau, \mathbf{y}) = f(\tau, -\mathbf{y})$ and assuming the independent motion of ink particle with identical distribution, the function $f(\tau, \mathbf{y})$ can be written as $f(\tau, \mathbf{y}) = \prod_{i=1}^{d} f_{\mathbf{y}}(\tau, y_i)$. Now, applying these assumptions and using the facts $\int_{\mathbb{R}^d} f(\tau, \mathbf{y}) dy = 1$, $\int_{\mathbb{R}} y_i f(\tau, \mathbf{y}) dy = 0, \int_{\mathbb{R}} y_i y_j f(\tau, \mathbf{y}) dy = 0, \ for \ i \neq j$ in the equation (9) to get

$$\int_{\mathbb{R}^d} \rho(t, \mathbf{x} + \mathbf{y}) f(\tau, \mathbf{y}) d\mathbf{y} = \rho(t, \mathbf{x}) + \frac{1}{2} \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} \rho(t, \mathbf{x}) \int_{\mathbb{R}^d} y_i^2 f(\tau, \mathbf{y}) d\mathbf{y} + O(\|\mathbf{y}\|^3) \tag{10}$$

Neglecting the higher orders terms from the equations (8) and (10), then substituting in the equation (7) to get the diffusion equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D \nabla \rho), \tag{11}$$

where $\int_{\mathbb{R}^d} y_i^2 f(\tau, \mathbf{y}) d\mathbf{y} = 2\tau D$.

2.3 Using Fokker-Plank description of Brownian motion

The motion of a small particles suspended in a moving liquid is subjected to random molecular bombardments. If $\mathbf{u}(t, \mathbf{x})$ denotes the velocity of fluid at the position $\mathbf{x}$ at time t, then the reasonable mathematical model for the position $\mathbf{X}_t$ of the particle at time t would be described by the stochastic differential equation in the form [3, 9]

$$d\mathbf{X}_t = \mathbf{u}(t, \mathbf{X}_t) dt + \sigma(t, \mathbf{X}_t) d\mathbf{W}_t, \tag{12}$$

where $\mathbf{W}_t \in \mathbb{R}^3$ denotes the Brownian motion [6] (or also known as Wiener Process) and $\sigma(t, \mathbf{x})$ is the strength of Brownian motion and some times called diffusion coefficient. The solution of the stochastic differential equation (12) may be thought of as a mathematical description of the motion of the small particles in a moving fluid.
Let $f(t, \mathbf{x})$ denotes the probability density of the position $\mathbf{X}_t$ of the particle in a moving fluid, then the Fokker-Plank equation [3, 10] of the SDE (12) is given by

$$\frac{\partial}{\partial t} f(t, \mathbf{x}) + \nabla \cdot (\mathbf{u} f(t, \mathbf{x})) = \nabla \cdot (D \nabla f(t, \mathbf{x})), \tag{13}$$

where $D = \frac{\sigma^2}{2}$ is the diffusion coefficient. Assuming the fluid is stationary, that means, $\mathbf{u} = 0$. if the amount of particles in the fluid is m_0 units, then the density of the particle $\rho(t, \mathbf{x}) = m_0 f(t, \mathbf{x})$ the equation (13) is reduces to the diffusion equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D \nabla \rho). \tag{14}$$

3 Monte Carlo Method and Estimation of Root Mean Square Error

In this section, the Monte Carlo method [7, 12] is presented to solve the diffusion equation with constant diffusion coefficient D

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho, \text{ where } \rho = \rho(t, \mathbf{x}) \tag{15}$$

For that, the stochastic differential equation (SDE) (12) is taken with $\mathbf{u} = 0$ and constant coefficient σ, that means,

$$d\mathbf{X}_t = \sigma d\mathbf{W}_t, \tag{16}$$

Then, the diffusion equation (15) is the corresponding Fokker-Plank equation of SDE (16).

The domain Ω is partitioned by non-overlapping finite number m of partitioning sets A such that $\Omega = \cup A$. The n number of independent and identically distributed random vectors $\mathbf{X}_i$ are generated that follow the normal distribution with mean $\mathbf{0}$ and co-variance matrix $2Dt\mathbb{I}$, that means, $X_i \sim N(\mathbf{0}, 2Dt\mathbb{I})$, where $\mathbb{I}$ denotes the identity matrix. Then, the approximated solution of the equation (15) $\hat{\rho}$ at the center $\mathbf{x}$ of A is calculated from

$$\hat{\rho}(\mathbf{x}) = \Big(\frac{m_0}{n} \sum_{\mathbf{X}_i \in \Omega} I_A(\mathbf{X}_i)\Big) \Big/ |A|\,, \tag{17}$$

where I_A denotes the indicator function and $|A|$ denotes the volume of set A.
The estimator $\hat{\rho}$ given in (17) is an unbiased estimator because

$$\begin{aligned} E(\hat{\rho}(\mathbf{x})) &= \Big(\frac{m_0}{n} \sum_{\mathbf{X}_i \in \Omega} E(I_A(\mathbf{X}_i))\Big) \Big/ |A| \\ &= \Big(\frac{m_0}{n} \sum_{\mathbf{X}_i \in \Omega} P(A)\Big) \Big/ |A| \\ &= \Big(\frac{m_0}{n} nP(A)\Big) \Big/ |A| \\ &= \frac{m_0 P(A)}{|A|} \\ \implies E(\hat{\rho}(\mathbf{x})) &= \rho(\mathbf{x}) \end{aligned} \tag{18}$$

The indicator function are $I_A(\mathbf{X}_i), i = 1, 2 \cdots, n$ are independent random variable, so the variance of the estimator $\hat{\rho}$ given in (17) is

$$\begin{aligned} V(\hat{\rho}) &= \Big(\frac{m_0^2}{n} V(I_A(\mathbf{X}_1))\Big) \Big/ |A|^2 \\ &= \frac{m_0^2}{n|A|^2} V(I_A(\mathbf{X}_1))\big) \\ &= \frac{m_0^2}{n|A|^2} \big(E(I_A^2) - E(I_A)^2\big)\big) \\ &= \frac{m_0^2}{n|A|^2} \big(P(A) - P^2(A)\big)\big) \\ \implies V(\hat{\rho}) &= \frac{m_0^2}{n|A|^2} P(A)\big(1 - P(A)\big)\big) \end{aligned} \tag{19}$$

The root mean square error ϵ of the Monte Carlo estimator is defined by

$$\begin{aligned}
\epsilon &= \sqrt{E\big([\rho-\hat{\rho}]^2\big)} \\
&= \sqrt{E\big([\rho^2-2\rho\hat{\rho}+\hat{\rho}^2]\big)} \\
&= \sqrt{\rho^2-2\rho E(\hat{\rho})+E(\hat{\rho}^2)} \\
&= \sqrt{\rho^2-2\rho^2+E(\hat{\rho}^2)}, \quad \text{using equation (18)} \\
&= \sqrt{E(\hat{\rho}^2)-\rho^2} \\
&= \sqrt{E(\hat{\rho}^2)-E(\hat{\rho})^2}, \quad \text{using equation (18)} \\
&= \sqrt{V(\hat{\rho})} \\
&= \sqrt{\frac{m_0^2 P(A)\big(1-P(A)\big)}{|A|^2}}\frac{1}{\sqrt{n}}, \quad \text{using equation (19)} \\
&\leq \sqrt{\frac{m_0^2 P_{max}(A)\big(1-P_{max}(A)\big)}{|A|^2}}\frac{1}{\sqrt{n}} \\
\implies \epsilon &\leq C\frac{1}{\sqrt{n}}, \text{ where } C=\sqrt{\frac{m_0^2 P_{max}(A)\big(1-P_{max}(A)\big)}{|A|^2}}.
\end{aligned} \tag{20}$$

Equation (20) tells that the root mean square error is inversely proportional to the square root of number n of randomly generated sample points X_i. It can be concluded that the estimated solution $\hat{\rho}$ converges to the exact solution when n is large enough.

3.1 Numerical Results and Discussions

The numerical experiment is performed in 1-dimensional open domain $(-a,a), a>0$ by dividing it into m number of sub-intervals. Initially, m_0 units of particles are placed at the location $x_0 \in (-a,a)$, i.e., $\rho(0,x_0)=\delta(x_0)$ or $\int_{-a}^{a}\delta(x_0)dx = m_0$. The motion of particles follow the SDE (16) and position of the particle at any time t is given by

$$X(t) = x_0 + \sigma W_t, \tag{21}$$

where W_t is the Brownian motion or Wiener process that follows the normal distribution with mean 0 and variance t, i.e., $W_t \sim N(0,t)$, so it can be generated by $W_t = \sqrt{t}z, z \sim N(0,1)$. Then, approximated solution $\hat{\rho}(t,x)$ of 1-dimensional diffusion equation by using the equation (17) at each point x and time t.

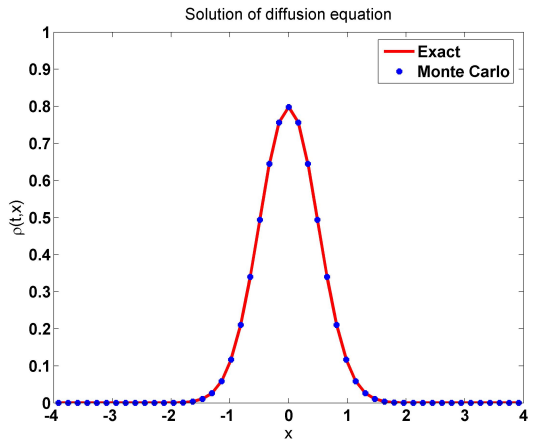

Figure 1: Solution at time t=0.25

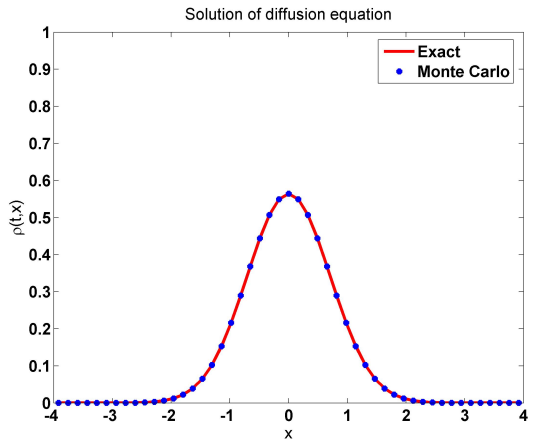

Figure 2: Solution at time t=0.50

Figures 1,2,3 and 4 show the solutions of the 1-dimensional diffusion equation (15) at the times t =

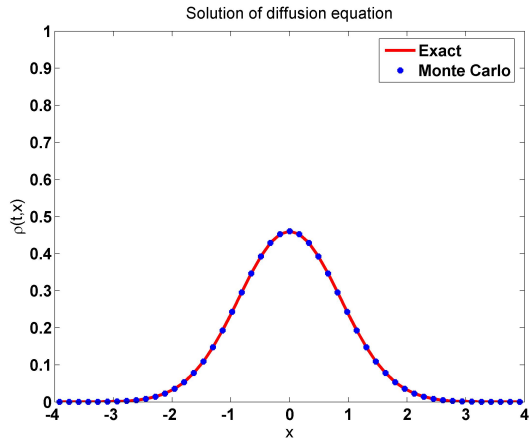

Figure 3: Solution at time t=0.75

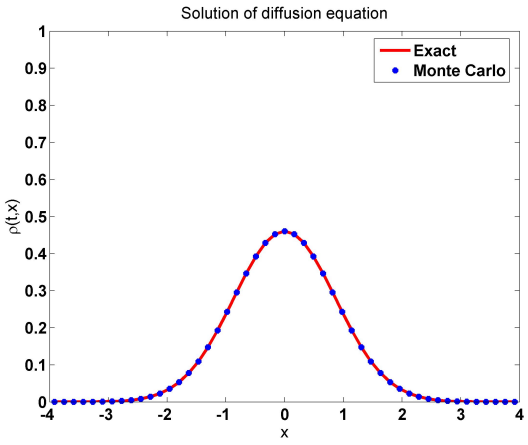

Figure 4: Solution at time t=1.0

$0.25, t = 0.50, t = 0.75$ and $t = 1.0$ seconds respectively. In each figure, the red solid curve represents the exact solution given in [4] and blue dots represent the approximated solutions computed by using Monte Carlo method. It can be seen from these results that the approximated solutions match perfectly with the exact solutions.

3.2 Error Analysis

The diffusion equation (15) is solved numerically by using the Monte Carlo method (17) at the end of the time point $t = 1$ second by increasing the number n of simulated points. Then, the maximum error $\|\epsilon\|_\infty$ and L_2-error $\|\epsilon\|_2$ are calculated using

$$\|\epsilon\|_\infty = max_{x\in(-a,a)} |\rho(x) - \hat{\rho}(x)| \tag{22}$$

$$\|\epsilon\|_2 = \sqrt{\int_{-a}^{a} |\rho(x) - \hat{\rho}(x)|^2 \, dx} \tag{23}$$

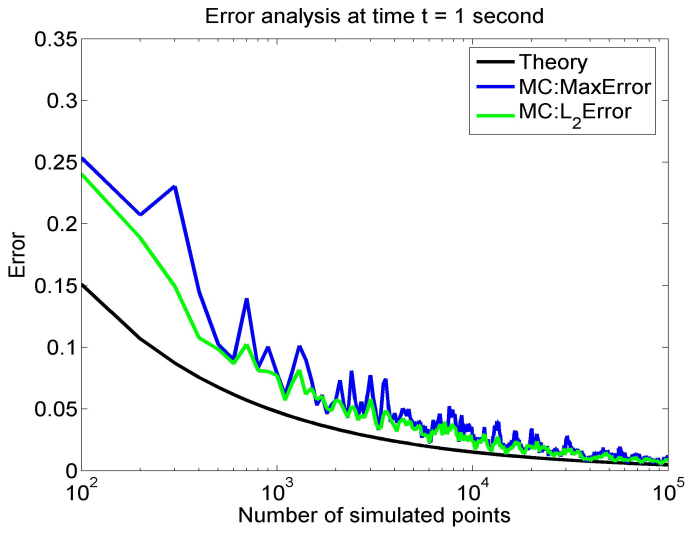

Figure 5: Various errors at time t=1 second

The figure 5 shows the plot of the various errors calculated from the equations (20), (22) and (23) at time point $t = 1$ when number of simulated points are increased from the range of small values to large values. The black solid curve is the theoretical root mean square error ϵ given by the equation (20), the solid blue curve is the maximum error $\|\epsilon\|_\infty$ calculated from (22) and the solid green curve is the L_2-error $\|\epsilon\|_2$ calculated using (23). It is clear from the above results that these errors are decreasing with increasing the number of simulated points. It can be seen that the when number of simulated points are higher than 10^5, the errors in all cases approach to zero.

4 Conclusions

Three different approaches, namely, the principle of conservation law, probability distribution procedure, and through the stochastic differential equation (SDE) driven by Brownian motion are discussed to derive the diffusion equation. This paper is mostly focused on the stochastic approach where Monte Carlo method is implemented to approximate the solution of the diffusion equation. The solutions obtained by the Monte Carlo method correctly approximated the exact solutions which are shown graphically at four different values time t. The root mean square error, maximum error and L_2-error are computed and presented graphically. It can be concluded that larger the number of simulated points better the approximated solutions computed using Monte Carlo method. The Monte Carlo method can be extended to higher dimensional space with irregular spatial domain.

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