Diffusion

Literature. J.D. Murray, “Mathematical Biology” Sec. 11.

Fickian diffusion

Let us consider some molecules (or small particles, or microbes, etc) with concentration c (concentration is the number of particles per unit volume). If we consider that all particles are on a line, the concentration, $c = c(x,t)$, is the number of particles per unit length.
Now, consider that they are in motion with flux $J(x,t)$ (flux is the number of particles passing across a certain point x per unit time).
In Fickian diffusion

$$J \sim \frac{\partial c}{\partial x} \Rightarrow J = -D\frac{\partial c}{\partial x} \quad (1)$$

(The flux is proportional to the gradient of the concentration and particles flow from higher to lower concentration.)

Let us consider a region from x_1 to x_2 and consider the change in the number of particles

$$\frac{\partial}{\partial t}\int_{x_1}^{x_2} c(x,t)\,dx = J(x_1,t) - J(x_2,t)$$

Let us now consider an infinitesimal region $x_2 - x_1 = \Delta x \to 0$ to get

$$\frac{\partial c}{\partial t}dx = J(x_1,t) - J(x_2,t) \Rightarrow \frac{\partial c}{\partial t} = -\frac{J(x_2,t)-J(x_1,t)}{dx} \Rightarrow \frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}$$

Using Fick’s law we obtain the Diffusion equation

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$$

For constant D we have the simpler equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \quad (2)$$

This is a linear partial differential equation.

See this tool for solving the diffusion equation online.

The solution of the diffusion equation

Example. (a) Show that the following is a solution of the diffusion equation (2),

$$c(x,t) = \frac{Q}{2(\pi D t)^{1/2}}\,e^{-x^2/(4Dt)}, \quad t > 0, \quad Q : const.$$

(b) Plot the solution for various values of t. (See here.)

(c) Note that the boundary conditions satisfied by the above solution at $c(\pm\infty) = 0$, and the initial condition is $c(x, t=0) \;=\; Q\delta(x)$. ($\delta$ is the Dirac delta-function.)

Let us consider an assemblage of objects (particles), for example, bacteria, animals, molecules etc. These may move around (e.g., animals in the woods, molecules in a chemical reaction, even people in a city) in an irregular way. Their motion is done in small steps, but, in the long run, they spread in the way of simple diffusion.

Solution by Fourier transform

We can find a solution $c(x, t)$ of (2) by starting from its Fourier transform

$$\hat{c}(k, t) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} c(x, t)\, dx$$

We have that (integrate by parts twice)

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \frac{\partial^2 c}{\partial x^2} dx = \frac{1}{\sqrt{2\pi}}(-ik) \int_{-\infty}^{\infty} e^{ikx} \frac{\partial c}{\partial x} dx = -k^2 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} c(x, t)\, dx = -k^2\, \hat{c}(k, t)$$

And

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \frac{\partial c}{\partial t} dx \;=\; \frac{\partial \hat{c}}{\partial t}$$

Using the last two equations, the diffusion equation gives

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \Rightarrow \frac{\partial \hat{c}}{\partial t} = -k^2 D\;\; \hat{c}(k, t)$$

that is, a differential equation with only time derivative.

We have to choose initial condition, and we choose $\hat{c}(k, t=0) \;=\; Q/\sqrt{2\pi}$. We get the solution

$$\hat{c}(x, t) \;=\; \frac{Q}{\sqrt{2\pi}}\, e^{-k^2 Dt}$$

We apply the inverse Fourier transform and have the solution of the diffusion equation

$$c(x, t) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \hat{c}(k, t)\, dk \;=\; \frac{Q}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} e^{-k^2 Dt}\, dk$$

Exercise. Show that $k^2 Dt + ikx \;=\; Dt(k + i\frac{x}{2Dt})^2 + \frac{x^2}{4Dt}$.

Use the result of the last exercise to write

$$\int_{-\infty}^{\infty} e^{-ikx} e^{-k^2 Dt}\, dk = e^{-x^2/(4Dt)} \int_{-\infty}^{\infty} e^{-Dt(k + i\frac{x}{2Dt})^2} dk = \sqrt{\frac{\pi}{Dt}}\, e^{-x^2/(4Dt)}.$$

Exercise. Show that (and use it in the above calculation) $\int_{-\infty}^{\infty} e^{-az^2} dz = \sqrt{\frac{\pi}{a}}$.

Combining the results we find

$$c(x,t) \;=\; \frac{Q}{\sqrt{4\pi D t}}\; e^{-x^2/(4Dt)}$$

[Thursday 9/4/2020]

Random walk

Suppose that a particle is released at $x = 0$ at the time $t = 0$ and let $p(x,t)$ the probability for the particle to be at position x at the time t. Suppose that our particle moves by Δx in a time interval Δt.

Let the particle be at position x at the time instance t. Then at the time $t - \Delta t$ it should have been either at $x - \Delta x$ or at $x + \Delta x$.

We suppose that the particle moves right with a probability a and left with a probability b. Of course, $a + b = 1$.

We have

$$p(x,t) \;=\; a\, p(x - \Delta x,\; t - \Delta t) \;+\; b\, p(x + \Delta x,\; t - \Delta t)$$

We consider this random walk with $a = b = \frac{1}{2}$ (unbiased random walk).

Write the Taylor expansion

$$p(x + \Delta x, t + \Delta t) \;=\; p(x,t) \;+\; \Delta t\, \frac{\partial p}{\partial t} + \; \Delta x\, \frac{\partial p}{\partial x} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 p}{\partial t^2} + \frac{1}{2}(\Delta x)^2\, \frac{\partial^2 p}{\partial x^2} + \ldots$$

We substitute and have

$$p(x,t) \;=\; a\,[p(x,t) \;-\; \Delta t\, \frac{\partial p}{\partial t} - \; \Delta x\, \frac{\partial p}{\partial x} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 p}{\partial t^2} + \frac{1}{2}(\Delta x)^2\, \frac{\partial^2 p}{\partial x^2}\;] \;+\; b\,[p(x,t) \;-\; \Delta t\, \frac{\partial p}{\partial t} + \; \Delta x\, \frac{\partial p}{\partial x} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 p}{\partial t^2} + \frac{1}{2}(\Delta$$

$$p(x,t) \;=\; (a+b)\, p(x,t) - (a+b)\Delta t\; \frac{\partial p}{\partial t} + \frac{1}{2}(a+b)(\Delta t)^2 \frac{\partial^2 p}{\partial t^2} + (-\,a + b)\Delta x\, \frac{\partial p}{\partial x} + \frac{1}{2}(a+b)(\Delta x)^2\, \frac{\partial^2 p}{\partial x^2} \Rightarrow$$

$$0 = -\,\Delta t\; \frac{\partial p}{\partial t} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 p}{\partial t^2} + \frac{1}{2}(\Delta x)^2\, \frac{\partial^2 p}{\partial x^2}$$

We want to obtain a *continuous* model in space and time, and we thus let $\Delta x \to 0$, $\Delta t \to 0$.

We choose

$$\lim_{\Delta x, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} = D$$

where we assume that D is a constant.

We obtain the diffusion equation for the probability p,

$$-\,\frac{\partial p}{\partial t} + (\Delta t)\, \frac{\partial^2 p}{\partial t^2} + \;\frac{(\Delta x)^2}{2\Delta t}\, \frac{\partial^2 p}{\partial x^2} = 0 \Rightarrow \frac{\partial p}{\partial t} \;=\; D \frac{\partial^2 p}{\partial x^2}$$

Exercise. The solution of this equation is $p(x,t) \;=\; \frac{Q}{2\sqrt{\pi D t}}\;\; e^{-x^2/(4Dt)}$. Show that

$$\int_{-\infty}^{\infty} p(x,t)\, dx \;=\; Q$$

for every time t. We can choose $Q = 1$ when p is to be interpreted as probability. If $Q \neq 1$ we can interpret it as the number of particles released at $x = 0$ at the time $t = 0$.

Animal dispersal model

- Insect dispersal.
- Biological invasions of mammals, birds, insects and plants.
- Immigration of people.

There may be an increase in the animal dispersal due to population pressure

$$J = -D(n)\,\partial_x n, \quad \frac{dD}{dn} > 0$$

that is, D is an increasing function of population density n.

Let us choose

$$D(n) \;=\; D_0\left(\frac{n}{n_0}\right)^m, \quad D_0, n_0 > 0 \quad \text{and} \quad m > 0 \text{ integer.}$$

Question. What phenomena does the above form take into account?
(Population pressure has an effect faster than linear.)

Let us see the diffusion equation in one dimension

$$\frac{\partial n}{\partial t} = D_0 \frac{\partial}{\partial x}\left[\left(\frac{n}{n_0}\right)^m \frac{\partial n}{\partial x}\right]$$

This has an analytic solution

$$n(x,t) \;=\; \frac{n_0}{\lambda(t)}\left[1 - \left(\frac{x}{r_0\lambda(t)}\right)^2\right]^{1/m}, \quad |x| \leq r_0\lambda(t) \text{ and } n(x,t) = 0, \quad |x| > r_0\lambda(t)$$

where

$$\lambda(t) \;=\; (t/t_0)^{1/(2+m)}, \quad r_0 > 0, \quad t_0 = \frac{r_0^{\,2} m}{2D_0(m+2)}$$

For $m = 1$ we have

$$n(x,t) = \frac{n_0}{\lambda(t)}\left[1 - \left(\frac{x}{r_0\lambda(t)}\right)^2\right], \quad \lambda(t) = (t/t_0)^{1/3}, \quad t_0 = \frac{r_0^{\,2}}{6D_0}, \quad r_0 > 0$$

For $m = 2$ we have

$$n(x,t) \;=\; \frac{n_0}{\lambda(t)}\left[1 - \left(\frac{x}{r_0\lambda(t)}\right)^2\right]^{1/2}, \quad \lambda(t) \;= (t/t_0)^{1/4}, \quad t_0 = \frac{r_0^{\,2}}{4D_0}, \quad r_0 > 0$$

Exercise. Plot $n(x,t)$ for successive values of t.
(a) For $m = 1$. Let us choose $D_0 = 1,\ n_0 = 100$ and $r_0^{\,2} = 48$ thus $t_0 = 8,\ \lambda(t) = t^{1/3}/2.$ For these values, the end of the front is at $x_f = r_0\lambda(t) \;=\; 2\sqrt{3}\cdot t^{1/3}$. Graph.
(b) For $m = 2$. Let us choose $D_0 = 1,\ n_0 = 10$ and $r_0^{\,2} = 8$ thus $t_0 = 2,\ \lambda = (t/2)^{1/4}$. For these values, the end of the front is at $x_f = \sqrt{8}\ (t/2)^{1/4}$.

Graph.

Note that

- The population extends up to $x_f = r_0\lambda(t)$, it is zero for $x > r_0\lambda(t)$.
- The solution represents a wave with front at $x = r_0\lambda(t)$.
- The derivative of n_f is discontinuous at the end of the front.
- The propagation speed of the front is $dx_f/dt = dx_f/dt = r_0 d\lambda/dt$. Note that this will be a decreasing function of time.

Remark. The dispersal patterns for grasshoppers exhibit a behavior similar to this model.

Exercise. Verify the solution for the above model for $m = 1$.

Question. In which cases would we expect higher values of the integer m in the animal dispersion model?

Diffusion in 3D

In the 3D space we write the law of conservation of mass in a volume V as

$$\frac{\partial}{\partial t}\int_V c(\vec{r}, t)\, dv = -\int_S \vec{J} \cdot d\vec{s}$$

where S is the surface enclosing the volume V (on the left side is the rate of change of the mass and on the right side is the flux through the surface).
We apply the divergence theorem (*) to the surface integral and have the volume integral $\int_S \vec{J} \cdot d\vec{s} = \int_V \vec{\nabla} \cdot \vec{J} dv$.
Using the latter result, we obtain

$$\int_V \frac{\partial c}{\partial t}\, dv = -\int_V \vec{\nabla} \cdot \vec{J} dv \Rightarrow \int_V (\frac{\partial c}{\partial t} + \vec{\nabla} \cdot \vec{J})\, dv = 0$$

Since the volume V is arbitrary the integrand must be zero (we obtain a continuity equation)

$$\frac{\partial c}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0.$$

Fick's law in 3D would be

$$\vec{J} = -D\vec{\nabla} c$$

Substitute this in the continuity equation and obtain the Diffusion equation in 3D

$$\frac{\partial c}{\partial t} = \vec{\nabla}(D\vec{\nabla}c)$$

or

$$\frac{\partial c}{\partial t} = D\,\Delta c\,, \quad \text{if } D \text{ is constant.}$$

Example. (Animal dispersal)

Let n the population density.

There may be an increase in dispersion due to population pressure

$$\vec{J} = -D(n)\,\vec{\nabla}n, \quad \frac{dD}{dn} > 0$$

that is D is an increasing function of population density n.

Let us choose

$$D(n) = D_0\left(\frac{n}{n_0}\right)^m, \qquad D_0,\ n_0 > 0 \text{ and } m > 0 \text{ integer.}$$

Exercise. Write the animal dispersal model for grasshoppers that disperse radially on the plane. Give the solution of the model.

In the solutions that we studied, the total population remains constant, $\int_V n\,dv = N$.

Gauss' divergence theorem (*)

[Marsden, Tromba, Sec. 8.4]

Let W be a symmetric elementary region in space. Denote by ∂W the oriented closed surface that bounds W. Let $\vec{F}$ be a smooth vector field defined on W. Then

$$\int_W (\vec{\nabla}\cdot\vec{F})\,dV = \int_{\partial W} \vec{F}\cdot d\vec{S}.$$

(Elements of the proof.)

Let $\vec{F} = P\vec{i} + Q\hat{j} + R\hat{k}$, thus $\vec{\nabla}\cdot\vec{F} = \frac{\partial Q}{\partial x} + \frac{\partial P}{\partial y} + \frac{\partial R}{\partial z}$.

Assume a cubic volume V and let two parts of the surface S_1 and S_2 that have opposite orientations, for example, $\hat{k}S_1 = -\hat{k}S_2$.

We have the following

$$\int_V\iint \frac{\partial R}{\partial z}dx\,dy\,dz = \int_S (R_1 - R_2)\,dx\,dy = \int_{S_1} R\,dx\,dy + \int_{S_2} R\,dx\,dy = \int_S \vec{F}\cdot\hat{k}\,dS = \int_S \vec{F}\cdot d\vec{S}.$$

where $d\vec{S} = \hat{k}S_1$ on S_1 and $d\vec{S}_2 = -\hat{k}S_2$ on S_2.

Reaction-Diffusion equations

Derivation

When mass can be created or annihilated in the volume V, then the law conservation of mass is

$$\frac{\partial}{\partial t}\int_V c(\vec{r},t)\,dv = -\int_S \vec{J}\cdot d\vec{s} + \int_V f\,dv$$

where f is a source of mass (for example, for $f=1$ and $J=0$, we have $dc/dt = 1$, i.e., constant increase of concentration).
In general, $f=f(c,\vec{x},t)$.
We apply the divergence theorem (*) to the surface integral and have the volume integral

$$\int_V \left(\frac{\partial c}{\partial t} + \vec{\nabla}\cdot\vec{J} - f\right) dv = 0$$

Since the volume V is arbitrary the integrand must be zero

$$\frac{\partial c}{\partial t} + \vec{\nabla}\cdot\vec{J} = f$$

Thus, we have a more general differential law of mass conservation.

If we assume Fick's law, then we obtain

$$\frac{\partial c}{\partial t} = f + \vec{\nabla}(D\vec{\nabla}c)$$

Example. We have applications in the following.

- In an ecological context, where c is the population density, f could represent the birth and death processes.
- In an epidemic, c may be the infected and f could represent the new infections and the recoverings.
- In cancer models involving mutating cancer cells.
- In animal dispersal models.

Make sure you understand the parameters of the problem. Consider that (and explain why)

- D can be a function of $\vec{r}$ and c.
- f can be a function of $\vec{r}$, t and c, that is, $f=f(c,\vec{r},t)$.

Generalization. We can imagine a system with many species and the respective concentrations c_i, so that the concentration is a vector $\vec{c}$. We then have a system of equations as a reaction diffusion system. Note that, in this case, D is a matrix.

Fisher-Kolmogorov equation

For logistic growth of a population n,

$$\frac{dn}{dt} = f(n), \quad f(n) = r\, n\, (1 - \frac{n}{K})$$

where r is the linear reproduction rate and K is the carrying capacity of the environment.

Exercise. Plot the solution of the logistic model and show graphically its dependence on $r,\ K$.

The solution is $n(t) = \frac{n_0 K\, e^{rt}}{K + n_0(e^{rt} - 1)}$. Note that $n(t = 0) = n_0$. [Graph.]

Let us consider a model with diffusion where the population follows the logistic growth. For diffusion parameter D and for f giving logistic growth we have the reaction-diffusion model

$$\frac{\partial n}{\partial t} = rn\, (1 - \frac{n}{K}) + D\, \Delta n, \quad n = n(\vec{r}, t)$$

known as the Fisher-Kolmogorov equation (Fisher (1937) proposed the one-dimensional version as a model for the spread of an advantageous gene in a population and Kolmogorov et al (1937) studied the equation).