5/26/04

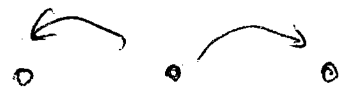
lecture 4

Spatial patterns / waves

- Spatial patterns in development
  Ca waves in fly embryo
- diffusion equation
  random walk / diffusion
  a simple solution of 1D diffusion eq.
  time scale, No wave possible
- reaction - diffusion eq.
  Fisher - kolmogoroff eq.
    the derivation of Fisher
      logistic growth
      spread of disease
      auto catalysis
  Analysis of Fisher - kolmogoroff eq.
    traveling wave solution
    phase plane analysis / minimum speed
    initial condition dependence
    shape of ~~the~~ wave
    simple argument on speed

diffusion / random walk

△ random walker in 1D



each step size l

N steps

typical distance traveled d.

$$x = x_1 + x_2 + \cdots x_N$$

where $x_i = \pm l$ equal prob.

$$\overline{x} = \overline{x_1} + \overline{x_2} + \cdot \overline{x_N} = 0$$

$$\overline{x^2} = \overline{\left(\sum x_i\right)^2} = \sum_i \sum_j \overline{x_i x_j}$$

$$= N \sum_i \overline{x_i^2} = N l^2$$

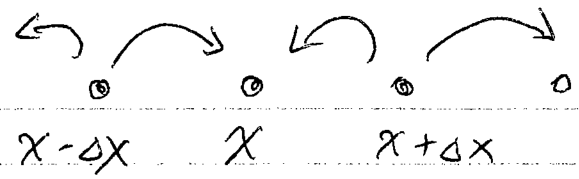
typical distance

$$d = \sqrt{\overline{x^2}} = N^{1/2} l$$

△ diffusion eq.

1D lattice, population

$u(x,t)$ particle density at position x and time t



$$u(x, t+\Delta t) = \frac{1}{2}\left[u(x+\Delta x, t) + u(x-\Delta x, t)\right]$$

$$u(x,t) + \frac{\partial u}{\partial t}\Delta t$$ partial derivative hold x fixed

$$= \frac{1}{2}\Big[u(x,t) + \frac{\partial u}{\partial x}(x,t)\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 + \cdots$$

$$+ u(x,t) - \frac{\partial u}{\partial x}(x,t)\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 \cdots$$

$$= \frac{1}{2}\cdot 2u(x,t) + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2$$

$$\frac{\partial u}{\partial t} = \frac{\Delta x^2}{2\Delta t}\frac{\partial^2 u}{\partial x^2}$$

define

$$D = \frac{\Delta x^2}{2\Delta t}$$

diffusion coefficient

$$\boxed{\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}}$$ diffusion equation

can also be obtained by using

Fick's law $J = -D\dfrac{\partial u}{\partial x}$

and mass conservation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}J = 0$$

$\triangle$ existence of diffusion coefficient

$$D = \frac{\Delta x^2}{2\Delta t} \quad \Delta t \to 0 \quad \text{exist}$$

when $\tau \ll \Delta t \ll t$

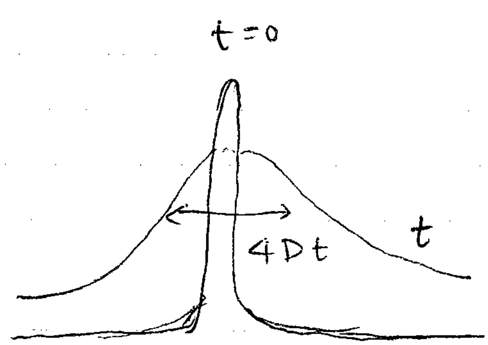
where τ is the microscopic time scale on which particle change its direction due to random collision

l : typical length particle travel before changing direction

$$\Delta x^2 = N l^2, \quad N = \frac{\Delta t}{\tau}$$

$$\Delta x^2 = \frac{\Delta t}{\tau} l^2, \quad \frac{\Delta x^2}{\Delta t} \to \frac{l^2}{\tau}$$

$\triangle$ a typical solution of 1D diffusion eq.



start with concentration concentrated at $x=0$

$$u(x, t=0) = \delta(x)$$

what's the solution $u(x,t)$?

dimensional analysis

length scale : $\begin{cases} x \\ \sqrt{Dt} \end{cases}$

$$u(x,t) = \frac{1}{\sqrt{Dt}}\, g\left(\frac{x}{\sqrt{Dt}}\right) = \frac{1}{\sqrt{Dt}}\, g(z)$$

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \qquad z = \frac{x}{\sqrt{Dt}}$$

$$\downarrow$$

$$-\tfrac{1}{2} t^{-3/2}\frac{1}{\sqrt{D}}\, g(z) + \frac{1}{\sqrt{Dt}}\, g'(z)\,\frac{x}{\sqrt{D}}\left(-\tfrac{1}{2}t^{-3/2}\right)$$

$$= D\cdot g''(z)\,\frac{1}{Dt}\cdot\frac{1}{\sqrt{Dt}}$$

$$g''(z) + \frac{1}{2}g(z) + \frac{1}{2}z\,g'(z) = 0$$

$$\frac{d}{dz}\left[g'(z) + \frac{1}{2}z\,g(z)\right] = 0$$

$$g'(z) + \frac{1}{2}z\,g(z) = A \rightarrow \text{const}$$

$z=0$, $g'(z)=0$, (symmetric)

$\hookrightarrow A = 0$

$$\frac{g'(z)}{g(z)} = -\frac{1}{2}z$$

$$g(z) = \text{const} \cdot e^{-\frac{z^2}{4}}$$

$$u(x,t) \propto \frac{1}{\sqrt{Dt}} e^{-\frac{x^2}{4Dt}}$$

normalization $\int_{-\infty}^{+\infty} u(x,t)\,dx = 1$

↓

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

⟶ can be obtained from random walker model + central limit theorem

given time t,

particle diffuse to a region of size $\sim \sqrt{Dt}$

△ time scale estimate

given length L

time it takes to diffuse

$$t \sim \frac{L^2}{D}$$

$D \sim 0.1 \times 10^{-9}\ m^2/s$, $L \sim 1mm$ fly egg

for Ca in cytoplasm

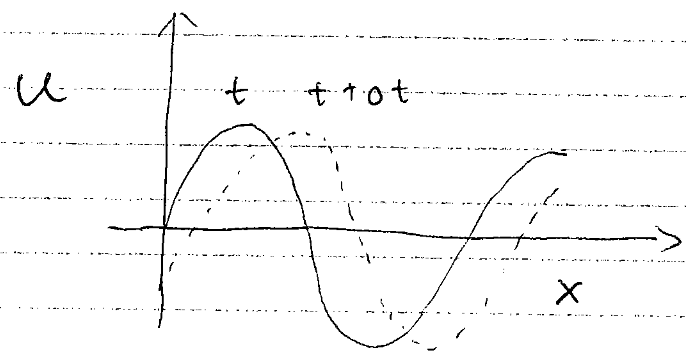
$$t \sim \frac{(1\ mm)^2}{0.1 \times 10^{-9}\ m^2/s} \sim 3 \text{ hours}$$

in general, diffusion is too slow for signal propagation

△ diffusion eq does not have traveling wave solution

a general traveling wave

$u(x,t) = u(z) = u(x - ct)$



e.g. sine wave

$u = A \sin(kx - \omega t)$

if $u = u(x - ct)$

$$D \frac{d^2 u}{dz^2} + c \frac{du}{dz} = 0$$

$$u = A + B e^{-\frac{c}{D} z}$$

to be bounded as $z \to -\infty$

$B = 0$

u is uniform everywhere

reaction - diffusion eq.

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u) \rightarrow \text{growth term}$$

△ Fisher - kolmogoroff eq.

Advance of advantageous genes

allele A_1 : p advantageous

A_2 : q

Genotype	$A_1 A_1$	$A_1 A_2$	$A_2 A_2$
	p^2	$2pq$	q^2
relative fitness	1	$1-\frac{s}{2}$	$1-s$
freq after selection	$\frac{p^2}{\bar{w}}$	$\frac{2pq(1-s/2)}{\bar{w}}$	$\frac{q^2(1-s)}{\bar{w}}$

$$\bar{w} = p^2 + 2pq(1-s/2) + q^2(1-s)$$

normalization

$$= 1 - pqs - q^2 s$$

after selection

$$p' = \frac{p^2}{\bar{w}} + \frac{pq(1-s/2)}{\bar{w}}$$

(A_1A_2 has only one A_1 allele)

$$\Delta p = p' - p$$

$$= \frac{p - \frac{pqs}{2}}{1 - pqs - q^2 s} - p \approx \frac{1}{2}pqs$$

$$\frac{dp}{dt} = \frac{s}{2\Delta t} p(1-p) \equiv k p(1-p)$$

$$\downarrow$$

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + k u(1-u)$$

⚠ Fisher eq. in other context

* auto-catalysis

$$A + B_0 \underset{k_R}{\overset{k_F}{\rightleftharpoons}} A + A$$

$$\frac{d[A]}{dt} = k_F [A][B_0] - k_R [A]^2$$

$$= k_F [A][B_0] \left(1 - \frac{k_R [A]}{k_F [B_0]}\right)$$

$$u = \frac{[A]}{[B_0]} \frac{k_R}{k_F}$$

$$\frac{du}{dt} = k_F [B_0] u(1-u)$$

$$\equiv k u(1-u)$$

* logistic growth
species invasion

$$\frac{dn}{dt} = kn\left(1 - \frac{n}{N}\right)$$ — growth

\# disease propagation

$$\frac{dS}{dt} = \alpha S H = \alpha S (T - S)$$

total

sick   Heathy

(a) behavior of Fisher - kolmogoroff eq.

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + k u (1-u)$$

dimensions: $[k] = \frac{1}{[T]}$

$$[D] = \frac{[L]^2}{[T]}$$

$$\left[\sqrt{\frac{D}{k}}\right] = [L]$$

$t' \Rightarrow kt$

$x' \rightarrow x\sqrt{\frac{k}{D}}$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u)$$

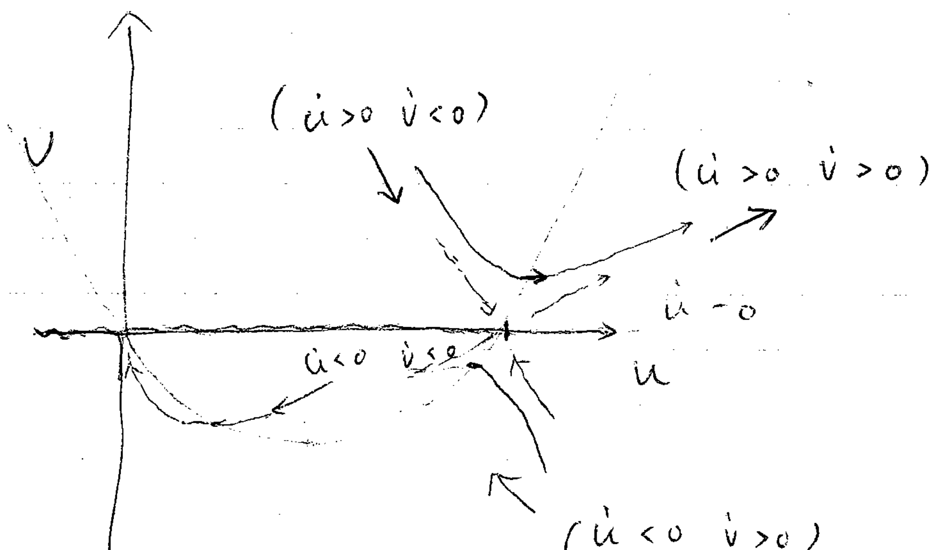
traveling wave solution

$$u = u(x-ct) = u(z)$$

$$-c\frac{du}{dz} = \frac{d^2 u}{dz^2} + u(1-u)$$

$$\boxed{\begin{aligned}\dot{u} &= v \\ \dot{v} &= -cv - u(1-u)\end{aligned}}$$

phase plane analysis



$\dot{u} = 0 \longrightarrow v = 0$ null-cline

$\dot{v} = 0 \qquad v = -\frac{1}{c}u(1-u)$

stability analysis

$$J = \begin{bmatrix} \frac{\partial \dot{u}}{\partial u} & \frac{\partial \dot{u}}{\partial v} \\ \frac{\partial \dot{v}}{\partial u} & \frac{\partial \dot{v}}{\partial v} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 2u-1 & -c \end{bmatrix}$$

evaluated at $(0, 0)$

$$J = \begin{bmatrix} 0 & 1 \\ -1 & -c \end{bmatrix} \qquad Tr = -c \qquad \Delta = 1$$

$$\lambda_{1,2} = \frac{Tr \pm \sqrt{Tr^2 - 4\Delta}}{2} = \frac{-c \pm \sqrt{c^2 - 4}}{2}$$

$(0, 0)$ is stable node $c^2 > 4$

stable spiral $c^2 < 4$

evaluated at $(1, 0)$

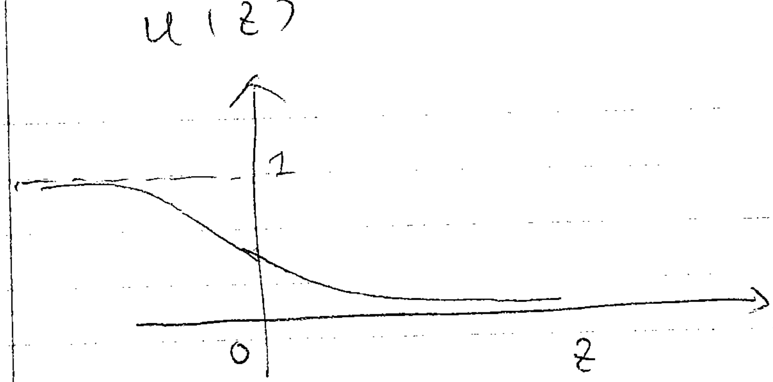
$$J = \begin{bmatrix} 0 & 1 \\ 1 & -c \end{bmatrix} \qquad Tr = -c \qquad \Delta = -1$$

$$\lambda_{1,2} = \frac{-c \pm \sqrt{c^2 + 4}}{2} \qquad \lambda_1 > 0, \quad \lambda_2 < 0$$

saddle point

when $(0, 0)$ is stable spiral, solution unphysical as u becomes negative

when $(0, 0)$ is stable node there is one unique trajectory connecting $(1, 0) \to (0, 0)$



solution for the wave front

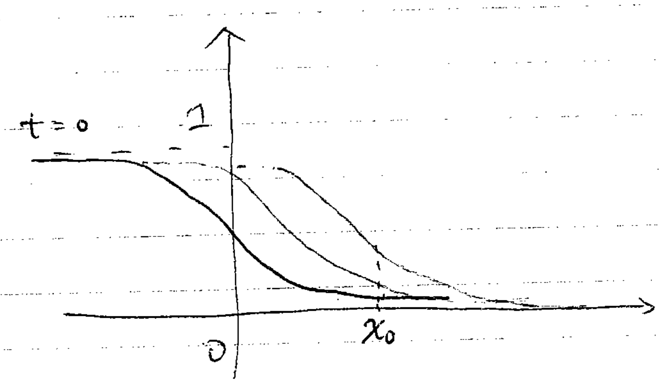
* minimum wave speed

$c \geq 2$

in term of original parameter

$c \geq 2\sqrt{KD}$

traveling wave



simple argument for wave speed

time it takes to grow a wave front $x_0 \to u \approx \frac{1}{2}$

$\sim \frac{1}{K}$

when $u(x_0) \sim \frac{1}{2}$

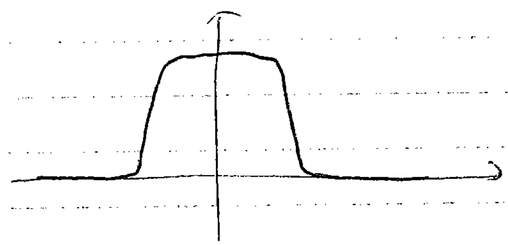
the new wave front diffused to $\sqrt{\frac{D}{K}}$

wave speed $\sqrt{\frac{D}{K}} / \frac{1}{K} \sim \sqrt{DK}$

* dependence of wave speed on initial conditions

if initially only a finite domain $u = 1$, $\rightarrow$ $c = c_{min}$

$= 2\sqrt{KD}$



if initially $u(x, 0) \sim Ae^{-ax}$

and $a < 1$

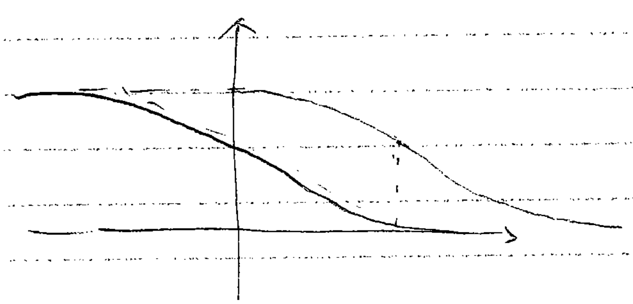
$u(x, t) = Ae^{-a(x-ct)}$ for the wave front

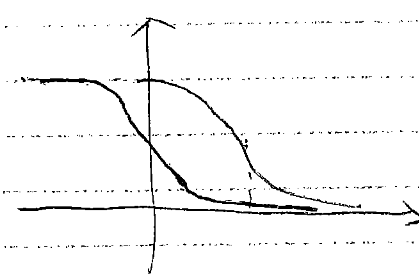
ignore nonlinear term

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

$$ca = 1 + a^2 \qquad c = a + \frac{1}{a}$$

flatter wave, faster speed





reaction-diffusion eq. are
widely used for modeling waves

e.g. with growth term

$$f(u) = Au(1-u)(u-c)$$

model Ca waves

Fitzhugh-Nagumo eq.

to model action-potential
propagation in a nerve axon