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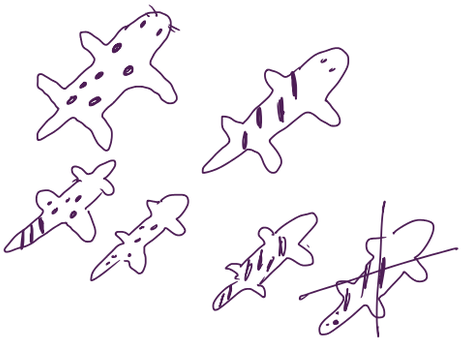
Chapter 1
The reaction-diffusion systems



Ref: JAMES MURRAY
MATHEMATICAL BIOLOGY

In a biological context, they have been introduced by ALAN TURING (1952) to study morphogenesis (start of the forms) where forms seem to appear out of "nothing" (ex: somitogenesis) clock and wavefronts

Turing showed that these types of form appearances occur in "very simple" systems like chemical mixes submitted to diffusion and reaction

These forms or structures are called Turing <u>patterns</u> and they have been used since the 1970's in a large number of biomaths works!
The mathematical modelling is a little bit abstract but we'll see it as a simplified model allowing to understand the basic organisation (or self-organisation) of a complex system.

For this purpose, we will use what we call reaction-diffusion systems.

<u>Question</u>: what are reaction diffusion systems?

TURING
- ① single equation
  - ⓐ diffusion only
  - ⓑ reaction diffusion
- ② system of 2 equations
- ③ Travelling waves / fronts

1. <u>Diffusion</u>

The "classical" equation of diffusive phenomena is:

$$\frac{\partial}{\partial t} u(t,x) = d \cdot \Delta u(t,x)$$: heat equation introduced by <u>FOURIER</u>

u : quantity that diffuses

t : time $(t \geq 0)$

x : space $x \in \Omega$, Ω: domain $(\Omega \subset \mathbb{R}, \mathbb{R}^2, \mathbb{R}^3)$

$\frac{\partial}{\partial t}$: partial derivative with respect to time

Δ : diffusion operator LAPLACIAN

in 1D: $\Delta u(t,x) = \frac{\partial^2}{\partial x^2} u(t,x)$

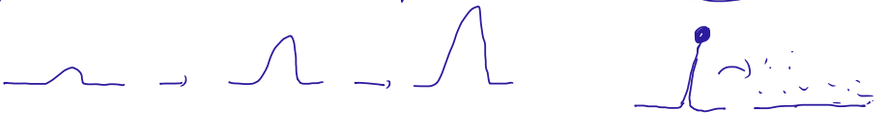
$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ in 2D $\Delta u(t,x) = \frac{\partial^2}{\partial x_1^2} u(t,x) + \frac{\partial^2}{\partial x_2^2} u(t,x)$

d : $d > 0$ diffusion coefficient

<u>what is diffusion?</u> it is a phenomenon for which "the flux is proportional to the gradient"

so diffusion "flattens" the "bumps" a fast a d and the gradient are large.

<u>Remark</u>: if $d < 0$ we call the phenomenon: <u>concentration</u>



heat equation: $\frac{\partial}{\partial t} u(t,x) = d \, \Delta u(t,x)$

in 1D $\frac{\partial}{\partial t} u(t,x) = d \cdot \frac{\partial^2}{\partial x^2} u(t,x)$

① <u>Conditions</u>

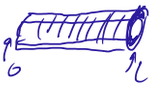
For the problem to be complete, it is necessary to specify what are: ⓐ - <u>the initial condition</u> : $u(0,x) \in \Omega$ $(u(t=0,x))$

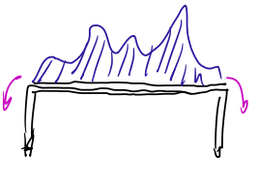
ⓑ - the <u>boundary conditions</u> for 1D: $\Omega = [0,L]$ $(L>0)$

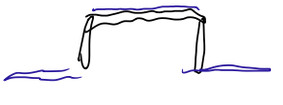
There exist 2 very well known boundary conditions:

ⓘ <u>DIRICHLET</u> homogeneous conditions:

$u(t,0) = u(t,L) = 0$





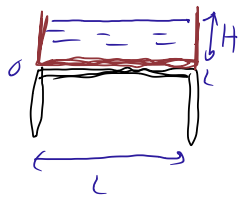


$\lim_{t \to +\infty} u(t,x) = 0$

② NEUMANN homogeneous conditions

$$\frac{\partial}{\partial x} u(t,0) = \frac{\partial}{\partial x} u(t,L) = 0$$

$\rightsquigarrow$



$$\lim_{t \to +\infty} u(t,x) = K = \int_0^L u(t,x)\,dx$$

$$\int_0^L u(t,x)\,dx = L \cdot H \Rightarrow H = \frac{1}{L} \cdot \int_0^L u(t,x)\,dx$$

Summary: to summarize, we have now the full problem:

$$\frac{\partial}{\partial t} u(t,x) = d \cdot \Delta u(t,x)$$

$+ \quad u(0,x) = \underbrace{f(x)}_{\text{given}}$ initial condition

$+ \quad$ DIRICHLET $u(t,0) = u(t,L) = 0$

OR NEUMANN $\frac{\partial}{\partial x} u(t,0) = \frac{\partial}{\partial x} u(t,L) = 0$ } boundary conditions

How do we solve such a problem?
we need for that a mathematical tool: eigen functions (FONCTIONS PROPRES)

② Eigenfunctions

The eigenfunctions of the diffusion operator Δ (with boundary conditions) is a "shape" that is a function depending only on the space variable x, we denote it $\boxed{w(x)}$ such that

① w is 2 times differentiable (w', w'')

② w, w' and w'' are defined on $[0,L]$

③ w satisfies the boundary conditions: $w(0) = w(L) = 0$ (DIRICHLET)
or $w'(0) = w'(L) = 0$ (NEUMANN)

④ w cannot equal to 0 everywhere
($w \not\equiv 0$) (not identically equal to 0)

⑤ $\Delta w(x) = \lambda w(x)$, $\lambda \in \mathbb{R}$

(when applying diffusion on w you do not modify the shape, you just shrink or enlarge it.

λ is called: the eigen value associated to w.

Exercise : what are the eigenfunctions of Δ with DIRICHLET conditions?

we look for functions satisfying:
- w, w', w'' exist on $[0,L]$
- $w \not\equiv 0$
- $w(0) = w(L) = 0$
- $\Delta w(x) = \lambda w(x)$, $\lambda \in \mathbb{R}$

that is $\boxed{w''(x) = \lambda w(x)}$

second order equation:

we look for solutions of the form: e^{rx}, $r \in \mathbb{C}$.

$w(x) = e^{rx}$
$w'(x) = re^{rx}$
$w''(x) = r^2 e^{rx}$

$$w''(x) = \lambda w(x) \iff r^2 e^{rx} = \lambda e^{rx}$$
$$\iff (r^2 - \lambda) e^{rx} = 0 \quad \forall x \in [0,L]$$
$$\iff \boxed{r^2 = \lambda}$$

$\boxed{\text{CASE 1}}$ $\boxed{\text{if } \lambda > 0}$

then there are 2 possible r: $r_1 = \sqrt{\lambda}$ $\quad r_2 = -\sqrt{\lambda}$

Then all the solutions w are a (LINEAR) combinations of $e^{r_1 x}$ and $e^{r_2 x}$ that is:

$$w(x) = c_1 e^{r_1 x} + c_2 e^{r_2 x}$$

with the DIRICHLET CONDITIONS we GET:

- $w(0) = 0 \iff c_1 e^0 + c_2 e^0 = 0$
$$\iff c_1 + c_2 = 0$$
$$\iff \boxed{c_2 = -c_1}$$

thus: $w(x) = c_1 (e^{r_1 x} - e^{r_2 x})$ $\left(\begin{array}{l} r_1 = \sqrt{\lambda} \\ r_2 = -\sqrt{\lambda} \\ \lambda > 0 \end{array} \right) \longrightarrow r_1 = -r_2$

- $w(L) = 0 \iff c_1 (e^{r_1 L} - e^{r_2 L}) = 0$
$$\iff c_1 (e^{r_1 L} - e^{-r_1 L}) = 0$$
$$\iff \begin{cases} c_1 = 0 \\ \text{or} \\ e^{r_1 L} = e^{-r_1 L} \end{cases} \Rightarrow \cancel{w(x) = 0} \ \forall x \in [0,L] \quad w \not\equiv 0!$$

$\hookrightarrow e^{r_1 L} = \frac{1}{e^{r_1 L}} \iff (e^{r_1 L})^2 = 1$
$$\iff e^{r_1 L} = 1$$
$$\iff r_1 \underbrace{L}_{>0} = 0$$
$$\boxed{r_1 = 0} \Rightarrow \cancel{w(x) = 0}$$

$\lambda > 0 \Rightarrow$ does not imply the existence of an eigen function

$\boxed{\text{CASE 2}}$ $\boxed{\lambda = 0}$ then $w''(x) = 0$, $x \in [0,L]$, $L > 0$

that is $w'(x) = c_1$

and $w(x) = c_1 x + c_2$

To estimate c_1 and c_2 we use the Dirichlet conditions:

$w(0) = w(L) = 0$ $\qquad w(0) = 0 \Rightarrow c_1 \cdot 0 + c_2 = 0$
$$\iff \boxed{c_2 = 0}$$

Then $w(x) = c_1 x$ $\qquad w(L) = 0 \Rightarrow c_1 L = 0$ with $L > 0$

$\Rightarrow c_1 = 0 \Rightarrow w(x) = 0$ $(w \equiv 0)$ identically equal to

IMPOSSIBLE for an eigen function

$\boxed{\text{CASE 3}}$ $\boxed{\lambda<0}$ $\quad r^2 = \lambda = -|\lambda| = i^2|\lambda| \Rightarrow r = \pm i\sqrt{|\lambda|}$ $\quad r_1 = i\sqrt{|\lambda|}$, $r_2 = -i\sqrt{|\lambda|}$

$r_1 = \alpha + i\beta$
$r_2 = \bar{r}_1 = \alpha - i\beta$ $\Rightarrow u(x) = e^{\alpha x}\left(c_1\cos(\beta x) + c_2\sin(\beta x)\right)$

here $\alpha = 0$ and $\beta = \sqrt{|\lambda|}$ then

$$w(x) = c_1\cos(x\sqrt{|\lambda|}) + c_2\sin(x\sqrt{|\lambda|})$$

with the Dirichlet conditions:

$w(0) = 0$ then $c_1\cos(0) + c_2\sin(0) = 0$
$\Leftrightarrow c_1 \cdot 1 + 0 = 0$
$\Leftrightarrow \boxed{c_1 = 0}$

we have $w(x) = c_2\sin(x\sqrt{|\lambda|})$

$w(L) = 0 \Leftrightarrow \boxed{c_2\sin(L\sqrt{|\lambda|})} = 0$ → either $c_2 = 0 \Rightarrow w \equiv 0$ IMPOSSIBLE
→ $\sin(L\sqrt{|\lambda|}) = 0 \Leftrightarrow L\sqrt{|\lambda|} = k\pi$, $k \in \mathbb{Z}$

since $L > 0$, $\sqrt{|\lambda|} > 0$, $\pi > 0$ $\Big\} \Rightarrow k \in \mathbb{N}^*$ $\quad k \in \{1, 2, 3, \dots\}$

then: $\boxed{\sqrt{|\lambda|} = \frac{k\pi}{L}} \Rightarrow |\lambda| = \left(\frac{k\pi}{L}\right)^2$
$\Rightarrow -\lambda = \left(\frac{k\pi}{L}\right)^2$ ($\lambda < 0$)
$\Leftrightarrow \boxed{\lambda = -\left(\frac{k\pi}{L}\right)^2}$, $k \in \mathbb{N}^*$

$c_2\sin(L\sqrt{|\lambda|})$

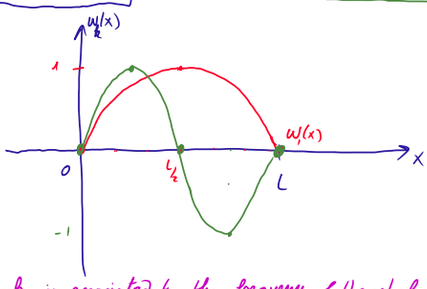
and $w(x) = c_2 \cdot \sin\left(\frac{k\pi x}{L}\right)$

since: $\Delta w(x) = \lambda w(x)$
$c_2 \neq 0$ $\quad c_2\Delta w(x) = \lambda c_2 w(x)$
$\Leftrightarrow \Delta(c_2 w(x)) = \lambda(c_2 w(x))$

without any loss of generality we take $\boxed{c_2 = 1}$

then, there exist an infinite number of eigen functions

$\boxed{w_k(x) = \sin\left(\frac{k\pi x}{L}\right)}$, $k \in \mathbb{N}^*$ and $\boxed{\lambda_k = -\left(\frac{k\pi}{L}\right)^2}$



$k = 1$ $\quad w_1(x) = \sin\left(\frac{\pi x}{L}\right)$
$k = 2$ $\quad w_2(x) = \sin\left(\frac{2\pi x}{L}\right)$

Remark: k is associated to the frequency of the shape of w_k.
that is if k is large
if k is small

Exercise: what are the eigenfunctions of Δ with the NEUMANN conditions?

we look for function w such that
- w, w', w'' exist on $[0, L]$, $L > 0$
- $w \not\equiv 0$ on $[0, L]$
- $w'(0) = w'(L) = 0$
- $\Delta w(x) = \lambda w(x)$, $\lambda \in \mathbb{R}$
  $\Leftrightarrow w''(x) = \lambda w(x)$

Let $x \in [0, L]$ $\quad w''(x) = \lambda w(x)$

we look first for solutions of the form e^{rx} with $r \in \mathbb{C}$

that is $r^2 e^{rx} = \lambda e^{rx}$, for all $x \in [0, L]$
$\Leftrightarrow r^2 = \lambda$

$\boxed{\text{CASE 1}}$ $\boxed{\text{if } \lambda > 0}$ there are 2 solutions $r_1 = \sqrt{\lambda}$ and $r_2 = -\sqrt{\lambda}$ $\quad (r_1 = -r_2)$

then $w(x) = c_1 e^{r_1 x} + c_2 e^{r_2 x}$

with the Neumann conditions: $w'(x) = c_1 r_1 e^{r_1 x} + c_2 r_2 e^{r_2 x}$

$w'(0) = 0 \Rightarrow c_1 r_1 + c_2 r_2 = 0$

$\Leftrightarrow c_1 r_1 - c_2 r_1 = 0$

$\Leftrightarrow (c_1 - c_2) r_1 = 0$ $\nearrow r_1 \neq 0$ because $\lambda > 0$, $r_1 = \sqrt{\lambda} > 0$

$\Leftrightarrow \boxed{c_1 = c_2}$

then $w(x) = c_1 \left(e^{r_1 x} + e^{-r_1 x}\right)$

$w'(L) = 0 \Rightarrow c_1 r_1 e^{r_1 L} + c_1 (-r_1) e^{-r_1 L} = 0$

$\Rightarrow c_1 \underbrace{r_1}_{\neq 0} \left(e^{r_1 L} - e^{-r_1 L}\right) = 0$ $\nearrow c_1 = 0 \Rightarrow w \equiv 0$ IMPOSSIBLE

$\searrow e^{r_1 L} = e^{-r_1 L}$

$\Leftrightarrow e^{r_1 L} = \frac{1}{e^{r_1 L}}$

$\Leftrightarrow \left(e^{r_1 L}\right)^2 = 1$

$\Rightarrow \overset{>0}{r_1} \overset{>0}{L} = 0$ NOT POSSIBLE

so, the case $\lambda > 0$ does not accept eigenfunctions

$\boxed{\text{CASE 2: } \lambda = 0}$ $w''(x) = 0$

$\Rightarrow w'(x) = c_1$ $\longrightarrow$ $w'(0) = w'(L) = 0 \Rightarrow c_1 = 0$

$\Rightarrow w(x) = c_1 x + c_2$

so $\boxed{w(x) = c_2}$ $\rightarrow$ without any loss of generality we take $\boxed{c_2 = 1}$

so $\boxed{w_0(x) = 1}$ is one eigenfunction

$\boxed{\text{CASE 3: } \lambda < 0}$ $w''(x) = \lambda w(x)$

$r^2 = \lambda = -|\lambda| = i^2 |\lambda|$ $\Rightarrow r_1 = i\sqrt{|\lambda|}$ and $r_2 = \bar{r}_1 = -i\sqrt{|\lambda|}$

so $w(x) = c_1 \cos\left(x\sqrt{|\lambda|}\right) + c_2 \sin\left(x\sqrt{|\lambda|}\right)$

$w'(x) = -c_1 \cdot \sqrt{|\lambda|} \cdot \sin\left(x\sqrt{|\lambda|}\right) + c_2 \cdot \sqrt{|\lambda|} \cdot \cos\left(x\sqrt{|\lambda|}\right)$

if $x = 0$ $w'(0) = -c_1 \sqrt{|\lambda|} \cdot \underbrace{\sin(0)}_{0} + c_2 \underbrace{\sqrt{|\lambda|}}_{>0} \cdot \underbrace{\cos(0)}_{1} = 0 \Rightarrow \boxed{c_2 = 0}$

then $\boxed{w(x) = c_1 \cos\left(x\sqrt{|\lambda|}\right)}$

and $w'(L) = -c_1 \underbrace{\sqrt{|\lambda|}}_{>0} \sin\left(L\sqrt{|\lambda|}\right) = 0$

$\nearrow c_1 = 0$ $w \equiv 0$ NOT POSSIBLE

$\searrow \sin\left(L\sqrt{|\lambda|}\right) = 0 \Rightarrow L\sqrt{|\lambda|} = k\pi,\ k \in \mathbb{Z}$

since $\left.\begin{array}{l} L > 0 \\ \sqrt{|\lambda|} > 0 \\ \pi > 0 \end{array}\right\} \Rightarrow k = \frac{L \cdot \sqrt{|\lambda|}}{\pi} \in \mathbb{N}^*$

then $\sqrt{|\lambda|} = \frac{k\pi}{L}$ $\Rightarrow |\lambda| = \left(\frac{k\pi}{L}\right)^2$ $\Rightarrow -\lambda = \left(\frac{k\pi}{L}\right)^2$

$\Rightarrow \boxed{\lambda_k = -\left(\frac{k\pi}{L}\right)^2},\ k \in \mathbb{N}^*$

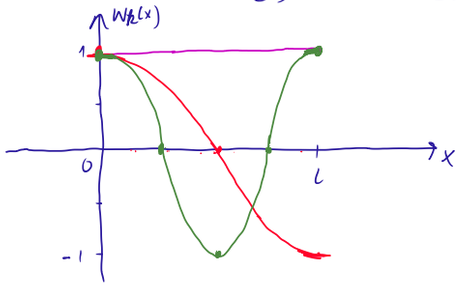
so $w_k(x) = c_2 \cos\left(\frac{k\pi x}{L}\right)$ $k \in \mathbb{N}^*$ we can take $c_2 = 1$ $\boxed{w_k(x) = \cos\left(\frac{k\pi x}{L}\right)}$

and $\boxed{\lambda_k = -\left(\frac{k\pi}{L}\right)^2}$

To summarize: eigenfunctions of Δ with NEUMANN:

are $\begin{cases} w_0(x) = 1 & , \lambda_0 = 0 \\ w_k(x) = \cos\left(\frac{k\pi x}{L}\right), k \in \mathbb{N}^*, & \lambda_k = -\left(\frac{k\pi}{L}\right)^2 \end{cases}$

we can write: $w_k(x) = \cos\left(\frac{k\pi x}{L}\right)$, $\lambda_k = -\left(\frac{k\pi}{L}\right)^2$ with $k \in \mathbb{N}$ ← no * !!



$k = 0$ $w_0(x) = 1$

$k = 1$ $w_1(x) = \cos\left(\frac{\pi x}{L}\right)$

$k = 2$ $w_2(x) = \cos\left(\frac{2\pi x}{L}\right)$

③ Solving the heat equation

ⓐ If the initial condition $u(0,x)$ is an eigenfunction of Δ, w_k

$$(E) \begin{cases} \frac{\partial}{\partial t} u(t,x) = d \cdot \Delta u(t,x) & t \geq 0,\ x \in [0,L] \\ u(0,x) = w_k(x) \ (*) & x \in [0,L] \\ + \text{ boundary conditions (Dirichlet or Neumann)} \end{cases}$$

Remark: since $u(0,x)$ is an eigenfunction, the solution $u(t,x)$ will evolve in time without changing its shape that is:
we look for solutions of the form $u(t,x) = \alpha(t) \cdot w_k(x)$
(that is called method of separation of variables).
Let's replace it in (E):

$$\frac{\partial}{\partial t}(\alpha(t)\, w_k(x)) = d \cdot \Delta(\alpha(t)\, w_k(x))$$

$$\Leftrightarrow \quad w_k(x) \cdot \frac{\partial}{\partial t}\alpha(t) = d \cdot \alpha(t) \cdot \Delta w_k(x) \quad \rightsquigarrow \quad \Delta w_k(x) = \lambda w_k(x)$$

$$\Leftrightarrow \quad \cancel{w_k(x)} \cdot \alpha'(t) = d \cdot \lambda_k\, \alpha(t)\, \cancel{w_k(x)}$$

$$\Leftrightarrow \quad \alpha'(t) = d\lambda_k\, \alpha(t)$$

$$\Leftrightarrow \quad \alpha(t) = K \cdot e^{d \cdot \lambda_k \cdot t} \qquad t \geq 0 \qquad d > 0 \qquad \lambda_k \leq 0$$

Then $\boxed{u(t,x) \underset{(**)}{=} K e^{d\lambda_k t} w_k(x)}$

$$u(0,x) \underset{(*)}{=} w_k(x) \underset{\substack{(**)\\ t=0}}{=} K w_k(x) \quad \Rightarrow \quad K = 1$$

$$\boxed{u(t,x) = e^{d \cdot \lambda_k t} w_k(x)}$$

Remark: ① eigenfunctions and eigenvalues:

for any dimension (1D, 2D, 3D, ...) with all the standard boundary conditions we could show that there exist an infinite number of eigenfunctions denoted $(w_0), w_1, w_2, w_3, \ldots$
associated with eigenvalues $(\lambda_0), \lambda_1, \lambda_2, \ldots$ always ≤ 0
And we start to tag them starting with the greatest one:

$$0 \geq \lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3 \ldots$$

And $k \in \mathbb{N}$ or $\mathbb{N}^*$ is associated to the frequency of the eigenfunction.

② the solution of the heat equation when $u(0,x) = w_k(x)$
is $u(t,x) = e^{d \cdot \lambda_k t} w_k(x)$

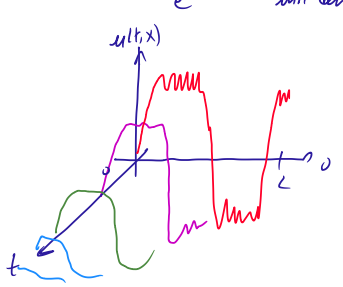
if NEUMANN and if $k=0$ then $u(t,x) \xrightarrow[t \to +\infty]{} e^0 \cdot 1 = 1$

if $\left\{ \begin{array}{l} \text{"} \\ \text{DIRICHLET} \end{array} \right.$ " $k > 0$ $\quad u(t,x) = e^{d \cdot \underbrace{\lambda_k}_{<0} t} w_k(x) \xrightarrow[t \to +\infty]{} 0$

③ If initial condition $u(0,x)$ is a mix of 2 eigenfunctions

$$u(0,x) = \alpha_{k_1} w_{k_1}(x) + \alpha_{k_2} w_{k_2}(x)$$

Then, thanks to the superposition principle

$$u(t,x) = \alpha_{k_1} e^{d\lambda_{k_1} t} w_{k_1}(x) + \alpha_{k_2} e^{d\lambda_{k_2} t} w_{k_2}(x)$$

Remark: this can be generalized to the sum of any linear combination of eigenfunctions
and as $\lambda_k = -\left(\frac{k\pi}{L}\right)^2$ if k increases (frequency)
$e^{d \cdot \lambda_k t}$ will decrease faster!