Reaction-Diffusion Equation and Its Applications

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This project aims at studying the Reaction-Diffusion equation from both analytic and numerical perspectives. Starting from the Diffusion equation, we derive the analytic solution to the problem with Dirichlet boundary conditions. In terms of numerical analysis, we use Monte Carlo Simulation and Finite Difference Method to study the front propagation and traveling waves.

1 Reaction-Diffusion Equation

The standard form of the Reaction-Diffusion equation is given as follows:

$$\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t) + F(\rho(x,t)) \tag{1}$$

where ρ is the probability density function of the population at time t and space x, D is the diffusion coefficient and $F(\rho)$ is the reaction term describing how particles or individuals react or interact at the same time undergo diffusion.

1.1 The Diffusion Equation

Let's first consider the diffusion equation where the reaction term is set to be zero (i.e., $F(\rho) = 0$).

$$\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t), \qquad x \in \mathbb{R}, t \geq 0. \tag{2}$$

The analytic solution of the above equation with initial condition $\rho(x,0) = \delta_0(x)$ is given as:

$$\rho(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right), t > 0 \tag{3}$$

Note that $\delta_0(x)$ is known as the Dirac delta function (a distribution over the real line) whose value is zero everywhere except at zero, and whose integral over the entire real line is one.

Another way to understand $\delta_0(x)$ is described in the following way. We define a sequence of functions $f_n(x)$, $f_n : \mathbb{R} \to \mathbb{R}$, $n \in \mathbb{N}^+$, as follows:

$$f_n(x) = \begin{cases} 0 & \text{if } x \in (-\infty, -\frac{1}{n}] \cup [\frac{1}{n}, \infty) \\ n^2 x + n & \text{if } x \in (-\frac{1}{n}, 0] \\ -n^2 x + n & \text{if } x \in (0, \frac{1}{n}) \end{cases}$$

Then, $\delta_0(x) = \lim_{n \to +\infty} f_n(x)$.

1.1.1 The Boundary Condition of the Diffusion Equation

In this section, we explicitly solve the Diffusion equation with Dirichlet boundary conditions.

We suppose x lies in a fixed interval, for convenience, let's suppose $x \in [0, 1]$. Consider the boundary conditions $\rho(0, t) = \rho(1, t) = 0$, and as an example, we consider the initial condition $\rho(x, 0) = \sin \pi x$, we then have:

$$\begin{cases} \dfrac{\partial}{\partial t}\rho(x,t) = \dfrac{\partial^2}{\partial x^2}\rho(x,t) \\ \rho(x,0) = \sin \pi x \ (\textit{initial condition}) \\ \rho(0,t) = 0 \\ \rho(1,t) = 0 \end{cases} \tag{4}$$

To solve this equation, we use separation of variables and assume

$$\rho(x, t) = A(x)B(t)$$

We then rewrite the diffusion equation as follows:

$$\begin{aligned} \frac{\partial}{\partial t}A(x)B(t) &= \frac{\partial^2}{\partial x^2}A(x)B(t) \\ AB' &= A''B \\ \frac{A''}{A}(x) &= \frac{B'}{B}(t) \end{aligned}$$

Suppose

$$\frac{A''}{A}(x) = \frac{B'}{B}(t) = \lambda(x, t)$$

We have

$$\begin{cases} \dfrac{\partial}{\partial t}\lambda = \dfrac{\partial}{\partial t}\dfrac{A''}{A}(x) = 0 \\ \dfrac{\partial}{\partial x}\lambda = \dfrac{\partial}{\partial x}\dfrac{B'}{B}(t) = 0 \end{cases}$$

Hence, $\lambda(x,t) = \lambda$ is constant. We then solve for the following:

$$\begin{cases} \dfrac{A''}{A}(x) = \lambda \\ \dfrac{B'}{B}(t) = \lambda \\ \rho(x,t) = A(x)B(t) \\ \rho(0,t) = \rho(1,t) = 0 \end{cases}$$

Let's first look at A(x).

$$\begin{cases} \dfrac{A''}{A}(x) = \lambda \\ A(0) = 0 \\ A(1) = 0 \end{cases}$$

If $\lambda \geq 0$, we will end up having a trivial solution $A(x) = 0$. Hence, $\lambda < 0$.

Let $\lambda = -\beta^2$,

$$\begin{cases} \dfrac{A''}{A}(x) + \beta^2 A = 0 \\ A(0) = A(1) = 0 \end{cases}$$

$\Rightarrow A(x) = c_1 sin\beta x + c_2 cos\beta x$.

Since $A(0) = A(1) = 0$, we have $c_2 = 0$ and $\beta = k\pi (k \in \mathbb{Z}, k \neq 0)$. That is to say, $\lambda = -k^2\pi^2$, and we have

$$A(x) = c_1 sink\pi x$$

Now, we look at $B(t)$ and we have

$$\frac{B'_k}{B_k} = \lambda = -k^2\pi^2$$

which gives

$$B(t) = c_2 e^{-k^2\pi^2 t}$$

$$\Rightarrow \rho_k(x,t) = A_k(x)B_k(t) = c_k e^{-k^2\pi^2 t} sink\pi x$$

The final solution to equation (4) should be a linear combination of all the possible ρ_k's. Hence,

$$\rho(x,t) = \sum_{k=1}^{\infty} c_k e^{-k^2\pi^2 t} sink\pi x$$

From the initial condition $\rho(x,0) = sin\pi x$, we can easily derive that $c_1 = 0, c_k = 0 (k > 1)$. Therefore, we now have the solution to equation (4):

$$\Rightarrow \rho(x,t) = e^{-\pi^2 t} sin\pi x$$

2 Numerical Analysis

In this section, we describe the two approaches we used to conduct the numerical analysis.

2.1 Monte Carlo Simulation

In Monte Carlo simulation, we approximate the initial total population by some large number N. At each time step, we let every individual perform random walk according to certain policy. We apply the random walk for a large number of trials to simulate the evolution of our model. By tracking the location of each individual at each time step, we can study the change of population density.

2.1.1 Monte Carlo Simulation for Solving the Diffusion Equation

To simulate the diffusion of a population of N individuals, we set every individual to stay at the zero point initially. Let x_n^i denote the location of the n^{th} individual at time step i (when $t = i\Delta t$), where $n = 1, 2, 3, ..., N$ and $i = 0, 1, 2, 3, ...$ We have $x_n^0 = 0$ for all $n's$. The random movement of each individual is given as (recall that D is the diffusion coefficient):

$$x_n^{i+1} = x_n^i + z_n^i, \ where\ z^i \sim \sqrt{D\Delta t} \cdot \mathcal{N}(0, 1)$$

As an example, we choose $D = 1$ and solve for $\frac{\partial}{\partial t}\rho(x,t) = \frac{\partial^2}{\partial x^2}\rho(x,t)$. Apply equation (3), we know that the analytic solution is given by:

$$\rho(x,t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right)$$

In our Monte Carlo simulation, we choose $N = 10000$ and $\Delta t = 0.1$. Figure 1 shows our numerical solution together with the analytic solution at $t = 500$.

2.1.2 Monte Carlo Simulation for Solving the Reaction-Diffusion Equation

Based on our approach to solve the Diffusion equation, all we need to do for solving Reaction-Diffusion equation is to involve a reaction term. We here consider the reaction term to be the logistic growth.

In order to simulate the reaction, we first divide the whole space into some number of small intervals. In each interval, we add a logistic growth term based on the current population of the interval. We calculate the new births of the interval based on the current interval population and let the new births be equally distributed within the interval.

2.2 Finite Difference Method

Note that we assumed $x \in [0, 1]$, we now assume that $x_0 = 0$ and $x_M = 1$, $x_m = m\Delta x$ where $\Delta x = \frac{1}{M}$ for $m = 0, 1, 2, 3, ..., M$. Similarly, we write $t_n = n\Delta t$ where $n = 0, 1, 2, 3, ..., N$. Then, we write $\rho_m^{(n)} = \rho(x_m, t_n) = \rho(m\Delta x, n\Delta t)$.

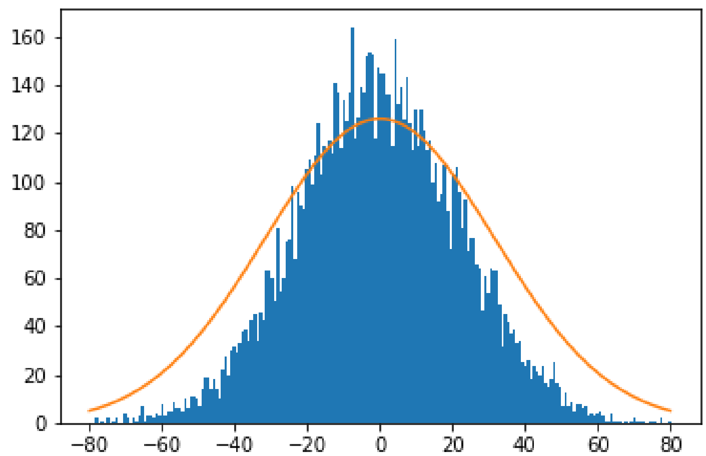

Figure 1: Numerical solution using Monte Carlo simulation and analytic solution of the one-dimensional Diffusion equation. Numerical solution is represented by blue bins (we divide the whole space into 200 bins) and analytic solution is represented by the orange line. x-axis represents the location and y-axis represents the population.

2.2.1 Finite Difference for First Order Derivative

For a function $u(t)$, we write $u_0 = u(0), u_1 = u(\Delta t), ..., u_k = u(k\Delta t)$. We solve $\frac{du}{dt}$ at $k\Delta t$, we have three approaches to approximate the derivative:

$$\frac{d}{dt}u_k \approx \frac{u_k - u_{k-1}}{\Delta t}$$
$$\frac{d}{dt}u_k \approx \frac{u_{k+1} - u_k}{\Delta t}$$
$$\frac{d}{dt}u_k \approx \frac{u_{k+1} - u_{k-1}}{2\Delta t}$$

By Taylor expansion, we have:

$$u_{k+1} = u(k\Delta t + \Delta t) = u_k + u'(k\Delta t)\Delta t + \frac{u''(k\Delta t)\Delta t^2}{2} + O(\Delta t^3)$$
$$u_{k-1} = u(k\Delta t - \Delta t) = u_k - u'(k\Delta t)\Delta t + \frac{u''(k\Delta t)\Delta t^2}{2} + O(\Delta t^3)$$

Then,

$$\frac{u_k - u_{k-1}}{\Delta t} = u'(k\Delta t) + O(\Delta t)$$
$$\frac{u_{k+1} - u_k}{\Delta t} = u'(k\Delta t) + O(\Delta t)$$
$$\frac{u_{k+1} - u_{k-1}}{2\Delta t} = u'(k\Delta t) + O(\Delta t^2)$$

The first two are both first-order method while the third approximation gives a second-order method which is more accurate.

2.2.2 Finite Difference for Second Order Derivative

We then do the similar in the space dimension, for a function $u(x)$, we write $u_0 = u(0), u_1 = u(\Delta x), ..., u_n = u(n\Delta x)$.

$$u_{n+1} = u(n\Delta x + \Delta x) = u_n + u'(n\Delta x)\Delta x + \frac{u''(n\Delta x)\Delta x^2}{2} + \frac{u'''(n\Delta x)\Delta x^3}{6} + O(\Delta x^4)$$
$$u_{n-1} = u(n\Delta x - \Delta x) = u_n - u'(n\Delta x)\Delta x + \frac{u''(n\Delta x)\Delta x^2}{2} - \frac{u'''(n\Delta x)\Delta x^3}{6} + O(\Delta x^4)$$

Adding the above two equations, we get

$$u_{n+1} + u_{n-1} = 2u_n + 2 \cdot \frac{u''(n\Delta x)\Delta x^2}{2} + 2 \cdot O(\Delta x^4)$$
$$u''(n\Delta x) = \frac{u_{n+1} + u_{n-1} - 2u_n}{\Delta x^2} + O(\Delta x^2)$$
$$\Rightarrow \frac{d^2}{dx^2} u_n \approx \frac{u_{n+1} + u_{n-1} - 2u_n}{\Delta x^2}$$

In fact, this can also be obtained by applying the finite difference method for the first order derivation twice:

$$\frac{d^2}{dx^2} u_n \approx \frac{\frac{u_{n+1} - u_n}{\Delta x} - \frac{u_n - u_{n-1}}{\Delta x}}{\Delta x} = \frac{u_{n+1} + u_{n-1} - 2u_n}{\Delta x^2}$$

2.2.3 Finite Difference Method for Solving Diffusion Equation

Let's now go back to our diffusion equation with $\frac{\partial}{\partial t}\rho(x,t) = \frac{\partial^2}{\partial x^2}\rho(x,t)$ where $\rho_m^{(n)} = \rho(x_m, t_n) = \rho(m\Delta x, n\Delta t)$. We now have

$$\rho_m^{(n+1)} = \rho_m^{(n)} + \frac{\Delta t}{\Delta x^2}(\rho_{m-1}^{(n)} + \rho_{m+1}^{(n)} - 2\rho_m^{(n)}) \tag{5}$$

For a general case with $\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t)$, the finite difference approximation is given as:

$$\rho_m^{(n+1)} = \rho_m^{(n)} + D\frac{\Delta t}{\Delta x^2}(\rho_{m-1}^{(n)} + \rho_{m+1}^{(n)} - 2\rho_m^{(n)}) \tag{6}$$

And the error of the above approximation is $\approx O(\Delta t + \Delta x^2)$.

Recall that we're given an initial condition $\rho(x, 0)$, i.e., $\rho_m^{(0)}$ is known for all m. Then, from equation (5), we can calculate $\rho_m^{(1)}$, which can be used to calculate $\rho_m^{(2)}$, and so on, $\rho_m^{(n)}$ are then known $\forall m, n$. Note that for $m = 0$ or $m = M$, $\rho_{m-1}^{(n)}$ and $\rho_{m+1}^{(n)}$ are not applicable, and we use the given boundary conditions to calculate $\rho_m^{(n)}$ when $m \in \{0, M\}$.

In practice, since $m = 0, 1, 2, 3, ..., M$ and $n = 0, 1, 2, 3, ..., N$, we use a $(N+1) \times (M+1)$ matrix to store the approximated function values where the $(n, m)^{th}$ entry records the value of $\rho_m^{(n)}$.

2.2.4 Stability Condition

The Courant–Friedrichs–Lewy(CFL) condition is a necessary condition for convergence while solving the partial differential equations numerically using the finite difference methods. Specifically, the stability condition for our diffusion equation is $\Delta t < C \cdot \Delta x^2$ where C is called the CFL number.

In our example in equation (4), the stability condition to be satisfied is $\Delta t < \frac{1}{2}\Delta x^2$ when choosing Δt and Δx.

2.2.5 Finite Difference Method for Solving Reaction-Diffusion Equation

Recall our Reaction-Diffusion equation:

$$\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t) + F(\rho(x,t))$$

We now consider the reaction term $F(\rho(x,t)) = R\rho(1-\rho)$. Namely, we would like to solve the following equaion using Finite Difference Method:

$$\frac{\partial}{\partial t}\rho(x,t) = D\frac{\partial^2}{\partial x^2}\rho(x,t) + R\rho(x,t)(1-\rho(x,t)) \tag{7}$$

We apply the Finite Difference Method as before and get the following approximation:

$$\rho_m^{(n+1)} = \rho_m^{(n)} + D\frac{\Delta t}{\Delta x^2}(\rho_{m-1}^{(n)} + \rho_{m+1}^{(n)} - 2\rho_m^{(n)}) + R \cdot \Delta t \cdot \rho_m^{(n)}(1 - \rho_m^{(n)}) \tag{8}$$

Now let's consider the following example.

Let $u(x,t)$ be the population density at time t and space x where $x \in [0, 20]$ and $t \in [0, 10]$. We want to solve for

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2u(1-u)$$

with initial condition

$$u(x,0) = \begin{cases} 1 & \text{if } x \leq 0.2 \\ 0 & \text{otherwise} \end{cases}$$

and boundary condition

$$u(0,t) = 1, u(20,t) = 0$$

Choosing $\Delta t = 0.0005$ and $\Delta x = 0.05$, we apply Equation (8) by plugging in $D = 1$ and $R = 2$. Figure 2 shows the front propagation of the population density approximated from finite difference method.

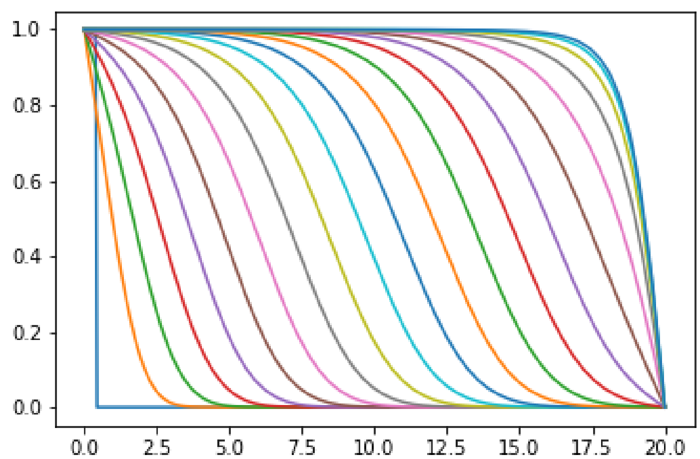

Figure 2: Front propagation of Reaction-Diffusion equation using Finite Difference approximation. x-axis direction represents space and y-axis direction represents population density. The density distribution plots of different timestamps are represented by different colors.

To further study the travelling waves, we want to observe the wave speed of the front propagation. We observe the wave speed by studying the travelling speed of the front propagation of the 0.5 level set (i.e., we study the change in space where the population density is 0.5).

Figure 3 shows the location of the 0.5 population density as a function of timestamps (note that we consider time interval $t \in [0, 10]$ and choose $\Delta t = 0.0005$, hence we have 20000 timestamps in total). As we can see from the graph, the majority of the line plot is approximately a straight line, indicating that the 0.5 level set travels at a constant velocity. We do not pay much attention to the space close to the boundaries because our boundary condition largely influence the travelling waves close to the boundaries.

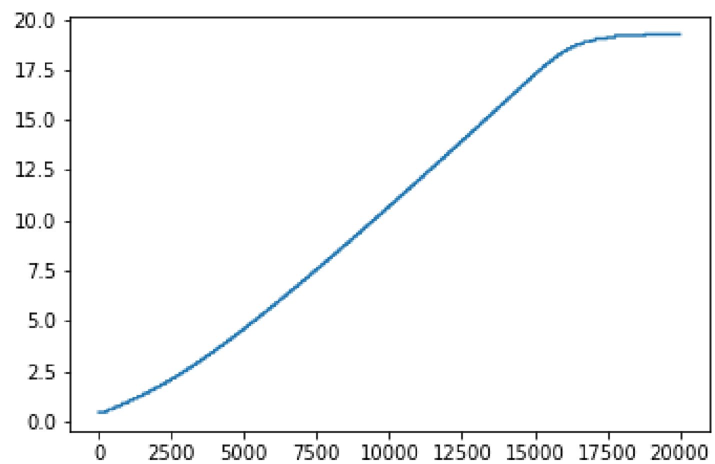

Figure 3: Line plot of space against time of 0.5 level set of travelling wave. x-axis direction represents timestamps and y-axis direction represents the distance of 0.5 level set of the front propagation.

3 Conclusion and Discussion

In this study, we closely studied the Reaction-Diffusion equation from both analytic and numerical perspectives. We solved the diffusion equation with Dirichlet boundary conditions from scratch using separation of variables. Then, we numerically simulated the diffusion equation and the reaction-diffusion equation using both the Monte Carlo method and the Finite Difference method. In addition, we closely observed the front propagation and studied the traveling waves of the reaction-diffusion equation via Finite Difference method.

Due to time restrictions, however, there are still many parts of this project that worth further study. We here also include some of our future perspective. First, we currently have only chosen some simple examples for both numerical simulation approaches. It's better if we can keep our numerical simulations coherent and compare the two numerical methods using the same set of parameters. Second, by examining the 0.5 density level set, we've observed the constant traveling speed of the front propagation. However, we haven't included a thorough study of the traveling speed analytically. It's better if we can get consistent results of deriving the traveling speed both analytically and numerically. Last but not least, there are many real life scenarios that can be modeled by the reaction-diffusion equation. It would be interesting and also more realistic if we can solve any real-world problems by the equation using some real-world data.

References

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