Parabolic PDEs

Diffusion Equation: Consider the second-order parabolic partial differential equation (PDE) of the form

$$\begin{cases} u_t & = & k\Delta u + g, & t > 0, \ \mathbf{x} \in \Omega \\ u(\mathbf{x},t) & = & h(\mathbf{x},t), & t \geq 0, \mathbf{x} \in \partial\Omega \\ u(\mathbf{x},0) & = & \phi(\mathbf{x}), & t = 0, \mathbf{x} \in \Omega. \end{cases}$$

The domain $\Omega \subset \mathbb{R}^n$ and h is given on the boundary $\partial\Omega$. The initial conditions are $\phi(\mathbf{x})$ for $\mathbf{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$. The term $g(\mathbf{x})$ models sources/sinks in Ω. The Δ denotes the *Laplacian* given by $\Delta u = u_{x_1x_1} + u_{x_2x_2} + \cdots + u_{x_nx_n}$.

We will consider here the specialized case when we are in one dimension and $\Omega = \mathbb{R}$. The PDE becomes

$$\begin{cases} u_t & = & ku_{xx}, & t > 0, \ -\infty < x < \infty \\ u(x,0) & = & \phi(x), & t = 0. \end{cases}$$

This avoids the need for boundary conditions and simplifies many of the derivations. We can then later extend many of the techniques to the case of boundaries, sources/sinks, and higher dimensions.

Derivation of Representations for Solutions: We consider the initial value problem having $\phi(x) = Q(x,0)$ with

$$Q(x,0) = \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases}$$

We will make use of the following properties of solutions of the PDE, (i) if u is a solution then so is $u_t, u_x, u_{xx}, \ldots$, (ii) if S is a solution then so is the integral $v(x,t) = \int S(x-y)g(y)dy$ for any smooth enough function g, (iii) if $u(x,t)$ is a solution and $a > 0$, then $u(\sqrt{a}x, at)$ is also a solution.

We use that the initial condition also has the behavior $Q(x,0) = Q(\sqrt{a}x, 0)$. This scale invariance means that the solution $Q(x,t)$ can only depend on (x,t) through the grouping $p = cx/\sqrt{t}$, where c is any constant with $c > 0$. This allows us to express Q as $Q(x,t) = g(p)$. We will find it convenient to choose $c = 1/\sqrt{4k}$. From these properties, we obtain that

$$\begin{aligned} Q_t - kQ_{xx} &= -\frac{1}{2t}pg'(p) - \frac{k}{4kt}g''(p) = 0 \Rightarrow g''(p) = -2pg'(p) = 0 \\ &\Rightarrow g'(p) = c_1 \exp\left(-p^2\right) \Rightarrow g(p) = c_1 \int \exp\left(-p^2\right) dp + c_2. \end{aligned}$$

This follows from substituting in the expressions for $g(p)$ and differentiating. The ODE in $g''(p)$ was solved using the method of integrating factors with $\exp(p^2)$. In terms of definite integrals, this gives the solution

$$g(p) = c_1 \int_0^p \exp(-q^2)dq + c_2.$$

By substituting $p = x/\sqrt{4kt}$, this gives the solution in (x,t)

$$Q(x,t) = c_1 \int_0^{x/\sqrt{4kt}} \exp(-q^2)dq + c_2.$$

A few useful identities for the integrals in the limit $p \to \infty$ are

$$\begin{aligned}
\int_{-\infty}^{\infty} \exp(-q^2)dq &:= \lim_{p\to\infty} \int_{-p}^{p} \exp(-q^2)dq = \sqrt{\pi} \\
\int_{0}^{\infty} \exp(-q^2)dq &:= \lim_{p\to\infty} \int_{0}^{p} \exp(-q^2)dq = \frac{1}{2}\sqrt{\pi} \\
\int_{-\infty}^{0} \exp(-q^2)dq &:= \lim_{p\to\infty} \int_{-p}^{0} \exp(-q^2)dq = \frac{1}{2}\sqrt{\pi}.
\end{aligned}$$

We can determine c_1, c_2 by using the initial conditions to obtain

$$\begin{cases} x > 0: & 1 = \lim_{t\to 0} c_1 \int_0^{x/\sqrt{4kt}} \exp(-q^2)dq + c_2 = c_1 \int_0^{\infty} \exp(-q^2)dq + c_2 = \frac{\sqrt{\pi}}{2}c_1 + c_2 \\ x < 0: & 0 = \lim_{t\to 0} c_1 \int_0^{x/\sqrt{4kt}} \exp(-q^2)dq + c_2 = -c_1 \int_{-\infty}^{0} \exp(-q^2)dq + c_2 = -\frac{\sqrt{\pi}}{2}c_1 + c_2. \end{cases}$$

This gives the linear system for c_1, c_2

$$\left\{ \begin{array}{lcl} \frac{\sqrt{\pi}}{2}c_1 + c_2 & = & 1 \\ -\frac{\sqrt{\pi}}{2}c_1 + c_2 & = & 0 \end{array} \right\} \Rightarrow \left\{ \begin{array}{lcl} \frac{\sqrt{\pi}}{2}c_1 + c_2 & = & 1 \\ c_2 & = & \frac{1}{2} \end{array} \right\} \Rightarrow \left\{ \begin{array}{lcl} c_1 & = & \frac{1}{\sqrt{\pi}} \\ c_2 & = & \frac{1}{2} \end{array} \right\}$$

This gives that

$$Q(x,t) = \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4kt}} \exp(-q^2)dq + \frac{1}{2}.$$

We now use that derivatives of solutions of the diffusion equation are again solutions. We also use that integrals using convolutions with a solution is again a solution. With this in mind, we consider $S(x,t) = \frac{\partial}{\partial x}Q(x,t)$ and

$$v(x,t) = \int_{-\infty}^{\infty} S(x-y,t)f(y)dy.$$

Here, we are integrating against the function

$$S(x-y,t) = \frac{1}{\sqrt{4\pi kt}} \exp\left(-\left(x-y\right)^2/4kt\right).$$

This is referred to as the *Green's Function.* As we have discussed, this specific function S has some important properties. First, note the function S is in fact the probability density of a Gaussian distribution $\eta(y;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-(y-\mu)^2/2\sigma^2\right)$ with mean $\mu = x$ and variance $\sigma^2 = 2kt$, $S(x-y,t) = \eta(y;x,2kt)$. As a result, we have $S > 0$ for any x and t. It also will integrate to one in the case $f(x) \equiv 1$ for any choice of t. Second, note the integral gives an average of f under this distribution. Since the distribution has variance $2kt$ and integrates to one, the averaging will become more and more narrowly concentrated around x and $t \to 0$. As a consequence, if f is continuous this suggests that $\lim_{t\to 0} v(x,t) = f(x)$.

We make a few additional remarks before proceeding with the derivation. One can think about the expressions above also intuitively in terms of probability theory. In fact, there are close connections between diffusion equations and the evolution over time of the probabilities associated with stochastic processes. The integral above gives an average of f under the Gaussian distribution, which can be viewed as the expectation $\mathbb{E}[f(X)] = \int S(x-y,t)f(y)dy$, where the random variable is the Gaussian $X \sim \eta(y;\mu,\sigma^2)$. Since $\sigma^2 = 2kt$ we have as $t \to 0$ the averaging occurs on smaller and smaller neighborhoods around the mean $\mu = x$ so that $\lim_{t\to 0} \mathbb{E}[f(X)] = \lim_{t\to 0} \int S(x-y,t)f(y)dy = f(x)$. That is the probability density of the Gaussian with variance $2kt$ concentrates at x as $t \to 0$. Again, this suggests that as $t \to 0$ that $v(x,t) \to f(x)$.

We now perform derivations to show this indeed holds. Consider

$$\begin{aligned}
\lim_{t\to 0} v(x,t) &= \lim_{t\to 0} \int_{-\infty}^{\infty} S(x-y,t)f(y)dy = \lim_{t\to 0} \int_{-\infty}^{\infty} \frac{\partial Q}{\partial x}(x-y,t)f(y)dy \\
&= -\lim_{t\to 0} \int_{-\infty}^{\infty} \frac{\partial Q}{\partial y}(x-y,t)f(y)dy \\
&= \lim_{t\to 0} -\left[\frac{\partial Q}{\partial y}(x-y,t)f(y)\right]_{y=-\infty}^{y=\infty} + \int_{-\infty}^{\infty} \lim_{t\to 0} Q(x-y,t)f'(y)dy \\
&= \int_{-\infty}^{x} f'(y)dy = [f(y)]_{y=-\infty}^{y=x} = f(x).
\end{aligned}$$

We assume here that f decays, so that the terms in the integration by parts and evaluation term go to zero as $|x| \to \infty$. We also assume that the integral of f' converges well enough that we can interchange the integration and limit. With the choice $f(x) = \phi(x)$, this shows that v satisfies the initial conditions

$$v(x,0) = \phi(x).$$

This provides the solution to our initial value problem. We remark that since S already decays some of the conditions on f above can be relaxed by using other techniques for the analysis.

Summary: Putting this together, we obtain the *solution representation* for the diffusion equation

$$u(x,t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} \exp\left(-(x-y)^2/4kt\right)\phi(y)dy.$$

Dirac δ-Functions and Green's Functions
In practice in PDEs, it is often a useful analytic approach to consider a fictitious function $\delta(x - x_0)$ which has the following formal property when integrated

$$\int \delta(y - x_0) f(y) dy = f(x_0),$$

for any function f that is sufficiently smooth. The $\delta(z)$ is referred to as the *Dirac δ-Function.*

While we will proceed formally for now, many arguments made based on this formal approach often can be made into more mathematically rigorous derivations. The main idea is to try to replace in derivations the fictitious function $\delta(z)$ with a corresponding measure μ and Lebesgue integrals which yields similar behaviors. This would correspond to the replacement $\delta(y - x_0)dy = d\mu(y)$. For those who are interested, you can look up topics in real analysis on the *theory of distributions.*

Throughout, we will primarily make use of the formal property above whenever referring to the Dirac δ-Function. In our derivation of the solution representation for the diffusion equation we used convolution with the function

$$S(x - y, t) = \frac{1}{\sqrt{4\pi k t}} \exp\left(-(x - y)^2/(4kt)\right).$$

This is referred to as the *Green's Function* of the diffusion equation. It is useful to denote this by $G(y; x, t) = S(x - y, t)$. Formally, we can view $S(x_0 - \cdot, t)$ and $G(\cdot; x_0, t)$ as solving

$$\begin{cases} u_t & = & k u_{xx}, & t > 0, \ -\infty < x < \infty \\ u(x, 0) & = & \delta(x - x_0), & t = 0. \end{cases}$$

This follows formally since if we integrate any function f against S we would obtain

$$\int S(x_0 - y, 0) f(y) dy = \int \lim_{t \to 0} S(x_0 - y, t) f(y) dy = \lim_{t \to 0} \int S(x_0 - y, t) f(y) dy = f(x_0).$$

The last equality follows from our derivations above. This gives formally that $S(x, 0) = G(x; x_0, 0) = \delta(x - x_0)$. We can also express this as

$$\int G(y; x_0, 0) f(y) dy = f(x_0).$$

This is a useful perspective, since we can use this in conjunction with the property that for many linear PDEs the linear combination of solutions is again a solution. For the diffusion equation, suppose we weigh the linear combination of G for different values of x_0 by using our initial condition $\phi(x)$. Let

$$v(x', t) = \int G(x'; x_0, t) \phi(x_0) dx_0.$$

Since this is a linear combination of the solutions $G(\cdot; x_0, t)$, we have $v_t = k v_{xx}$. Formally, we would have

$$v(x, 0) = \lim_{t \to 0} v(x, t) = \lim_{t \to 0} \int G(x; x_0, t) \phi(x_0) dx_0 = \int G(x; x_0, 0) \phi(x_0) dx_0 = \phi(x).$$

This indicates that $v(x,0)$ would satisfy the initial conditions. This suggests the representations for solutions of the diffusion equation of the general form

$$u(x,t) = \int G(x;x_0,t)\phi(x_0)dx_0.$$

This approach reduces the problem of finding solutions of the PDE to that of finding the appropriate *Green's Function* for the given initial conditions and boundary conditions. These techniques are also useful in gaining intuition for how information propagates in such PDEs. The strategy above arises frequently when developing solution techniques for parabolic and elliptic PDEs.

Numerical Methods for Simulations of 1D Diffusion: The representations above for the solutions involve primarily performing integration of the initial conditions. We can obtain a numerical approximation of the solutions by approximating these integrals. We consider the diffusion equation $u_t = k_0 u_{xx}$, where k_0 denotes the parameter to avoid confusion with numerical indices k. We can model initial conditions specified over a finite interval $[-L, L]$ by the values of ϕ at a collection of n equally spaced points. This can be obtained by using grid points $x_m = -L + m\Delta x$, where $\Delta x = 2L/(n-1)$ with $m \in [0, 1, \ldots, n-1]$. We consider representing the solution at times $t_k = k\Delta t$ with $k_0\Delta t \gg \Delta x^2$. To compute a numerical approximation of the solution at $u(x_m, t_k)$ we use

$$\begin{aligned} u(x_m,t_k) &= \frac{1}{\sqrt{4\pi k_0 t}} \int_{-\infty}^{\infty} \exp\left(-\left(x-y\right)^2/4k_0 t\right)\phi(y)dy \\ &\approx \sum_{\ell=0}^{n} q_\ell \frac{1}{\sqrt{4\pi k_0 t}} \exp\left(-\left(x-y\right)^2/4k_0 t\right)\phi(x_\ell). \end{aligned}$$

The main approximation is in replacing the integration with a finite sum using the function evaluations of $\phi(x_\ell)$ at the grid points x_ℓ. This is referred to as a *quadrature* approximation of the integral and almost any method could be used here. For simplicity, we will use the trapezoid method where the integral is approximated by the sum

$$\int_{-\infty}^{\infty} g(y)dy \approx \int_{-L}^{L} g(y)dy \approx \frac{\Delta x}{2}\left(g(x_0) + 2\sum_{\ell=1}^{n-1} g(x_\ell) + g(x_n)\right).$$

This would be the same as approximating the area under the curve of the integrand $g(x)$ by the Riemann sum approximation where trapezoids are used to approximate the areas on each sub-interval $[x_{m-1}, x_m)$. In summary, we obtain the numerical method

$$\tilde{u}(x_m,t_k) = \frac{\Delta x}{2}\left(g(x_0;x_m,t_k) + 2\sum_{\ell=0}^{n-1} g(x_\ell;x_m,t_k) + g(x_n;x_m,t_k)\right),$$

where

$$g(x_\ell;x_m,t_k) = \frac{1}{\sqrt{4\pi k_0 t_k}} \exp\left(-\left(x_\ell - x_m\right)^2/(4k_0 t_k)\right)\phi(x_\ell).$$

Again, the k_0 is the parameter in $u_t = k_0 u_{xx}$ to avoid confusion with index k of the numerical approximation.

For a fixed time $t = t_k$ an approximate solution $\tilde{u}(x,t)$ can be obtained by sweeping over the grid points x_m. By looking at these solutions at successive times by increasing k, the evolution of solutions of the diffusion equation can be studied numerically. I encourage everyone to implement this in your preferred programming language, such as python, and to give this a try. In python, this can be done using the packages: *numpy* and *matplotlib*. A good study would be to investigate empirically the different roles that ϕ and parameter k_0 play in the solution of the resulting diffusions and how it evolves over time. The ϕ gives the initial configuration and k_0 specifies the rate of diffusion. A good exercise to build intuition is to study how different choices of the initial conditions and parameter k_0 impact the evolution of the solutions. These results can also be compared to other PDEs to help further build intuition into the behaviors of solutions.