CS520: Introduction (Ch. 1)

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Introduction

- 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 indenpendent variable ("**time**").
- Partial differential equation (PDE): several independent variables.

Partial differential equations

- 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.

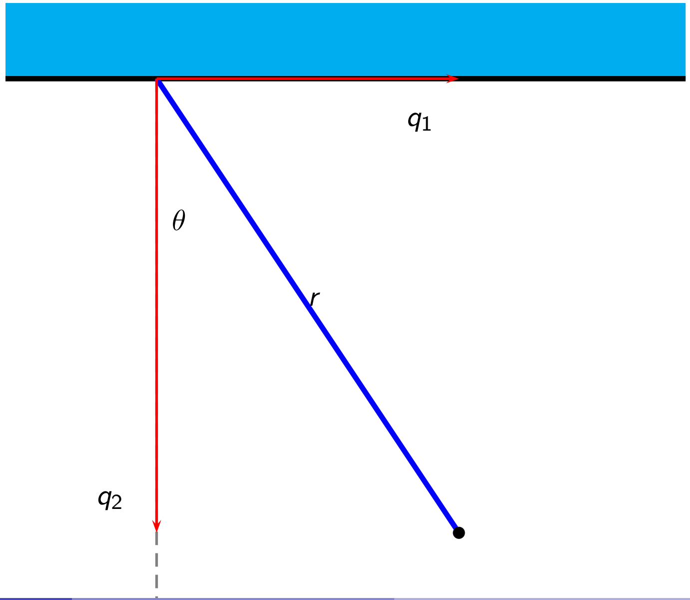
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

- 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:

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad a < t < b.$$

For the pendulum

$$\mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} y_2 \\ -g \sin(y_1) \end{pmatrix}.$$

Side conditions

e.g.

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

- Initial value problem: $\mathbf{y}(a)$ given. (In the pendulum example: $\theta(0)$ and $\theta'(0)$ given.)
- Boundary value problem: relations involving $\mathbf{y}$ 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 ν 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

$$u(t, 0) = g_0(t), \;\; u(t, b) = g_b(t).$$

Simple analysis

- Ignore boundary conditions, seek special solution of the form

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

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

- ξ is wave number; $e^{\imath\xi x}$ is mode; $|\hat{u}(t,\xi)|$ is amplitude.
- For this special solution

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

- Obtain ODE

$$\hat{u}_t = -\left(\nu\xi^2 + 3\imath\xi\right)\hat{u}.$$

Simple analysis cont.

- The solution of the initial value ODE problem

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

  is

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

- 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 ν

- 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:

$$\hat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\imath \xi x} v(x) dx.$$

- The corresponding inverse transform:

$$v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\imath \xi x} \hat{v}(\xi) d\xi.$$

- ξ 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

$$\begin{aligned} u_x(t,x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\imath \xi) e^{\imath \xi x} \hat{u}(t,\xi) d\xi, \\ u_{xx}(t,x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\imath \xi)^2 e^{\imath \xi x} \hat{u}(t,\xi) d\xi, \\ u_t(t,x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\imath \xi x} \hat{u}_t(t,\xi) d\xi. \end{aligned}$$

- So, our simple PDE can be written as

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

Return to simple PDE cont.

- To satisfy

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

 for all x, what's in square brackets must vanish, so we obtain the ODE

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

 for each wavenumber ξ.

- The symbol of this PDE is

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

 so

$$P(\imath\xi) = -(\nu\xi^2 + 3\imath\xi).$$

Well-posed initial-value problems

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

$$\begin{aligned} u_t &= P(\partial_x)u, \qquad -\infty < x < \infty,\ t > 0 \\ u(t,0) &= u_0(x). \end{aligned}$$

- The initial value problem is well-posed if there are constants K and α such that

$$\|u(t)\| \le Ke^{\alpha t}\|u(0)\| = Ke^{\alpha t}\|u_0\|, \quad \forall u_0 \in \mathcal{L}_2.$$

Condition using Fourier transform

- To check well-posedness, apply Fourier transform as before.
- Obtain well-posedness iff there are constants K and α such that

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

Heat equation

- The simplest parabolic PDE:

$$u_t = u_{xx}.$$

- we get the symbol

$$P(\imath\xi) = -\xi^2.$$

- Hence

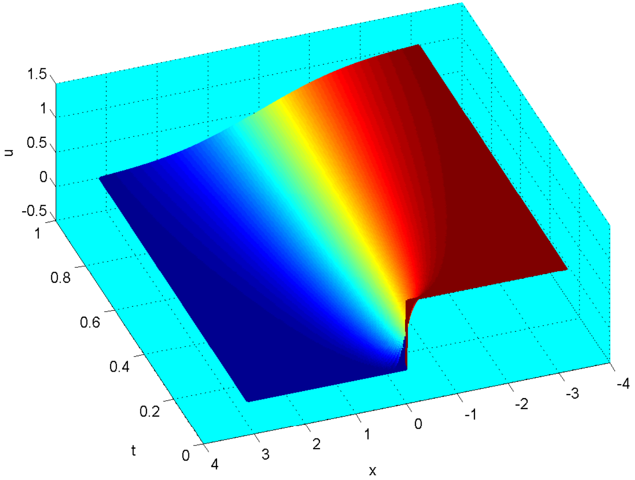
$$|e^{P(\imath\xi)t}| = |e^{-\xi^2 t}| \leq 1 \quad \forall\xi.$$

  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:

$$u_t + a u_x = 0$$

- we get

$$P(\imath\xi) = -a\imath\xi.$$

  Hence

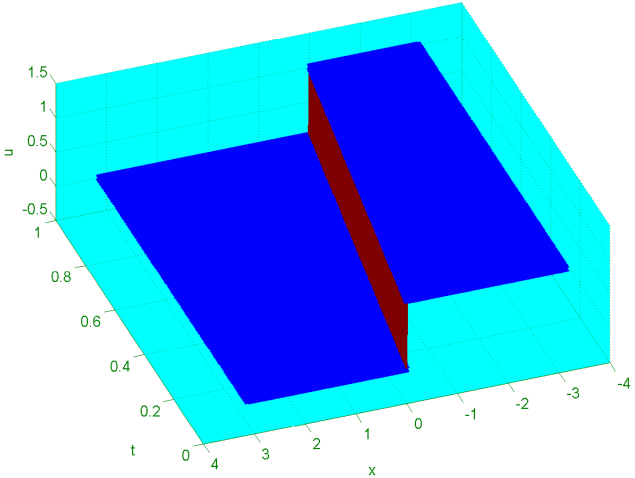
$$|e^{P(\imath\xi)t}| = |e^{-\imath a\xi t}| = 1 \quad \forall \xi.$$

- 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

fig1_3



Wave equation

- A better behaved hyperbolic PDE, the classical wave equation:

$$w_{tt} - c^2 w_{xx} = 0.$$

- Define $u_1 = w_t,\ u_2 = c w_x,\ \mathbf{u} = (u_1, u_2)^T$, obtain

$$\mathbf{u}_t - \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} \mathbf{u}_x = 0.$$

- 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 $c = \imath$ 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.

Systems of PDEs

- Consider the PDE system

$$\mathbf{u}_t = A\mathbf{u}_{xx}.$$

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

$$\mathbf{u}_t = A\mathbf{u}_x$$

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

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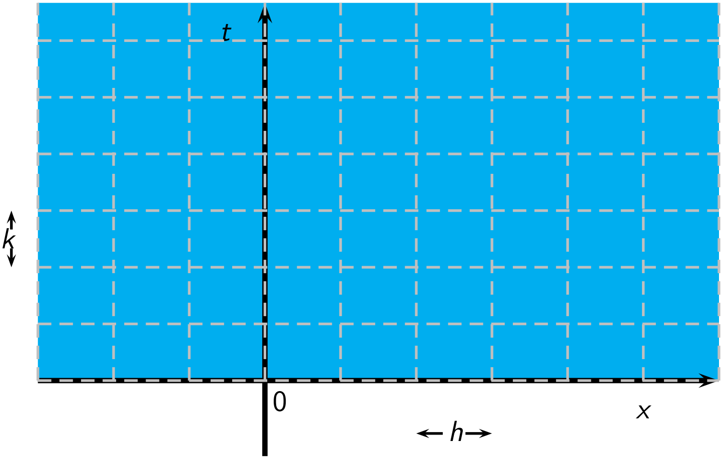
Discretization mesh

Step sizes $\Delta t = k,\ \Delta x = h$

$$v_j^n = v(t_n, x_j) \equiv v(nk, jh) \approx u(nk, jh)$$



Three discretizations for advection equation

Advection equation: $u_t + au_x = 0.$

1. One sided

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

2. Centered in x

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

3. Leap-frog

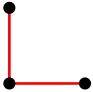
$$\frac{1}{2k}(v_j^{n+1} - v_j^{n-1}) + \frac{a}{2h}(v_{j+1}^n - v_{j-1}^n) = 0.$$

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

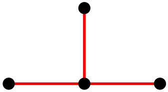
Three discretizations: molecular representation

Set $\mu = k/h$.

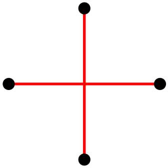
$$v_j^{n+1} = v_j^n - \mu a(v_{j+1}^n - v_j^n)$$



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



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



Simple example

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

$$u(0,x) = u_0(x) = \begin{cases} 1, & x \le 0 \\ 0, & x > 0 \end{cases}.$$

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

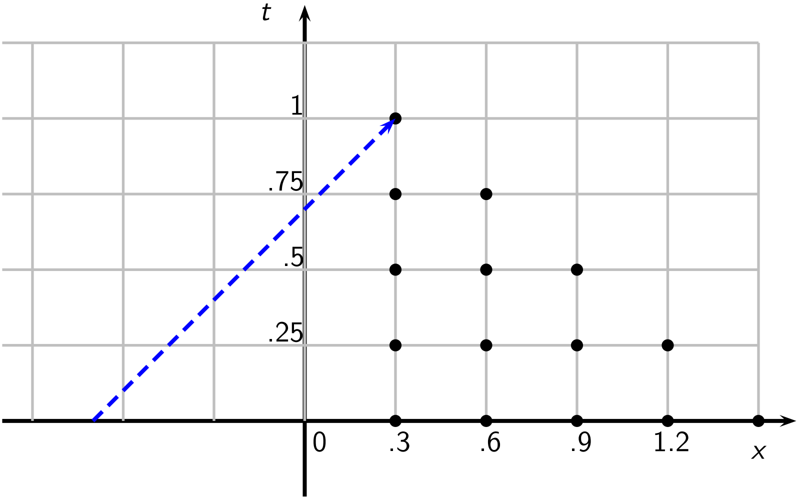
$$u(1,x) = \begin{cases} 1, & x \le 1 \\ 0, & x > 1 \end{cases}.$$

- 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 $v_j^N = 0, \quad \forall\, j > 0$, which has the error

$$|v_j^N - u(1,x_j)| = 1 \quad \text{for} \quad 0 < x_j \le 1.$$

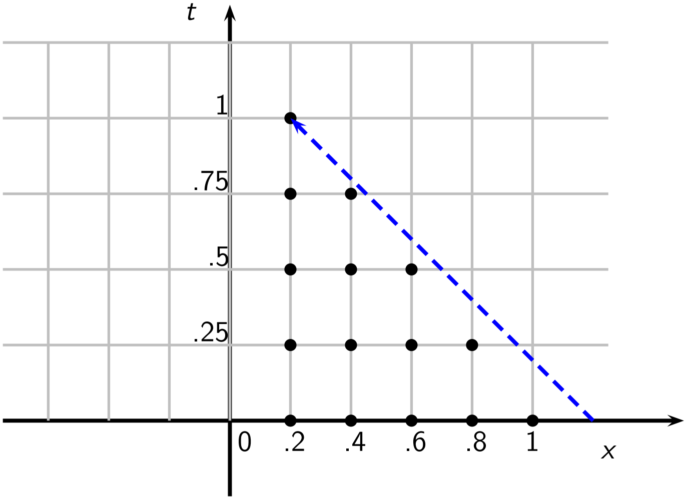
Simple example cont.

Note domain of dependence (triangle spanned by black dots) of numerical method. The charactristic line arrives from outside it.



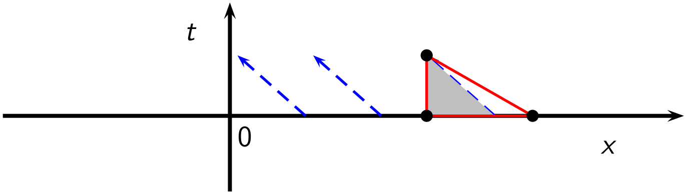
Another simple example

Setting $a = -1$, so $u_t - u_x = 0$, likewise have inconsistency if $\mu > 1$.



Courant-Friedrichs-Lewy (CFL) condition

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 $h >$ small enough, solution norm should not increase in time: as $k \to 0,\ nk \le t_f$, must have $\|v^{n+1}\| \le \|v^n\|$.

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

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

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

Stability of one-sided scheme

- For advection equation $u_t + au_x = 0$ consider one-sided scheme.
- Substituting in one-sided scheme,

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

- Integrands must agree:

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

- Set $\zeta = \xi h$ and $g(\zeta) = 1 - \mu a\left(e^{\imath\zeta} - 1\right)$. So, each Fourier mode is multiplied by a $g(\zeta)$ over each time step.
- For stability, require amplification factor to satisfy

$$|g(\zeta)| \le 1,\ \forall\zeta.$$

Stability of one-sided scheme cont.

- Need $|g(\zeta)| = |1 - \mu a(e^{\imath\zeta} - 1)| \leq 1, \; -\pi \leq \zeta \leq \pi$.
- 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!

Stability of space-centred scheme

- 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

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

- So,

$$g(\zeta) = 1 - \frac{\mu a}{2}\left(e^{\imath\zeta} - e^{-\imath\zeta}\right) = 1 - \imath\mu a \sin\zeta.$$

- 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

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

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

$$\hat{v}(t+k,\xi) = \hat{v}(t-k,\xi) - \mu a\big(e^{\imath\xi h} - e^{-\imath\xi h}\big)\hat{v}(t,\xi).$$

- Ansatz: try to solve this with $\hat{v}(t_n,\xi) = \kappa^n$.
 Substitute and divide by κ^{n-1}, obtaining

$$\kappa^2 = 1 - 2\big(\imath\mu a \sin\zeta\big)\kappa.$$

- Solve quadratic equation:

$$g(\zeta) \sim \kappa = -\imath\mu a \sin\zeta \pm \sqrt{-\mu^2 a^2 \sin^2\zeta + 1}.$$

Stability of leap-frog scheme cont.

- Ansatz: try to solve this with $\hat{v}(t_n, \xi) = \kappa^n$.
  Substitute and divide by κ^{n-1}, obtaining

$$\kappa^2 = 1 - 2(\imath \mu a \sin \zeta)\kappa.$$

- Solve quadratic equation:

$$g(\zeta) \sim \kappa = -\imath \mu a \sin \zeta \pm \sqrt{-\mu^2 a^2 \sin^2 \zeta + 1}.$$

- 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).

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 η.
- Check stability and accuracy
- See Figure 1.12 and Table 1.1 in text.