Finite difference method for heat equation

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Heat equation: Initial value problem

- Partial differential equation, $\mu > 0$

$$\begin{aligned} u_t &= \mu u_{xx}, \quad (x,t) \in \mathbb{R} \times \mathbb{R}^+ \\ u(x,0) &= f(x), \quad x \in \mathbb{R} \end{aligned}$$

- Exact solution

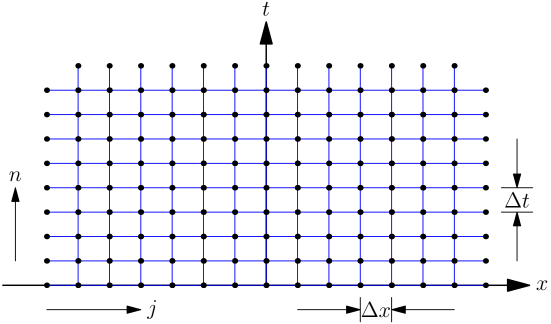
$$u(x,t) = \frac{1}{\sqrt{4\pi\mu t}} \int_{-\infty}^{+\infty} \mathrm{e}^{-y^2/4\mu t} f(x-y)\mathrm{d}y =: (E(t)f)(x)$$

- Solution bounded in maximum norm

$$\|u(t)\|_{\mathcal{C}} = \|E(t)f\|_{\mathcal{C}} \leq \|f\|_{\mathcal{C}} = \sup_{x\in\mathbb{R}} |f(x)|$$

- Finite difference mesh in space and time: partition space $\mathbb{R}$ by a uniform mesh of size h and time $\mathbb{R}^+$ by a uniform mesh of size Δt

$$
\begin{aligned}
x_j &= jh, \quad j = \ldots, -2, -1, 0, +1, +2, \ldots \\
t_n &= n\Delta t, \quad n = 0, 1, 2, \ldots
\end{aligned}
$$



- Let the numerical approximation be

$$
U_j^n \approx u(x_j, t_n)
$$

- Finite difference in space
  First derivative:

$$D_x^+ U_j^n = \frac{U_{j+1}^n - U_j^n}{h}, \quad D_x^- U_j^n = \frac{U_j^n - U_{j-1}^n}{h}, \quad D_x^0 U_j^n = \frac{U_{j+1}^n - U_{j-1}^n}{2h}$$

  Second derivative:

$$D_x^+ D_x^- U_j^n = \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2}$$

- Finite difference in time

$$D_t^+ U_j^n = \frac{U_j^{n+1} - U_j^n}{\Delta t}$$

- Finite difference scheme: forward time and central space (FTCS)

$$D_t^+ U_j^n = \mu D_x^+ D_x^- U_j^n, \quad n = 0, 1, 2, \ldots$$

i.e.,

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \mu \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2}$$

- Update equation: Solve for U_j^{n+1}

$$U_j^{n+1} = (E_h U^n)_j = \lambda U_{j-1}^n + (1 - 2\lambda) U_j^n + \lambda U_{j+1}^n$$

where

$$\boxed{\lambda = \frac{\mu \Delta t}{h^2}}$$

- Explicit scheme

$$U^{n+1} = H(U^n)$$

Maximum principle

- If $\lambda \leq 1/2$, then U_j^{n+1} is given by a convex linear combination of $U_{j-1}^n, U_j^n, U_{j+1}^n$. Hence

$$\min(U_{j-1}^n, U_j^n, U_{j+1}^n) \leq U_j^{n+1} \leq \max(U_{j-1}^n, U_j^n, U_{j+1}^n)$$

$$\min_k U_k^n \leq U_j^{n+1} \leq \max_k U_k^n, \quad \forall j$$

- Hence solution at any time level n is bounded by initial data

$$\min_k U_k^0 \leq U_j^n \leq \max_k U_k^0, \quad \forall j, \quad \forall n$$

- Maximum norm

$$\|U\|_\infty = \sup_j |U_j|$$

- Maximum stability: If $\lambda \leq 1/2$, then

$$\left\|U^{n+1}\right\|_\infty = \|E_h U^n\|_\infty \leq \|U^n\|_\infty \leq \ldots \leq \left\|U^0\right\|_\infty$$

  and hence

$$\|U^n\|_\infty \leq \left\|U^0\right\|_\infty = \|f\|_\infty, \quad \forall n$$

Maximum principle

- We have

$$\|E_h V\|_\infty \le \|V\|_\infty \qquad \|E_h^n V\|_\infty \le \|V\|_\infty$$

- $\lambda \le 1/2$ is necessary: Consider initial condition

$$f_j = f(x_j) = (-1)^j \epsilon, \qquad 0 < \epsilon \ll 1$$

so that $\|f\|_\infty = \epsilon$

- After one time step

$$U_j^1 = [\lambda(-1)^{j-1} + (1-2\lambda)(-1)^j + \lambda(-1)^{j+1}]\epsilon = (1-4\lambda)(-1)^j \epsilon$$

and after n time steps

$$U_j^n = (1-4\lambda)^n (-1)^j \epsilon$$

If $\lambda > 1/2$, then

$$\|U^n\|_\infty = |1-4\lambda|^n \epsilon \to \infty \quad \text{as} \quad n \to \infty$$

Maximum principle

Remark: The condition $\lambda \leq \frac{1}{2}$ implies that the allowed time step Δt depends on the space step h as

$$\Delta t \leq \frac{h^2}{2\mu} \qquad \Longrightarrow \qquad \Delta t = \mathcal{O}\left(h^2\right)$$

The scheme is said to be ***conditionally stable***.

Truncation error and consistency

- If $u(x,t)$ is exact solution then with $u_j^n = u(x_j, t_n)$, the local truncation error

  $$\boxed{\tau_j^n := D_t^+ u_j^n - \mu D_x^+ D_x^- u_j^n}$$

  Using Taylor's formula, for some $\bar{x}_j \in (x_{j-1}, x_{j+1})$ and $\bar{t}_n \in I_n = (t_n, t_{n+1})$

  $$\tau_j^n = \frac{1}{2}\Delta t u_{tt}(x_j, \bar{t}_n) - \frac{1}{12}\mu h^2 u_{xxxx}(\bar{x}_j, t_n)$$

  Using the PDE, we get $u_{tt} = \mu^2 u_{xxxx}$ and from the exact solution, we have $|u_{xxxx}|_C \leq |f_{xxxx}|_C$. The truncation error is bounded as

  $$\begin{aligned} \|\tau^n\|_\infty &\leq C\Delta t \max_{t\in I_n} |u_{tt}(t)|_{\mathcal{C}} + Ch^2 |u_{xxxx}(t_n)|_{\mathcal{C}} \\ &\leq Ch^2 \max_{t\in I_n} |u_{xxxx}(t)|_{\mathcal{C}}, \quad \text{since} \quad \lambda \leq 1/2 \\ &\leq Ch^2 |f_{xxxx}|_{\mathcal{C}} \end{aligned}$$

Error estimate

Let U^n and u^n be the numerical and exact solutions, and let $\lambda \leq 1/2$. Then there is a constant C such that

$$\|U^n - u^n\|_\infty \leq C t_n h^2 |f_{xxxx}|_{\mathcal{C}}, \quad t_n \geq 0$$

Proof: Set $e^n = U^n - u^n$. Then

$$D_t^+ e_j^n - \mu D_x^+ D_x^- e_j^n = -\tau_j^n$$

and hence

$$e_j^{n+1} = (E_h e^n)_j - \Delta t \ \tau_j^n$$

Iterating over time

$$\begin{aligned} e_j^n &= (E_h^n e^0)_j - \Delta t \sum_{l=0}^{n-1} (E_h^{n-1-l} \tau^l)_j \\ &= -\Delta t \sum_{l=0}^{n-1} (E_h^{n-1-l} \tau^l)_j \qquad \text{since} \quad e^0 = U^0 - u^0 = 0 \end{aligned}$$

Using the stability estimate and truncation error estimate

$$\begin{aligned}
\|e^n\|_\infty &\le \Delta t \sum_{l=0}^{n-1} \left\|E_h^{n-1-l}\tau^l\right\|_\infty \\
&\le \Delta t \sum_{l=0}^{n-1} \left\|\tau^l\right\|_\infty, \qquad\qquad \left\|E_h^{n-1-l}\tau^l\right\|_\infty \le \left\|\tau^l\right\|_\infty \le Ch^2|f_{xxxx}|_{\mathcal{C}} \\
&\le C(n\Delta t)h^2|f_{xxxx}|_{\mathcal{C}} \\
&= Ct_n h^2|f_{xxxx}|_{\mathcal{C}}
\end{aligned}$$

Remark: The FTCS scheme has first order accuracy in time and second order accuracy in space $\tau_j^n = \mathcal{O}\left(\Delta t + h^2\right)$. Since $\Delta t = \mathcal{O}\left(h^2\right)$ under the stability condition $\lambda \le 1/2$, the scheme has second order accuracy with respect to the mesh width h. If h is halved, then the error reduces by 1/4. But number of time steps increases by a factor of 4.

Symbol of E_h

- FTCS scheme

$$U_j^{n+1} = \lambda U_{j-1}^n + (1-2\lambda)U_j^n + \lambda U_{j+1}^n$$

- General finite difference scheme

$$U_j^{n+1} = \sum_p a_p(\lambda) U_{j-p}^n$$

How does scheme modify one Fourier mode: $U_j^n = g^n \mathrm{e}^{-\mathrm{i}j\xi}$

$$g = \text{ amplitude} \qquad\qquad g^{n+1}(\xi) = \tilde{E}_h(\xi) g^n(\xi)$$

ξ is called the wave number.

- *Symbol* or *characteristic polynomial* of E_h

$$\tilde{E}_h(\xi) = \sum_p a_p \mathrm{e}^{-\mathrm{i}p\xi}, \quad \xi \in \mathbb{R}$$

- Useful in stability analysis: Fourier stability

Necessary condition for maximum stability

A necessary condition for stability of the operator E_h with respect to the discrete maximum norm is that

$$|\tilde{E}_h(\xi)| \leq 1, \quad \forall\, \xi \in \mathbb{R}$$

Proof: Assume that E_h is stable in maximum norm and that $|\tilde{E}_h(\xi_0)| > 1$ for some $\xi_0 \in \mathbb{R}$. Then with initial condition $f_j = \mathrm{e}^{\mathrm{i}j\xi_0}\epsilon$, the numerical solution after one time step is

$$U_j^1 = \sum_p a_p \mathrm{e}^{\mathrm{i}(j-p)\xi_0}\epsilon = \left(\sum_p a_p \mathrm{e}^{-\mathrm{i}p\xi_0}\right)\mathrm{e}^{\mathrm{i}j\xi_0}\epsilon = \tilde{E}_h(\xi_0) f_j$$

By iterating in time, we get $U_j^n = [\tilde{E}_h(\xi_0)]^n f_j$ and

$$\|U^n\|_\infty = |\tilde{E}_h(\xi_0)|^n \epsilon \to \infty \quad \text{as} \quad n \to \infty$$

Since $\|f\|_\infty = \epsilon$, this contradicts the stability of the scheme and hence the theorem is proved.

FTCS scheme

$$U_j^{n+1} = \lambda U_{j-1}^n + (1-2\lambda)U_j^n + \lambda U_{j+1}^n$$

Symbol

$$\tilde{E}_h(\xi) = \lambda \mathrm{e}^{-\mathrm{i}\xi} + (1-2\lambda)\mathrm{e}^0 + \lambda \mathrm{e}^{\mathrm{i}\xi} = 1 - 2\lambda + 2\lambda\cos(\xi)$$

Since $\cos(\xi) \in [-1, +1]$, the maximum value is attained for $\cos(\xi) = -1$

$$\max_\xi |\tilde{E}_h(\xi)| = |1 - 4\lambda| \leq 1 \qquad \Longrightarrow \qquad \lambda \leq \frac{1}{2}$$

which is the condition previously derived for maximum stability.

Discrete Fourier transform

- For any grid function $V = \{V_j\} \in \mathbb{R}^\infty$ define discrete l_2 norm

$$\|V\|_{2,h} = \left(h \sum_{j=-\infty}^{j=+\infty} |V_j|^2 \right)^{1/2}$$

- Space of bounded grid functions

$$l_{2,h} = \{V \in \mathbb{R}^\infty : \|V\|_{2,h} < \infty\}$$

- Discrete Fourier transform

$$\widehat{V}(\xi) = h \sum_{j=-\infty}^{+\infty} V_j \mathrm{e}^{-\mathrm{i}j\xi}$$

- Inverse transform

$$V_j = \frac{1}{2\pi h} \int_{-\pi}^{+\pi} \widehat{V}(\xi) \mathrm{e}^{\mathrm{i}j\xi} \mathrm{d}\xi$$

Discrete Fourier transform

- Parseval relation

$$\|V\|_{2,h}^2 = \frac{1}{2\pi h}\int_{-\pi}^{+\pi} |\widehat{V}(\xi)|^2 \mathrm{d}\xi = \frac{1}{2\pi}\int_{-\pi/h}^{+\pi/h} |\widehat{V}(\xi h)|^2 \mathrm{d}\xi$$

Definition: Stability in $l_{2,h}$

The discrete solution operator E_h is said to be stable in the norm $\|\cdot\|_{2,h}$ if

$$\|E_h V\|_{2,h} \leq \|V\|_{2,h}\,, \qquad V \in l_{2,h}$$

Von Neumann stability condition

A necessary and sufficient condition for E_h to be stable in $l_{2,h}$ is given by

$$|\tilde{E}_h(\xi)| \le 1, \quad \xi \in \mathbb{R}$$

<u>Proof</u>: For any $V \in l_{2,h}$,

$$\begin{aligned}
\widehat{E_h V}(\xi) &= h \sum_{j=-\infty}^{\infty} (E_h V)_j \mathrm{e}^{-\mathrm{i}j\xi} \\
&= h \sum_j \sum_p a_p V_{j-p} \mathrm{e}^{-\mathrm{i}j\xi} \\
&= \sum_p a_p \mathrm{e}^{-\mathrm{i}p\xi} h \sum_j V_{j-p} \mathrm{e}^{-\mathrm{i}(j-p)\xi} \\
&= \tilde{E}_h(\xi) \widehat{V}(\xi)
\end{aligned}$$

and iterating in time

$$\widehat{E_h^n V}(\xi) = [\tilde{E}_h(\xi)]^n \widehat{V}(\xi)$$

Using Parseval relation, stability of E_h in $l_{2,h}$ is equivalent to

$$\int_{-\pi}^{+\pi} |\widehat{E_h^n V}(\xi)|^2 \mathrm{d}\xi = \int_{-\pi}^{+\pi} |\tilde{E}_h(\xi)|^{2n} |\widehat{V}(\xi)|^2 \mathrm{d}\xi \leq \int_{-\pi}^{+\pi} |\widehat{V}(\xi)|^2 \mathrm{d}\xi$$

which holds if and only if

$$|\tilde{E}_h(\xi)|^n \leq 1, \quad n \geq 0, \quad \xi \in \mathbb{R}$$

Remark: If the problem is in the time interval $(0, T)$, then a less restrictive notion of stability is given by the condition

$$\|E_h^n V\| \leq C_T \|V\|, \quad 0 \leq n \leq T/\Delta t$$

If the finite difference scheme satisfies

$$\|E_h V\| \leq (1 + K\Delta t) \|V\|, \quad K \geq 0$$

then this implies

$$\|E_h^n V\| \leq (1 + K\Delta t)^n \|V\| \leq \mathrm{e}^{Kn\Delta t} \|V\| \leq \mathrm{e}^{KT} \|V\|$$

Fourier transform in space

Define numerical scheme at all $x \in \mathbb{R}$, not just at the mesh points

$$U^{n+1}(x) = (E_h U^n)(x) = \sum_p a_p(\lambda) U^n(x - x_p)$$

Advantage: All the U^n lie in same function space, $L^2(\mathbb{R})$ or $\mathcal{C}(\mathbb{R})$, independently of h. Define usual L^2 norm

$$\|v\| = \left(\int_{-\infty}^{+\infty} |v(x)|^2 \mathrm{d}x \right)^{1/2}$$

Fourier transform

$$\widehat{v}(\xi) = \int_{-\infty}^{+\infty} v(x) \mathrm{e}^{-\mathrm{i}x\xi} \mathrm{d}x$$

Parseval relation

$$\|v\|^2 = \frac{1}{2\pi} \|\widehat{v}\|^2$$

Then

$$\widehat{E_h v}(\xi) = \sum_p a_p \widehat{v(\cdot - ph)}(\xi) = \left(\sum_p a_p \mathrm{e}^{-\mathrm{i}ph\xi} \right) \widehat{v}(\xi) = \tilde{E}_h(h\xi) \widehat{v}(\xi)$$

For the numerical scheme, we thus find

$$\|U^n\| = \frac{1}{\sqrt{2\pi}} \left\| [\tilde{E}_h(h\xi)]^n \widehat{U^0} \right\| \leq \frac{1}{\sqrt{2\pi}} \sup_{\xi\in\mathbb{R}} |\tilde{E}_h(h\xi)|^n \left\| \widehat{U^0} \right\| = \sup_{\xi\in\mathbb{R}} |\tilde{E}_h(h\xi)|^n \left\| U^0 \right\|$$

Stability in L^2 norm holds if

$$\sup_{\xi\in\mathbb{R}} |\tilde{E}_h(h\xi)| \leq 1$$

Accuracy of order r

The finite difference scheme E_h is accurate of order r if

$$\tilde{E}_h(\xi) = \mathrm{e}^{-\lambda\xi^2} + \mathcal{O}\left(|\xi|^{r+2}\right), \quad \xi \to 0$$

Example: FTCS scheme

$$\begin{aligned}
\tilde{E}_h(\xi) &= 1 - 2\lambda + 2\lambda\cos(\xi) \\
&= 1 - \lambda\xi^2 + \frac{1}{12}\lambda\xi^4 + \mathcal{O}\left(\xi^6\right) \\
&= \mathrm{e}^{-\lambda\xi^2} + \left(\frac{1}{12}\lambda - \frac{1}{2}\lambda^2\right)\xi^4 + \mathcal{O}\left(\xi^6\right)
\end{aligned}$$

FTCS is accurate of order 2; For the choice $\lambda = \frac{1}{6}$ it is accurate of order 4.

Convergence in L^2

Assume that the scheme E_h with $\lambda = \frac{\Delta t}{h^2}$ = constant and is accurate of order r and stable in L^2. Then

$$\|U^n - u^n\| \leq C t_n h^r |f|_{r+2}, \qquad t_n \geq 0$$

<u>Proof</u>: Since $\tilde{E}_h(\xi)$ is bounded in $\mathbb{R}$, we have from accuracy property

$$|\tilde{E}_h(\xi) - \mathrm{e}^{-\lambda\xi^2}| \leq C|\xi|^{r+2}, \qquad \xi \in \mathbb{R}$$

By stability and $a^n - b^n = (a-b)(a^{n-1} + a^{n-2}b + \ldots + b^n)$ it follows that

$$|[\tilde{E}_h(\xi)]^n - \mathrm{e}^{-n\lambda\xi^2}| \leq \left| (\tilde{E}_h(\xi) - \mathrm{e}^{-\lambda\xi^2}) \sum_{j=0}^{n-1} [\tilde{E}_h(\xi)]^{n-1-j} \mathrm{e}^{-j\lambda\xi^2} \right| \leq Cn|\xi|^{r+2}$$

Take Fourier transform of heat equation in x variable

$$\frac{\mathrm{d}\widehat{u}}{\mathrm{d}t}(\xi, t) = -\xi^2 \widehat{u}(\xi, t), \qquad t > 0, \qquad \widehat{u}(\xi, 0) = \widehat{f}(\xi)$$

so that

$$\widehat{u}(\xi, t) = \mathrm{e}^{-\xi^2 t}\widehat{f}(\xi)$$

Fourier transform of error in numerical solution is

$$(\widehat{U}^n - \widehat{u}^n)(\xi) = ([\tilde{E}_h(h\xi)]^n - \mathrm{e}^{-n\Delta t \xi^2})\widehat{f}(\xi)$$

From Parseval relation

$$\|U^n - u^n\|^2 = \frac{1}{2\pi}\left\|\widehat{U}^n - \widehat{u}^n\right\|^2 = \frac{1}{2\pi}\left\|([\tilde{E}_h(h\xi)]^n - \mathrm{e}^{-n\Delta t \xi^2})\widehat{f}(\xi)\right\|^2$$

But

$$|[\tilde{E}_h(h\xi)]^n - \mathrm{e}^{-n\Delta t \xi^2}| \leq Cnh^{r+2}|\xi|^{r+2}$$

and using the fact that

$$\widehat{\frac{\mathrm{d}f}{\mathrm{d}x}} = -\mathrm{i}\xi\widehat{f}(\xi), \qquad \widehat{\frac{\mathrm{d}^r f}{\mathrm{d}x}} = (-\mathrm{i}\xi)^r\widehat{f}(\xi), \qquad \lambda = \frac{\Delta t}{h^2} = \mathrm{const}$$

we get

$$\begin{aligned}
\|U^n - u^n\| &\leq \frac{1}{\sqrt{2\pi}} C n h^{r+2} \left\| \xi^{r+2} \widehat{f}(\xi) \right\| \\
&\leq C(n\Delta t) h^r \left\| f^{(r+2)} \right\|, \qquad h^2 = \mathcal{O}\left(\Delta t\right) \\
&= C t_n h^r |f|_{r+2}
\end{aligned}$$

Multi-level scheme

- Higher order accuracy in time

$$D_t^0 U_j^n = \mu D_x^+ D_x^- U_j^n$$

or

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = \mu \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2}$$

Formally second order in t and x, but unstable

- Dufort-Frankel scheme: stable for any λ

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = \mu \frac{U_{j-1}^n - 2\left(\frac{U_j^{n+1} + U_j^{n-1}}{2}\right) + U_{j+1}^n}{h^2}$$

Note: You need to get U^1 by some other scheme.
Second order accurate (need $\Delta t/h \to 0$, ok if $\Delta t/h^2$ =constant)

$$\tau_h^n = \mathcal{O}\left(\Delta t^2\right) + \mathcal{O}\left(h^2\right) + \frac{\Delta t^2}{h^2} u_{tt}(x_j, t_n) + \mathcal{O}\left(\frac{\Delta t^4}{h^2}\right)$$

Initial-boundary value problem

$$
\begin{aligned}
u_t &= \mu u_{xx}, \quad (x,t) \in (0,1) \times \mathbb{R}^+ \\
u(x,0) &= f(x) \\
u(0,t) &= 0 \\
u(1,t) &= 0
\end{aligned}
$$

IBVP: Forward Euler scheme

Consider a uniform grid of $M+1$ points, indexed from 0 to M.

$$D_t^+ U_j^n = \mu D_x^+ D_x^- U_j^n, \quad j = 1, \ldots, M-1$$

or

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2}$$

or

$$U_j^{n+1} = \lambda U_{j-1}^n + (1-2\lambda) U_j^n + \lambda U_{j+1}^n, \quad j = 1, \ldots, M-1$$
$$U_0^{n+1} = U_M^{n+1} = 0$$

Maximum norm

$$\|U\|_{\infty,h} = \max_{0 \le j \le M} |U_j|$$

IBVP: Forward Euler scheme

Maximum stability

The forward Euler scheme for the IBVP is stable in maximum norm iff $\lambda \le 1/2$.

$\lambda \le 1/2$ is necessary: Consider initial condition

$$U_j^0 = f_j = (-1)^j \sin(\pi j h), \quad j = 0, 1, \ldots, M$$

so that $\|f\|_{\infty,h} = 1$. Then

$$U_j^n = [1 - 2\lambda - 2\lambda \cos(\pi h)]^n f_j, \quad j = 0, 1, \ldots, M$$

If $\lambda > 1/2$, then for sufficiently small h

$$|1 - 2\lambda - 2\lambda \cos(\pi h)| \ge \gamma > 1$$

which implies

$$\|U^n\|_{\infty,h} \ge \gamma^n \|f\|_{\infty,h} = \gamma^n \to \infty, \quad h \to 0$$

IBVP: Forward Euler scheme

Local truncation error: (for any fixed λ)

$$|\tau_j^n| \leq Ch^2 \max_{t \in I_n} |u_{xxxx}(t)|_{\mathcal{C}}, \quad I_n = (t_n, t_{n+1})$$

Error estimate

If $\lambda \leq 1/2$, then the FTCS scheme for IBVP has error estimate given by

$$\|U^n - u^n\|_{\infty,h} \leq Ct_n h^2 \max_{t \leq t_n} |u_{xxxx}(t)|_{\mathcal{C}}$$

Numerical example: FTCS (forward Euler)

PDE

$$u_t = \mu u_{xx} \qquad x \in (0,1)$$

Initial condition

$$u(x,0) = f(x) = \sin(\pi x)$$

Exact solution

$$u(x,t) = \mathrm{e}^{-\mu\pi^2 t}\sin(\pi x)$$

Try with

$$\lambda = 0.5, \quad 0.6$$

Matlab code: `heat_1d_fe.m`

Implicit scheme for IBVP: Backward Euler

Explicit scheme (Forward Euler/FTCS)

$$D_t^+ U_j^n = \mu D_x^+ D_x^- U_j^n$$

Implicit scheme (Backward Euler/BTCS)

$$D_t^+ U_j^n = \mu D_x^+ D_x^- U_j^{n+1}$$

or

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \mu \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{h^2}$$

$$-\lambda U_{j-1}^{n+1} + (1 + 2\lambda) U_j^{n+1} - \lambda U_{j+1}^{n+1} = U_j^n, \quad j = 1, \ldots, M-1$$

$$U_0^{n+1} = U_M^{n+1} = 0$$

In matrix notation

$$BU^{n+1} = U^n$$

where $U = [U_1, U_2, \ldots, U_{M-1}]^\top$ and

Implicit scheme for IBVP: Backward Euler

$$B = \begin{bmatrix} 1+2\lambda & -\lambda & 0 & \dots & 0 \\ -\lambda & 1+2\lambda & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\lambda & 1+2\lambda & -\lambda \\ 0 & \dots & 0 & -\lambda & 1+2\lambda \end{bmatrix}$$

Maximum stability

The backward Euler scheme is stable in maximum norm for any value of λ. The scheme is unconditionally stable.

Proof: At time level $n+1$, let the maximum be achieved at grid point $j = j_0$. Then

$$U_{j_0}^{n+1} = \frac{1}{1+2\lambda}\left[\lambda U_{j_0-1}^{n+1} + \lambda U_{j_0+1}^{n+1} + U_{j_0}^{n}\right]$$

Implicit scheme for IBVP: Backward Euler

and

$$\begin{aligned} \left\|U^{n+1}\right\|_{\infty,h} &= |U_{j_0}^{n+1}| \\ &\le \frac{1}{1+2\lambda}\left[\lambda|U_{j_0-1}^{n+1}| + \lambda|U_{j_0+1}^{n+1}| + |U_{j_0}^{n}|\right] \\ &\le \frac{2\lambda}{1+2\lambda}\left\|U^{n+1}\right\|_{\infty,h} + \frac{1}{1+2\lambda}\left\|U^{n}\right\|_{\infty,h} \end{aligned}$$

which implies that $\left\|U^{n+1}\right\|_{\infty,h} \le \|U^n\|_{\infty,h}$.

Remark: If we write

$$BU^{n+1} = U \qquad \text{as} \qquad U^{n+1} = B^{-1}U^n =: E_\Delta U^n$$

then maximum norm stability implies that

$$\|E_\Delta U\|_{\infty,h} \le \|U\|_{\infty,h} \qquad \Longrightarrow \qquad \|E_\Delta\|_{\infty,h} \le 1$$

Implicit scheme for IBVP: Backward Euler

Error estimate

The backward Euler scheme has the error estimate

$$\|U^n - u^n\|_{\infty,h} \leq C t_n(\Delta t + h^2) \max_{t \leq t_n} |u_{xxxx}(t)|_{\mathcal{C}}$$

Proof: Define the error $e^n = U^n - u^n$.

$$\begin{aligned}
\frac{U_j^{n+1} - U_j^n}{\Delta t} &= \mu \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{h^2} \\
\frac{u_j^{n+1} - u_j^n}{\Delta t} &= \mu \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{h^2} + \tau_j^n
\end{aligned}$$

The local truncation error can be bounded as

$$\|\tau^n\|_{\infty,h} \leq C(\Delta t + h^2) \max_{t \in I_{n-1}} |u(t)|_{\mathcal{C}^4}, \qquad I_{n-1} = (t_{n-1}, t_n)$$

Implicit scheme for IBVP: Backward Euler

Then the error satisfies

$$\frac{e_j^{n+1} - e_j^n}{\Delta t} = \mu \frac{e_{j-1}^{n+1} - 2e_j^{n+1} + e_{j+1}^{n+1}}{h^2} - \tau_j^n$$

In terms of matrix B and discrete evolution operator E_Δ

$$Be^{n+1} = e^n - \Delta t \; \tau^n \qquad \Longrightarrow \qquad e^{n+1} = E_\Delta e^n - \Delta t E_\Delta \tau^n$$

Iterating over time

$$\begin{aligned} e^n &= E_\Delta^n e^0 - \Delta t \sum_{l=0}^{n-1} E_\Delta^{n-l} \tau^l, \quad n \geq 1 \\ &= -\Delta t \sum_{l=0}^{n-1} E_\Delta^{n-l} \tau^l \qquad \text{since} \quad e^0 = 0 \end{aligned}$$

Implicit scheme for IBVP: Backward Euler

Therefore

$$
\begin{aligned}
\|e^n\|_{\infty,h} &\leq \Delta t \sum_{l=0}^{n-1} \left\|E_\Delta^{n-l}\tau^l\right\|_{\infty,h} \\
&\leq \Delta t \sum_{l=0}^{n-1} \left\|\tau^l\right\|_{\infty,h}, \qquad \text{from stability of } E_\Delta \\
&\leq (n\Delta t) \max_{0\leq l\leq n-1} \left\|\tau^l\right\|_{\infty,h} \\
&\leq t_n C(\Delta t + h^2) \max_{t\leq t_n} |u(t)|_{\mathcal{C}^4} \quad \square
\end{aligned}
$$

Remark: The Backward Euler scheme is first order accurate in time and second order accurate in space.

Implicit scheme for IBVP: Crank-Nicholson

$$D_t^+ U_j^n = \mu D_x^+ D_x^- \left(\frac{U_j^n + U_j^{n+1}}{2} \right)$$

$$-\frac{\lambda}{2} U_{j-1}^{n+1} + (1+\lambda) U_j^{n+1} - \frac{\lambda}{2} U_{j+1}^{n+1} = \frac{\lambda}{2} U_{j-1}^n + (1-\lambda) U_j^n + \frac{\lambda}{2} U_{j+1}^n$$

$$U_0^{n+1} = U_M^{n+1} = 0$$

In matrix notation

$$BU^{n+1} = AU^n$$

where

Implicit scheme for IBVP: Crank-Nicholson

$$B = \begin{bmatrix} 1+\lambda & -\frac{1}{2}\lambda & 0 & \dots & 0 \\ -\frac{1}{2}\lambda & 1+\lambda & -\frac{1}{2}\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\frac{1}{2}\lambda & 1+\lambda & -\frac{1}{2}\lambda \\ 0 & \dots & 0 & -\frac{1}{2}\lambda & 1+\lambda \end{bmatrix} \qquad A = \begin{bmatrix} 1-\lambda & \frac{1}{2}\lambda & 0 & \dots & 0 \\ \frac{1}{2}\lambda & 1-\lambda & \frac{1}{2}\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \frac{1}{2}\lambda & 1-\lambda & \frac{1}{2}\lambda \\ 0 & \dots & 0 & \frac{1}{2}\lambda & 1-\lambda \end{bmatrix}$$

$$U^{n+1} = B^{-1}AU^n =: E_\Delta U^n$$

Maximum stability

The Crank-Nicholson scheme is stable in maximum norm for $\lambda \leq 1$

Proof: Similar to backward Euler scheme

Remark: Backward Euler scheme was unconditionally stable in maximum norm.

Implicit scheme for IBVP: Crank-Nicholson

Remark: If $\lambda > 1$, then

$$\left\|U^{n+1}\right\|_{\infty,h} \leq (2\lambda - 1)\left\|U^{n}\right\|_{\infty,h}$$

But since $2\lambda - 1 > 1$, this does not yield stability in maximum norm.

Error estimate

For $\lambda \leq 1$, the Crank-Nicholson scheme has the error estimate

$$\left\|U^{n} - u^{n}\right\|_{\infty,h} = \mathcal{O}\left(\Delta t^2 + h^2\right)$$

Remark: The condition $\lambda \leq 1$ is too restrictive. This can be relaxed if we use a weaker norm for stability.

IBVP: Fourier stability

Vector $V = (V_0, V_1, \ldots, V_M) \in \mathbb{R}^{M+1}$
Inner product

$$(V, W)_h := h \sum_{j=0}^{M} V_j W_j$$

and corresponding norm

$$\|V\|_{2,h} = \sqrt{(V,V)_h}$$

Space of vectors

$$l^0_{2,h} = \{V \in \mathbb{R}^{M+1} : \|V\|_{2,h} < \infty,\ V_0 = V_M = 0\}$$

Orthonormal basis vectors for $l^0_{2,h}$: $\phi_p \in \mathbb{R}^{M+1}$, $p = 1, \ldots, M-1$

$$\phi_{p,j} = \sqrt{2}\sin(\pi p j h), \quad j = 0, 1, \ldots, M \qquad\qquad (\phi_p, \phi_q)_h = \delta_{pq}$$

ϕ_p are eigenfunctions of finite difference operator $-D_x^+ D_x^-$

$$-D_x^+ D_x^- \phi_{p,j} = \frac{2}{h^2}[1 - \cos(\pi p h)]\phi_{p,j}, \quad j = 1, 2, \ldots, M-1$$

IBVP: Fourier stability

Let $f \in l^0_{2,h}$ be initial data. Then

$$f = \sum_{p=1}^{M-1} \hat{f}_p \phi_p, \qquad \hat{f}_p = (f, \phi_p)_h$$

Parseval relation

$$\|f\|_{2,h} = \|\hat{f}\|_2$$

Forward Euler method (FTCS): Consider one time step

$$\begin{aligned} U_j^1 &= f_j + \mu \Delta t D_x^+ D_x^- f_j \\ &= \sum_{p=1}^{M-1} \hat{f}_p [1 - 2\lambda(1 - \cos(\pi p h))] \phi_{p,j}, \quad j = 1, 2, \ldots, M-1 \end{aligned}$$

and

$$U_0^1 = U_M^1 = 0$$

IBVP: Fourier stability

or more generally

$$U_j^n = \sum_{p=1}^{M-1} \hat{f}_p[\tilde{E}_h(\pi ph)]^n \phi_{p,j}, \quad j = 0, 1, \ldots, M$$

where $\tilde{E}_h(\xi)$ is the symbol of the operator E_h

$$\tilde{E}_h(\xi) = 1 - 2\lambda[1 - \cos(\xi)]$$

By orthogonality of $\{\phi_p\}$ and Parseval's relation

$$\|U^n\|_{2,h} = \left(\sum_{p=1}^{M-1} \hat{f}_p^2 [\tilde{E}_h(\pi ph)]^{2n} \right)^{1/2} \leq \max_p |\tilde{E}_h(\pi ph)|^n \, \|f\|_{2,h}$$

Check that $|\tilde{E}_h(\xi)| \leq 1$ for $\xi \in [0, \pi]$ iff $\lambda \leq 1/2$. In that case, we have stability

$$\|U^n\|_{2,h} \leq \|f\|_{2,h}, \quad \text{iff} \quad \lambda \leq 1/2$$

IBVP: Fourier stability

This condition is identical to the condition for maximum norm stability of FTCS scheme.

Backward Euler method

$$\tilde{E}_h(\xi) = \frac{1}{1 + 2\lambda[1 - \cos(\xi)]}$$

and $0 \leq \tilde{E}_h(\xi) \leq 1$ for all $\xi \in [0, \pi]$ and any $\lambda > 0$. Hence we have unconditional stability.

Crank-Nicholson method

$$\tilde{E}_h(\xi) = \frac{1 - \lambda[1 - \cos(\xi)]}{1 + \lambda[1 - \cos(\xi)]}$$

and $|\tilde{E}_h(\xi)| \leq 1$ for $\xi \in [0, \pi]$ and for any $\lambda > 0$. Thus the CN scheme is unconditionally stable in $l^0_{2,h}$.

IBVP: Fourier stability

Convergence of CN scheme in $l^0_{2,h}$

Let U^n and u^n be numerical and exact solutions. Then for any $\lambda > 0$

$$\|U^n - u^n\|_{2,h} \leq C t_n (h^2 + \Delta t^2) \max_{t \leq t_n} |u(t)|_{\mathcal{C}^6}$$

Proof: The local truncation error

$$\begin{aligned}
\tau_j^n &= D_t^+ u_j^n - \mu D_x^+ D_x^- \left(\frac{u_j^n + u_j^{n+1}}{2} \right) \\
&= \left[D_t^+ u_j^n - u_t(x_j, t_{n+\frac{1}{2}}) \right] - \mu D_x^+ D_x^- \left[\frac{u_j^n + u_j^{n+1}}{2} - u_j^{n+\frac{1}{2}} \right] \\
&\quad - \mu \left[D_x^+ D_x^- u_j^{n+\frac{1}{2}} - u_{xx}(x_j, t_{n+\frac{1}{2}}) \right]
\end{aligned}$$

and using Taylor formula we get

$$\|\tau^n\|_{2,h} \leq C(\Delta t^2 + h^2) \max_{t \in I_n} |u(t)|_{\mathcal{C}^6}$$

IBVP: Fourier stability

The error $e = U^n - u^n$ satisfies the difference equation

$$e^{n+1} = E_\Delta e^n - \Delta t \ B^{-1} \tau^n$$

or

$$e^n = -\Delta t \sum_{l=0}^{n-1} E_\Delta^{n-1-l} B^{-1} \tau^l$$

The result follows from the stability of E_Δ and the boundedness of B^{-1}, i.e.,

$$\|E_\Delta V\|_{2,h} \leq \|V\|_{2,h} \qquad \text{and} \qquad \left\|B^{-1} V\right\|_{2,h} \leq \|V\|_{2,h}$$

θ-scheme

$$D_t^+ U^n = \mu D_x^+ D_x^- \left[(1-\theta)U^n + \theta U^{n+1}\right]$$

$\theta = 0$	Forward Euler	Explicit	$\mathcal{O}\left(\Delta t + h^2\right)$
$\theta = 1$	Backward Euler	Implicit	$\mathcal{O}\left(\Delta t + h^2\right)$
$\theta = 1/2$	Crank-Nicholson	Implicit	$\mathcal{O}\left(\Delta t^2 + h^2\right)$

Symbol of the scheme

$$\tilde{E}_h(\xi) = \frac{1 - 2(1-\theta)\lambda(1-\cos\xi)}{1 + 2\theta\lambda(1-\cos\xi)}$$

For $0 \le \theta \le 1$, we have $\tilde{E}_h(\xi) \le 1$ for all ξ. Stability requires that

$$\min_{\xi} \tilde{E}_h(\xi) = \frac{1 - 4(1-\theta)\lambda}{1 + 4\theta\lambda} \ge -1 \quad \Longrightarrow \quad (1-2\theta)\lambda \le \frac{1}{2}$$

$\theta < 1/2$: stable in $l_{2,h}^0$ only if $\lambda < \frac{1}{2(1-2\theta)}$
$\theta \ge 1/2$: unconditionally stable in $l_{2,h}^0$

Numerical example

Initial and boundary condition same as in (29)
Matlab codes:

- Backward euler scheme: `heat_1d_be.m`
- Crank-Nicholson scheme: `heat_1d_cn.m`