Lecture 6: Finite difference methods

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Finite difference methods

- Finite difference methods: basic numerical solution methods for partial differential equations.
- Obtained by replacing the derivatives in the equation by the appropriate numerical differentiation formulas.
- Numerical scheme: accurately approximate the true solution.
- Basic finite difference schemes for the heat and the wave equations.

Finite difference methods

- Numerical algorithms for the heat equation
  Finite difference approximations
- Consider the heat equation

$$\begin{cases} \dfrac{\partial u}{\partial t} - \gamma \dfrac{\partial^2 u}{\partial x^2} = 0, \quad x \in [0,1], t \geq 0, \\ u(t,0) = u(t,1) = 0, \quad t \geq 0, \\ u(0,x) = u_0(x), \quad x \in [0,1], \end{cases}$$

$\gamma > 0$: thermal conductivity.

Finite difference methods

- Numerical approximation to the solution u:
  - Rectangular mesh consisting of points (t_k, x_j) with

    $$0 = t_0 < t_1 < t_2 < \dots \quad \text{and} \quad 0 = x_0 < x_1 < \dots < x_{N+1} = 1.$$

  - Uniform time step and spatial mesh sizes:

    $$\Delta t = t_{k+1} - t_k, \quad \Delta x = x_{j+1} - x_j = \frac{1}{N}.$$

Finite difference methods

- Numerical approximation of u at the mesh point (t_k, x_j):

$$u_j^k \approx u(t_k, x_j) \quad \text{where } t_k = k\Delta t, \quad x_j = j\Delta x.$$

- Dirichlet boundary conditions $u(t,0) = u(t,1) = 0,\ t \geq 0 \Rightarrow$

$$u_0^k = u_{N+1}^k = 0 \quad \text{for all } k > 0.$$

Finite difference methods

- Finite difference approximations for the derivatives.
- Approximation of the second order space derivative:

$$\frac{\partial^2 u}{\partial x^2}(t_k, x_j) \approx \frac{u(t_k, x_{j-1}) - 2u(t_k, x_j) + u(t_k, x_{j+1})}{(\Delta x)^2} + O((\Delta x)^2)$$

$$\approx \frac{u_{j-1}^k - 2u_j^k + u_{j+1}^k}{(\Delta x)^2} + O((\Delta x)^2).$$

Finite difference methods

- Approximation of the time derivative:

$$\frac{\partial u}{\partial t}(t_k, x_j) \approx \frac{u(t_{k+1}, x_j) - u(t_k, x_j)}{\Delta t} + O(\Delta t) \approx \frac{u_j^{k+1} - u_j^k}{\Delta t} + O(\Delta t).$$

Finite difference methods

- Explicit scheme:

$$\frac{u_j^{k+1} - u_j^k}{\Delta t} + \gamma \frac{-u_{j-1}^k + 2u_j^k - u_{j+1}^k}{(\Delta x)^2} = 0$$

  for $k \geq 0$ and $j \in \{1, \ldots, N\}$.

- $$\mu := \frac{\gamma \Delta t}{(\Delta x)^2};$$

- Vector whose entries are the numerical approximations to the solution values at time t_k at the interior nodes:

$$u^{(k)} := (u_1^k, u_2^k, \ldots, u_N^k)^\top \approx (u(t_k, x_1), u(t_k, x_2), \ldots, u(t_k, x_N))^\top.$$

Finite difference methods

- Matrix form:

$$u^{(k+1)} = Au^{(k)};$$

- $$A := \begin{pmatrix} 1-2\mu & \mu & & & & \\ \mu & 1-2\mu & \mu & & & \\ & \mu & 1-2\mu & \mu & & \\ & \ddots & \ddots & \ddots & & \\ & & \mu & 1-2\mu & \mu \\ & & & \mu & 1-2\mu \end{pmatrix}.$$

- A: symmetric and tridiagonal.

Finite difference methods

- Consistency, stability, and convergence
- General finite difference method:

$$F_{\Delta t, \Delta x}(\{u_{j+n}^{k+m}\}_{m^- \leq m \leq m^+, n^- \leq n \leq n^+}) = 0,$$

$m^{\pm}, n^{\pm}$: width of the stencil of the scheme.

Finite difference methods

- DEFINITION: Consistency and order

  - Finite difference scheme: consistent with $F(u) = 0$ if, for any smooth solution $u(x, t)$, truncation error:

$$F_{\Delta t, \Delta x}(\{u(t_{k+m}, x_{j+n})\}_{m^- \leq m \leq m^+, n^- \leq n \leq n^+}) \to 0$$

    as Δt and $\Delta x \to 0$ independently.
  - Scheme: of order p in time and order q in space if truncation error: of the order of $O((\Delta t)^p + (\Delta x)^q)$ as Δt and $\Delta x \to 0$.

Finite difference methods

- THEOREM:
  - Explicit scheme: consistent with the heat equation, of order one in time and two in space.
  - Moreover, if

$$(*) \qquad \frac{\gamma \Delta t}{(\Delta x)^2} = \frac{1}{6},$$

then, explicit scheme: of order two in time and four in space.

Finite difference methods

- PROOF:
  - Taylor expansion of $v(t,x) \in \mathcal{C}^6$ evaluated at (t,x),

$$\frac{v(t+\Delta t,x)-v(t,x)}{\Delta t} + \gamma \frac{-v(t,x-\Delta x)+2v(t,x)-v(t,x+\Delta x)}{(\Delta x)^2}$$
$$= (\frac{\partial v}{\partial t} - \gamma \frac{\partial^2 v}{\partial x^2})(t,x) + \frac{\Delta t}{2}\frac{\partial^2 v}{\partial t^2}(t,x) - \frac{\gamma(\Delta x)^2}{12}\frac{\partial^4 v}{\partial x^4}(t,x) + O((\Delta t)^2 + (\Delta x)^4).$$

Finite difference methods

- v: solution of the heat equation $\Rightarrow$ truncation error goes to zero as $\Delta t, \Delta x \to 0$ $\Rightarrow$ explicit scheme: consistent.
- Scheme: of order 1 in time and 2 in space.
- Suppose that $(*)$ holds $\Rightarrow$ terms in Δt and $(\Delta x)^2$ cancel out since

$$\frac{\partial^2 v}{\partial t^2} = \gamma \frac{\partial^3 v}{\partial t \partial x^2} = \gamma^2 \frac{\partial^4 v}{\partial x^4}.$$

- Explicit scheme: of order 2 in time and 4 in space.

Finite difference methods

- DEFINITION: Stability
  - Finite difference scheme: stable with respect to the norm $\| \|_r$ defined by

$$\|u^{(k)}\|_r := \left(\sum_{j=1}^{N} \Delta x |u_j^k|^r \right)^{\frac{1}{r}}, \quad 1 \leq r \leq +\infty,$$

$u^{(k)}$, if there exists a positive constant C independent of Δt and Δx s.t.

$$\|u^{(k)}\|_r \leq C \|u^{(0)}\|_r \quad \text{for all } k \geq 0.$$

Finite difference methods

- DEFINITION: Linear scheme
  - Finite difference scheme: linear if scheme: linear with respect to its arguments u_{j+n}^{k+m}.
- Linear finite difference scheme:

$$u^{(k+1)} = Au^{(k)},$$

A: iteration matrix.

Finite difference methods

- $\Rightarrow$

$$u^{(k+1)} = A^{k+1} u^{(0)}.$$

- Stability $\Leftrightarrow$

$$\|A^k u^{(0)}\|_r \leq C \|u^{(0)}\|_r, \quad \text{for all } k \geq 0 \text{ and } u^{(0)} \in \mathbb{R}^N.$$

- Matrix norm

$$\|M\|_r = \sup_{u \in \mathbb{R}^N, u \neq 0} \frac{\|Mu\|_r}{\|u\|_r}.$$

- Stability $\Leftrightarrow$

$$\|A^k\|_r \leq C, \quad \text{for all } k \geq 0.$$

Finite difference methods

- Stability in the L^∞ norm
- L^∞-norm:

$$\|u^{(k)}\|_\infty := \sup_{1\le j\le N} |u_j^k|.$$

- Implicit scheme:

$$\frac{u_j^{k+1} - u_j^k}{\Delta t} + \gamma \frac{-u_{j-1}^{k+1} + 2u_j^{k+1} - u_{j+1}^{k+1}}{(\Delta x)^2} = 0$$

  for $k \ge 0$ and $j \in \{1, \dots, N\}$.

- Implicit scheme well defined: $u^{(k+1)}$ can be obtained from $u^{(k)}$ by inverting the definite positive matrix

$$\begin{pmatrix} 1+2\mu & -\mu & & & & \\ -\mu & 1+2\mu & -\mu & & & \\ & -\mu & 1+2\mu & -\mu & & \\ & \ddots & \ddots & \ddots & & \\ & & -\mu & 1+2\mu & -\mu \\ & & & -\mu & 1+2\mu \end{pmatrix}.$$

Finite difference methods

- THEOREM:

  (i) Explicit scheme: stable with respect to the L^∞ norm iff the Courant-Friedrichs-Lewy (CFL) condition holds:

  $$2\gamma \Delta t \leq (\Delta x)^2.$$

  (ii) Implicit scheme: unconditionally stable with respect to the L^∞ norm.

Finite difference methods

- Stability in the L^2 norm
- Consider the heat equation with the periodic boundary conditions

$$u(t, x+1) = u(t, x) \quad \text{for all } x \in [0,1], \quad t \geq 0.$$

- For any $u^{(k)} = (u_j^k)_{j=0,\ldots,N}$, we associate a piecewise constant function $u^{(k)}(x)$, periodic with period 1, defined on $[0,1]$ by

$$u^{(k)}(x) := u_j^k \quad \text{for } x_{j-\frac{1}{2}} < x < x_{j+\frac{1}{2}},$$

$$x_{j+\frac{1}{2}} = (j+\frac{1}{2})\Delta x, \quad j = 0, \ldots, N, \quad x_{-\frac{1}{2}} = 0, x_{N+1+\frac{1}{2}} = 1.$$

Finite difference methods

- Fourier series of $u^{(k)}$:

$$u^{(k)}(x) = \sum_{n\in\mathbb{Z}} \hat{u}_n^{(k)} e^{2\pi inx},$$

$$\hat{u}_n^{(k)} := \int_0^1 u^{(k)}(x) e^{-2\pi inx}\, dx.$$

- Plancherel's formula $\Rightarrow$

$$\int_0^1 |u^{(k)}(x)|^2\, dx = \sum_{n\in\mathbb{Z}} |\hat{u}_n^{(k)}|^2.$$

- Property of Fourier series of periodic functions:

$$v^{(k)}(x) = u^{(k)}(x+\Delta x) \Rightarrow \hat{v}_n^{(k)} = \hat{u}_n^{(k)} e^{2\pi in\Delta x}.$$

Finite difference methods

- Explicit scheme:

$$\frac{u^{k+1}(x) - u^k(x)}{\Delta t} + \gamma \frac{-u^k(x-\Delta x) + 2u^k(x) - u^k(x+\Delta x)}{(\Delta x)^2} = 0.$$

- Fourier transform $\Rightarrow$

$$\hat{u}_n^{(k+1)} = \left(1 - \frac{\gamma \Delta t}{(\Delta x)^2}(e^{-2\pi i n \Delta x} + 2 - e^{2\pi i n \Delta x})\right) \hat{u}_n^{(k)}.$$

Finite difference methods

- Equivalently,
$$\hat{u}_n^{(k+1)} = \alpha(n)\hat{u}_n^{(k)} = \alpha(n)^{k+1}\hat{u}^{(0)}(n)$$
with
$$\alpha(n) := 1 - \frac{4\gamma\Delta t}{(\Delta x)^2}(\sin(\pi n\Delta x))^2.$$
- $\Rightarrow \hat{u}_n^{(k)}$: bounded as $k \to +\infty$ iff the amplification factor $\alpha(n)$ satisfies
$$|\alpha(n)| \leq 1 \quad \text{for all } n \in \mathbb{Z}.$$
- Plancherel's formula $\Rightarrow$
$$\|u^{(k)}\|_2^2 = \int_0^1 |u^{(k)}(x)|^2\,dx = \sum_{n\in\mathbb{Z}} |\hat{u}_n^{(k)}|^2 \leq \sum_{n\in\mathbb{Z}} |\hat{u}_n^{(0)}|^2 = \|u^{(0)}\|_2^2,$$
- $\Rightarrow$ Conditional stability with respect to the L^2 norm.
- CFL condition:
$$\frac{2\gamma\Delta t}{(\Delta x)^2} \leq 1.$$

Finite difference methods

- Implicit scheme:

$$\frac{u^{k+1}(x) - u^k(x)}{\Delta t} + \gamma \frac{-u^{k+1}(x - \Delta x) + 2u^{k+1}(x) - u^{k+1}(x + \Delta x)}{(\Delta x)^2} = 0.$$

- Fourier transform $\Rightarrow$

$$\hat{u}_n^{(k+1)} = \beta(n)\hat{u}_n^{(k)} = \beta(n)^{k+1}\hat{u}^{(0)}(n),$$

$$\beta(n) := \left(1 + \frac{4\gamma\Delta t}{(\Delta x)^2}(\sin(\pi n \Delta x))^2\right)^{-1}.$$

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- Plancherel's formula $\Rightarrow$ Unconditional stability with respect to the L^2 norm.

Finite difference methods

- THEOREM:

  (i) Explicit scheme: stable with respect to the L^2 norm iff the CFL condition

  $$2\gamma\Delta t \leq (\Delta x)^2$$

  holds.

  (ii) Implicit scheme: unconditionally stable with respect to the L^2 norm.

Finite difference methods

- Convergence
- THEOREM: Lax theorem
  - u: smooth solution of the heat equation.
  - Suppose that the finite difference scheme for computing the numerical solution u_j^k: linear, consistent, and stable with respect to the norm $\| \|_r$.
  - Let $e_j^k := u_j^k - u(t_k, x_j)$ and $e^{(k)} = (e_1^k, e_2^k, \ldots, e_N^k)^\top$.
  - Assume that $u_j^0 = u_0(x_j)$.

Finite difference methods

- Then,

$$\lim_{\Delta t, \Delta x \to 0} \Big(\sup_{t_k \le T} \|e^{(k)}\|_r \Big) = 0 \quad \text{for all } T > 0.$$

- Moreover, if the scheme: of order p in time and q in space, then there exists a constant $C_T > 0$ s.t.

$$\sup_{t_k \le T} \|e^{(k)}\|_r \le C_T \big((\Delta t)^p + (\Delta x)^q \big).$$

Finite difference methods

- PROOF:
  - $u^{(k+1)} = Au^{(k)}$; A: iteration matrix; $\widetilde{u}_j^k = u(t_k, x_j)$.
  - Consistency $\Rightarrow$ there exists $\epsilon^{(k)}$ s.t.

$$\widetilde{u}^{(k+1)} = A\widetilde{u}^{(k)} + (\Delta t)\epsilon^{(k)} \quad \text{and} \quad \lim_{\Delta t, \Delta x \to 0} \|\epsilon^{(k)}\|_r = 0,$$

    uniformly in k.
  - Scheme: of order p in time and q in space $\Rightarrow$

$$\|\epsilon^{(k)}\|_r \leq C\big((\Delta t)^p + (\Delta x)^q\big).$$

Finite difference methods

- $\Rightarrow$
$$e^{(k+1)} = Ae^{(k)} - \Delta t \epsilon^{(k)}.$$
- By induction,
$$e^{(k)} = A^k e^{(0)} - \Delta t \sum_{l=1}^{k} A^{k-l} \epsilon^{(l-1)}.$$
- Stability $\Rightarrow$
$$\|A^k\|_r \leq C'$$
for some positive constant C'.
- $\Rightarrow$
$$\|e^{(k)}\|_r \leq (\Delta t) k C C'((\Delta t)^p + (\Delta x)^q) \leq T C C'((\Delta t)^p + (\Delta x)^q).$$

Finite difference methods

- Numerical algorithms for the one-way wave equation

$$\begin{cases} \dfrac{\partial u}{\partial t} = c\dfrac{\partial u}{\partial x}, \\ u(0,x) = u_0(x), \end{cases}$$

- $c > 0$: wave speed.
- Solution given by $u(t,x) = u_0(x+ct)$.
- Identity:

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

Finite difference methods

Finite difference methods

- There are three finite difference approximations of the solution:

$$\frac{u_j^{k+1} - u_j^k}{\Delta t} = \begin{cases} c\,\dfrac{u_{j+1}^k - u_j^k}{\Delta x} & \textbf{upwind scheme}, \\ c\,\dfrac{u_j^k - u_{j-1}^k}{\Delta x} & \textbf{downwind scheme}, \\ c\,\dfrac{u_{j+1}^k - u_{j-1}^k}{2\Delta x} & \textbf{centered scheme}. \end{cases}$$

Finite difference methods

- Taylor expansions of a smooth solution u:

$$\frac{u(t+\Delta t, x) - u(t,x)}{\Delta t} = \frac{\partial u}{\partial t}(t,x) + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(t,x) + O((\Delta t)^2),$$

$$\frac{u(t, x+\Delta x) - u(t,x)}{\Delta x} = \frac{\partial u}{\partial x}(t,x) + \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}(t,x) + O((\Delta x)^2),$$

$$\frac{u(t, x+\Delta x) - u(t,x-\Delta x)}{\Delta x} = \frac{\partial u}{\partial x}(t,x) + O((\Delta x)^2),$$

- $\Rightarrow$ truncation error in the upwind scheme is $O(\Delta t + \Delta x)$.
- Analogously, the truncation error in the downwind scheme is $O(\Delta t + \Delta x)$, while the one in the centered is $O(\Delta t + (\Delta x)^2)$.
- If

$$c = \frac{\Delta x}{\Delta t},$$

then the truncation error in the upwind scheme is $O((\Delta t)^2 + (\Delta x)^2)$.

Finite difference methods

- Stability analysis: one can easily see that the upwind scheme is stable with respect to the L^2 norm provided that the following CFL condition holds:

$$\frac{c\Delta t}{\Delta x} \leq 1.$$

- Downwind and the centered schemes are unstable.
- One way to fix the stability issue for the centered scheme is to add diffusion. One replaces the centered scheme with

$$\frac{u_j^{k+1} - u_j^k}{\Delta t} = c\,\frac{u_{j+1}^k - u_{j-1}^k}{2\Delta x} + \theta\,\frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{(\Delta x)^2},$$

where $\theta > 0$, or equivalently, with

$$\frac{u_j^{k+1} - (\frac{\lambda}{2}u_{j+1}^k + (1-\lambda)u_j^k + \frac{\lambda}{2}u_{j-1}^k)}{\Delta t} = c\,\frac{u_{j+1}^k - u_{j-1}^k}{2\Delta x}.$$

Here, λ is defined by

$$\lambda = \frac{2\Delta t}{(\Delta x)^2}\theta.$$

Finite difference methods

Finite difference methods

- Numerical algorithms for the wave equation
- Consider the wave equation

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = c^2 \dfrac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad t \geq 0, \\ u(t, x+1) = u(t, x), \quad 0 < x < 1, \quad t \geq 0, \\ u(0, x) = u_0(x), \quad 0 < x < 1, \\ \dfrac{\partial u}{\partial t}(0, x) = u_1(x), \quad 0 < x < 1, \end{cases}$$

$c > 0$: wave speed.

- Suppose

$$(**) \qquad \int_0^1 u_1(x)\, dx = 0.$$

Finite difference methods

- Similar to the numerical schemes for the heat equation, we can use differentiation formulas to arrive at a numerical scheme for the wave equation.
- Since both time and space derivatives are of second order, we use centered differences to approximate them:

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2}(t_k, x_j) &\approx \frac{u(t_{k-1}, x_j) - 2u(t_k, x_j) + u(t_{k+1}, x_j)}{(\Delta t)^2} + O((\Delta t)^2) \\ &\approx \frac{u_j^{k-1} - 2u_j^k + u_j^{k+1}}{(\Delta t)^2} + O((\Delta t)^2).\end{aligned}$$

- Then up to an error of order $O((\Delta x)^2 + (\Delta t)^2)$ the solution to the wave equation can be approximated by the following explicit finite difference scheme:

$$\frac{u_j^{k+1} - 2u_j^k + u_j^{k-1}}{(\Delta t)^2} = c^2 \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{(\Delta x)^2}.$$

- One can prove that the scheme is stable in the L^2 norm provided that $c(\Delta t)/(\Delta x) \leq 1$.

Finite difference methods

- Another standard finite difference scheme for solving the wave equation: θ-centered scheme

$$\left\{ \begin{array}{l} \dfrac{u_j^{k+1} - 2u_j^k + u_j^{k-1}}{(\Delta t)^2} + \theta c^2 \dfrac{-u_{j-1}^{k+1} + 2u_j^{k+1} - u_{j+1}^{k+1}}{(\Delta x)^2} \\ \quad + (1-2\theta) c^2 \dfrac{-u_{j-1}^{k} + 2u_j^{k} - u_{j+1}^{k}}{(\Delta x)^2} + \theta c^2 \dfrac{-u_{j-1}^{k-1} + 2u_j^{k-1} - u_{j+1}^{k-1}}{(\Delta x)^2} = 0, \end{array} \right.$$

$0 \leq \theta \leq 1/2$.

Finite difference methods

- If $\theta = 0$, then the scheme: explicit;
- Scheme: implicit if $\theta \neq 0$.
- Initial conditions expressed by

$$u_j^0 = u_0(x_j) \quad \text{and} \quad \frac{u_j^1 - u_j^0}{\Delta t} = \int_{x_{j-1/2}}^{x_{j+1/2}} u_1(x)\, dx;$$

- $\Rightarrow$ $(**)$: satisfied by the numerical solution.

Finite difference methods

- THEOREM:
  - If $1/4 \leq \theta \leq 1/2$, then the θ-centered scheme: unconditionally stable with respect to the L^2 norm.
  - If $0 \leq \theta < 1/4$, scheme: stable provided that the CFL condition

$$\frac{c\Delta t}{\Delta x} < \sqrt{\frac{1}{1-4\theta}}$$

holds and unstable if $c\Delta t/\Delta x > 1/\sqrt{1-4\theta}$.