# *PDEs in Mathematical Biology*
# *& Numerical Methods to Solve Them*

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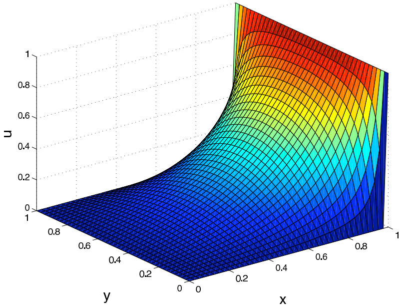


# PDEs in Math Biology

- Wave equation (*hyperbolic PDE*)
- Diffusion or heat equation (*parabolic PDE*)
- Laplace's & Poisson's equations (*elliptic PDEs*)
  - for electrostatic potential
- Cable equation (*parabolic diffusion PDE with source term*)
  - models electrical impulses along axons & dendrites
- Advection-diffusion equation (*parabolic PDE*)
  - models fluid transport of ions (coupled to Poisson's equation)
  - or of bacteria & nutrients, etc.

# Derivatives & Notation

Second-order accurate central difference approx. to first derivative

$$\left(\frac{df}{dx}\right)_i \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

Second-order accurate central difference approx. to second derivative

$$\left(\frac{d^2 f}{dx^2}\right)_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

First-order accurate one-sided difference approx. to first derivative

$$\left(\frac{df}{dx}\right)_i \approx \frac{f_{i+1} - f_i}{\Delta x} \quad \text{or} \quad \frac{f_i - f_{i-1}}{\Delta x}$$

Approximate solution

$$u_i^n \approx u(x_i, t_n)$$

# Taylor Series

To verify formulas, use Taylor series

$$f_{i\pm1} = f(x_i \pm \Delta x) = f_i \pm \Delta x\, f_i' + \frac{\Delta x^2}{2!} f_i'' \pm \frac{\Delta x^3}{3!} f_i''' + \cdots$$

Then

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f_i' + \frac{\Delta x^2}{6} f_i''' + \cdots$$

# First-Order Wave (Advection) Equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \quad u(x, t = 0) = u_0(x)$$

Solution is

$$u(x,t) = u_0(x - ct)$$

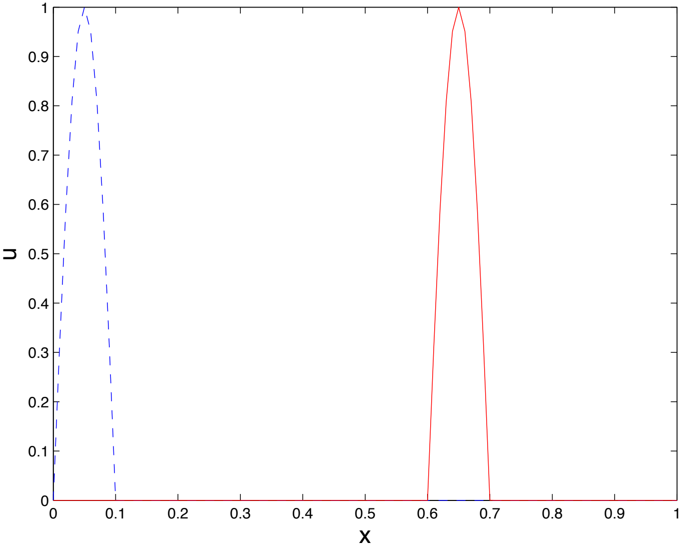
Numerical method: *upwind*

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c\frac{u_i^n - u_{i-1}^n}{\Delta x}$$

$$u_i^{n+1} = u_i^n - c\frac{\Delta t}{\Delta x}\left(u_i^n - u_{i-1}^n\right)$$

First-order accurate & stable for $\Delta t \leq \frac{\Delta x}{c}$ (CFL condition)

# Wave Equation



# Diffusion Equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \;\; u(x, t=0) = u_0(x), \;\; u(x=-1,t) = 0 = u(x=1,t)$$

Numerical method: *backward Euler*

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = D\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2}$$

$$u_i^{n+1} = u_i^n + D\frac{\Delta t}{\Delta x^2}\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right)$$

A-stable & first-order accurate

In matrix form with $u = [u_2, u_3, \ldots, u_N]^t$ & $u_1 = 0 = u_{N+1}$,

$$u^{n+1} = u^n + \frac{D\Delta t}{\Delta x^2}Au^{n+1}$$

$$\left(I - \frac{D\Delta t}{\Delta x^2}A\right)u^{n+1} = u^n$$

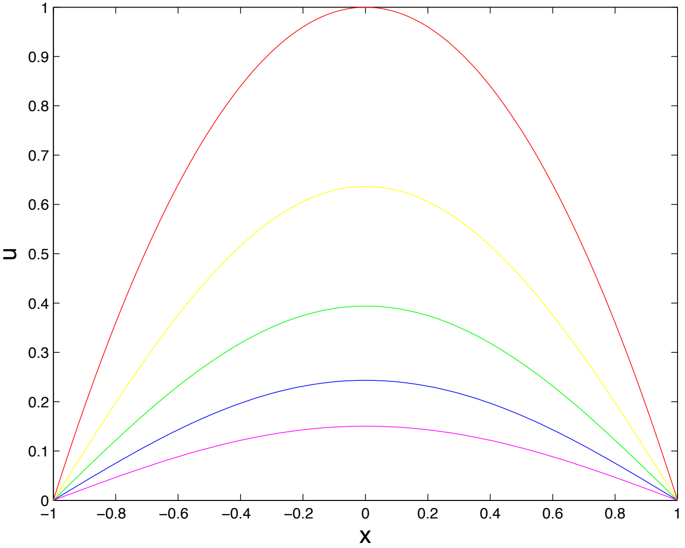
# Diffusion Equation

$$\left(I - \frac{D\Delta t}{\Delta x^2} A\right) u^{n+1} = u^n$$

where (for $N = 10$)

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

# Diffusion Equation



# Poisson's Equation & Laplace's Equation

Poisson equation

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(x,y)$$

Laplace equation

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Numerical method: *second-order accurate central differences & Gauss-Seidel iteration*

Dirichlet BCs on unit square with $u = 0$ on three sides & $u(x = 1, y) = 1$

Define residual (set $\Delta x = \Delta y = h$)

$$r_{ij} = \left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}\right)/h^2 \rightarrow 0$$

Jacobi iteration

$$u_{ij}^{(k+1)} = \frac{1}{4}\left(u_{i+1,j}^{(k)} + u_{i-1,j}^{(k)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k)}\right) = u_{ij}^{(k)} + \frac{h^2}{4} r_{ij}^{(k)}$$

# Laplace’s Equation