CS520: Introduction (Ch. 1)

Uri Ascher

Department of Computer Science
University of British Columbia
asher@cs.ubc.ca
people.cs.ubc.ca/~asher/520.html
Differential equations: ODEs and PDEs
PDE example
Well-posed initial value PDE problems
Numerical methods: a taste of finite differences
Differential equations

### Arise in all branches of science and engineering, economics, computer science.

### Relate physical state to rate of change. e.g., rate of change of particle is velocity

\[
\frac{dx}{dt} = v(t) = g(t, x), \quad a < t < b.
\]

- **Ordinary differential equation (ODE):** one independent variable ("time").
- **Partial differential equation (PDE):** several independent variables.
Simplest elliptic PDE: Poisson.

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g(x, y).
\]

Simplest parabolic PDE: heat.

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.
\]

Simple hyperbolic PDE: wave.

\[
\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0.
\]
ORDINARY DIFFERENTIAL EQUATIONS

e.g., pendulum.
Ordinary differential equations

e.g., pendulum.

\[ \frac{d^2 \theta}{dt^2} \equiv \theta'' = -g \sin(\theta), \]

where \( g \) is the scaled constant of gravity, e.g., \( g = 9.81 \), and \( t \) is time.

- Write as first order ODE system: \( y_1(t) = \theta(t), \ y_2(t) = \theta'(t) \). Then \( y_1' = y_2, \ y_2' = -g \sin(y_1) \).
- ODE in standard form:

\[ y' = f(t, y), \quad a < t < b. \]

For the pendulum

\[ f(t, y) = \begin{pmatrix} y_2 \\ -g \sin(y_1) \end{pmatrix}. \]
SIDE CONDITIONS

e.g.

\[ y' = -y \quad \Rightarrow \quad y(t) = c \cdot e^{-t}. \]

- **Initial value problem**: \( y(a) \) given. (In the pendulum example: \( \theta(0) \) and \( \theta'(0) \) given.)
- **Boundary value problem**: relations involving \( y \) at more than one point given. (In the pendulum example: \( \theta(0) \) and \( \theta(\pi) \) given.)

We stick to initial value ODEs!
A SIMPLE PDE

Consider

\[ u_t = \nu u_{xx} - 3u_x. \]

- \( t \) and \( x \) are independent variables, \( t \geq 0 \) time, \( 0 \leq x \leq b \) space, and \( \nu \) is a parameter.
- Subscripts denote partial derivatives, so PDE is

\[ \frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} - 3 \frac{\partial u}{\partial x}. \]

- Initial conditions:

\[ u(0, x) = u_0(x), \quad 0 \leq x \leq b. \]

- Boundary conditions: e.g. Dirichlet

\[ u(t, 0) = g_0(t), \quad u(t, b) = g_b(t). \]
Simple analysis

- Ignore boundary conditions, seek special solution of the form

$$u(t, x) = \hat{u}(t, \xi) e^{i\xi x},$$

where $$i = \sqrt{-1}$$.

- $$\xi$$ is wave number; $$e^{i\xi x}$$ is mode; $$|\hat{u}(t, \xi)|$$ is amplitude.

- For this special solution

$$u_x = i\xi \hat{u} e^{i\xi x}; \quad u_{xx} = -\xi^2 \hat{u} e^{i\xi x}; \quad u_t = \hat{u}_t e^{i\xi x}.$$

- Obtain ODE

$$\hat{u}_t = - (\nu \xi^2 + 3i\xi) \hat{u}.$$
The solution of the initial value ODE problem

\[ \hat{u}_t = -\left(\nu \xi^2 + 3\nu \xi\right) \hat{u}, \]

is

\[ \hat{u}(t, \xi) = e^{-\left(\nu \xi^2 + 3\nu \xi\right) t} \hat{u}(0, \xi). \]

Hence

\[ |\hat{u}(t, \xi)| = e^{-\nu \xi^2 t} |\hat{u}(0, \xi)|, \]

so also

\[ |u(t, x)| = e^{-\nu \xi^2 t} |u(0, x)|. \]
Different cases of $\nu$

- If $\nu > 0$, the solution magnitude decays in time, faster for larger wave numbers (typical for **parabolic PDEs**).
- If $\nu = 0$, the solution magnitude remains constant in time (typical for **hyperbolic PDEs**).

**But...** why do we care so much about such a special solution?!
ASIDE: FOURIER TRANSFORM

- The continuous version of the Fourier transform:
  \[ \hat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi x} v(x) \, dx. \]

- The corresponding inverse transform:
  \[ v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi x} \hat{v}(\xi) \, d\xi. \]

- \( \xi \) is called wave number when \( x \) is a space variable, and frequency when \( x \) is time.

- Note Parseval equality
  \[ \| v \|^2 = \int_{-\infty}^{\infty} |v(x)|^2 \, dx = \int_{-\infty}^{\infty} |\hat{v}(\xi)|^2 \, d\xi = \| \hat{v} \|^2. \]
Return to simple PDE

- Apply Fourier transform in $x$

\[ u(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\imath \xi x} \hat{u}(t, \xi) d\xi. \]

- Then

\[ u_x(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\imath \xi) e^{\imath \xi x} \hat{u}(t, \xi) d\xi, \]

\[ u_{xx}(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\imath \xi)^2 e^{\imath \xi x} \hat{u}(t, \xi) d\xi, \]

\[ u_t(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\imath \xi x} \hat{u}_t(t, \xi) d\xi. \]

- So, our simple PDE can be written as

\[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\imath \xi x} \left[ \hat{u}_t + (\nu \xi^2 + 3 \imath \xi) \hat{u} \right] d\xi = 0. \]
To satisfy

\[
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i \xi x} \left[ \hat{u}_t + (\nu \xi^2 + 3i \xi) \hat{u} \right] d\xi = 0
\]

for all \( x \), what’s in square brackets must vanish, so we obtain the ODE

\[
\hat{u}_t = -(\nu \xi^2 + 3i \xi) \hat{u},
\]

for each wavenumber \( \xi \).

The symbol of this PDE is

\[
P(s) = \nu s^2 - 3s,
\]

so

\[
P(\nu \xi) = -(\nu \xi^2 + 3i \xi).
\]
Well-posed initial-value problems

Next, consider the more general case – a constant-coefficient Cauchy problem

\[ u_t = P(\partial_x)u, \quad -\infty < x < \infty, \ t > 0 \]
\[ u(t, 0) = u_0(x). \]

The initial value problem is well-posed if there are constants \( K \) and \( \alpha \) such that

\[ \|u(t)\| \leq Ke^{\alpha t}\|u(0)\| = Ke^{\alpha t}\|u_0\|, \quad \forall u_0 \in \mathcal{L}_2. \]
To check well-posedness, apply \textbf{Fourier transform} as before.

Obtain well-posedness iff there are constants $K$ and $\alpha$ such that

$$
\sup_{-\infty < \xi < \infty} |e^{P(\xi)t}| \leq Ke^{\alpha t}.
$$


**Heat Equation**

- The simplest parabolic PDE:
  \[ u_t = u_{xx}. \]
  
- we get the symbol
  \[ P(\imath \xi) = -\xi^2. \]
  
- Hence
  \[ |e^{P(\imath \xi)t}| = |e^{-\xi^2 t}| \leq 1 \quad \forall \xi. \]

So, \( K = 1, \alpha = 0. \)

- Moreover, higher wave numbers are attenuated more! Thus, the heat equation operator is a smoother.

- Note ill-posedness for \( t < 0 \): heat equation is not reversible.
Example: Heat Equation Smoothing Effect

fig1_4
Advection equation

- A simple hyperbolic PDE:

\[ u_t + au_x = 0 \]

- we get

\[ P(\xi) = -a\xi. \]

Hence

\[ |e^{P(\xi)t}| = |e^{-a\xi t}| = 1 \quad \forall \xi. \]

- Note no attenuation of any wave number. No smoothing of solution in time. Also, advection equation is reversible.

- Solution is constant along characteristics \( x = at \) with wave speed \( \frac{dx}{dt} = a \), so exact solution is:

\[ u(t, x) = u_0(x - at). \]
Example: Advection Equation Solution

\[ u(x, t) \]
Wave equation

- A better behaved hyperbolic PDE, the classical wave equation:
  \[ w_{tt} - c^2 w_{xx} = 0. \]

- Define \( u_1 = w_t, \ u_2 = c w_x, \ u = (u_1, u_2)^T \), obtain
  \[ u_t - \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} u_x = 0. \]

- The eigenvalues of this matrix are \( \pm c \). They are real, hence the wave equation is hyperbolic.
Laplace Equation

- The simplest elliptic equation is
  \[ w_{tt} + w_{xx} = 0. \]

- Same analysis as above but \( c = i \) not real.
- the initial-value problem for Laplace and other elliptic PDEs is not well-posed.
- But the boundary-value problem for elliptic equations is well-posed.
Consider the PDE system

\[ u_t = Au_{xx}. \]

This is a parabolic system if \( A \) is symmetric positive definite (SPD). Then the initial value problem (IVP) is well-posed.

The PDE system

\[ u_t = Au_x \]

is a hyperbolic system if \( A \) is diagonalizable and has real eigenvalues (like the wave equation). Then IVP is well-posed.
Introduction

- Differential equations: ODEs and PDEs
- PDE example
- Well-posed initial value PDE problems
- Numerical methods: a taste of finite differences
Step sizes $\Delta t = k$, $\Delta x = h$

$$v^n_j = v(t^n, x_j) \equiv v(nk, jh) \approx u(nk, jh)$$
THREE DISCRETIZATIONS FOR ADVECTION EQUATION

Advection equation: $u_t + au_x = 0$.

1. One sided

$$\frac{1}{k}(v_{j+1}^n - v_j^n) + \frac{a}{h}(v_{j+1}^n - v_j^n) = 0.$$ 

2. Centered in $x$

$$\frac{1}{k}(v_{j+1}^n - v_j^n) + \frac{a}{2h}(v_{j+1}^n - v_{j-1}^n) = 0.$$ 

3. Leap-frog

$$\frac{1}{2k}(v_{j+1}^n - v_j^{n-1}) + \frac{a}{2h}(v_{j+1}^n - v_{j-1}^n) = 0.$$ 

These schemes are all explicit: knowing $\{v^n\}$ march forward to $\{v^{n+1}\}$.
THREE DISCRETIZATIONS: MOLECULAR REPRESENTATION

Set $\mu = k/h$.

\[ v_j^{n+1} = v_j^n - \mu a (v_{j+1}^n - v_j^n) \]

\[ v_j^{n+1} = v_j^n - \frac{\mu a}{2} (v_{j+1}^n - v_{j-1}^n) \]

\[ v_j^{n+1} = v_j^{n-1} - \mu a (v_{j+1}^n - v_{j-1}^n) \]
**Simple Example**

- Set \( a = 1 \), so \( u_t + u_x = 0 \); consider **Cauchy problem** (pure IVP on half space)

\[
    u(0, x) = u_0(x) = \begin{cases} 
    1, & x \leq 0 \\
    0, & x > 0 
    \end{cases}.
\]

- The exact solution is \( u(t, x) = u_0(x - t) \), so

\[
    u(1, x) = \begin{cases} 
    1, & x \leq 1 \\
    0, & x > 1 
    \end{cases}.
\]

- Consider the **one-sided** difference scheme.
  
  If \( x_0 = 0 \) then \( v_{j}^0 = 0, \ \forall \ j > 0 \), implying \( v_{j}^1 = 0, \ \forall \ j > 0 \), then \( v_{j}^2 = 0, \ \forall \ j > 0 \), etc.

- So for \( Nk = 1 \) obtain \( v_{j}^N = 0, \ \forall \ j > 0 \), which has the error

\[
    |v_{j}^N - u(1, x_j)| = 1 \quad \text{for} \quad 0 < x_j \leq 1.
\]
Simple example cont.

Note **domain of dependence** (triangle spanned by black dots) of numerical method. The characteristic line arrives from outside it.
Another simple example

Setting $a = -1$, so $u_t - u_x = 0$, likewise have inconsistency if $\mu > 1$. 
The domain of dependence of the PDE must be contained in the domain of dependence of the difference scheme.
Stability of numerical method

- CFL condition is necessary but not sufficient for scheme to be well-behaved.
- Require stability: For fixed $h > 0$ small enough, solution norm should not increase in time: as $k \to 0$, $nk \leq t_f$, must have $\|v^{n+1}\| \leq \|v^n\|$. 

$$\|v^n\| = \sqrt{h \sum_j (v^n_j)^2}.$$ 

- This condition for the numerical method parallels well-posedness for the PDE problem.
- So, consider the same sort of analysis for

$$v(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi x} \hat{v}(t, \xi) d\xi.$$
Stability of one-sided scheme

For advection equation \( u_t + au_x = 0 \) consider one-sided scheme.

Substituting in one-sided scheme,

\[
\int_{-\infty}^{\infty} e^{i\xi x} \hat{\nu}(t + k, \xi) d\xi = \int_{-\infty}^{\infty} \left[ e^{i\xi x} - \mu a \left( e^{i\xi(x+h)} - e^{i\xi x} \right) \right] \hat{\nu}(t, \xi) d\xi.
\]

Integrands must agree:

\[
\hat{\nu}(t + k, \xi) = \left[ 1 - \mu a e^{i\xi h} - 1 \right] \hat{\nu}(t, \xi).
\]

Set \( \zeta = \xi h \) and \( g(\zeta) = 1 - \mu a (e^{i\zeta} - 1) \). So, each Fourier mode is multiplied by \( g(\zeta) \) over each time step.

For stability, require amplification factor to satisfy

\[
|g(\zeta)| \leq 1, \forall \zeta.
\]
Stability of one-sided scheme cont.

- Need $|g(\zeta)| = |1 - \mu a(e^{\zeta} - 1)| \leq 1, -\pi \leq \zeta \leq \pi$.
- Must have $a \leq 0$.
- For $a \leq 0$, circle centred at $1 + \mu a$ with radius $-\mu a$ must be contained in unit disk.
- This implies $(-a)\mu \leq 1$, obtaining stability iff CFL condition holds!
For the scheme

\[(v_j^{n+1} - v_j^n) + \frac{\mu a}{2} (v_{j+1}^n - v_{j-1}^n) = 0,\]

(forward in time, centred in space), apply same analysis.

Obtain

\[\hat{v}(t + k, \xi) = \left[1 - \frac{\mu a}{2} (e^{i\xi h} - e^{-i\xi h})\right] \hat{v}(t, \xi).\]

So,

\[g(\zeta) = 1 - \frac{\mu a}{2} (e^{i\zeta} - e^{-i\zeta}) = 1 - \mu a \sin \zeta.\]

Here, \( |g|^2 = 1 + \mu^2 a^2 \sin^2 \zeta > 1 \) so this scheme is unconditionally unstable.
Stability of leap-frog scheme

For the leap-frog scheme

\[(v_j^{n+1} - v_j^{n-1}) + \mu a(v_{j+1}^n - v_{j-1}^n) = 0,\]

(centred in time, centred in space), apply same analysis.

Obtain

\[\hat{v}(t + k, \xi) = \hat{v}(t - k, \xi) - \mu a(e^{i\xi h} - e^{-i\xi h})\hat{v}(t, \xi).\]

Ansatz: try to solve this with \(\hat{v}(t_n, \xi) = \kappa^n\).

Substitute and divide by \(\kappa^{n-1}\), obtaining

\[\kappa^2 = 1 - 2(\mu a \sin \xi)\kappa.\]

Solve quadratic equation:

\[g(\xi) \sim \kappa = -\mu a \sin \xi \pm \sqrt{-\mu^2 a^2 \sin^2 \xi + 1}.\]
Stability of leap-frog scheme cont.

- **Ansatz**: try to solve this with \( \hat{\nu}(t_n, \xi) = \kappa^n \).
  Substitute and divide by \( \kappa^{n-1} \), obtaining
  \[
  \kappa^2 = 1 - 2(\nu a \sin \xi) \kappa.
  \]

- Solve quadratic equation:
  \[
  g(\xi) \sim \kappa = -\nu a \sin \xi \pm \sqrt{-\mu^2 a^2 \sin^2 \xi + 1}.
  \]

- To get \( |\kappa| \leq 1 \), must have nonnegative argument under square root sign. Obtain **stability** iff
  \[
  \mu |a| \leq 1
  \]
  (which again agrees with the CFL condition).
Finite differences

**Numerical example**

\[ u_t = u_x, \quad u_0(x) = \sin(\eta x), \text{ periodic BC}. \]

- Run `fig1_12`
- Play with step sizes \( k, h \), oscillation parameter \( \eta \).
- Check stability and accuracy
- See Figure 1.12 and Table 1.1 in text.