2.1

PDE perspective derivation

density : # per unit of area

concentration : # per unit of volume

non-uniform distribution $\Rightarrow$ idealization

does it look uniform at a certain scale ?

example : cars on a highway $\leftarrow$ 1-dim

u density $u(t,x) = \frac{\#\text{ cars}}{\text{km}}$

c speed $c(x) = \frac{\text{km}}{\text{hour}}$

J flux $c(x)\,u(t,x) = \frac{\#\text{ cars}}{\text{hour}}$ thas pass x from left to right

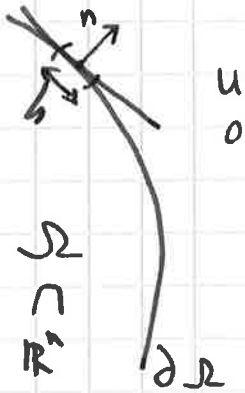
no creaction, no destruction only redistribution

conservation law $\quad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(cu) = 0$

derivation $\quad \underset{a}{\overset{J}{\rightarrow}}\!\!\text{———}\!\!\underset{b}{\overset{J}{\rightarrow}} \quad \frac{d}{dt}\int_a^b u(t,\xi)\,d\xi = J(t,a) - J(t,b)$

Now $J(t,a) - J(t,b) = -\int_a^b \frac{\partial J}{\partial x}(t,\xi)\,d\xi$

Hence $\int_a^b \left(\frac{\partial u}{\partial t} + \frac{\partial J}{\partial x}\right) d\xi = 0$. Arbitrariness of a,b $\square$



unit vector n outward pointing

$\frac{\text{number}}{\text{time}}$ passing $\partial\Omega$ from inside to outside in a small neighbourhood of size h $(\dim h = (\text{length})^{n-1})$

$= J \cdot n\, h + o(h)$ as $h \downarrow 0$

2.2 **Gauss-Green formula** $\int_\Omega \frac{\partial v}{\partial x_i}\, dx = \int_{\partial\Omega} v\, n_i\, ds$

Divergence $\nabla \cdot J = \sum_{i=1}^{n} \frac{\partial J_i}{\partial x_i}$

Divergence Theorem $\int_\Omega \nabla \cdot J\, dx = \int_{\partial\Omega} J \cdot n\, ds$

conservation law $\frac{\partial u}{\partial t} + \nabla \cdot J = 0$

deterministic motion (transport, drift)

$$J(t,x) = c(x)\, u(t,x)$$

scalar

vector: velocity ~ speed + direction

1855 Physiologist Fick
1822 Fourier heat flow (based on Newton's law of cooling)

$$J(t,x) = -d(x)\, \nabla u(t,x) \qquad \begin{pmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_n} \end{pmatrix} = \nabla u$$

diffusion coefficient

gradient

$$\frac{\#}{\text{time}\,(\text{length})^{n-1}} = \dim d \, \frac{\#}{(\text{length})^{n+1}} \implies \dim d = \frac{(\text{length})^2}{\text{time}}$$

~~Side remark~~ Now the divergence theorem yields $\underbrace{\frac{\partial u}{\partial t} = \nabla \cdot (d \nabla u)}_{\text{divergence form of diffusion equation}}$

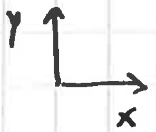
and, if d is constant: $\frac{\partial u}{\partial t} = d\, \Delta u$

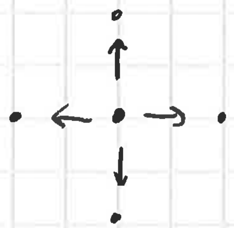
Side remark: $\int_\Omega \Delta u = \int_{\partial\Omega} \frac{\partial u}{\partial n}$

2.3 Section 4.2 Various ways to motivate Fick's Law

two-dim anisotropic random walk ← (not in text)

lattice

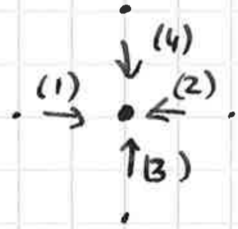




vertical prob. $\frac{1-q}{4}$ $q \in (-1,1)$

horizontal prob. $\frac{1+q}{4}$

distance λ time interval τ



$$u(t+\tau, x, y) = \frac{1+q}{4} u(t, x-\lambda, y)$$
$$+ \frac{1+q}{4} u(t, x+\lambda, y) + \frac{1-q}{4} u(t, x, y-\lambda) + \frac{1-q}{4} u(t, x, y+\lambda)$$

$$\text{lhs} = \cancel{u(t,x,y)} + \tau \frac{\partial u}{\partial t}(t,x,y) + O(\tau^2)$$
$$\text{rhs} = \frac{1+q}{2} \cancel{u(t,x,y)} + \frac{1+q}{4} 2 \frac{\lambda^2}{2} \frac{\partial^2 u}{\partial x^2}(t,x,y) + O(\lambda^4)$$
$$+ \frac{1-q}{2} \cancel{u(t,x,y)} + \frac{1-q}{4} 2 \frac{\lambda^2}{2} \frac{\partial^2 u}{\partial y^2}(t,x,y) + O(\lambda^4)$$

by symmetry, odd derivative terms cancel

Limit $\tau \downarrow 0$, $\lambda \downarrow 0$, $\frac{\lambda^2}{\tau} \frac{1+q}{4} \to d_1$, $\frac{\lambda^2}{\tau} \frac{1-q}{4} \to d_2$

So NB that speed $\frac{\lambda}{\tau} \to \infty$

$$\frac{\partial u}{\partial t} = d_1 \frac{\partial^2 u}{\partial x^2} + d_2 \frac{\partial^2 u}{\partial y^2}$$

D.G. Aronson Skellam revisited

general form $d_1 \frac{\partial^2 u}{\partial x^2} + 2 d_m \frac{\partial^2 u}{\partial x \partial y} + d_2 \frac{\partial^2 u}{\partial y^2}$

with matrix $\begin{pmatrix} d_1 & d_m \\ d_m & d_2 \end{pmatrix}$ positive definite, i.e.

$$(x_1\ x_2) \begin{pmatrix} d_1 & d_m \\ d_m & d_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} > 0 \quad \forall \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Leftrightarrow \text{all ev. of matrix are positive}$$

2.4 / Connection between PDE and Stochastic perspective : see vi

Consider $\frac{\partial u}{\partial t} = d \Delta u$ on all of $\mathbb{R}^n$ (so no b.c.)

Fundamental Solution

§ 5.1

$$\Phi(t,x) = \frac{1}{(4\pi d t)^{n/2}} e^{-\frac{|x|^2}{4td}}$$

Gauss distribution with mean zero, variance 2td

i) $\int_{\mathbb{R}^n} \Phi(t,x)\,dx = 0$ for all $t>0$ $\Leftarrow$ unit mass

ii) $\lim_{t \downarrow 0} \Phi(t,\cdot) = \delta$ Dirac in the sense of distributions

iii) interpretation — prob. distr. for one particle / density of particles

(iv) self-similar, i.e., invariant under scaling

$x = \varepsilon x^*$ $\quad t = \varepsilon^2 t^*$ $\quad \Phi = \frac{1}{\varepsilon^n} \Phi^*$ $\quad \int \Phi\, dx = \int \Phi^* dx^*$

v) building block for superposition

$$u(t,x) = \int_{\mathbb{R}^n} \Phi(t, x-y)\, u_0(y)\, dy$$

vi) $Q_t(x, \Gamma) = \int_\Gamma \Phi(t, y-x)\, dy$

space is homogeneous, so only the relative position $y-x$ matters; in fact only the distance $|y-x|$ since there is also isotropy

2.5 vii) $n=1$ $\Omega = [0,\infty)$ b.c. $u=0$ in $x=0$ fund. sol.

$$\Phi(t, x-y) - \Phi(t, x+y)$$

which corresponds to extending u_0 to $(-\infty,\infty)$ according to

$$u_0(-y) = -u_0(y) \qquad \text{odd}$$

If the b.c. is $u'=0$ in $x=0$ then fund. sol.

$$\Phi(t, x-y) + \Phi(t, x+y)$$

which corresponds to extending u_0 to $(-\infty,\infty)$ according to

$$u_0(-y) = u_0(y) \qquad \text{even}$$

viii) Note that $\Phi > 0$ for arbitrarily large $|x|$, no matter how small $t>0$

$\Rightarrow$ infinite speed of propagation

<u>but</u> Gaussian is <u>extremely small</u> for large $|x|$!

Ignoring the normalizing first factor, we can postulate that

$$\frac{|x|^2}{4td} = \text{constant}$$

tells us where particles arrive in reasonable quantities in time interval of length t

Rule of Thumb

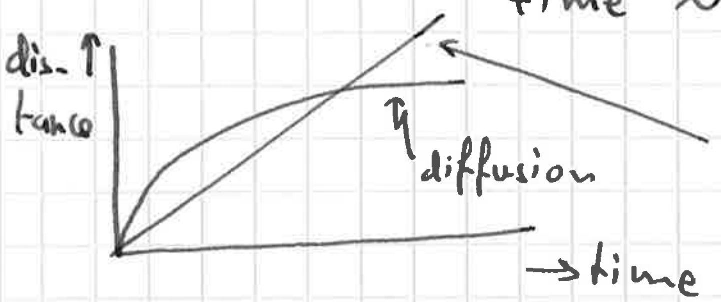
Physical aspects of diffusion

"particles" undergoing diffusion travel

distance $\sim \sqrt{dt}$ in time t

so they need

time $\sim \dfrac{|x|^2}{d}$ to travel over distance $|x|$



deterministic transport: dist = speed · time

Corollary provided there is a surplus of particles (e.g., messenger molecules) diffusion is a very efficient transport mechanism for small distances, but very inefficient for large distances

- circulatory blood system for active transport, but very last part of transport often by diffusion
- neurotransmitter diffuses across a small gap (called synapse) between two neurons
- a virus in a host has no need for active transport

Exercise Section 4.4 How to determine the diffusion coefficient experimentally?

General observation Section 4.5 $N = F\tau$

steady situation

N: amount present

F: amount that enters per unit of time

τ: expected sojourn time

2.7 / Section 4.6 How long does it take, on average, to cover distance x ?

steady state $\left.\begin{array}{l} d\frac{d^2u}{dx^2}=0 \\ u(0)=0 \\ u(L)=u_0 \end{array}\right\} \Rightarrow u(x) = u_0\frac{x}{L}$

$\Rightarrow J_{in}$ = influx $= -d\frac{du}{dx}\Big]_{x=L}$

$= d\frac{u_0}{L}$

$$N = \int_0^L u(x)dx = \frac{u_0}{L}\left[\tfrac{1}{2}x^2\right]_0^L = \frac{u_0 L}{2}$$

independence

$$\tau = \frac{N}{J_{in}} = \frac{\cancel{u_0}L}{2}\,\frac{L}{d\cancel{u_0}} = \frac{L^2}{2d}$$

Example: small molecule in air $d \approx 10^{-5}\frac{m^2}{sec}$

room of 5 m $\Rightarrow \tau \approx \frac{25}{2}10^5$ sec $\approx 14\frac{1}{2}$ day

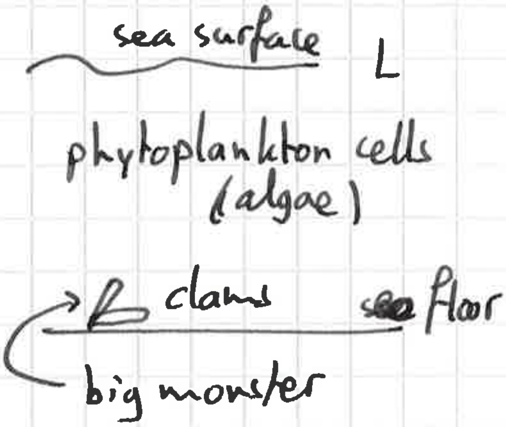
But turbulent air motion enhances the diffusion coeff. by approx. a factor 10^4 (still 2 min ?)

NB dimension ($n=1,2,3$) and shape are important too

diffusion along membrane

Macrophages use chemical clues to actively "hunt" bacteria $\Leftarrow$ chemotaxis (Edelstein-Keshet)

A very similar problem



$T(x)$ = expected time till absorption at $x=0$

Claim $0 = 1 + d\,T''(x)$

$T(0)=0 \quad T'(L)=0$ (reflecting)

2.8

consistency $T(x) = t + \int_{-\infty}^{\infty} \Phi(t, y-x)\, T(y)\, dy + o(t)$

$\Rightarrow \quad 0 = 1 + d \int_{-\infty}^{\infty} [\Phi(t, y-x)]_{xx \leftarrow yy}\, T(y)\, dy$ integrate by parts twice and let $t \downarrow 0$

<u>solution</u> $T(x) = \frac{x}{d}\left(L - \frac{x}{2}\right)$ max for $x = L$: $\frac{L^2}{2d}$ see above

For $x = \frac{L}{2}$: $T = \frac{3L^2}{8d}$ vertical eddy diffusivity in the ocean's mixed Layer $\approx 10^{-4} \frac{m^2}{sec}$

$L \approx 10\ m \Rightarrow \approx 4$ days

2.9

Appendix

Fundamental solution   self-similar   scale invariant

$$u(t,x) = \lambda^{\alpha} u(\lambda t, \lambda^{\beta} x) \qquad \lambda > 0 \qquad (\lambda \to \xi)$$

Choose $\lambda = t^{-1} \Rightarrow$ function of one-variable $t^{-\beta}x$

$$u(t,x) = t^{-\alpha}\phi(t^{-\beta}x)$$

$$\frac{\partial u}{\partial t}(t,x) = -\alpha t^{-\alpha-1}\phi(t^{-\beta}x) + t^{-\alpha}\phi'(t^{-\beta}x)\left(-\beta t^{-\beta-1}x\right)$$

$$\frac{\partial u}{\partial x}(t,x) = t^{-\alpha}\phi'(t^{-\beta}x)\, t^{-\beta} \Rightarrow \frac{\partial^2 u}{\partial x^2}(t,x) = t^{-\alpha-2\beta}\phi''(t^{-\beta}x)$$

$$\frac{\partial u}{\partial t} = d\frac{\partial^2 u}{\partial x^2} \Leftrightarrow -\alpha t^{-1}\phi(\xi) - \beta t^{-1}\xi\phi'(\xi) = d\, t^{-2\beta}\phi''(\xi) \qquad \xi := t^{-\beta}x$$

choose $\beta = \frac{1}{2} \Rightarrow$ factor t^{-1} drops out

$$d\,\phi''(\xi) + \tfrac{1}{2}\xi\phi'(\xi) + \alpha\phi(\xi) = 0$$

$$1 = \int_{-\infty}^{\infty} u(t,x)\,dx = t^{-\alpha}\int_{-\infty}^{\infty}\phi(t^{-\frac{1}{2}}x)\,dx = t^{\frac{1}{2}-\alpha}\int_{-\infty}^{\infty}\phi(\xi)\,d\xi \Rightarrow \text{choose } \alpha = \tfrac{1}{2}$$

$$d\,\phi''(\xi) + \frac{d}{d\xi}\left[\tfrac{1}{2}\xi\phi(\xi)\right] = 0 \Rightarrow d\,\phi'(\xi) + \tfrac{1}{2}\xi\phi(\xi) = \text{const.}$$

symmetry $x \to -x \Rightarrow \phi'(0) = 0 \Rightarrow$ const $= 0$

$$\Rightarrow \phi(\xi) = A e^{-\frac{\xi^2}{4d}} \qquad \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{4d}}\,d\xi = 2\sqrt{\pi d}$$

$\Rightarrow$ choose $A = \dfrac{1}{2\sqrt{\pi d}}$

$$\Rightarrow u(t,x) = \frac{1}{2\sqrt{\pi d t}}\, e^{-\frac{x^2}{4dt}}$$