LTCC Mathematical Biology – Lecture Notes

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Adapted from lecture notes by Dr Freya Bull and various authors (see MIT Nonlinear Dynamics Notes).

Contents

1 Motivation

Diffusive processes are part of our everyday lives. When we add a dash of milk to a cup of tea or coffee, the process by which the milk mixes with the dark liquid is diffusive. It happens slowly, reducing the milk's density from an initially localised drop to a homogeneous mixture. This passive process is driven by the inherent kinetic energy of the system and the *random motion* of particles down a concentration gradient.

Diffusion is an important transport mechanism. It is the same mechanism by which an ideal gas fills an empty room, and it is particularly important in biology. First, it does not require extra energy to be added to the system. Second, cells depend on diffusive processes to transport various molecules such as glucose, oxygen (e.g., gas exchange in the lungs) and ions, relaying cellular processes and facilitating the mixing of reactants in chemical reactions. Plants, for example, absorb water and nutrients from the soil through diffusion. Heat transfer also occurs through diffusion.

Mathematically, diffusion is very simple to describe and appears naturally everywhere, as we will see in the upcoming sections. Before we get our hands dirty, here is a quick outline of this lecture: first, we are going to derive the diffusion equation from random walks. Then, we will see methods to solve the Diffusion Equation. Finally, we are going to look at applications of diffusive processes to understand its properties. This will lead to Lecture 2, where we will study pattern formation.

2 Random Walks

Random walks are the simplest models for diffusive processes. You can get a lot of insight about diffusion from a simple random walk example.

Example 1: Drunken-sailor

Imagine a pub by the edge of a cliff. Drunken sailors leave the pub planning to walk home, but their walk is *erratic*: they take a step to the right with probability q, and left with probability $1-q$. Each step is independent of the previous—a property we call **Markovian** or **memoryless**.

If the pub is one step away to the right of the cliff (it takes one step left from the pub to fall off), what is the probability that the sailor arrives home safe?

Sol.: Define the position of the cliff as $x=0$, the pub is at $x=1$. Let $P_{\text{cliff}}(x)$ be the probability that the sailor walks off the cliff *at some time in the future* starting at position x. We want to know the value of $1-P_{\text{cliff}}(1)$.

From $x=1$, the sailor can take a step either left or right,

$$P_{\text{cliff}}(1) = \underbrace{(1-q)}_{\text{1st step left}} + \underbrace{q \cdot P_{\text{cliff}}(2)}_{\text{1st step right}} .$$

What is $P_{\text{cliff}}(2)$? It is the probability that the sailor eventually walks from $x=2$ to $x=1$ and subsequently moves from $x=1$ to $x=0$. Since each step is independent, by translation symmetry, the probability of eventually walking from $x = 2$ to $x = 1$ is the same as the probability of eventually walking from $x = 1$ to $x = 0$ (total displacement 1 step to the left). Hence,

$$P_{\text{cliff}}(1) = (1 - q) + q \cdot P_{\text{cliff}}(1) \cdot P_{\text{cliff}}(1).$$

This is a quadratic equation with solutions

$$P_{\text{cliff}}(1) = 1 \quad \text{or} \quad P_{\text{cliff}}(1) = \frac{1-q}{q}.$$

When $q = 0$, $P_{\text{cliff}}(1) = 1$ as the sailor immediately steps left, off the cliff. When $q = 1$, $P_{\text{cliff}}(1) = 0$, as the sailor only walks away from the cliff. For $q = \frac{1}{2}$, the two solutions intersect. Thus, the solution is,

$$P_{\text{cliff}}(1) = \begin{cases} 1, & \text{if } q \leq \frac{1}{2}, \\ \frac{1-q}{q}, & \text{if } q > \frac{1}{2}. \end{cases}$$

And the probability that the sailor gets home safe is

$$1 - P_{\text{cliff}}(1) = \begin{cases} 0, & \text{if } q \leq \frac{1}{2}, \\ \frac{2q-1}{q}, & \text{if } q > \frac{1}{2}. \end{cases} \tag{1}$$

This example, however simple, holds parallels with more interesting problems, such as the removal probability of a gas molecule through a semipermeable membrane in a cell.

2.1 Random walk definition

The drunken sailor problem is an example of a more general class of processes called *random walks* which are closely connected to transport phenomena, in particular, diffusion, as we will see later.

Definition: Random Walk

Consider a sequence of independent and identically distributed (i.i.d) random variables, Δ_1, Δ_2, ..., each representing a step in $\mathbb{R}^d$. Setting the starting point $X_0 = z$ (for some vector $z \in \mathbb{R}^d$), the position after n steps is given by

$$X_n = X_0 + \sum_{i=1}^{n} \Delta_i,$$

or recursively, $X_n = X_{n-1} + \Delta_n$.

The drunken sailor is an example of a random walk with $\mathbb{P}(\Delta_i = 1) = q$, $\mathbb{P}(\Delta_i = -1) = 1-q$, and $X_0 = 1$. In the drunken sailor problem, we also defined an *absorbing boundary condition* at $x = 0$.

Exercise 1: Consider a random walk such that $\mathbb{P}(\Delta_i = 1) = q$, $\mathbb{P}(\Delta_i = -1) = 1 - q$ on $\mathbb{R}$. Find $P(x, t \,|\, y, s)$, the probability that a particle reaches position x at step t given it was at position y at step s.

Sol.: The particle must take $n = t - s$ steps in total. Additionally, $n = n_R + n_L$ as each step is either right or left. The total rightwards displacement required is then $x - y = n_R - n_L$. Hence,

$$
\begin{aligned}
n_L &= n_R - x + y, \\
n_R &= n - n_L = t - s + x - y - n_R, \\
n_R &= \frac{1}{2}\left(t - s + x - y\right).
\end{aligned}
$$

This is now just a combinatorial problem. Out of n steps, what is the probability that the particle performs n_R right steps?

$$
\begin{aligned}
P(x, t \,|\, y, s) &= P[n_R \text{ right steps out of } n], \\
&= \binom{n}{n_R} q^{n_R} (1-q)^{n-n_R}.
\end{aligned}
$$

If the particle starts at $x_0 = 0$, the probability of finding the particle at position x at time t is

$$
P(x,t) = \binom{t}{\frac{t+x}{2}} q^{\frac{t+x}{2}} (1-q)^{\frac{t-x}{2}}.
$$

Note that $t + x$ must be even! If $t + x$ is odd, then $P(x,t) = 0$. The reason is that each step reverses the parity of the position of the particle, such that it reaches even positions at even steps and odd positions at odd steps. Thus, the sum of position and step number must be even for any valid path of the particle.

Exercise 2: Find the probability that the sailor survives N steps.

Hint: Find the probability that the sailor reaches the cliff exactly at step t using the *Method of Images*.

3 Random Walks and Diffusion

The symmetric discrete random walk has the probability of stepping left or right equal to $\frac{1}{2}$. Each step has size δ and the interval between each step is τ. The position of a particle starting at $x = 0$ after n steps is

$$
X(n) = \sum_{i=1}^{n} \Delta_i, \quad \text{where} \quad \Delta_i = \begin{cases} +\delta, & \text{w/ prob.} \frac{1}{2}, \\ -\delta, & \text{w/ prob.} \frac{1}{2}. \end{cases}
$$

3.1 Mean displacement

Suppose we have a group of N identical particles, all starting at the same time from $x = 0$. What is the average position of the group?

Definition: Ensemble average
If Y is a property of a particle, the ensemble mean of Y is defined as

$$\langle Y \rangle = \frac{1}{N} \sum_{i=1}^{N} y_i,$$

where y_i is the value of property Y of the i-th particle.

For Y the position of the particle, we get

$$\langle x_i(n) \rangle = \sum_{i=1}^{n} \langle \Delta_i \rangle = \sum_{i=1}^{n} \left\{ \delta \cdot \underbrace{\mathbb{P}(\Delta_i = \delta)}_{\frac{1}{2}} + (-\delta) \cdot \underbrace{\mathbb{P}(\Delta_i = -\delta)}_{\frac{1}{2}} \right\} = 0.$$

On average, the particle is "going nowhere"! This reflects the fact that the particle has no preferred direction of movement. It does not mean that the particle is not moving!

Similarly, for the ensemble average,

$$\langle X(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle x_i(n) \rangle = 0.$$

This means that, while the particles might be distancing themselves from the origin, the average position of the centre of mass does not.

3.2 Mean squared displacement

We can now evaluate the particle's mean squared displacement, which gives an idea of how spread out its trajectory becomes. This is similar to the particle's variance in position.

$$\begin{aligned}
\langle x^2(n) \rangle &= \left\langle \sum_{i=1}^{n} \Delta_i \sum_{j=1}^{n} \Delta_j \right\rangle, \\
&= \left\langle \sum_{i=1}^{n} \Delta_i^2 + \sum_{i=1}^{n} \sum_{j \neq i}^{n} \Delta_i \Delta_j \right\rangle, \\
&= \sum_{i=1}^{n} \langle \Delta_i^2 \rangle + \sum_{i=1}^{n} \sum_{j \neq i}^{n} \langle \Delta_i \Delta_j \rangle, \\
&= n \left\{ \delta^2 \cdot \mathbb{P}(\Delta_i = \delta) + \delta^2 \cdot \mathbb{P}(\Delta_i = -\delta) \right\} + \sum_{i=1}^{n} \sum_{j \neq i}^{n} \langle \Delta_i \Delta_j \rangle, \\
&= n\delta^2 + 0,
\end{aligned}$$

where we used the independency of the steps to decouple $\langle \Delta_i \Delta_j \rangle = \langle \Delta_i \rangle \langle \Delta_j \rangle$.

By writing $n = t/\tau$, we now have the **mean squared displacement (MSD)**

$$\langle \Delta x^2 \rangle = \frac{\delta^2}{\tau} t,$$

and the **root mean squared displacement (RMSD)**,

$$\sqrt{\langle \Delta x^2 \rangle} = \sqrt{\frac{\delta^2}{\tau} t}.$$

That is, the displacement of the particles (or the spread of the ensemble) is proportional to $\sqrt{t}$, meaning that, as time passes, the ensemble becomes more spread out. This is a **key property** of **diffusion processes**.

4 Fick's Laws (of diffusion)

4.1 Fick's first law

Let $N(x)$ be the number of particles at position x. Consider a line at $x + \frac{\delta}{2}$. The flux of particles through the line in an interval τ is

$$J(x)\tau = \frac{1}{2}N(x) - \frac{1}{2}N(x+\delta),$$

where the first term comes from particles at x going right and the second comes from particles at $x + \delta$ going left.

Define $n(x) = \frac{N(x)}{\delta}$ to be a particle density. Multiplying the previous equation by δ/δ, we can write it as

$$J(x) = -\frac{\delta^2}{2\tau}\left(\frac{n(x+\delta) - n(x)}{\delta}\right).$$

Now we take the limits $\delta, \tau \to 0$ such that the ratio $\frac{\delta^2}{2\tau} \to D$, constant. Then

$$J(x) = -D\frac{\partial n}{\partial x}. \qquad \text{(Fick's first law)}$$

The constant D is called the **diffusion constant**.

Recalling our expression for the mean square displacement, we can write

$$\langle \Delta x^2 \rangle = 2dDt,$$

where d is the number of dimensions of the random walk.

4.2 Fick's second law

Consider the change in particle number within the region $[x - \delta/2, x + \delta/2]$ during an interval τ:

$$N(x, t+\tau) - N(x, \tau) = J\left(x - \tfrac{\delta}{2}, t\right)\tau - J\left(x + \tfrac{\delta}{2}, t\right)\tau.$$

Dividing by $\tau\delta$, we can write it in terms of the particle density $n = \frac{N}{\delta}$

$$\frac{n(x, t+\tau) - n(x,t)}{\tau} = \frac{J\left(x - \frac{\delta}{2}, t\right) - J\left(x + \frac{\delta}{2}, t\right)}{\delta}.$$

In the limit $\delta, \tau \to 0$,

$$\frac{\partial n}{\partial t} = -\frac{\partial J}{\partial x} = D\frac{\partial^2 n}{\partial x^2}. \qquad \text{(Fick's second law)}$$

This is the (1D) diffusion equation, which describes how a cloud of particles evolves in time.

5 A probabilistic approach

We can also derive the time evolution of a cloud of N_0 particles from the probability states, $P(x,t)$. The number of particles in the interval $[x - \delta/2, x + \delta/2]$ is

$$N(x,t) = N_0 P(x,t) = N_0 p(x,t)\delta,$$

where $p(x,t)$ is the probability density function (pdf).

To find the equation describing the probability states $P(x,t)$, we consider the possible changes in density at position x:

$$\underbrace{P(x,t)}_{\text{Probability at } t+\tau} = \underbrace{\frac{1}{2}P(x-\delta,t)}_{\text{Particles at } x-\delta \text{ move right}} + \underbrace{\frac{1}{2}P(x+\delta,t)}_{\text{Particles at } x+\delta \text{ move left}}.$$

Dividing by δ and taking a Taylor expansion for $\tau, \delta \ll 1$,

$$\begin{aligned}
p(x,t) + \frac{\partial p}{\partial t}\tau &\approx \frac{1}{2}\left[p(x,t) - \delta\frac{\partial p}{\partial x} + \frac{1}{2}\delta^2\frac{\partial^2 p}{\partial x^2} + p(x,t) + \delta\frac{\partial p}{\partial x} + \frac{1}{2}\delta^2\frac{\partial^2 p}{\partial x^2}\right], \\
p(x,t) + \frac{\partial p}{\partial t}\tau &\approx p(x,t) + \frac{1}{2}\delta^2\frac{\partial^2 p}{\partial x^2}, \\
\frac{\partial p}{\partial t} &\approx \frac{\delta^2}{2\tau}\frac{\partial^2 p}{\partial x^2} = D\frac{\partial^2 p}{\partial x^2}.
\end{aligned}$$

Since $n(x,t) = N_0 p(x,t)$, this recovers the diffusion equation.

Exercise 3: Repeat the previous derivations now for a biased random walk in which $\mathbb{P}(\Delta_i = \delta) = q$ and $\mathbb{P}(\Delta_i = -\delta) = 1 - q$. What happens to the first derivatives in x?

Suggested Reading: For more information about how Random Walks are used in biological modelling, a good textbook is *Random Walks in Biology* by Howard C. Berg.

6 Solving the Diffusion Equation

We have shown through two different arguments that the density of random walkers in a one-dimensional line follows the Diffusion Equation

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2}.$$

We are interested in knowing the solution of this equation subject to the initial condition $n(x,0) = n_0(x)$ and $\lim_{x\to\pm\infty} n(x,t) = 0$.

6.1 Fourier method

The Fourier method to solve this equation relies on the fact that we can decompose $n(x,t)$ in planar waves

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\hat{n}(k,t)\,\mathrm{d}k.$$

The coefficients $\hat{n}(k,t)$ are found using the Fourier Transform,

$$\hat{n}(k,t) = \int_{-\infty}^{\infty} e^{-ikx}n(x,t)\mathrm{d}x.$$

We define $\hat{n}_0(k)$ to be the Fourier Transform of $n_0(x)$.

Taking the Fourier Transform of the Diffusion Equation,

$$\int_{-\infty}^{\infty} e^{-ikx}\frac{\partial n}{\partial t}\mathrm{d}x = D\int_{-\infty}^{\infty} e^{-ikx}\frac{\partial^2 n}{\partial x^2}\mathrm{d}x,$$

gives

$$\frac{\partial \hat{n}}{t} = (ik)^2 D\hat{n} = -k^2 D\hat{n}.$$

This is a simple ODE with solution

$$\hat{n}(k,t) = \hat{n}_0(k)e^{-k^2 Dt}.$$

Therefore, the solution of the Diffusion Equation is

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{n}_0(k)e^{ikx-k^2 Dt}\,\mathrm{d}k. \tag{2}$$

Note that the higher wave numbers are rapidly damped, emphasising the smoothing property of diffusion.

Example: Consider the Gaussian initial distribution

$$n_0(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{x^2}{2\sigma^2}}. \tag{3}$$

The Fourier Transform of the above distribution is

$$\hat{n}_0(k) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(\frac{x^2}{2\sigma^2}+ikx\right)}\,\mathrm{d}x.$$

Completing the square,

$$\hat{n}_0(k) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x+ik\sigma^2)^2}{2\sigma^2}} e^{-\frac{k^2\sigma^2}{2}}\,\mathrm{d}x.$$

Now we need a bit of Complex Analysis. The Cauchy Formula states that, for a function $f(z) \in \mathbb{C}$, $z \in \mathbb{C}$,

$$\oint f(z)\,\mathrm{d}z = 0,$$

provided there are no poles in the interior of the integration path.

Introducing $z = x + ik\sigma^2$, $dz = dx$, the previous integral becomes

$$\hat{n}_0(k) = \frac{e^{-\frac{k^2\sigma^2}{2}}}{\sqrt{2\pi\sigma^2}} \lim_{R\to\infty} \int_{-R+ik\sigma^2}^{R+ik\sigma^2} e^{-\frac{z^2}{2\sigma^2}}\,dz \tag{4}$$

Let's keep R finite for the moment. We can then think of the integral as one segment of a closed curve with rectangular shape:

$$\begin{aligned}0 &= \oint e^{-\frac{z^2}{2\sigma^2}}\,dz \\ &= \int_{-R+ik\sigma^2}^{R+ik\sigma^2} e^{-\frac{z^2}{2\sigma^2}}\,dz + \int_{R+ik\sigma^2}^{R} e^{-\frac{z^2}{2\sigma^2}}\,dz + \int_{R}^{-R} e^{-\frac{z^2}{2\sigma^2}}\,dz + \int_{-R}^{-R+ik\sigma^2} e^{-\frac{z^2}{2\sigma^2}}\,dz\end{aligned}$$

In the limit $R \to \infty$, the second as well as the last integral vanish due to the exponential damping with large R, leading to

$$\lim_{R\to\infty} \int_{-R+ik\sigma^2}^{R+ik\sigma^2} e^{-\frac{z^2}{2\sigma^2}}\,dz = \lim_{R\to\infty} \int_{-R}^{R} e^{-\frac{z^2}{2\sigma^2}}\,dz\ .$$

Inserting this into Eq. (4), we obtain

$$\hat{n}_0(k) = \frac{e^{-\frac{k^2\sigma^2}{2}}}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}\,dx.$$

This means that we can basically drop the imaginary part in the original integral.

Given the integral of a Guassian

$$\int_{-\infty}^{\infty} e^{-x^2} = \sqrt{\pi},$$

so by making a change of variable $y = x/\sqrt{2\sigma^2}$ we have that

$$\hat{n}_0(k) = e^{-\frac{k^2\sigma^2}{2}}.$$

This result is worth keeping in mind: The Fourier transform of a Gaussian is a Gaussian.

To obtain the full solution of the diffusion equation in real space, we have to insert $\hat{n}_0(k)$ into Eq. (2),

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-Dk^2t-k^2\sigma^2/2}dk.$$

We can do a bit of rearranging to get

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-k^2\left(Dt+\sigma^2/2\right)}dk\ .$$

As before we complete the square for the exponent,

$$k^2\left(Dt+\frac{\sigma^2}{2}\right)-ikx = \left(Dt+\frac{\sigma^2}{2}\right)\left\{\left[k-\frac{ix}{2(Dt+\sigma^2/2)}\right]^2+\frac{x^2}{4\left(Dt+\sigma^2/2\right)^2}\right\},$$

so that the integral becomes

$$n(x,t) = \frac{e^{-\frac{x^2}{4(Dt+\sigma^2/2)}}}{2\pi}\int_{-\infty}^{\infty} e^{-(Dt+\sigma^2/2)\left[k-\frac{ix}{2(Dt+\sigma^2/2)}\right]^2}dk.$$

This is essentially the same integral that we had before, so we drop the imaginary part and change the integration variable, giving the result

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

This is the solution of the diffusion equation starting from a Gaussian distribution at time $t=0$.

Note:

- Introducing $\tilde{\sigma}^2 = 2(Dt+\sigma^2/2)$, the solution is a Gaussian with a standard deviation $\tilde{\sigma}$, i.e. the width of the solution grows like $\sqrt{Dt}$ in time. Similarly, the amplitude decreases like $\frac{1}{\sqrt{Dt}}$.

- Let us substitute $t_d = \sigma^2/(2D)$. The solution then can be written as

$$n(x,t) = \frac{e^{-\frac{x^2}{4D(t+t_d)}}}{\sqrt{4\pi D(t+t_d)}}. \tag{5}$$

  Remember that in the limit $t_d = \frac{\sigma^2}{2D} \to 0$ the initial condition Eq. (3) corresponds to a Dirac delta function. Thus an initially Gaussian distribution of particles that is diffusing may be viewed as having originated from a delta function a time t_d ago. Indeed, it can be shown that diffusion will cause any form of particle distribution initially localised about zero to eventually look like a Gaussian.

6.2 Green's function method

This method relies on another trick for representing the solution, which is somewhat more intuitive. Now, instead of representing n in a basis of plane wave states, we will express it as a basis of states which are localised in *position*. This is done by using the so-called Dirac delta function, denoted $\delta(x - x_0)$. You should think of this of a large spike of unit area that is centered exactly at the position x_0. The definition of δ is that given any function[1] $f(x)$,

$$\int_{-\infty}^{\infty} f(x')\,\delta(x - x')dx' = f(x).$$

We can represent the initial distribution of particles $n(x, 0) = n_0(x)$ as a superposition of δ-functions

$$n_0(x) = \int_{-\infty}^{\infty} n_0(x')\,\delta(x - x')\,dx'.$$

This formula decomposes n_0 into a continuous series of "spikes". The idea is to then understand how each spike individually evolves and then superimpose the evolution of each spike to find the final density distribution. We define the Green's function $G(x - x', t)$ so that $G(x - x', 0) = \delta(x - x')$, and

$$n(x, t) = \int_{-\infty}^{\infty} G(x - x', t)\; n_0(x')\,dx'.$$

Plugging this into the diffusion equation we see that

$$\int_{-\infty}^{\infty} n_0(x')\,\frac{\partial G(x - x', t)}{\partial t}\;dx' = D\int_{-\infty}^{\infty} n_0(x')\,\frac{\partial^2 G(x - x', t)}{\partial x^2}\;dx'.$$

Thus $G(x - x', t)$ *obeys the diffusion equation* and we have reduced the problem to the mathematics of solving the diffusion equation for the localised initial condition $\delta(x - x')$.

This problem can be solved by using the Fourier decomposition of $\delta(x - x')$ and solving the equation in Fourier space, and then transforming back into real space.

[1]Intuitively, one can obtain the Dirac δ-function from the normalized Gaussian (3) by letting $\sigma \to 0$. Derivatives of order n of the δ-function, denoted by $\delta^{(n)}$, can be defined by partial integration

$$\int_{-\infty}^{\infty} f(x')\,\delta^{(n)}(x - x')\,dx' = (-1)^n \int_{-\infty}^{\infty} f^{(n)}(x')\,\delta(x - x')\,dx'.$$

The Fourier transformation of the δ-function is given by

$$\hat{\delta}(k) = \int_{-\infty}^{\infty} e^{-ikx}\delta(x)\,dx = 1.$$

Applying the inverse transformation yields a useful integral representation of the Dirac δ-function

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\hat{\delta}(k)\,dk = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dk.$$

7 Pattern Formation

In the first lecture, we studied diffusive systems as a limit of random walks, deriving the diffusion equation, solving and obtaining insight into its properties.

In the second lecture, we will model a biological system with diffusion and understand its effects on pattern formation. Before diving into the modelling aspect, we need a short background on stability analysis.

7.1 (Linear) Stability analysis for PDEs

Consider a scalar density $n(x,t)$ on the interval $[0,L]$, governed by the Diffusion Equation,

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2},$$

with reflecting boundary conditions,

$$\frac{\partial n}{\partial t}(0,t) = \frac{\partial n}{\partial t}(L,t) = 0.$$

Under these dynamics, the 'total mass' of the system is conserved, i.e.,

$$N(t) = \int_0^L n(x,t)\,\mathrm{d}x \equiv N_0,$$

and a spatially homogeneous stationary solution is given by

$$n_0 = N_0/L.$$

To evaluate its stability, we can consider wave-like perturbations,

$$n(x,t) = n_0 + \delta n(x,t), \quad \delta n(x,t) = \epsilon e^{\sigma t - ikx}.$$

Inserting this ansatz into the Diffusion Equation gives the dispersion relation

$$\sigma(k) = -Dk^2 \geq 0,$$

signaling that n_0 is a stable solution, because all modes with $|k| > 0$ become exponentially damped.

7.2 Reaction-diffusion (RD) systems

RD systems provide another generic way of modeling structure formation in chemical and biological systems. The idea that RD processes could be responsible for morphogenesis goes back to a 1952 paper by Alan Turing (see class slides), and it seems fair to say that this paper is the most important one ever written in mathematical biology.

RD system can represented in the form

$$\partial_t \boldsymbol{q}(t,\boldsymbol{x}) = D\nabla^2 \boldsymbol{q} + \boldsymbol{R}(\boldsymbol{q}), \tag{6}$$

where

- $\boldsymbol{q}(t, \boldsymbol{x})$ as an n-dimensional vector field describing the concentrations of n chemical substances, species etc.
- D is a *diagonal* $n \times n$-diffusion matrix, and
- the n-dimensional vector $\boldsymbol{R}(\boldsymbol{q})$ accounts for all *local* reactions.

7.2.1 Two species in one space dimension

As a specific example, let us consider $\boldsymbol{q}(t, \boldsymbol{x}) = (u(t, x), v(t, x))$, $D = \mathrm{diag}(D_u, D_v)$ and $\boldsymbol{R} = (F(u, v), G(u, v))$, then

$$u_t = D_u u_{xx} + F(u, v) \tag{7a}$$

$$v_t = D_v v_{xx} + G(u, v) \tag{7b}$$

In general, (F, G) can be derived from the reaction/reproduction kinetics, and conservation laws may impose restrictions on permissible functions (F, G). The fixed points (u_*, v_*) of (7) are determined by the condition

$$\boldsymbol{R}(u_*, v_*) = \begin{pmatrix} F(u_*, v_*) \\ G(u_*, v_*) \end{pmatrix} = \mathbf{0}. \tag{8}$$

Expanding (7) for small plane-wave perturbations

$$\begin{pmatrix} u(t, x) \\ v(t, x) \end{pmatrix} = \begin{pmatrix} u_* \\ v_* \end{pmatrix} + \boldsymbol{\epsilon}(t, x) \tag{9a}$$

with

$$\boldsymbol{\epsilon} = \hat{\boldsymbol{\epsilon}}\, e^{\sigma t - ikx} = \begin{pmatrix} \hat{\epsilon} \\ \hat{\eta} \end{pmatrix} e^{\sigma t - ikx}, \tag{9b}$$

we find the linear equation

$$\sigma \hat{\boldsymbol{\epsilon}} = -\begin{pmatrix} k^2 D_u & 0 \\ 0 & k^2 D_v \end{pmatrix} \hat{\boldsymbol{\epsilon}} + \begin{pmatrix} F_u^* & F_v^* \\ G_u^* & G_v^* \end{pmatrix} \hat{\boldsymbol{\epsilon}} \equiv M \hat{\boldsymbol{\epsilon}}, \tag{10}$$

where

$$F_u^* = \partial_u F(u_*, v_*), \quad F_v^* = \partial_v F(u_*, v_*), \quad G_u^* = \partial_u G(u_*, v_*), \quad G_v^* = \partial_v G(u_*, v_*).$$

Solving this eigenvalue equation for σ, we obtain

$$\sigma_\pm = \frac{1}{2} \left\{ -(D_u + D_v)k^2 + (F_u^* + G_v^*) \pm \sqrt{4 F_v^* G_u^* + [F_u^* - G_v^* + (D_v - D_u)k^2]^2} \right\}.$$

In order to have an instability for some finite value k, at least one of the two eigenvalues must have a positive real part. This criterion can be easily tested for a given reaction kinetics (F, G). We still consider a popular example.

7.2.2 Lotka-Volterra model

This model describes a simple predator-prey dynamics, defined by

$$F(u,v) = Au - Buv, \tag{11a}$$
$$G(u,v) = -Cv + Euv \tag{11b}$$

with positive rate parameters $A, B, C, E > 0$. The field $u(t,x)$ measures the concentration of prey and $v(t,x)$ that of the predators. The model has two fixed points

$$(u_0, v_0) = (0,0), \quad (u_*, v_*) = (C/E, A/B), \tag{12}$$

with Jacobians

$$\begin{pmatrix} F_u(u_0,v_0) & F_v(u_0,v_0) \\ G_u(u_0,v_0) & G_v(u_0,v_0) \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & -C \end{pmatrix} \tag{13a}$$

and

$$\begin{pmatrix} F_u(u_*,v_*) & F_v(u_*,v_*) \\ G_u(u_*,v_*) & G_v(u_*,v_*) \end{pmatrix} = \begin{pmatrix} A - \frac{BC}{E} & -A \\ C & -C + \frac{AE}{B} \end{pmatrix}. \tag{13b}$$

It is straightforward to verify that, for suitable choices of A, B, C, D, the model exhibits a range of unstable k-modes.

8 Coding Exercises

The following repositories contain coding exercises focused on deepening the understanding of the topics covered in these lecture notes. The questions are open-ended, and students are free to work on the tasks at their own pace. To run the code, open the Jupyter notebook locally or in Google Colab.

Random Walkers: `https://github.com/philip-pearce/randomwalkers/`
Pattern Formation: `https://github.com/amsontag/pattern_formation/`