Facilitated Diffusion PDEs

Unveiling Valid Probability Distributions

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Motivation

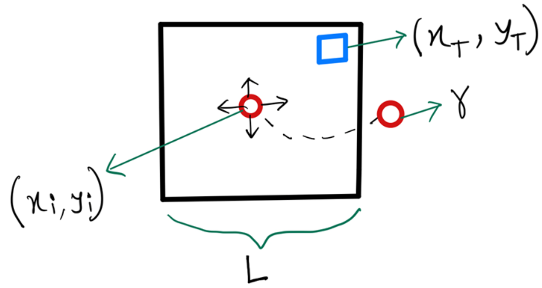

Figure 1: Facilitated Diffusion in 2 spatial dimensions

Imagine a 2D square lattice where a diffusing particle has four degrees of movement and we add an additional freedom by letting the particle (red circle) fall off the lattice into 3D with probability γ. The ultimate goal is for the particle at initial position (x_i, y_i) to reach the target (x_T, y_T)–as fast as it can.

Why should we care about this picture in Figure 1? This picture represents a particular type of diffusion called *Facilitated Diffusion*. The 1D model for facilitated diffusion has been studied rigorously by biologists and biophysicists [2]. The same could not be said for the 2D model. In my undergraduate physics thesis [1], I have studied how facilitated diffusion can accelerate search times for bacteria and then proposed a 2-dimensional model for facilitated surface diffusion. Understanding the efficacy of the 2-dimensional model requires us to understand solutions to two particular PDEs which evolved in the derivation of [1].
Consider the following two partial differential equations, where a and Γ are positive scalars, and $\Delta = \partial_x^2 + \partial_y^2$:

$$\partial_t p(x, y, t) = a\Delta p(x, y, t) - \Gamma \tag{1}$$

with initial conditions: $p(x, y, 0) = \delta((x, y) - (x_0, y_0))$. and[1]:

$$\Delta p(x, y) = ap(x, y) \tag{2}$$

Here a is related with a normalized diffusion coefficient and Γ is the falling-off rate from a 2-dimensional surface. For more on this, please refer to [1].

PDEs can admit many solutions but in this case we are interested in infinite domain solutions that represent probability distributions or if they admit such solutions at all. If they do not admit any such valid probability functions under our modeled initial conditions, then it's a sign that we are probably not modeling accurately. Spoiler: This happens in our thesis as well, oops.

Throughout the thesis, we want to study Equation 1 as it is really close to the classical heat equation. It is a parabolic PDE when in the 1-dimensional case.[2] For the one-spatial dimensional version of Equation 1, we get the PDE:

$$\partial_t p(x,t) = a\partial_x^2 p(x,t) - \Gamma. \tag{3}$$

Recognize that 3 is a linear inhomogeneous partial differential equation with the linear operator: $L = \partial_t - a\Delta_x$. This calls for a reminder of a useful theorem in linear algebra.

Proposition I.1. *Let $v_1, \cdots, v_k$ be solutions to the inhomogeneous linear systems $L[v_1] = f_1, \cdots L[v_k] = f_k$, involving the same linear operator L. Then, given any constants $c_1, \cdots c_k$, the linear combination $v = c_1v_1 + \cdots c_kv_k$ solves the inhomogeneous system $L[v] = f$ for the combined forcing function $f = c_1f_1 + \cdots + c_kf_k$.*

Proof. An inhomogeneuous linear differential equation looks like: $L[v] = f$

$$\begin{aligned} L[v] &= L[c_1v_1 + \cdots c_kv_k] \\ &= L[c_1v_1] + \cdots L[c_kv_k][\text{L is a linear operator}] \\ &= c_1L[v_1] + \cdots c_kL[v_k] \\ &= c_1f_1 + \cdots + c_kf_k \\ &= f \end{aligned}$$

□

Proposition I.1 is useful in solving any inhomogeneous PDE. [3] But first, we want to compute an example of the homogeneous case.

Problem 1.2. *We want to demonstrate how to solve $u_t = u_{xx}$ with boundary conditions $u(t,0) = 0$ and $u(t,\pi) = 0$.*

We consider the heat equation

$$u_t = u_{xx}, \tag{4}$$

with boundary conditions $u(t,0) = 0$ and $u(t,\pi) = 0$.
Solution
Assume $u(x,t) = X(x)T(t)$. This gives

$$X(x)T'(t) = X''(x)T(t). \tag{5}$$

Dividing by XT, we get

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = -\lambda. \tag{6}$$

This leads to two ODEs:

$$T'(t) + \lambda T(t) = 0, \tag{7}$$
$$X''(x) + \lambda X(x) = 0. \tag{8}$$

We want to consider negative eigenvalues because we expect some decay in the process of diffusion and positive eigenvalues are not useful for this context. With boundary conditions $X(0) = X(\pi) = 0$, we find that $X(x)$ must be in the form of an odd function. The eigenvalues λ_n are n^2, where n is a positive integer.

The general solution is

$$u(x,t) = \sum_{n=1}^{\infty} B_n e^{-n^2 t} \sin(nx), \tag{9}$$

where B_n are constants determined by the initial condition.

To incorporate the initial condition $u(x, 0)$ into the general solution of the heat equation, the coefficients B_n are determined using the Fourier sine series. The projection of the initial condition onto the orthogonal basis formed by $\sin(nx)$ is calculated as follows:

$$B_n = \frac{2}{\pi} \int_0^{\pi} u(x,0) \sin(nx)\, dx,$$

where $u(x, 0)$ is the initial condition. This integral computes the component of the initial condition corresponding to the frequency n by calculating the overlap between $u(x, 0)$ and the eigenfunction $\sin(nx)$. The coefficient B_n represents the amplitude of the n-th sinusoidal component in the initial condition, allowing the solution $u(x, t)$ to satisfy the initial condition at $t = 0$. This familiarity with fourier series is important in understanding Fourier Transforms which is later applied in this thesis.

This sets us up to start finding analytic solutions to Equation. 3. This equation is really similar to the heat equation we just solved in Problem 1.2 except that now we have a sink term $-\Gamma$.

Heat PDE with Sink: Uniqueness and Solution

Consider the partial differential equation (PDE):

$$\partial_t p(x,t) = a\partial_x^2 p(x,t) - \Gamma \tag{10}$$

with the initial condition $p(x, 0) = \delta(x - x_0)$, where δ is the Dirac delta function and Γ is a constant. For convenience, we can normalize by setting $a = 1$ and solve the equation.

What the initial condtition represents
The Dirac delta function, $\delta(x - x_0)$, is a mathematical construct designed to model a "point" source or an initial condition that is infinitely concentrated at a single point x_0 and zero everywhere else. Its integral over the entire real line is equal to one, making it perfect for representing an initial condition where the entire probability mass is localized at x_0 at time $t = 0$. This approach is particularly useful for modeling phenomena where a distribution

starts from a perfectly known state and evolves over time according to a specific partial differential equation (PDE). In the context of the given PDE, using the Dirac delta function as an initial condition allows us to explore how a probability distribution, initially concentrated at a location, spreads out over time while being influenced by a constant sink term Γ.

Proposition I.2. *Solutions to*

$$\partial_t p(x,t) = \partial_x^2 p(x,t) - \Gamma \tag{11}$$

are unique under the given initial condition: $p(x,0) = \delta(x - x_0)$ *and boundary conditions:* $p(-\infty,t) = p(\infty,t) = 0$.

Proof. Assume there exists more than one solution to Equation 11 : u and v are such two solutions. Call $u - v = w$, we get another solution satisfying the conditions:

$$\begin{cases} \partial_t w - \partial_x^2 w = 0 \\ w(x,0) = 0 \\ w(-\infty,t) = w(\infty,t) = 0 \end{cases} \tag{12}$$

We want to show that $u(t,x) = 0$ for $(t,x) \in [0,T] \times (-\infty,\infty)$. We perform the following super-important and very commonly used strategy: we multiply both sides of (1.0.6) by w and integrate dx over the interval $(-\infty,\infty)$ to derive

$$\int_{-\infty}^{\infty} w\partial_t w\,dx = \int_{-\infty}^{\infty} w\partial_x^2 w\,dx \tag{13}$$

differentiate under the integral

$$\Rightarrow \frac{d}{dt}\frac{1}{2}\int_{-\infty}^{\infty} w^2(t,x)\,dx = \int_{-\infty}^{\infty} w\partial_t w\,dx = \int_{-\infty}^{\infty} w\partial_x^2 w\,dx \tag{14}$$

integrate by parts

$$= -\int_{-\infty}^{\infty} \left(\partial_x w(t,x)\right)^2\,dx + w(t,x)\partial_x w(t,x)\Big|_{x=-\infty}^{x=\infty} \leq 0. \tag{15}$$

So if we define the *energy*

$$E(t) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} w^2(t,x)\,dx, \tag{16}$$

then we have shown that

$$\frac{dE}{dt} \leq 0. \tag{17}$$

But $E(0) = 0$ by the initial conditions of u. Therefore, $E(t) = 0$ for $t \in [0,T]$. But since $w^2(t,x)$ is continuous and non-negative, it must be that $w^2(t,x) = 0$ for $(t,x) \in [0,T] \times (-\infty,\infty)$.

□

Proposition I.2 uses the energy concept by showing that if the energy of the difference between any two solutions starts at zero ($E(0) = 0$, given that $w(x, 0) = 0$) and if this energy cannot increase over time (showed by $\frac{dE}{dt} \leq 0$), then the energy must remain zero for all times. This implies that the difference w itself must be identically zero across the entire domain and for all time points, proving that the two solutions u and v are in fact the same. This quantity is similar to energy in traditional sense because it quantifies the 'strength' or 'intensity' of the solution w across the spatial domain, similar to how kinetic or potential energy quantifies the capacity for motion or positional change in physical systems.

Now that we know the solution to Equation 11 is unique, it's time to find it.

Step 1: Solving the Homogeneous Equation

The reader is encouraged to familiarize themselves with Section 8.1 of [3] to understand the general solution to the homogeneous heat equation in one dimension:

$$\partial_t p(x,t) = a\partial_x^2 p(x,t), \tag{18}$$

subject to the initial condition $p(x, 0) = \delta(x - x_0)$ and boundary conditions $p(-\infty, t) = p(\infty, t) = 0$. [3] presents a solution involving Fourier transforms, which we will explore in greater depth.

The Fourier transform is an essential tool in solving partial differential equations (PDEs) like the heat equation. It allows us to convert a PDE from the physical space into frequency space, where differential operators become algebraic, and thus, more tractable. In particular, for the heat equation, the Fourier transform simplifies the analysis of diffusion processes by transforming the spatial derivatives into multiplicative factors in the frequency domain.

We now derive Equation 8.14 from Olver [3], which is crucial for understanding the diffusion of heat from a point source at position ξ:

$$p(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-\xi)-k^2t}\, dk. \tag{19}$$

Here, ξ represents the position of the initial heat concentration. Specifically, it is where the initial condition is not zero, indicative of a spike or impulse at that location. In our case, we have $\xi = 0$, meaning a localized initial condition at the origin.

To understand the integral in Equation 19, we rewrite it by focusing on $\xi = 0$:

$$p(x,t;\xi = 0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-k^2t}e^{ikx}\, dk.$$

Completing the square within the exponent yields:

$$-k^2t + ikx = -t\left(k - \frac{ix}{2t}\right)^2 + \frac{x^2}{4t},$$

leading to the integral's evaluation:

$$I = e^{\frac{x^2}{4t}} \int_{-\infty}^{\infty} e^{-t\left(k - \frac{ix}{2t}\right)^2} \, dk.$$

Identifying the Gaussian integral and its solution allows us to express the result as:

$$I = \sqrt{\frac{\pi}{t}} e^{\frac{x^2}{4t}}.$$

Incorporating the $\frac{1}{2\pi}$ scaling factor, we arrive at the fundamental solution to the heat equation. This is what we call the homogeneous solution in our context:

$$p(x, t; \xi = 0) = p_{homogeneous} = \frac{1}{2\sqrt{\pi t}} e^{-\frac{x^2}{4t}}.$$

Understanding these Fourier transforms is vital because they underscore the method through which solutions to the heat equation are obtained. This function, represented by $p(x, t; \xi)$, describes the evolution of temperature distribution in a medium over time. It illustrates the innate nature of the heat equation—diffusion—which is central to the physical phenomena being modeled.

Step 2: Finding the Particular Solution

For the inhomogeneous term $-\Gamma$, we assume a particular solution $p_{\text{particular}}(x, t)$ and determine it by solving:

$$\frac{dp_{particular}(t)}{dt} = -\Gamma \tag{20}$$

which leads to:

$$p_{\text{particular}}(t) = -\Gamma t + C' \tag{21}$$

where C' is an integration constant. $p_{particular}$ has no dependence on x and only dependent on t. So when $t = 0$, we have:

$$p_{particular}(0) = 0 + C' \tag{22}$$

$$C' = 0 \tag{23}$$

C' goes to 0 due to our solution being defined for $t > 0$.

Step 3: Combining the Solutions

Proposition I.1 allows us to write the general solution to the PDE $p(x, t)$ is the sum of the homogeneous and particular solutions:

$$p(x, t) = p_{\text{homogeneous}}(x, t) + p_{\text{particular}}(x, t) \tag{24}$$

$$\Rightarrow p(x,t) = \frac{e^{\frac{-x^2}{4t}}}{2\sqrt{\pi t}} - \Gamma t \tag{25}$$

which represents our proposed solution. Let's see if it is indeed a valid probability distribution.

Proposition I.2. *Prove that $p(x,t)$ Cannot Represent a Probability Distribution.*

Proof. For $p(x,t)$ to be a probability distribution, it must be non-negative for all values of x. Claim that there exists t for some $\Gamma > 0$ value for which $p(x,t) < 0$ and hence no longer qualifies to be a probability distribution.

Now it's not possible to algebraically solve for t in because it leads to an equation where it's impossible to seperate t in Equation 25. But what we can do is: evaluate the function at $x = 0$.

$$p(x = 0, t) = \frac{1}{2\sqrt{\pi t}} - \Gamma t \tag{26}$$

Now we can solve for the case where equation $\frac{1}{2\sqrt{\pi t}} - \Gamma t < 0$.

Pick t such that $t > (\frac{1}{2\Gamma\sqrt{\pi}})^{2/3}$, we have $p(x = 0, t) < 0$. This violates the condition of a probability distribution being non-negative and we are done.

$\square$

Although the solution $p(x,t) = \frac{e^{-\frac{x^2}{4t}}}{2\sqrt{\pi t}} - \Gamma t$ doesn't describe any probability distribution, it could describe the diffusion of heat in a medium over time, modified by a linear decay term Γt. The Gaussian component $\frac{e^{-\frac{x^2}{4t}}}{2\sqrt{\pi t}}$ reflects the fundamental solution to the heat equation, capturing the dispersion of heat from a point source with time and the inherent smoothing effect of the equation. The term $-\Gamma t$ introduces a time-dependent decay, potentially representing energy loss or absorption in the medium at a rate proportional to Γ. This combined solution suggests a balance between diffusion-driven spread and a linearly increasing absorption or loss, which could model realistic physical scenarios where external forces or fields influence heat distribution.

Generalizing for n-dimensions

We want to write the solution to the n-dimensional analog of Equation 3:

$$\partial_t p(X,t) = a\Delta p(X,t) - \Gamma. \tag{27}$$

where $X = (x^1, \cdots, x^n)$ representing n-spatial dimensions and $\Delta = \sum_{i=1}^n \partial_i^2$. MIT course notes solve the problem through the derived fundamental solution in their lecture note 5. Following the strategy we used in the case of 1 dimension, we can write the solution to be:

$$p(X,t) = \frac{1}{(4\pi a t)^{n/2}} e^{-\frac{|x|^2}{4at}} - \Gamma t \tag{28}$$

where $|x|^2 = \sum_{i=1}^{n} (x^i)^2$.

For Equation 1, the solution we get in case of 2-spatial dimensions is:

$$p(x,y,t) = \frac{1}{4\pi a t} e^{\frac{-(x^2+y^2)}{4at}} - \Gamma t \tag{29}$$

Proposition I.2 can be extended to proving that Equation 29 cannot represent a valid probability distribution as well.

Conclusions and Further Work

Throughout the thesis I wasn't able to uncover any valid probability distribution that could describe the 2D Facilitated Diffusion model in [1]. But I was able to find distributions that don't describe the process and come up with some generalized predictions about their nature. Further work lies in being able to identify probability distributions that are solutions to both Equations 1 and 2. This requires me to propose valid models to the facilitated diffusion process and continuing the approach to solve corresponding PDEs.

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Appendix

1. An iterative approach of guessing and checking leads us to the following solution to Equation 2:

$$p(x,y) = \frac{1}{2} \exp\left(-\sqrt{a}(\sqrt{x^2} + \sqrt{y^2})\right) \tag{30}$$

Upon scrutinizing this solution, however, we discern a fundamental inconsistency with physical principles: the derived probability distribution exhibits spherical asymmetry within our two-dimensional context. For a probability distribution over $\mathbb{R}^2$ that is supposed to model phenomena symmetric around a point (in this case, the origin), the distribution must be a function of the radial distance $r = \sqrt{x^2+y^2}$ only. This ensures that all points equidistant from the origin have the same probability density. The given $p(x,y)$, however, sums the square roots of the squared coordinates, which does not correspond to the radial distance

and breaks this spherical symmetry. Hence, it treats different points at the same distance from the origin differently, which is conceptually incorrect for such phenomena.
For our thesis, however, we did not delve into finding alternative solutions to Equation 2 due to limited time and scope.

2. This necessitates the categorization of PDEs. For the mentioned 1-D case, we have a scalar-valued function $u(t, x)$. We know that the most general partial differential equation has the form:

$$L[u] = Au_{tt} + Bu_{tx} + Cu_{xx} + Du_t + Eu_x + Fu = G \tag{31}$$

The discriminant that determines the type of such a partial differential equation is :

$$\Delta = B^2 - 4AC \tag{32}$$

For Equation 3, we get $B = A = 0$ but $C = a$. Hence satisfying $\Delta(x, t) = 0$ while $A^2 + B^2 + C^2 \neq 0$ and qualifying to be a parabolic PDE by the Definition 4.12 of [3]. The categorization is important because the Equation 3 we are studying is a variant of a parabolic heat PDE with a constant sink. So if we are able to find something interesting about the solutions to Equation 3, we can make predictions about Parabolic PDEs with sinks in general, hence the categorization.

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