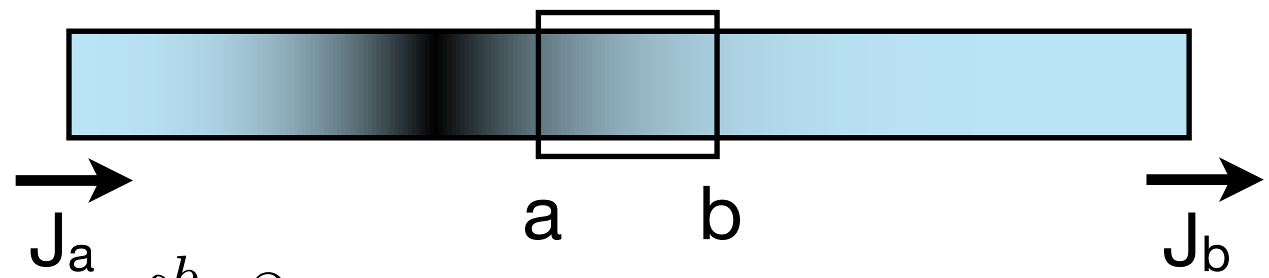
Today

- Diffusion equation -
  - derivation (transport eqns in general)
  - initial conditions, boundary conditions
  - steady state
  - separation of variables

Conservation equations

c(x,t) is linear mass density of ink in a long narrow tube.

$$Q_{ab}(t) = \int_a^b c(x,t)\ dx$$



$$\frac{dQ_{ab}}{dt}(t) = \frac{d}{dt}\int_a^b c(x,t)\ dx \ = \int_a^b \frac{\partial}{\partial t} c(x,t)\ dx$$

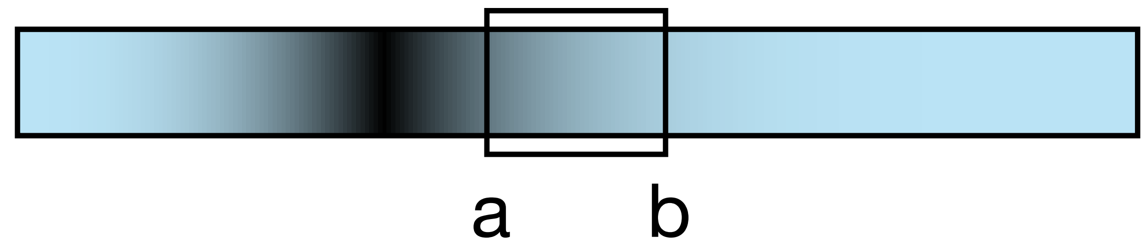
Define the flux J_a to be the amount of mass crossing the line x=a per unit of time (particles moving right count as positive flux) .

In that case, the change of Q inside the a-b box can also be counted watching flux, that is, flux at a - flux at b:

$$\frac{dQ_{ab}}{dt}(t) = \ -J_b + J_a$$

Conservation equations - Transport equation

$$Q_{ab}(t) = \int_a^b c(x,t)\ dx$$



$$\frac{dQ_{ab}}{dt}(t) = \frac{d}{dt}\int_a^b c(x,t)\ dx\ = \int_a^b \frac{\partial}{\partial t}c(x,t)\ dx$$

$$\frac{dQ_{ab}}{dt}(t) = \ -J_b + J_a$$

Need a model for flux. Let’s consider simpler case first (not diffusion yet!)

If fluid in pipe is moving with velocity v, flux is vc: $J_a = vc(a,t)$

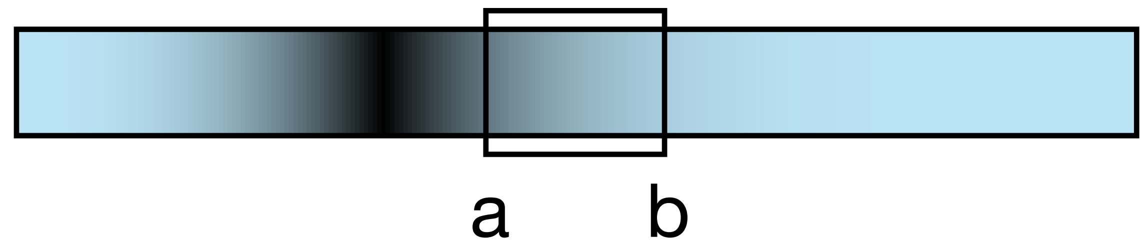
$$\frac{dQ_{ab}}{dt}(t) = -J_b + J_a\ = -vc(b,t) + vc(a,t) = -\ vc(x,t)\Big|_a^b = -\int_a^b v\frac{\partial c}{\partial x}\ dx$$

$$\int_a^b \frac{\partial}{\partial t}c(x,t)\ dx\ = -\int_a^b v\frac{\partial c}{\partial x}\ dx\ \Rightarrow\ \frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x}$$

Called Transport equation.

Conservation equations - Diffusion equation

$$Q_{ab}(t) = \int_a^b c(x,t)\ dx$$



$$\frac{dQ_{ab}}{dt}(t) = \frac{d}{dt}\int_a^b c(x,t)\ dx \ = \int^b \frac{\partial}{\partial} c(x,t)\ dx$$

$$\frac{dQ_{ab}}{dt}(t) = \ -J_b + J_a$$

The Diffusion Equation

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2}$$

Now lets consider diff ... from chemical potential but it also makes sense that for diffusion: $J_a = -D\ \left.\frac{\partial c}{\partial x}\right|_{x=a}$

$$\frac{dQ_{ab}}{dt}(t) = -J_b + J_a = D\ \left.\frac{\partial c}{\partial x}\right|_{x=b} - D\ \left.\frac{\partial c}{\partial x}\right|_{x=a} = D\ \left.\frac{\partial c}{\partial x}\right|_a^b$$

$$\int_a^b \frac{\partial}{\partial t}c(x,t)\ dx \ = \int_a^b D\frac{\partial^2 c}{\partial x^2}\ dx \quad \Rightarrow \quad \frac{\partial}{\partial t}c(x,t) = D\frac{\partial^2}{\partial x^2}c(x,t)$$

Initial and boundary conditions

- One derivative in time requires an initial condition in t.
- Two derivatives in space require two "initial conditions" in x (i.e. one at x=0 and one at x=L). Called boundary conditions (BCs).
- Initial condition: c(x,0) = f(x) where f(x) gives initial concentration profile.
- Boundary conditions:
  - $c(0,t) = c_0$ and $c(L,t) = c_L$ — Dirichlet conditions
  - $\frac{dc}{dx}(0,t) = m_0$ and $\frac{dc}{dx}(L,t) = m_L$ — Neumann conditions (no-flux conditions)
  - $c(0,t) = c_0$ and $\frac{dc}{dx}(L,t) = m_L$ — Mixed conditions
  - $a\frac{dc}{dx}(0,t) + bc(0,t) = m_0$ — Robin conditions

Recall flux: $J_a = -D\frac{dc}{dx}(a,t)$

Neumann conditions also called flux conditions (no-flux when $m_0 = m_L = 0$)

The Diffusion equation

The Diffusion Equation

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2}$$

- What does a steady state of the Diffusion equation look like?

$$0 = D\frac{d^2c}{dx^2}$$

$$c_{ss}(x) = Ax + B$$

- A and B can be determined using the BCs. Getting A from Neumann conditions requires using the IC as well (total mass conservation).

Separation of variables

- Doc cam

This pdf is also posted on the lecture slides page.

Deriving the FS coefficient formulae

Define the dot product for periodic functions (with period P)

$$f(x)\circ g(x) = \int_{\text{one period}} f(x)\cdot g(x)\,dx = \int_{-P/2}^{P/2} f(x)g(x)\,dx$$

Let $v_n(x) = \cos\left(\frac{2\pi n x}{P}\right)$, $w_n(x) = \sin\left(\frac{2\pi n x}{P}\right)$, $v_0(x) = 1$. $(n = 1, 2, \cdots)$

Recall (or calculate for yourself) that

$v_0(x)\circ v_0(x) = P$, $v_m(x)\circ v_n(x) = 0$ for $m \neq n$, $v_n(x)\circ v_n(x) = P/2$

$w_m(x)\circ v_n(x) = 0$, $w_m(x)\circ w_n(x) = 0$ for $m \neq n$, $w_n(x)\circ w_n(x) = P/2$

Suppose $f(x)$ can be represented exactly as a FS. Thus

$$f(x) = A_0 v_0(x) + \sum_{m=1}^{\infty} a_m v_m(x) + \sum_{m=1}^{\infty} b_m v_m(x).$$

Find its FS coefficients. As with vectors, use "$\circ$" to find A_0, a_n, b_n.

To find A_0,

$$f(x)\circ v_0(x) = A_0 v_0(x)\circ v_0(x) + \sum_{m=1}^{\infty} a_m v_m(x)\circ v_0(x) + \sum_{m=1}^{\infty} b_m w_m(x)\circ v_0(x) = A_0\cdot P$$

Thus, $A_0 = \frac{1}{P} f(x)\circ v_0(x) = \frac{1}{P}\int_{-P/2}^{P/2} f(x)\,dx.$

To find a_n,

$$f(x)\circ v_n(x) = A_0 v_0(x)\circ v_n(x) + \sum_{m=1}^{\infty} a_m v_m(x)\circ v_n(x) + \sum_{m=1}^{\infty} b_m w_m(x)\circ v_n(x) = a_n \underbrace{v_n(x)\circ v_n(x)}_{P/2}$$

Thus, $a_n = \frac{2}{P} f(x)\circ v_n(x) = \frac{2}{P}\int_{-P/2}^{P/2} f(x)\cos\frac{2n\pi x}{P}\,dx.$

Similarly, $b_n = \frac{2}{P}\int_{-P/2}^{P/2} f(x)\sin\frac{2n\pi x}{P}\,dx$

In many cases, we will have $P = 2L$ (but not always!) so

$$A_0 = \frac{1}{2L}\int_{-L}^{L} f(x)\,dx$$

$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{n\pi x}{L}\right)dx$$

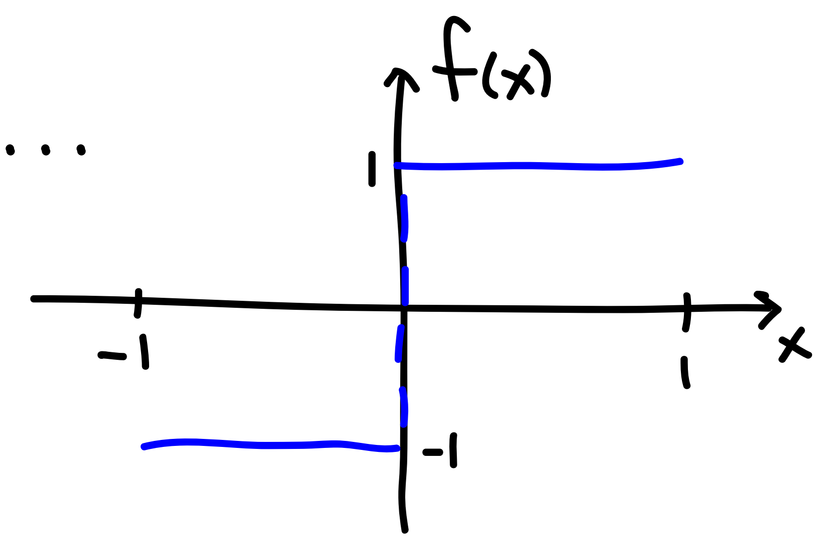
$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{n\pi x}{L}\right)dx$$

Fourier series

- Find the Fourier series for f(x) = $2u_0(x)$-1 on the interval [-1,1].

$$f_{FS}(x) = \frac{a_0}{2} + a_1 \cos\left(\frac{\pi x}{L}\right) + a_2 \cos\left(\frac{2\pi x}{L}\right) + \cdots$$

$$+ b_1 \sin\left(\frac{\pi x}{L}\right) + b_2 \sin\left(\frac{2\pi x}{L}\right) + \cdots$$



- Our hope is that f(x) = $f_{FS}(x)$ so we calculate coefficients as if they were equal:

$$A_0 = \frac{1}{2L}\int_{-L}^{L} f(x)\ dx$$

A_0 is the average value of f(x)!

$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{n\pi x}{L}\right)\ dx$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{n\pi x}{L}\right)\ dx$$

- To simplify formulas, usually define

$$a_0 = 2A_0 = \frac{1}{L}\int_{-L}^{L} f(x)\ dx$$

Fourier series

- Calculate the coefficients.

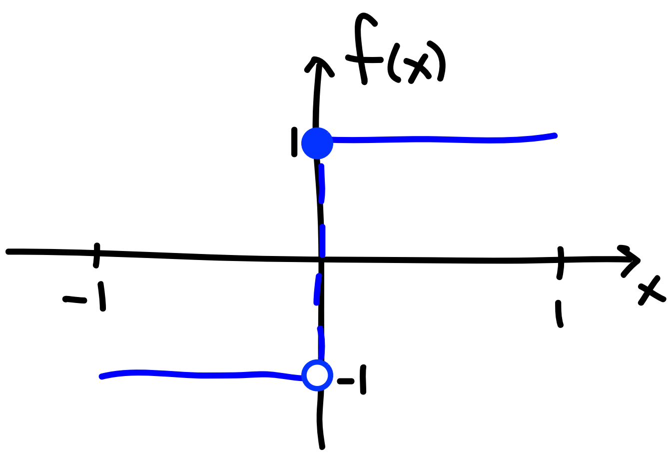
$$f_{FS}(x) = \frac{a_0}{2} + a_1 \cos\left(\frac{\pi x}{L}\right) + a_2 \cos\left(\frac{2\pi x}{L}\right) + \cdots$$
$$+ b_1 \sin\left(\frac{\pi x}{L}\right) + b_2 \sin\left(\frac{2\pi x}{L}\right) + \cdots$$

$$a_0 = \frac{1}{L}\int_{-L}^{L} f(x)\, dx$$
$$a_n = \frac{1}{L}\int_{-L}^{L} f(x) \cos\left(\frac{n\pi x}{L}\right)\, dx$$
$$b_n = \frac{1}{L}\int_{-L}^{L} f(x) \sin\left(\frac{n\pi x}{L}\right)\, dx$$

$a_0 = 0$

$a_n = 0$

$b_n = 2\,(1 - (-1)^n) / n\pi$



$$f_{FS}(x) = \frac{4}{\pi}\sin\left(\frac{\pi x}{L}\right) + \frac{4}{3\pi}\sin\left(\frac{3\pi x}{L}\right) + \frac{4}{5\pi}\sin\left(\frac{5\pi x}{L}\right)$$

https://www.desmos.com/calculator/tlvtikmi0y

Does $f(x) = f_{FS}(x)$ for all x?

Problems at jumps! x=-1, 0, 1

Fourier series

- **Theorem** Suppose f and f' are piecewise continuous on [-L,L] and periodic beyond that interval. Then f(x) = f_{FS}(x) at all points at which f is continuous. Furthermore, at points of discontinuity, f_{FS}(x) takes the value of the midpoint of the jump. That is,

$$f_{FS}(x) = \frac{f(x^+) + f(x^-)}{2}$$

Heat/Diffusion equation - example

- Find the solution to the heat/diffusion equation

$$u_t = 7u_{xx}$$

- subject to BCs

$$u(0,t) = 0 = u(4,t)$$

- and with IC

$$u(x,0) = \begin{cases} 1, & 0 \leq x \leq 2 \\ 0, & 2 < x \leq 4 \end{cases}$$

- The “warming up the milk bottle” example.

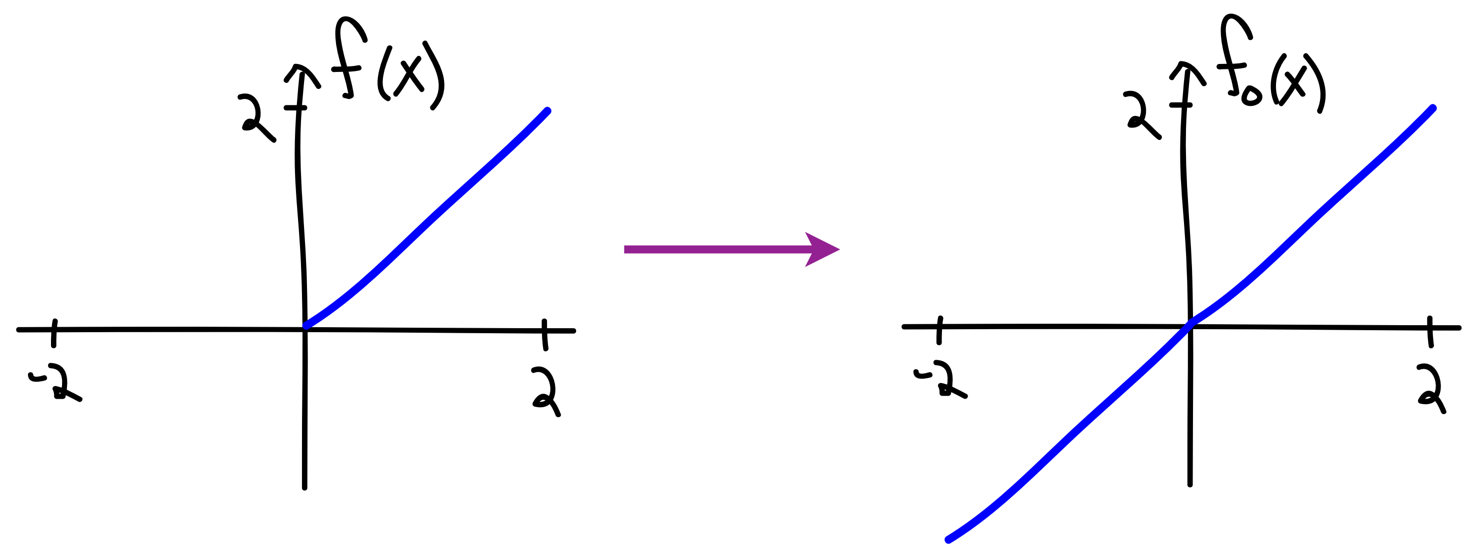
https://www.desmos.com/calculator/zvowjmu30g

Using Fourier Series to solve the Diffusion Equation

$u_t = 4u_{xx}$

$u(0,t) = u(2,t) = 0$

$u(x,0) = x$



(A) $$u(x,t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n e^{-n^2\pi^2 t} \cos\frac{n\pi x}{2}$$

$$a_0 = 1, \; a_n = -\frac{8}{n^2\pi^2} \text{ for } n \text{ even}$$
$$(0 \text{ for } n \text{ odd})$$

(B) $$u(x,t) = \sum_{n=1}^{\infty} b_n e^{-n^2\pi^2 t} \sin\frac{n\pi x}{2}$$

$$b_n = \frac{(-1)^{n+1}4}{n\pi}$$

- Show Desmos movies.

https://www.desmos.com/calculator/yt7kztckeu

https://www.desmos.com/calculator/wcdvgrveez

Using Fourier Series to solve the Diffusion Equation

$$u_t = 4u_{xx}$$

$$\left.\frac{du}{dx}\right|_{x=0,2} = 0$$

$$u(x,0) = \cos\frac{3\pi x}{2}$$

The IC is an eigenvector! Note that it satisfies the BCs.

$$v_3(x) = \cos\frac{3\pi x}{2}$$

$$v_n(x) = \cos\frac{n\pi x}{2}$$

$$u_n(x,t) = e^{\lambda_n t}\cos\frac{n\pi x}{2}$$

$$\frac{\partial}{\partial t}u_n(x,t) = \lambda_n e^{\lambda_n t}\cos\frac{n\pi x}{2}$$

$$4\frac{\partial^2}{\partial x^2}u_n(x,t) = -\frac{4n^2\pi^2}{4}e^{\lambda_n t}\cos\frac{n\pi x}{2}$$

$$\lambda_n = -n^2\pi^2$$

So the solution is

$$u(x,t) = e^{-9\pi^2 t}\cos\frac{3\pi x}{2}$$