Stochastic Modeling

Md Danish Ansari

(Stream Project under the Guidance of Prof. Dr. Subir Das)

Department of Mathematical Sciences
Indian Institute of Technology (BHU), Varanasi
Varanasi - 221 005.

8 May, 2024

Presentation Overview

Why do we require Sigma Algebra And Measure Theory ?

Consider the following example: Suppose you have a unit square in $\mathbb{R}^2$ you are interested in the probability of randomly selecting a point that is a member of a specific set in the unit square.

In many cases, determining this probability is straightforward by comparing the areas of various sets. For instance, one can draw circles, measure their areas, and then establish the probability as the fraction of the square contained within the circle. However, complications arise when the area of the set in question is not clearly defined.

Sigma Algebra And Measure Theory

Sigma Algebra

A sigma-algebra F (σ-algebra) is a set of subsets ω of (Ω is a set) such that the following conditions hold:

a.) $\phi \in F$

b.) If $\omega \in F \implies \omega^{\complement} \in F$

c.) If $\omega_1, \omega_2, \omega_3 \ldots\ \omega_n \in F \implies \bigcup_{i=1}^{n} \omega_i \in F$

Measure Theory

A set function μ defined on σ-algebra (Σ) is called a measure if and only if the following conditions hold:

a.) $0 \leq \mu(\mathrm{A}) \leq \infty$. for any $\mathrm{A} \in \Sigma$

b.) $\mu(\phi) = 0$.

c.) σ - additivity: For any seqeunce of pairwise disjoint set, $A_n \in \Sigma$ such that $\bigcup_{i=1}^{n} \mathrm{A}_i \in \Sigma \implies \mu(\bigcup_{i=1}^{n} \mathrm{A}_i) = \sum_{i=1}^{n} \mu(A_i)$

Kolmogorov's Axioms

Let P: E $\rightarrow$ [0,1] be the probability measure and E be some σ-algebra (events) generated by some set X. Then

a.) $0 \leq$ P(A) ≤ 1 for all A $\in E$

b.) P(X) = 1

c.) P($a_1 \bigcup a_2 \bigcup a_3 ... \bigcup a_n$) = P($a_1$) + P($a_2$) + P($a_3$) + ... + P($a_n$), where a_1, a_2, a_3 ... a_n are all disjoint sets in E.

Random Variable

A random variable X is a measurable function from the probability space (Ω, Σ, P) into the probability space (χ,A_x ,P_x), where χ in R is the range of X (which is a subset of the real line) A_x is a sigma field of X, and P_x is the probability measure on χ induced by X. Specifically, X: $\Omega \rightarrow \chi$.

Stochastic Process

A stochastic process $X(t)$, $t \in I$ is a time indexed collection of random variables, where I is the index set.

Examples:

- $X(t)$ might equal the total number of customers that have entered a supermarket by time t.
- $X(t)$ might equal the stock price of a company at time t.

The state space of the a stochastic process is defined as the set of all possible values that the random variables $X(t)$ can assume.

The index set I is called the parameter space of the process.

Classification of Stochastic Process on the basis of state space and parameter space:

- Discrete Time Discrete Space.
- Continuous Time Discrete Space.
- Discrete Time Continuous State.
- Continuous Time Continuous State.

Stochastic Process

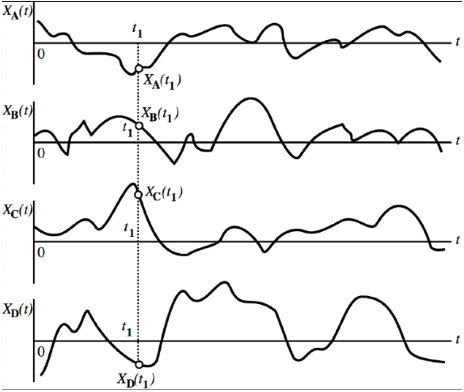

Figure: Realisation of the Stochastic processes

The Diffusion Equation

According to **Fick's Law** of diffusion: "The molar flux due to diffusion is proportional to the concentration gradient". The rate of change of concentration of the solution at a point in space is proportional to the second derivative of concentration with space.

1. Equation of continuity:

$$\underbrace{\frac{\partial \rho}{\partial t}}_{\text{change in concentration}} + \underbrace{\nabla \cdot \vec{J}}_{\text{divergence of current}} = 0. \tag{1}$$

2. Diffusion from a region of higher concentration to a region of lower concentration.

$$\vec{J}(\vec{r},t) = -D\nabla\rho(\vec{r},t). \tag{2}$$

- D represents the Diffusion Constant
- J represents the diffusion flux vector.
- ρ represents the concentration
- ∇ represents the del or the gradient operator.

The Diffusion Equation

$$\underbrace{\frac{\partial \rho}{\partial t} = D\nabla^2 \rho(\vec{r},t).}_{\text{This equation is of dimension 1st order in time and second order in space}} \tag{3}$$

Derivation of Diffusion equation using random walk

Consider a linear lattice with lattice constant 'a'. Let p be the probability that a particle is at position j and at time t.

Then the rate of change of probability of the particle is obtained as:

$$\frac{\partial p(ja,t)}{\partial t} = \frac{\Lambda}{2}(p(ja+a,t)+p(ja-a,t)-2p(ja,t)) \tag{4}$$

where Λ represents the average rate at which these jumps occur.

Consider the case when

$$\Lambda \to \inf, a \to 0 \tag{5}$$

Then variable ja $\to$ x (becomes a continuos variable).

The Diffusion Equation

Thus eqn (4) can be written as:

$$\lim_{\Lambda \to \inf, a \to 0} \frac{\partial p(j,t)}{\partial t} = \frac{\Lambda a}{2} \left(\frac{p(ja+a,t) - p(ja,t)}{a} - \frac{p(ja,t) - p(ja-a,t)}{a} \right) \tag{6}$$

Thus we finally obtain the diffusion equation from Discrete Random Walks.

$$\frac{\partial p(x,t)}{\partial t} = D\left(\frac{\partial^2 p(x,t)}{\partial x^2} \right) \tag{7}$$

where D $\equiv \lim_{\Lambda \to \mathrm{inf}}$,a $\to 0$ $\frac{\Lambda a^2}{2} = \mathit{finite}$.

Thus the above equation represents the Diffusion Equation, which obtained by taking the continuum limit of random walk.

Solution of the Diffusion equation

Considering the natural boundary condition as p($\vec{r}$,t) = 0, as r $\rightarrow$ inf.
Initial Condition: p($\vec{r}$,0) = $\delta^d(\vec{r})$.

Let's consider the following transformations.

$$\mathscr{L}(p(\vec{r},t)) = \underbrace{\tilde{p}(\vec{r},s)}_{\text{Laplace tranform}} \tag{8}$$

$$\tilde{p}(\vec{r},s) = \int \underbrace{f(\vec{k},s)}_{\text{Fourier transform of } \tilde{p}(\vec{r},s)} e^(i\vec{k}\cdot\vec{r}) \frac{1}{(2\pi)^d}(d^d)k \tag{9}$$

$$\tilde{f}(\vec{k},s) = \int \tilde{p}(\vec{r},s) exp(-i\vec{k}\cdot\vec{r})(d^d)r \tag{10}$$

The Diffusion Equation

Choosing Cartesian Co-ordinates for integration we obtain

$$p(\vec{r},t) = \frac{1}{(2\pi)^d}(\int_{-\inf}^{\inf} exp(ik_1x_1)exp(-Dk_1^2t)dk_1)....(\int_{-\inf}^{\inf} exp(ik_dx_d)exp(-Dk_d^2t)(dk_d)) \quad (11)$$

Calculating the first integral.

$$I_1 = \frac{1}{(2\pi)}(\int_{-\inf}^{\inf} exp(-\frac{x_1^2}{4Dt})exp(-Dt(k_1 - \frac{ix_1}{2Dt})^2)dk_1). \quad (12)$$

$$I_1 = exp(-\frac{x_1^2}{4Dt})\frac{1}{(2\pi)}\frac{\sqrt{\pi}}{\sqrt{Dt}}. \quad (13)$$

Similarly Calculating all the other values of I_2, I_3 ... we obtain.

$$\boxed{p(\vec{r},t) = \frac{exp(-\frac{r^2}{4Dt})}{(4\pi Dt)^{(\frac{d}{2})}}.} \quad (14)$$

Solution of diffusion Equation

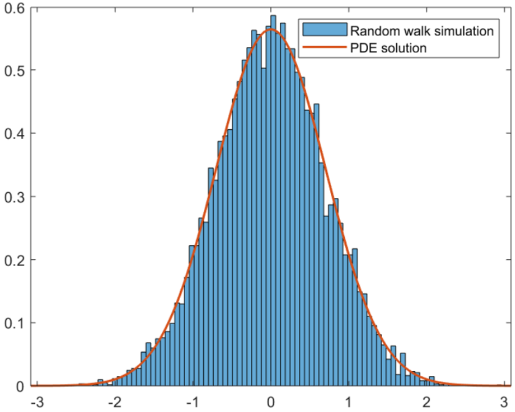

Figure: Random Walk simulation vs the solution of diffusion equation

Diffusion with Drift: Consider situations where the diffusion process incorporates drift caused by a constant force.

So we have

$$P(ja,n\tau) = \alpha P(ja-a,n\tau-\tau)+\beta P(ja+a,n\tau-\tau) \tag{15}$$

where α represents the rate of forward jump ans β represents the probability of backward jump ,also α+β = 1.

Solving this double recurrence relation we obtain the solution known as **The Smoluchowski Equation** :

$$\frac{\partial p(x,t)}{\partial t} = -c\frac{\partial p(x,t)}{\partial x} + D\frac{\partial^2 p(x,t)}{\partial x^2} \tag{16}$$

where c = a$\frac{(\alpha-\beta)}{\tau}$, D = $\frac{a^2\alpha}{\tau}$

The term c $\rightarrow$ represents Drift Velocity

D $\rightarrow$ represents Diffusion coefficient.

$\alpha-\beta \rightarrow$ represents the bias.

The Diffusion Equation

Solution of **Diffusion Convection Equation** by transformation of variables.

$$\frac{\partial f}{\partial t} = \underbrace{\frac{D\partial^2 f}{\partial x^2}}_{\text{Diffusion}} - \underbrace{\mu\frac{\partial f}{\partial x}}_{\text{Convection}} \tag{17}$$

Applying the transformation of the variables by y = x - μt, we obtain the following transformed equation we obtain the following.

$$\frac{\partial \tilde{f}}{\partial t} = D\frac{\partial^2 \tilde{f}}{\partial y^2} \tag{18}$$

Thus transalation of the spatial variable at speed μ , we obtain a pure diffusion equation whose solution have been derived before.

Consider the initial-boundary value problem for 1D diffusion as follows:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + f(x,t) \qquad x \in (0,L),\ t \in (0,T] \tag{19}$$

Initial condition:

$$u(x,0) = I(x) \tag{20}$$

Boundary conditions:

$$u(0,t) = 0, \quad t > 0$$
$$u(L,t) = 0, \quad t > 0$$

Discretizing the domain:

Mesh points:

$$x_i = i\Delta x,\ i = 0,\dots,N_x$$

Time points:

$$t_n = n\Delta t,\ n = 0,\dots,N_t$$

Mesh function: $u_i^n \approx u(x_i,t_n)$ for $i = 0,\dots,N_x$ and $n = 0,\dots,N_t$

Forward Euler scheme

Applying the PDE at mesh point (x_i, t_n):

$$\frac{\partial u(x_i,t_n)}{\partial t} = \alpha \frac{\partial^2 u(x_i,t_n)}{\partial x^2} + f(x_i,t_n) \tag{21}$$

Finite difference approximation using a forward difference in time and a central difference in space:

$$[D_t^+ u]_i^n = \alpha [D_x D_x u]_i^n + f(x_i,t_n) \tag{22}$$

where:

$$[D_t^+ u]_i^n \text{ denotes the forward difference approximation of } \frac{\partial u}{\partial t} \text{ at } (x_i,t_n)$$

$$[D_x D_x u]_i^n \text{ denotes the central difference approximation of } \frac{\partial^2 u}{\partial x^2} \text{ at } (x_i,t_n)$$

Forward Euler scheme

We obtain the following discrete equations.

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + f_i^n \tag{23}$$

The term $\alpha \frac{\Delta t}{\Delta x^2}$ is called as the mesh Fourier number (F).

F acts as the key parameter in the discrete diffusion equation

Note that F is a dimensionless number that lumps the key physical parameter in the problem, α, and the discretization parameters Δx and Δt into a single parameter. Properties of the numerical method are critically dependent upon the value of F.

Simulations with the Forward Euler scheme has the time step restriction, F ≤ 1, which means $\Delta t \leq \frac{\Delta x^2}{2\alpha}$, may be relevant in the beginning of the diffusion process.

By using implicit schemes, which lead to coupled systems of linear equations to be solved at each time level, any size of Δt is possible.

Backward Euler scheme: We now apply a backward difference in time in the diffusion equation but the same central difference in space:

$$[D_t^- u]_i^n = [D_x D_x u]_i^n + f(x_i, t_n) \tag{24}$$

which written out reads

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + f_i^n \tag{25}$$

Backward Euler scheme

Collecting the unknowns on the left-hand side eqn 23 can be written as

$$-Fu_{i-1}^{n} + (1+2F)u_i^n - Fu_{i+1}^n = u_i^{n-1} \tag{26}$$

for i = 1,2,..,$N_x - 1$.

Adding the boundary equations to the $N_x - 1$ equations in the above equation.

$$u_0^n = 0. \tag{27}$$

$$u_{N_x}^n = 0. \tag{28}$$

The above equations corresponds to the matrix equation

$$AU = b$$

where

$$U = (u_n^0, \ldots, u_{N_x}^n) \tag{29}$$

and A is a tridiagonal matrix.

The unifying Θ rule

For the equation

$$\frac{\partial u}{\partial t} = G(u),$$

where $G(u)$ is some spatial differential operator, the θ-rule looks like

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \theta G(u_i^{n+1}) + (1-\theta) G(u_i^n).$$

The choice of θ in the θ-rule affects the numerical scheme:

- $\theta = 0$ gives the Forward Euler scheme in time.
- $\theta = 1$ gives the Backward Euler scheme in time.
- $\theta = \frac{1}{2}$ gives the Crank-Nicolson scheme in time.

In the compact difference notation, we write the θ-rule as

$$[D_t u = \alpha D_x D_x u]^{n+\theta}.$$

We have that

$$t_{n+\theta} = \theta t_{n+1} + (1-\theta) t_n.$$

The unifying Θ rule

When applied to the diffusion problem, the θ-rule scheme leads to a matrix system $AU = b$ with entries:

$$A_{i,i-1} = -F\theta, \quad A_{i,i} = 1 + 2F\theta, \quad A_{i,i+1} = -F\theta.$$

while right-hand side entry b_i is:

$$b_i = u_i^n + F(1-\theta)\frac{u_{i+1}^n - 2u_i^n + u_i^{n-1}}{\Delta x^2} + \Delta t\theta f_i^{n+1} - \Delta t(1-\theta)f_i^n. \tag{30}$$

Diffusion in heterogeneous media normally implies a non-constant diffusion coefficient $\alpha = \alpha(x)$.

A diffusion model with such a variable diffusion coefficient reads

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial u}{\partial x}\right) + f(x,t), \quad x \in (0,L), \quad t \in (0,T] \tag{31}$$

$$u(x,0) = I(x), \quad x \in [0,L], \tag{32}$$

$$u(0,t) = U_0, \quad t > 0, \tag{33}$$

$$u(L,t) = U_L, \quad t > 0. \tag{34}$$

Discretization

We can discretize equation (31) by a Θ-rule in time and centered differences in space and thus solve the problem.

Time-dependent Advection-diffusion equation

Consider the following Advection-diffusion governing equation as

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2}$$

(35)

Analytical Solution:
The diffusion is now dominated by convection, a wave, and diffusion, a loss of amplitude. One possible analytical solution is a traveling Gaussian function

$$u(x,t) = B\exp\left(-\frac{x-vt}{4at}\right) \tag{36}$$

This function moves with velocity $v > 0$ to the right ($v < 0$ to the left) due to convection, but at the same time we have a damping $e^{-16a^2t^2}$ from diffusion.

Time-dependent Advection-diffusion equation

Numerical Schemes for equation governing the advection-diffusion system is given as follows:
Forward in time, upwind in space scheme : A good approximation for the pure advection equation is to use upwind discretization of the advection term. We also know that centered differences are good for the diffusion term, so combining these two discretizations results in a good-level approximations given by the equation as:

$$[D_t u + v D_x^- u = \alpha D_x D_x u + f]_i^n \quad v > 0 \tag{37}$$

However, In this case the physical diffusion and the extra numerical diffusion $v\frac{\Delta x}{2}$ will stabilize the solution, but give an overall too large reduction in amplitude compared with the exact solution.

We may also interpret the upwind difference as artificial numerical diffusion and centered differences in space everywhere, so the scheme can be expressed as:

$$[D_t u + v D_{2x}^- u = \alpha v \frac{\Delta x}{2} D_x D_x u + f]_i^n \tag{38}$$

Future Plans

- Derivation of Non-linear Fractional Diffusion Equation by system of interacting walkers.
- Analytical Solution of the non-linear fractional diffusion equation.
- Numerical Schemes for the approximation of fractional diffusion equation using various schemes of finite difference computing (finite element analysis).
- Solution of fractional diffusion equation with a moving boundary condition by well-known semi-analytical methods such as variational iteration method.

Acknowledgement and References I

I would like to express my sincere gratitude to my guide **Prof. Dr. Subir Das Sir** for your invaluable guidance and unwavering support throughout my project.

I am truly thankful for the time and effort you invested in mentoring me.

J Medhi (2002). An Introduction to Stochastic Processes. *Wiley*, New York.

Grigorios A. Pavliotis (2016). Stochastic Processes and Applications: Diffusion Processes, the Fokker-Planck and Langevin Equations: *Probab. Theory and Related Fields*,

Dr Qianqian Yang,R. Metzler, J. Klafter. (2007). The random walk's guide to anomalous diffusion: a fractional dynamics approach. Physics Reports 339 (2000) 1-77.

Gregory Lawler. (2014). Stochastic Calculus: An Introduction with Applications. *http://www.math.uchicago.edu/ lawler/finbook.pdf*.

David Williams (1991). Probability with Martingales. Cambridge University Press.

Martin Haugh. (2016). A Brief Introduction to Stochastic Calculus. http://www.columbia.edu/ mh2078/FoundationsFE/IntroStochCalc.pdf

Thank You