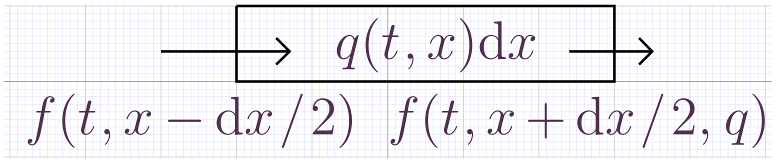
Overview

- First-order PDEs
  - advection equation
  - convection equation
  - characteristic solution
- Second-order PDE classification, canonical forms
  - hyperbolic, wave equation
  - parabolic, heat equation
  - elliptic, Poisson equation
- Reformulating second-order PDEs as first-order PDE system, eigenproblems
- Overview of numerical method development: finite differences, finite volume, finite element, spectral methods
- Finite difference example: leapfrog discretization of wave equation

- Many (most) phenomena depend on multiple independent variables
- Natural phenomena are governed by *conservation laws* (mass, momentum, energy, charge): change in quantity $q(t,x)$ in an infinitesimal volume at time t and position x equals difference of what is going out/in and what was produced



$$\frac{\partial q}{\partial t} = -\frac{\partial f(t,x,q)}{\partial x} + \sigma(t,x,q)$$

$f(t,x,q)$ is the *flux* of quantity q, $\sigma(t,x,q)$ is the *source* of quantity q.

- *Advection*: transport of quantity q in space x and time t by velocity field u
  - Constant velocity advection IBVP, $u=$ constant, flux $f=uq$

$$q_t + u q_x = 0,\ q(x,t=0) = f(x),\ q(x=0,t) = g(t),\ q(x=1,t) = h(t).$$

  - Variable velocity advection, $u(x,t)$, same equations as above

  Examples: transport of a pollutant in a river, drug in the blood stream
- *Convection*: transport of quantity q in space-time (x,t) by a velocity field that depends on q, e.g., Burgers' equation for $q(t,x)$, $q_t \equiv \partial q/\partial t$, $q_x \equiv \partial q/\partial x$

$$q_t + q q_x = 0\ (\text{nonlinear, similar IBVP conditions as above})$$

- Theory of conic sections highlights *quadratic forms* in (x, y) coordinates

$$Ax^2 + 2Bxy + Cy^2 + Dx + Ey - G = 0 \Rightarrow$$

$$\begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} D & E \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} - G = 0 \ , \boldsymbol{M} = \begin{bmatrix} A & B \\ B & C \end{bmatrix}, \boldsymbol{q} = \begin{bmatrix} x \\ y \end{bmatrix}$$

M symmetric $\Rightarrow$ orthogonal diagonalizable, real eigenvalues, $\boldsymbol{M} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$.

$$\boldsymbol{q}^T(\boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T)\boldsymbol{q} + \boldsymbol{c}^T\boldsymbol{q} = -F, \boldsymbol{z} = \boldsymbol{U}^T\boldsymbol{q} \Rightarrow \boldsymbol{z}^T\boldsymbol{\Lambda}\boldsymbol{z} + \boldsymbol{m}^T\boldsymbol{z} = -F$$

- Denote $\boldsymbol{\Lambda} = \mathrm{diag}(a, b)$, consider $G = 0$ (homogeneous), $\boldsymbol{m}^T = \boldsymbol{c}^T\boldsymbol{U} = \begin{bmatrix} 2s & 2t \end{bmatrix}$. Quadratic form becomes $\boldsymbol{z}^T\boldsymbol{\Lambda}\boldsymbol{z} + \boldsymbol{m}^T\boldsymbol{z} = 0$ under change of coordinates

$$\boldsymbol{z} = \begin{bmatrix} u \\ v \end{bmatrix} = \boldsymbol{U}^T\boldsymbol{q} = \boldsymbol{U}^T \begin{bmatrix} x \\ y \end{bmatrix}$$

  - $ab > 0 \Rightarrow \xi^2 + \eta^2 = 0$ an *ellipse*, $\xi = \sqrt{a}\,u + s/\sqrt{a}$, $\eta = \sqrt{b}\,v + t/\sqrt{b}$
  - $ab < 0 \Rightarrow \xi^2 - \eta^2 = 0$, a *hyperbola*
  - $ab = 0 \Rightarrow \xi^2 = \eta$, a *parabola*

- Mathematical physics highlights certain ubiquitous PDEs of form

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G$$

- Simplest case: $A, \ldots, G$ constant, linear PDE, classified similar to quadratics

$$\left(\begin{bmatrix} \partial_x & \partial_y \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix} + \begin{bmatrix} D & E \end{bmatrix} \begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix} + F \right) u = G$$

- As in case of quadratics, changes of variables lead to *canonical forms*
  - *Poisson equation* $u_{\xi\xi} + u_{\eta\eta} = f$, an *elliptical* PDE
  - *Wave equation* $u_{\xi\xi} - u_{\eta\eta} = f$, a *hyperbolic* PDE
  - *Heat equation* $u_{\xi\xi} - u_{\eta} = f$, a *parabolic* PDE
- The above classification is of special relevance to numerical analysis since different numerical methods are applicable for each type of equation

- Homogeneous wave equation $u_{tt} - u_{xx} = 0$, $v \equiv u_t, w = u_x, u_{tx} = u_{xt} \Rightarrow$

$$\begin{array}{l} v_t = w_x \\ w_t = v_x \end{array}, \boldsymbol{q} = \left[\begin{array}{c} v \\ w \end{array} \right], \boldsymbol{q}_t + \boldsymbol{A}\boldsymbol{q}_x = \boldsymbol{0}, \boldsymbol{A} = \left[\begin{array}{cc} 0 & -1 \\ -1 & 0 \end{array} \right]$$

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T = \frac{1}{\sqrt{2}}\left[\begin{array}{cc} 1 & 1 \\ -1 & 1 \end{array} \right]\left[\begin{array}{cc} -1 & 0 \\ 0 & 1 \end{array} \right]\frac{1}{\sqrt{2}}\left[\begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array} \right]$$

Second-order wave equation leads to a first order system with *real* eigenvalues

- Homogeneous Poisson equation $u_{xx} + u_{yy} = 0$, $v \equiv u_x, w = u_y, u_{xy} = u_{yx} \Rightarrow$

$$\begin{array}{l} v_y = w_x \\ w_y = -v_x \end{array}, \boldsymbol{q} = \left[\begin{array}{c} v \\ w \end{array} \right], \boldsymbol{q}_y + \boldsymbol{A}\boldsymbol{q}_x = \boldsymbol{0}, \boldsymbol{A} = \left[\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right]$$

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T = \frac{1}{\sqrt{2}}\left[\begin{array}{cc} i & 1 \\ -i & 1 \end{array} \right]\left[\begin{array}{cc} i & 0 \\ 0 & -i \end{array} \right]\frac{1}{\sqrt{2}}\left[\begin{array}{cc} i & -i \\ 1 & 1 \end{array} \right]$$

Second-order elliptic equation leads to a first order system with *imaginary* eigenvalues

- Basic ideas: discretize both operators (∂_t, ∂_x) or discretize only one operator (typically ∂_x) and reduce to an ODE system (typically in t)
- Approaches:
  - finite difference discretization of differentiation operators, $u_i^n = u(nk, ih)$

$$u_{tt} - u_{xx} = 0 \Rightarrow \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} - \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{k^2} = 0$$

  - finite difference discretization of ∂_{xx} operator only, $u_i(t) = u(t, ih)$

$$\frac{\mathrm{d}^2 u_i}{\mathrm{d}t^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

  - introduce a piecewise approximation in space for $u(t,x)$

$$u(t,x) \cong U_i(t) + [U_{i+1}(t) - U_i(t)](x - x_i)/(x_{i+1} - x_i)$$

    a *finite element method*.
- Different approximations of $u(t,x)$ lead to finite volume, spectral methods.

- Consider the wave equation $u_{tt} - u_{xx} = 0$ with initial, boundary conditions

$$u(0,x) = \sin x, u_t(0,x) = 0, u(t,0) = 0, u(t,\pi) = 0.$$

This is known as the plucked string problem, and models a guitar string plucked at midpoint.

- Construct a numerical method by introducing a centered derivative approximation in space, $x_j = jh$, $h = \pi/m$

$$u_{xx}(t,jh) \cong \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{h^2}, j = 1, \ldots, m-1$$

- Replace above approximation in wave equation at $x = x_j$

$$\frac{\mathrm{d}^2 u_j(t)}{\mathrm{d}t^2} = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{h^2}, j = 1, \ldots, m-1$$

- Transform second-order ODE into two first-order ODEs

$$\frac{\mathrm{d}v_j}{\mathrm{d}t} = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{h^2}, \frac{\mathrm{d}u_j}{\mathrm{d}t} = v_j$$

- Obtain a system of ODEs

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \boldsymbol{M}\boldsymbol{q},\ \boldsymbol{q} = \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix}, \boldsymbol{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_{m-1} \end{bmatrix}, \boldsymbol{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_{m-1} \end{bmatrix}, \boldsymbol{M} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{D} & \boldsymbol{0} \end{bmatrix}$$

- Note the block matrix structure with $\boldsymbol{I}$ the identity matrix, and

$$\boldsymbol{D} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}, \boldsymbol{I}, \boldsymbol{D} \in \mathbb{R}^{(m-1)\times(m-1)}$$

- Apply leap-frog to the ODE system with time step k, $\boldsymbol{q}^n = \boldsymbol{q}(nk)$

$$\frac{\boldsymbol{q}^{n+1} - \boldsymbol{q}^{n-1}}{2k} = \boldsymbol{M}\boldsymbol{q}^n$$

- Leap-frog has a stability region $z = \lambda k$ on the slit from $z = -i$ to $z = +i$
- Eigenvalues of $\boldsymbol{M}$ are required. These can be determined analytically

$$\boldsymbol{M}\boldsymbol{q} = \lambda \boldsymbol{q} \Rightarrow \left[\begin{array}{cc} \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{D} & \boldsymbol{0} \end{array}\right]\left[\begin{array}{c} \boldsymbol{u} \\ \boldsymbol{v} \end{array}\right] = \lambda \left[\begin{array}{c} \boldsymbol{u} \\ \boldsymbol{v} \end{array}\right] \Rightarrow \left\{\begin{array}{l} \boldsymbol{v} = \lambda \boldsymbol{u} \\ \boldsymbol{D}\boldsymbol{u} = \lambda \boldsymbol{v} \end{array}\right. \Rightarrow \boldsymbol{D}\boldsymbol{u} = \lambda^2 \boldsymbol{u} = \mu \boldsymbol{u}$$

- The eigenvalues of $\boldsymbol{D}$ are

$$\mu_l = -\frac{4}{h^2} \sin^2\left(\frac{l h}{2}\right), l = 1, 2, \ldots, m - 1, h = \pi / m$$

- The eigenvalues of $\boldsymbol{M}$ are therefore

$$\lambda_l = \sqrt{\mu_l} = \pm \frac{2i}{h} \sin\left(\frac{l h}{2}\right), l = 1, 2, \ldots, m - 1$$

and are purely imaginary, and therefore leap-frog numerical solutions can be made stable by an appropriate time step restriction.