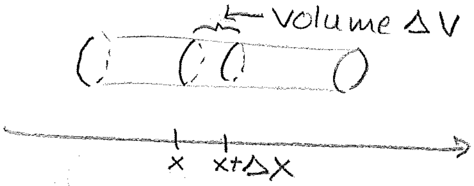
Modeling with partial differential equations (PDE's)

A PDE is an equation for an unknown function $u(t,x,\dots)$ of 2 or more variables that contains derivatives on at least two variables ($u'_x, u'_t, u''_{xx}, u''_{xt}, \dots$). They can describe fundamental laws of nature (physics) or empirical/engineering models. In biology, the heat or diffusion equation, $u'_t = k u''_{xx}$, is common and we focus on it, how to interpret and solve it, and applications.

Notation for derivative: $\frac{\partial u}{\partial x} = u'_x = u_x$ ← without prime

The conservation (continuity) equation

Consider a thin tube with particles inside



A = area of cross section (assume constant)

$\Delta V = A\Delta x$

The tube is so thin that we model the concentration of particles $u(t,x)$ as not varying on each cross section, only along x and in time t.

Let $\sigma(t,x)$ be sources/sinks ($\sigma>0$ if source), the number of particles created or eliminated per unit volume.

Let $J(t,x)$ be the flux of particles, the number of particles crossing a unit area in the positive x-direction per unit time.

If Δx is small so that $u(t,x)\approx u(t,x+\Delta x)$, the number of particles in ΔV is $u(t,x)\Delta V = u(t,x)A\Delta x$. Variation of this in time

$$\frac{\partial}{\partial t}(u(t,x)A\Delta x) = \underbrace{J(t,x)A}_{\text{particles coming in from left}} - \underbrace{J(t,x+\Delta x)A}_{\text{out to the right}} + \underbrace{\sigma(t,x)A\Delta x}_{\text{particles created or eliminated}}$$

Divide by $A\Delta x \Rightarrow$

$$\frac{\partial u}{\partial t} = -\frac{J(t,x+\Delta x)-J(t,x)}{\Delta x} + \sigma(t,x)$$

Let $\Delta x \to 0 \Rightarrow$

$$\frac{\partial u}{\partial t}(t,x) = -\frac{\partial J}{\partial x}(t,x) + \sigma(t,x)$$

conservation/continuity eq.

(important: understand signs of the terms)

Fick's law : the flux of particles is proportional to the change of concentration (in space) :

$$J(t,x) = -D\cdot\frac{\partial u}{\partial x}(t,x) \quad , \quad \text{positive flow if } \frac{\partial u}{\partial x}<0$$

$D>0$ = diffusion constant

Empirical law, but can be motivated by studying random motion

Then $\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x} + \sigma = D\frac{\partial^2 u}{\partial x^2} + \sigma$. With $\sigma=0$ this is the heat or diffusion equation $u_t = Du_{xx}$, a linear PDE of order 2 (and constant coeff.). It is used in many models in science.

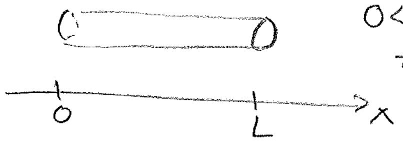
One can have more space dimensions, in 3D for $u(t,x,y,z)$

$$u_t = D(u_{xx}+u_{yy}+u_{zz}) = D\cdot\nabla^2 u = D\Delta u \ , \quad \nabla^2 = \Delta = \text{Laplace operator}$$

Another common PDE is the wave equation $u_{tt} = c^2 u_{xx}$

($u_{tt} = c^2\nabla^2 u$ in 3D)

How can we solve $u_t = Du_{xx}$?



$0<x<L$, $t>0$

We can have boundary conditions (BC) at $x=0$ and $x=L$ of different types

$$\begin{cases} u(t,0) = g_1(t) \\ u(t,L) = g_2(t) \end{cases}$$ Dirichlet conditions. Homogeneous if $g_1(t) = g_2(t) = 0$, means that u is kept to 0 at all times at the ends.

$$\begin{cases} u_x(t,0) = h_1(t) \\ u_x(t,L) = h_2(t) \end{cases}$$ Neumann conditions. $h_1(t) = h_2(t) = 0$ means no flow in or out at the ends.

One can also have combinations of these conditions.

Initial condition (IC) : the concentration in the tube at time $t=0$: $u(0,x) = f(x)$, $0<x<L$, f some given/observed function.

The problem

$$\begin{cases} u_t(t,x) = D u_{xx}(t,x) & , 0<x<L \, , t>0 \quad \text{(PDE)} \\ u(t,0) = g_1(t) & , t>0 \quad \text{(BC)} \\ u(t,L) = g_2(t) & , t>0 \quad \text{(BC)} \\ u(0,x) = f(x) & , 0<x<L \quad \text{(IC)} \end{cases}$$

is called an <u>initial-boundary</u> <u>value</u> <u>problem</u> (IBVP) for $u(t,x)$

Other types of BC's are possible. It should have a unique solution (correct number of BC's and IC, only <u>one</u> thing happens in nature)

We will use Fourier and sin/cos-series to solve IBVP's.

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Fourier, sin- , and cos - series

Consider real one-variable functions on an interval $(-L, L)$, and define

$$(f,g) = \int_{-L}^{L} f(x)g(x)\,dx \qquad \text{(other notations: } (f|g) \text{ or } \langle f|g\rangle)$$

Then $(f,g) = (g,f)$, $(f, c_1g_1 + c_2g_2) = c_1(f,g_1) + c_2(f,g_2)$, and $(f,f) \geq 0$ (and, if f is continuous, $= 0$ only if $f(x) = 0$ for all x). This means that (f,g) is a scalar product or an inner product (as defined in the linear algebra course).

Let $m \geq 0$ and $n \geq 0$ be integers and recall that $2\cos A \cos B = \cos(A+B) + \cos(A-B)$. Then

$$(\cos\frac{m\pi x}{L}, \cos\frac{n\pi x}{L}) = \int_{-L}^{L} \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}\,dx = \frac{1}{2}\int_{-L}^{L}(\cos\frac{(m+n)\pi x}{L} + \cos\frac{(m-n)\pi x}{L})\,dx =$$

$$= \Big[\frac{L}{(m+n)\pi}\sin\frac{(m+n)\pi x}{L} + \frac{L}{(m-n)\pi}\sin\frac{(m-n)\pi x}{L}\Big]_{-L}^{L} = 0 \qquad \text{if } m \neq n.$$

If $m = n \neq 0$, $\quad (\cos\frac{m\pi x}{L}, \cos\frac{m\pi x}{L}) = \frac{1}{2}\int_{-L}^{L}(\cos\frac{2m\pi x}{L} + 1)\,dx = L$,

and if $m = n = 0$, $\cos\frac{0\pi x}{L} = 1$ and $\quad (1,1) = \int_{-L}^{L} dx = 2L$.

Similarily, for $m \geq 0$ and $n \geq 1$, $\quad (\cos\frac{m\pi x}{L}, \sin\frac{n\pi x}{L}) = 0$,

and, for $m \geq 1$ and $n \geq 1$, $\quad (\sin\frac{m\pi x}{L}, \sin\frac{n\pi x}{L}) = 0$ if $m \neq n$ and $= L$ if $m = n$.

$\Rightarrow \quad 1, \cos\frac{\pi x}{L}, \sin\frac{\pi x}{L}, \cos\frac{2\pi x}{L}, \sin\frac{2\pi x}{L}, \ldots$ are all orthogonal. In fact, they form an orthogonal basis for the (infinite-dimensional) vector space of all "nice" functions. Any (nice) $f(x)$ can be written as an infinite linear combination

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n\cos\frac{n\pi x}{L} + b_n\sin\frac{n\pi x}{L}) \quad \text{on } (-L,L), \text{ called the } \underline{\text{Fourier series}} \text{ of } f.$$

To find the coefficients a_n for a given f, take the scalar product with $\cos\frac{n\pi x}{L}$:

$$(f(x), \cos\frac{n\pi x}{L}) = (\frac{a_0}{2} + \sum_{m=1}^{\infty}(a_m\cos\frac{m\pi x}{L} + b_m\sin\frac{m\pi x}{L}), \cos\frac{n\pi x}{L}) =$$

$$= \frac{a_0}{2}\underbrace{(1, \cos\frac{n\pi x}{L})}_{=0, n\geq 1,\ =2L, n=0} + \sum_{m=1}^{\infty}(a_m\underbrace{(\cos\frac{m\pi x}{L}, \cos\frac{n\pi x}{L})}_{=0, m\neq n,\ =L, m=n} + b_m\underbrace{(\sin\frac{m\pi x}{L}, \cos\frac{n\pi x}{L})}_{=0}) = a_nL$$

$$\Rightarrow \quad a_n = \frac{1}{L}(f(x), \cos\frac{n\pi x}{L}) = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}\,dx \quad \text{for } n \geq 0.$$

In the same way, $\quad b_n = \frac{1}{L}(f(x), \sin\frac{n\pi x}{L}) = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}\,dx \quad$ for $n \geq 1$.

Example. Let $L = \pi$ and $f(x) = x$. Then partial integration gives

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} x\sin nx\,dx = \Big[-\frac{x\cos nx}{n\pi}\Big]_{-\pi}^{\pi} + \int_{-\pi}^{\pi}\frac{\cos nx}{n\pi}\,dx = -\frac{2\pi\cos n\pi}{n\pi} + \Big[\frac{\sin nx}{n^2\pi}\Big]_{-\pi}^{\pi} = -\frac{2(-1)^n}{n} + 0$$

Similarly $a_n = 0$ for all $n \geq 0$ so

$$f(x) = x = -2\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\sin nx = 2(\sin x - \tfrac{1}{2}\sin 2x + \tfrac{1}{3}\sin 3x - \tfrac{1}{4}\sin 4x + \ldots) \quad \text{on } (-\pi,\pi)$$

More theory (convergence of series, integrals, function spaces, ...) in courses on Transform Theory or Fourier Analysis. One can also use $e^{i\pi nx/L}$ and write a complex version of the Fourier series.

Suppose now that $f(x)$ is defined on $(0, L)$ only. Extend f to an *even* function $\tilde{f}$ on $(-L, L)$. This means that $\tilde{f}(x) = f(x)$ on $(0, L)$ and that $\tilde{f}(-x) = \tilde{f}(x)$. The Fourier series of $\tilde{f}$ on $(-L, L)$ has all $b_n = 0$ since $\tilde{f}(x)$ even and $\sin\frac{n\pi x}{L}$ odd $\Rightarrow \tilde{f}(x)\sin\frac{n\pi x}{L}$ odd, and

$$b_n = \frac{1}{L}\int_{-L}^{L} \tilde{f}(x)\sin\frac{n\pi x}{L}\,dx = 0 \qquad \text{(since the interval is symmetric)}$$

Then $\tilde{f}(x) = \dfrac{a_0}{2} + \displaystyle\sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L}$ on $(-L, L)$, with

$$a_n = \frac{1}{L}\int_{-L}^{L} \underbrace{\tilde{f}(x)\cos\frac{n\pi x}{L}}_{even}\,dx = \frac{2}{L}\int_0^L \underbrace{\tilde{f}(x)}_{=f(x)}\cos\frac{n\pi x}{L}\,dx = \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}\,dx$$

Since $f = \tilde{f}$ on $(0, L)$ we have

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n\cos\frac{n\pi x}{L} \quad \text{on } (0, L), \text{ with } \quad a_n = \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}\,dx$$

This is called the <u>cos-series</u> of f on $(0, L)$.

In the same way (extend f to an odd function),

$$f(x) = \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L} \quad \text{on } (0, L), \text{ with } \quad b_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}\,dx\ ,$$

the <u>sin-series</u> of f on $(0, L)$.

TEST QUESTIONS

1. Find the Fourier series on $(-L, L)$ of $f(x) = \begin{cases} 1 & \text{om } x \geq 0 \\ 0 & \text{om } x < 0 \end{cases}$
2. Find the Fourier series of $f(x) = 8\sin 3x - 17\cos 7x$ on $(-\pi, \pi)$
3. Find the cos- and sin-series of $f(x) = x$ on $(0, 1)$

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SOLUTIONS

1. $\Rightarrow \quad a_n = \dfrac{1}{L}\displaystyle\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}\,dx = \frac{1}{L}\int_0^L \cos\frac{n\pi x}{L}\,dx = \frac{1}{L}\Big[\frac{L\sin\frac{n\pi x}{L}}{n\pi}\Big]_0^L = 0 \quad$ for $n \neq 0$,

$$a_0 = \frac{1}{L}\int_{-L}^{L} f(x)\,dx = \frac{1}{L}\int_0^L dx = 1 \quad ,$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}\,dx = \frac{1}{L}\int_0^L \sin\frac{n\pi x}{L}\,dx = \frac{1}{L}\Big[\frac{-L\cos\frac{n\pi x}{L}}{n\pi}\Big]_0^L = \frac{1-\cos n\pi}{n\pi} \quad \text{for } n \geq 1,$$

$$\Rightarrow\ f(x) = \frac{1}{2} + \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n}\sin\frac{n\pi x}{L} = \frac{1}{2} + \frac{2}{\pi}\Big(\sin\frac{\pi x}{L} + \frac{1}{3}\sin\frac{3\pi x}{L} + \frac{1}{5}\sin\frac{5\pi x}{L} + \dots\Big) \quad \text{on } (-L, L)$$

2. The Fourier series is unique so $f(x) = 8\sin 3x - 17\cos 7x$ has Fourier series $8\sin 3x - 17\cos 7x$

3. $a_n = 2\displaystyle\int_0^1 x\cos(n\pi x)\,dx = 2\Big[\frac{x\sin(n\pi x)}{n\pi}\Big]_0^1 - 2\int_0^1 \frac{\sin(n\pi x)}{n\pi}\,dx = 0 + 2\Big[\frac{\cos(n\pi x)}{n^2\pi^2}\Big]_0^1 = 2\frac{\cos(n\pi)-1}{n^2\pi^2}$

for $n \neq 0$, and $a_0 = 2\displaystyle\int_0^1 x\,dx = [x^2]_0^1 = 1 \quad \Rightarrow$ the cos-series is

$$x = \frac{1}{2} + \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n - 1}{n^2}\cos(n\pi x) = \frac{1}{2} - \frac{4}{\pi^2}\cos(\pi x) - \frac{4}{9\pi^2}\cos(3\pi x) - \frac{4}{25\pi^2}\cos(5\pi x) - \dots \text{ on } (0,1)$$

$$b_n = 2\int_0^1 x\sin(n\pi x)\,dx = -2\Big[\frac{x\cos(n\pi x)}{n\pi}\Big]_0^1 + 2\int_0^1 \frac{\cos(n\pi x)}{n\pi}\,dx = -2\frac{\cos(n\pi)}{n\pi} + 2\Big[\frac{\sin(n\pi x)}{n^2\pi^2}\Big]_0^1 = -2\frac{(-1)^n}{n\pi}$$

$\Rightarrow$ the sin-series is

$$x = \frac{-2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\sin(n\pi x) = \frac{2}{\pi}\big(\sin(\pi x) - \tfrac{1}{2}\sin(2\pi x) + \tfrac{1}{3}\sin(3\pi x) - \dots\big) \quad \text{on } (0,1)$$