REACTION-DIFFUSION EQUATIONS

ALEX NEILL

Abstract. Notes on reaction-diffusion equations and some biological applications. If unspecified, maps are assumed to be as smooth as necessary.

Contents

1. The Diffusion Equation

Let Ω be a domain of $\mathbb{R}^n$, and consider a map $u : \Omega \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ where we denote a point of the domain by (x, t) (representing spatial and time coordinates respectively). Then the general form of a single reaction-diffusion equation is

$$u_t = D\Delta u + f \circ u,$$

where $f : \mathbb{R} \to \mathbb{R}$ is a smooth map that describes the 'reaction', while $D > 0$ is the diffusion coefficient for the Laplace operator on the spatial coordinates. A solution u is a state variable that typically describes the concentration or density of a substance or population. For more general situations, f may depend explicitly on t, x, and the gradient of u.

Remark 1.1. Throughout these notes a domain is an open connected set while a region is a set whose interior is a domain.

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1.1. **Derivation.** Let $u : \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ represent a density and $J : \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \to \mathbb{R}^3$ its diffusion flux (amount of substance per unit volume per unit time). For a compact region $\Omega \subset \mathbb{R}^3$ with piecewise smooth boundary Γ, *ceteris paribus* (assuming only conservation of mass) we have

$$\frac{d}{dt}\int_\Omega u(x,t)dV = -\int_\Gamma J(x,t)\cdot dS.$$

The divergence theorem implies that

$$\int_\Gamma J \cdot dS = \int_\Omega \operatorname{div} J dV,$$

and so we obtain

$$\int_\Omega \left(u_t + \operatorname{div} J\right) dV = 0.$$

As this holds for all volumes Ω, we have

$$u_t + \operatorname{div} J = 0, \tag{2}$$

called the *continuity equation*. Now Fick's first law asserts that

$$J = -D\nabla u,$$

which says that the only flux is diffusive flux. Combining this with (2) we arrive at Fick's second law, bearing an uncanny resemblance to the heat equation:

$$u_t = D\Delta u. \tag{3}$$

This is a simple case of the diffusion equation where D is constant.

1.2. **Interlude on the Leibniz Integral Rule.** In PDE we often have occasion to differentiate integrals, and there are many different variations of this scattered throughout the literature. Here we make no attempt at generality; we only present a proof of the quite simple case required in the derivation above.

Proposition 1.4. *Let $\Omega \subset \mathbb{R}^3$ be a compact region with measure zero boundary and $u : \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ a smooth map. Then*

$$\frac{d}{dt}\int_\Omega u(x,t)dx = \int_\Omega u_t(x,t)dx.$$

Proof. First observe that since u is continuously differentiable, both integrals exist for all t. Now writing

$$\frac{d}{dt}\int_\Omega u(x,t)dx = \lim_{h\to 0}\int_\Omega \frac{u(x,t+h)-u(x,t)}{h}dx,$$

we want to show that for all $\epsilon > 0$ we can choose h such that

$$\left|\int_\Omega \left(\frac{u(x,t+h)-u(x,t)}{h} - u_t(x,t)\right)dx\right| < \epsilon.$$

Applying the mean value theorem and invoking the uniform continuity of u_t, we obtain the desired result. $\square$

1.3. **The Fundamental Solution.** Consider the problem

$$u_t = Du_{xx} \quad \text{for } x \in \mathbb{R},\ t > 0; \tag{5}$$

$$u(x,0) = \phi(x). \tag{6}$$

We first make some observations regarding the 'invariance' of solutions (ignoring the initial condition).

(i) Any linear combination of solutions is also a solution.
(ii) Any translation of a solution is also a solution.
(iii) Any scaling $u(\sqrt{a}x, at)$ for $a > 0$ of a solution $u(x,t)$ is also a solution.
(iv) Any derivative of a (sufficiently nice) solution is also a solution.
(v) Any integral of a solution is also a solution in the following way. If $u(x,t)$ is a solution, then so is the convolution

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

where f is sufficiently nice (so that the integral converges in a sufficiently nice manner).

To give an example of why these hold, we show (ii). Let $T : \mathbb{R} \to \mathbb{R}$ be a translation defined by $x \mapsto x - a$. If u solves $u_t = Du_{xx}$, consider $\bar{u}(x,t) = u(T(x),t)$. We then have

$$\bar{u}_t(x,t) = u_t(T(x),t)$$

and

$$\bar{u}_x(x,t) = u_x(T(x),t)T'(x) = u_x(T(x),t), \text{ so that } \bar{u}_{xx}(x,t) = u_{xx}(T(x),t).$$

Let us suppose for a moment that our initial condition is given by

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

To determine $Q(x,t)$, we begin with invariance under scaling (as this leaves the initial condition unchanged). In particular we want $Q(x,t)$ to remain unchanged under scaling. Of course, if the dependency of Q on x and t is only on the ratio $x/\sqrt{t}$ we have such an invariance, and hence we restrict Q to be of the following form (with an additional factor for convenience later):

$$Q(x,t) = g(p), \text{ where } p = \frac{x}{\sqrt{4Dt}}.$$

Now this allows us to turn (5) into an ordinary differential equation that we can solve. We have

$$\begin{aligned} Q_t &= \frac{dg}{dp}\frac{\partial p}{\partial t} = -\frac{x}{2t\sqrt{4Dt}} g'(p) \\ Q_x &= \frac{dg}{dp}\frac{\partial p}{\partial x} = \frac{1}{\sqrt{4Dt}} g'(p) \\ Q_{xx} &= \frac{dQ_x}{dp}\frac{\partial p}{\partial x} = \frac{1}{4Dt} g''(p), \end{aligned}$$

and hence

$$0 = Q_t - DQ_{xx} = -\frac{x}{2t\sqrt{4Dt}} g'(p) - \frac{1}{4t} g''(p) = \frac{1}{t}\left(-\frac{p}{2}g'(p) - \frac{1}{4}g''(p)\right).$$

We thus have the ODE
$$g'' + 2pg' = 0,$$
and a first integration yields
$$g' = c_1 e^{-p^2}.$$
Integrating once more we arrive at the solution
$$g(p) = c_1 \int e^{-p^2} dp + c_2.$$
To impose conditions on c_1 and c_2 we let
$$Q(x,t) = c_1 \int_0^{x/\sqrt{4Dt}} e^{-p^2} dp + c_2,$$
which is valid for all $t > 0$. Then the initial conditions must be satisfied in the limit $t \searrow 0$; for $x > 0$ we have
$$1 = c_1 \int_0^{\infty} e^{-p^2} dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2;$$
for $x < 0$ we have
$$0 = c_1 \int_0^{-\infty} e^{-p^2} dp + c_2 = -c_1 \frac{\sqrt{\pi}}{2} + c_2.$$
This implies that $c_1 = \frac{1}{\sqrt{\pi}}$ and $c_2 = \frac{1}{2}$, so that
$$Q(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4Dt}} e^{-p^2} dp.$$
Now let $S = Q_x$, which also solves (5). For an arbitrary smooth map ϕ where $\phi(x) = 0$ when $|x|$ is sufficiently large, let
$$u(x,t) = \int_{\mathbb{R}} S(x-y,t)\phi(y)dy.$$
We know that u solves (5), and want to show it satisfies (6) as well. To this end, we observe that integrating by parts gives
$$\begin{aligned} u(x,t) &= \int_{\mathbb{R}} \frac{\partial Q}{\partial x}(x-y,t)\phi(y)dy \\ &= -\int_{\mathbb{R}} \frac{\partial Q}{\partial y}(x-y,t)\phi(y)dy \\ &= -\phi(y)Q(x-y,t)\Big|_{-\infty}^{\infty} + \int_{\mathbb{R}} \phi'(y)Q(x-y,t)dy. \end{aligned}$$
Then
$$u(x,0) = \int_{\mathbb{R}} Q(x-y,0)\phi'(y)dy = \int_{-\infty}^{x} \phi'(y)dy = \phi(x).$$
Computing the spatial derivative of Q we find
$$S = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt},$$
and so
$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{\mathbb{R}} e^{-(x-y)^2/4Dt} \phi(y)dy. \tag{7}$$

This is called the *fundamental solution*, and while it is rare to be able to solve the integral explicitly, for some ϕ it may be written using the well-known error function

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-p^2} dp$$

that satisfies

$$\operatorname{erf}(0) = 0 \qquad \text{and} \qquad \lim_{x\to\infty} \operatorname{erf}(x) = 1.$$

1.4. **The Inhomogeneous Equation.** Here we solve

$$\begin{aligned} u_t - Du_{xx} &= f(x,t) \quad \text{for } x \in \mathbb{R},\ t > 0 \\ u(x,0) &= \phi(x) \end{aligned} \tag{8}$$

where ϕ describes the initial distribution and f is a 'source' or 'sink' term. But let us first consider the analogous problem for ordinary differential equations.

For constant $A \in \mathbb{R}^{n\times n}$, $f \in C((a,b), \mathbb{R}^n)$, and $0 \in (a,b)$ with $-\infty \le a < b \le \infty$, the initial-value problem

$$u' - Au = f,\ u(0) = u_0$$

is solved (using variation of parameters) by

$$u(t) = e^{At}u_0 + \int_0^t e^{A(t-s)} f(s)ds.$$

Indeed, with $f \equiv 0$, the solution reads $u(t) = S(t)u_0$ where $S(t) = e^{At}$. Then when $f \not\equiv 0$, we multiply the equation by integrating factor $S(-t)$:

$$S(-t)u'(t) - S(-t)Au(t) = \frac{d}{dt}\left[S(-t)u(t)\right] = S(-t)f(t).$$

Integrating this from 0 to t we obtain

$$S(-t)u(t) = u_0 + \int_0^t S(-s)f(s)ds$$

and then multiplying by $S(t)$ yields

$$u(t) = S(t)u_0 + \int_0^t S(t-s)f(s)ds.$$

In analogy to this, we want to show that

$$u(x,t) = \int_{\mathbb{R}} S(x-y,t)\phi(y)dy + \int_0^t \int_{\mathbb{R}} S(x-y,t-s)f(y,s)dyds \tag{9}$$

is a solution to (8). Note that it suffices to check the second term. We have

$$\begin{aligned} u_t &= \frac{\partial}{\partial t} \int_0^t \int_{\mathbb{R}} S(x-y,t-s)f(y,s)dyds \\ &= \int_0^t \int_{\mathbb{R}} S_t(x-y,t-s)f(y,s)dyds + \lim_{s\to t} \int_{\mathbb{R}} S(x-y,t-s)f(y,s)dy \\ &= \int_0^t \int_{\mathbb{R}} DS_{xx}(x-y,t-s)f(y,s)dyds + \lim_{\epsilon\to 0} \int_{\mathbb{R}} S(x-y,\epsilon)f(y,t)dy \\ &= D\frac{\partial^2}{\partial x^2} \int_0^t \int_{\mathbb{R}} S(x-y,t-s)f(y,s)dyds + f(x,t) \\ &= Du_{xx} + f \end{aligned}$$

Observing that

$$\lim_{t\to 0} u(x,t) = \phi(x),$$

we have the desired solution. This is often referred to as *Duhamel's principle.*

1.5. **Uniqueness on Cylindrical Domains.** Now let us consider the Dirichlet problem for the diffusion equation with inhomogeneity f:

$$\begin{aligned} u_t - Du_{xx} &= f(x,t) \quad \text{for } 0 < x < l \text{ and } t > 0; \\ u(x,0) &= \phi(x); \\ u(0,t) &= g(t); \\ u(l,t) &= h(t). \end{aligned} \tag{10}$$

Proposition 1.11. *The Dirichlet problem as given above has at most one solution.*

Proof. Assume u_1 and u_2 both satisfy (10), and let $w = u_1 - u_2$. Then w satisfies

$$\begin{aligned} w_t - Dw_{xx} &= 0 \quad \text{for } 0 < x < l \text{ and } t > 0; \\ w(x,0) &= 0; \text{ and} \\ w(0,t) &= 0, \ w(l,t) = 0. \end{aligned}$$

Now consider

$$\left(\frac{1}{2}w^2\right)_t - (Dw_x w)_x + Dw_x^2;$$

observe that this is zero and integrate with respect to x:

$$0 = \int_0^l \left(\frac{1}{2}w^2\right)_t dx + D\int_0^l w_x^2 dx.$$

Note that the middle term vanishes due to the boundary conditions, and by the Leibniz integral rule

$$\frac{d}{dt}\int_0^l \frac{1}{2}w^2 dx = -D\int_0^l w_x^2 dx \le 0.$$

This implies that the integral $\int_0^l w^2 dx$ is monotone decreasing in t, so that

$$0 \le \int_0^l w^2 dx \le \int_0^l w^2(x,0)dx = 0.$$

Hence $w = 0$, concluding the proof. The method of proof employed here is a common one in proving uniqueness of solutions, called the *energy method.* □

1.6. **A (Weak) Maximum Principle.**

Proposition 1.12. *Let $u(x,t)$ satisfy the diffusion equation in the rectangle $\mathcal{R} = [0,l] \times [0,T] = \{0 \le x \le l,\ 0 \le t \le T\}$. Then the maximum value of u on $\mathcal{R}$ is assumed either on the initial line $t = 0$ or the boundary lines $x = 0$, $x = l$.*

Proof. Let M denote the maximum of u on the three boundary lines $t = 0$, $x = 0$, and $x = l$, and for $\epsilon > 0$, define

$$v(x,t) = u(x,t) + \epsilon x^2.$$

It is clear that

$$v(x,t) \le M + \epsilon l^2$$

on the three boundary lines, and in addition we have the inequality

$$v_t - Dv_{xx} = u_t - Du_{xx} - 2\epsilon D = -2\epsilon D < 0. \tag{13}$$

If we assume that v achieves its maximum in the interior we know that $v_t = 0$ and $v_{xx} \le 0$, a contradiction to (13). Now, again for the sake of contradiction, assume the maximum is attained at (x_0, T) where $0 < x_0 < l$. We still have that $v_{xx} \le 0$, and

$$v_t(x_0, t_0) = \lim_{\delta \searrow 0} \frac{v(x_0, t_0) - v(x_0, t_0 - \delta)}{\delta} \ge 0,$$

another contradiction to (13). Hence

$$v(x,t) \le M + \epsilon l^2$$

on $\mathcal{R}$, so that

$$u(x,t) \le M + \epsilon(l^2 - x^2).$$

This concludes the proof. □

Corollary 1.14. *The analogous result holds for the minimum of u.*

Proof. Apply the maximum principle to $-u(x,t)$. □

1.7. **Relation to Brownian Motion.** Consider a 1-dimensional symmetric random walk with step length Δx, and suppose r steps are made per unit of time so that $\Delta t = \frac{1}{r}$ is the time of a single step.

Let $\xi_k \in \{-\Delta x, \Delta x\}$ be the step in the time interval $[(k-1)\Delta t, k\Delta t]$ for $k \in [n]$, and suppose $x_0 = 0$ is the initial point. Then after time $t = n\Delta t$ the position is given by the random variable

$$x_n = \sum_{k=1}^{n} \xi_k.$$

We define $u(x,t)$ to be the probability that the particle is at position x at time t, i.e.,

$$u(x,t) = P(x_n = x)$$

where $x = m\Delta x$ and $t = n\Delta t$ for $m \in \mathbb{Z},\ n \in \mathbb{N}$. To find this probability, first let n_l and n_r denote the number of left steps and right steps respectively. Then we have $n_l + n_r = n$ and $n_r - n_l = m$, which together give

$$n_r = \frac{n+m}{2}.$$

The probability being given by the binomial distribution is then

$$P(x_n = m\Delta x) = \binom{n}{n_r}\left(\frac{1}{2}\right)^{n_r}\left(\frac{1}{2}\right)^{n-n_r} = \frac{1}{2^n}\binom{n}{\frac{n+m}{2}}.$$

The expectation is

$$\begin{aligned} E(x_n) &= E\left(\sum_{k=1}^{n} \xi_k\right) = \sum_{k=1}^{n} E(\xi_k) \\ &= \sum_{k=1}^{n} \Big((-\Delta x) P(\xi_k = -\Delta x) + \Delta x P(\xi_k = \Delta x)\Big) = 0, \end{aligned}$$

while the variance is

$$\begin{aligned}V(x_n) &= V\left(\sum_{k=1}^{n}\xi_k\right) = \sum_{k=1}^{n}V(\xi_k)\\ &= \sum_{k=1}^{n}\Big((-\Delta x)^2P(\xi_k=-\Delta x)+(\Delta x)^2P(\xi_k=\Delta x)\Big) = (\Delta x)^2 n.\end{aligned}$$

Rewriting as $V(x_n)=(\Delta x)^2rt$ we note that $\sigma(x_n)=\sqrt{V(x_n)}\sim\sqrt{t}$, which has the physical interpretation that while the particle's expected position is its starting point due to symmetry, for growing t this probability decreases (slower than linearly).

To obtain Brownian motion, we let $\Delta x\to 0$ and $r\to\infty$ such that

$$\lim_{\Delta x\to 0, r\to\infty}(\Delta x)^2 r = 2D > 0.$$

Now our discrete formulation of the problem gives the following equation:

$$u(x,t+\Delta t) = \frac{1}{2}u(x-\Delta x,t)+\frac{1}{2}u(x+\Delta x,t).$$

If we consider the Taylor expansions

$$u(x,t+\Delta t) = u(x,t)+u_t\Delta t+\frac{1}{2}u_{tt}\Delta t^2+\cdots$$

and

$$u(x\pm\Delta x,t) = u(x,t)\pm u_x\Delta x+\frac{1}{2}u_{xx}\Delta x^2\pm\cdots,$$

we obtain

$$u_t\Delta t+\frac{1}{2}u_{tt}\Delta t^2+\cdots = \frac{1}{2}u_{xx}\Delta x^2+\frac{1}{4}u_{xxxx}\Delta x^4+\cdots.$$

Then dividing through by Δt and passing to the limit we get

$$u_t = Du_{xx},$$

which is precisely the diffusion equation! For our random walk we have initial condition $u(x,0)=\delta(x)$, and so our fundamental solution is

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-x^2/4\pi Dt}.$$

Remark 1.15. Of course, the assumption that

$$\frac{(\Delta x)^2}{2\Delta t}$$

tends to a finite limit implies that the velocity $(\Delta x)/(\Delta t)$ approaches infinity, which is not physically realizable. One can also observe this from the derived Gaussian (normal) solution (with mean 0 and variance $2Dt$). In particular, for all $x\in\mathbb{R}$ and $t>0$ we have $u(x,t)>0$, meaning the there is a positive probability that the particle will be located arbitrarily far away from the initial point immediately. Hence the model is really only valid for large t.

1.8. **Diffusion Variance.**

Proposition 1.16. *Let u solve*

$$u_t = Du_{xx}$$

and suppose that

$$C = \int_{\mathbb{R}} u(x,t)dx$$

is independent of t and

$$\lim_{x\to\pm\infty} xu(x,t) = 0 \quad \text{and} \quad \lim_{x\to\pm\infty} x^2 u_x(x,t) = 0.$$

Intuitively, this means that we have a constant population and the density is 'small at infinity'. Let

$$\sigma^2(t) = \frac{1}{C}\int_{\mathbb{R}} x^2 u(x,t)dx.$$

Then

$$\sigma^2(t) = 2Dt + \sigma^2(0)$$

for all t.

Proof. We apply integration by parts:

$$\begin{aligned}
\frac{C}{D}\frac{d\sigma^2}{dt} &= \frac{1}{D}\frac{d}{dt}\int_{\mathbb{R}} x^2 u dx \\
&= \frac{1}{D}\int_{\mathbb{R}} x^2 u_t dx \\
&= \int_{\mathbb{R}} x^2 u_{xx} dx \\
&= \Big[x^2 u_x\Big]_{-\infty}^{\infty} - \int_{\mathbb{R}} 2xu_x dx \\
&= -\big[2xu\big]_{-\infty}^{\infty} + \int_{\mathbb{R}} 2u dx \\
&= 2\int_{\mathbb{R}} u dx = 2C.
\end{aligned}$$

Hence

$$\frac{d\sigma^2(t)}{dt} = 2D$$

and integration gives

$$\sigma^2(t) = 2Dt + \sigma^2(0).$$

In the special case that the particles are initially concentrated around $x = 0$ (so that $u(x,0) = 0$ for all $|x| > \epsilon$), we obtain

$$\int_{\mathbb{R}} x^2 u(x,0)dx = \int_{-\epsilon}^{\epsilon} x^2 u(x,0)dx \le \epsilon^2 \int_{-\epsilon}^{\epsilon} u(x,0)dx = \epsilon^2 C.$$

Thus

$$\sigma^2(0) = \epsilon^2 \approx 0.$$

$\square$

2. Existence and Uniqueness

2.1. **Maximum and Comparison Principles.**

Consider the following problem:

$$u_t = D\Delta u + f(x,t,u) \text{ on } \Omega \times (0,T)$$
$$u = 0 \text{ on } \partial\Omega \times (0,T)$$
$$u = u_0 \text{ on } \Omega \times \{0\}$$

where Ω is a bounded domain.

References

[1] Christina Kuttler. `http://www-[]m6.ma.tum.de/~kuttler/script_reaktdiff.pdf`