other refs:
Heath: "Scientific Computing: An Introductory Survey"
Ferziger + Perić "Computational Methods for Fluid Dynamics"
Ascher + Petzold "Computer Methods for ODEs and DAEs"

2.3 Local Truncation Error

Def The *local truncation error* is the residual of the difference operator applied to the exact solution.

EXAMPLE

Euler's Method applied to the IVP

$$\begin{cases} y' = f(t,y) \\ y(0) = y_0 \end{cases}$$

$$\frac{y_{i+1} - y_i}{\Delta t} = f(t_i, y_i) \quad \leftarrow \text{Forward Euler}$$

Let $F(y_i) \equiv \dfrac{y_{i+1} - y_i}{\Delta t} - f(t_i, y_i)$

represent the difference operator

If $y(t)$ is the exact solution, then

$$\text{local truncation error} = F(y(t)) = \frac{y(t_{i+1}) - y(t_i)}{\Delta t} - f(t_i, y(t_i))$$

$$F(y(t)) = \frac{\cancel{y(t_i)} + \Delta t\, y'(t_i) + \frac{1}{2}\Delta t^2 y''(t_i) + \cdots \cancel{- y(t_i)}}{\Delta t} - f(t_i, y(t_i))$$

$$= \underbrace{y'(t_i) - f(t_i, y(t_i))}_{=0} + \frac{1}{2}\Delta t\, y''(t_i)$$

So local truncation error for Euler is $O(\Delta t)$.

For the heat equation

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

discretized with central differences in space + forward Euler in time, the difference operator is

$$F_{FE}(\phi_j^i) \equiv \frac{\phi_j^{i+1} - \phi_j^i}{k} - \frac{\phi_{j+1}^i - 2\phi_j^i + \phi_{j-1}^i}{h^2}$$

let Φ be an exact solution to $\frac{\partial \Phi}{\partial t} = \frac{\partial^2 \Phi}{\partial x^2}$

Then, the local truncation error is

$$\tau_j^i = F_{FE}(\Phi_j^i) = \frac{\Phi_j^{i+1} - \Phi_j^i}{k} - \frac{1}{h^2}\left(\Phi_{j+1}^i - 2\Phi_j^i + \Phi_{j-1}^i\right)$$

Using Taylor Expansions

$$\Phi_j^{i+1} = \Phi_j^i + k\left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{1}{2}k^2\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i + \ldots$$

$$\Phi_{j+1}^i = \Phi_j^i + h\left(\frac{\partial \Phi}{\partial x}\right)_j^i + \frac{1}{2}h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{h^3}{3!}\left(\frac{\partial^3 \Phi}{\partial x^3}\right)_j^i + \frac{h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \ldots$$

$$\Phi_{j-1}^{i} = \Phi_{j}^{i} - h\left(\frac{\partial \Phi}{\partial x}\right)_j^i + \frac{1}{2}h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i$$

$$- \frac{h^3}{3!}\left(\frac{\partial^3 \Phi}{\partial x^3}\right)_j^i + \frac{h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \cdots$$

then, after some cancellation

$$\tau_j^i = \left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i$$

$$-\frac{1}{h^2}\left(h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{2h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \cdots\right)$$

$$\tau_j^i = \underbrace{\left(\frac{\partial \Phi}{\partial t}\right)_j^i - \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i}_{=0} + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i - \frac{h^2}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i$$

since Φ is an exact sol.

so $\boxed{\tau_j^i = O(k) + O(h^2)}$ = local truncation error

$\therefore$ this scheme is first order accurate in time + second order accurate in space.

Local Truncation Error (Backward Euler)

$$F_{BE}(\phi_j^i) \equiv \frac{\phi_j^{i+1} - \phi_j^i}{k} - \frac{\phi_{j+1}^{i+1} - 2\phi_j^{i+1} + \phi_{j-1}^{i+1}}{h^2}$$

so

$$\tau_j^i = F_{BE}(\Phi_j^i) = \frac{\Phi_j^{i+1} - \Phi_j^i}{k} - \frac{\Phi_{j+1}^{i+1} - 2\Phi_j^{i+1} + \Phi_{j-1}^{i+1}}{h^2}$$

for exact solution Φ

similarly to the Forward Euler case...

$$\tau_j^i = \left(\left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i\right) - \frac{1}{h^2}\left(h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^{i+1} + \frac{h^4}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^{i+1} + \cdots\right)$$

$$= \cancel{\left(\frac{\partial \Phi}{\partial t}\right)_j^i} + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i - \left(\cancel{\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i} + k\left(\frac{\partial^3 \Phi}{\partial t \partial x^2}\right)_j^i + \cdots + \frac{h^2}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^{i+1}\right)$$

$$\boxed{\tau_j^i = O(k) + O(h^2)}$$

So the backward Euler scheme is also first order accurate in time and second order accurate in space.

Local Truncation Error (Crank-Nicolson)

[see exercise 2.12]

$$F_{CN}(\phi_j^i) \equiv \frac{\phi_j^{i+1} - \phi_j^i}{k} - \frac{1}{2h^2}\left(\left(\phi_{j+1}^i - 2\phi_j^i + \phi_{j-1}^i\right) + \left(\phi_{j+1}^{i+1} - 2\phi_j^{i+1} + \phi_{j-1}^{i+1}\right) \right)$$

So

$$\tau_j^i = F_{CN}(\Phi_j^i) = \frac{\Phi_j^{i+1} - \Phi_j^i}{k} - \frac{1}{2h^2}\left(\left(\Phi_{j+1}^i - 2\Phi_j^i + \Phi_{j-1}^i\right) + \left(\Phi_{j+1}^{i+1} - 2\Phi_j^{i+1} + \Phi_{j-1}^{i+1}\right) \right)$$

Taylor Expand everywhere...

$$\tau_j^i = \left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i + \frac{k^2}{3!}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + \ldots$$

$$- \frac{1}{2h^2}\left(\left[h^2 \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{h^4}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \ldots \right] + \left[h^2 \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^{i+1} + \frac{h^4}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^{i+1} + \ldots \right] \right)$$

$$\tau_j^i = \left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{1}{2}k\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i + \frac{k^2}{6}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + \ldots$$

$$-\frac{1}{2h^2}\left[\left(h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{h^4}{24}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \ldots\right)\right.$$

$$\left.+\left(h^2\left(\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + k\left(\frac{\partial^3 \Phi}{\partial x^2 \partial t}\right)_j^i + O(k^2)\right) + h^4\left(\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + O(k)\right)\right)\right]$$

$$= \cancel{\left(\frac{\partial \Phi}{\partial t}\right)_j^i} + \frac{1}{2}k\cancel{\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i} + \frac{k^2}{6}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + \ldots$$

$$-\cancel{\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i} - \frac{1}{2}k\cancel{\left(\frac{\partial^3 \Phi}{\partial x^2 \partial t}\right)_j^i} + O(k^2) + O(h^2)$$

So $\boxed{\tau_j^i = O(k^2) + O(h^2)}$

Crank-Nicolson is 2nd order accurate in space <u>and</u> time.

2.4 Consistency

For a numerical scheme to be consistent, the local truncation error must go to zero as the time step k (i.e. Δt) and grid spacing h (i.e. Δx) go to zero.

It is possible to write down a difference scheme (say for $u_t = u_{xx}$) that is inconsistent — the difference scheme has a solution that converges to the solution of a different PDE as $h, k \to 0$. NOT GOOD.

- see examples in textbook - p. 44-45.

EXAMPLE (exercise 2.16)

Examine the consistency of

$$\frac{\phi_j^{i+1} - \phi_j^{i-1}}{2k} = \frac{\phi_{j+1}^{i} - \phi_j^{i+1} - \phi_j^{i-1} + \phi_{j-1}^{i}}{h^2}$$

(model due to Du Fort + Frankel)

... examine local truncation error with Φ satisfying

$$\frac{\partial \Phi}{\partial t} = \frac{\partial^2 \Phi}{\partial x^2}$$

$$F(\Phi_j^i) \equiv \frac{\Phi_j^{i+1} - \Phi_j^{i-1}}{2k} - \frac{1}{h^2}\left(\Phi_{j+1}^{i} - \Phi_j^{i+1} - \Phi_j^{i-1} + \Phi_{j-1}^{i}\right)$$

$$\Phi_j^{i+1} = \Phi_j^i + k\left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{k^2}{2!}\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i + \frac{k^3}{3!}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + \ldots$$

$$\Phi_j^{i-1} = \Phi_j^i - k\left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{k^2}{2!}\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i - \frac{k^3}{3!}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + \ldots$$

$$\Phi_{j+1}^i = \Phi_j^i + h\left(\frac{\partial \Phi}{\partial x}\right)_j^i + \frac{h^2}{2}\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{h^3}{3!}\left(\frac{\partial^3 \Phi}{\partial x^3}\right)_j^i + \frac{h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i$$

$$\Phi_{j-1}^i = \Phi_j^i - h\left(\frac{\partial \Phi}{\partial x}\right)_j^i + \frac{h^2}{2}\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i - \frac{h^3}{3!}\left(\frac{\partial^3 \Phi}{\partial x^3}\right)_j^i + \frac{h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + \ldots$$

So

$$\tau_j^i = F(\Phi_j^i) = \frac{1}{2k}\left[2k\left(\frac{\partial \Phi}{\partial t}\right)_j^i + \frac{2k^3}{3!}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + O(k^5)\right]$$

$$-\frac{1}{h^2}\left[\left(h^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i + \frac{2h^4}{4!}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + O(h^6)\right) - \left(k^2\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i + \frac{2k^4}{4!}\left(\frac{\partial^4 \Phi}{\partial t^4}\right)_j^i + O(k^6)\right)\right]$$

$$\tau_j^i = \cancel{\left(\frac{\partial \Phi}{\partial t}\right)_j^i} + \frac{k^2}{3!}\left(\frac{\partial^3 \Phi}{\partial t^3}\right)_j^i + O(k^4)$$

$$- \cancel{\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_j^i} - \frac{h^2}{12}\left(\frac{\partial^4 \Phi}{\partial x^4}\right)_j^i + O(h^4)$$

$$+ \frac{k^2}{h^2}\left(\frac{\partial^2 \Phi}{\partial t^2}\right)_j^i - \frac{k^4}{24h^2}\left(\frac{\partial^4 \Phi}{\partial t^4}\right)_j^i + O\left(\frac{k^6}{h^2}\right)$$

$$\tau_j^i = O\left(k^2, h^2, \frac{k^2}{h^2}\right)$$

bad if $k = O(h)$!!

2.5 Convergence

- Let Φ be the exact solution to a PDE
- Let $\vec{\phi}^i$ represent the components ϕ_j^i of the solution of a finite difference scheme for the PDE ~~at time level i.~~
- Define discretization error $\vec{e}_j = \vec{\phi}_j - \vec{\Phi}_j$

  where $\vec{\Phi}_j$ is the exact sol. evaluated at $x = x_j$

The finite difference scheme is convergent in the norm $\| \cdot \|_h$ when

$$\lim_{h \to 0} \left(\max_{i=0,1,\ldots,i_{max}} \| \vec{e}_j \|_h \right)$$

where
$$\| \vec{e}_j \|_h = \left(h \sum_j |e_j|^2 \right)^{1/2}$$
grid dependent Euclidean Norm

Comments:

The Euler scheme is convergent as $h \to 0$

when $r = \frac{k}{h^2} \leq 1/2$. (see text p. 46-48).

2.6 Stability

Basically, a stable numerical scheme is one in which small errors that arise during numerical computation do not grow and eventually dominate the solution (usually as $t \to \infty$)

Lax Equivalency Thm: (e.g. Richtmyer + Morton 1967)

'Given a properly posed linear IVP and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence' (see Ferziger + Perić, "Computational Methods for Fluid Dynamics")

We'll examine stability of

- Euler
- Backward Euler
- Crank-Nicolson

schemes applied to the heat eq. $\begin{cases} u_t = u_{xx} \\ u=0 \text{ at } x=0,1 \\ u=f \text{ at } t=0 \end{cases}$

All of those schemes can be written in the form

$$\vec{\Phi}^{i+1} = A\,\vec{\Phi}^{i} \quad \text{where} \quad \vec{\Phi}^{i} = \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \phi_N \end{bmatrix}^{i}$$

- Forward Euler:

$$A = I + rT_{N-1}$$ (see p. 2.33 in notes)

- Backward Euler

$$A = (I - rT_{N-1})^{-1}$$ (see p. 2.34 in notes)

- Crank-Nicolson

$$A = (2I - rT_{N-1})^{-1}(2I + rT_{N-1})$$ (see p. 2.36 in notes)

Note:

$$\vec{\Phi}^{1} = A\,\vec{\Phi}^{0}$$

$$\vec{\Phi}^{2} = A\,\vec{\Phi}^{1} = A(A\vec{\Phi}^{0}) = A^{2}\vec{\Phi}^{0}$$

$$\vdots$$

$$\vec{\phi}^{i} = A^{i}\,\vec{\phi}^{0}$$

Consider a perturbation in the input

$$\vec{\Phi}^{0*} = \vec{\Phi}^{0} + \vec{e}^{\,0}$$

This results in a solution at time level i of the form

$$\vec{\Phi}^{i*} = A^i\left(\vec{\Phi}^{0} + \vec{e}^{\,0}\right) = A^i\vec{\Phi}^{0} + A^i\vec{e}^{\,0}$$

$$= \vec{\Phi}^{i} + A^i\vec{e}^{\,0}$$

Let $\vec{e}^{\,i} = \vec{\Phi}^{i*} - \vec{\Phi}^{i}$

then $\boxed{\vec{e}^{\,i} = A^i\vec{e}^{\,0}}$

so

$$\underbrace{\|\vec{e}^{\,i}\|}_{\text{vector norm}} \leq \underbrace{\|A^i\|}_{\text{matrix norm}}\,\underbrace{\|\vec{e}^{\,0}\|}_{\text{vector norm}}$$

A stable scheme can be defined as one where

$\|A^i\| \leq M$ for $i = 1, 2, \ldots, i_{MAX}$ (Lax)

This limits the growth of $\|\vec{e}^{\,i}\|$.

Since $\|A^i\| = \|A \cdot A \cdot \ldots \cdot A\| \leq \|A\|^i$ we shall require $\|A\| \leq 1$ (to avoid unlimited growth of error) so $$\rho(A) = \max_s \left| 1 - 4r\sin^2 \frac{s\pi}{2N} \right|$$

For stability, require

$$\underbrace{-1 \leq 1 - 4r\sin^2 \frac{s\pi}{2N} \leq 1}_{\text{always holds}} \qquad s = 1, 2, \ldots, N-1$$

$$r \leq \frac{1}{2\sin^2 \frac{s\pi}{2N}} \qquad s = 1, 2, \ldots, N-1$$

$\sin^2 \frac{s\pi}{2N}$ is largest when $s = N-1$

$\left(\frac{s\pi}{2N} \text{ closest to } \frac{\pi}{2} \right)$

so

$$r \leq \frac{1}{2\sin^2 \frac{(N-1)\pi}{2N}}$$

as $h \to 0$ and $N \to \infty$ $\Rightarrow$ $\boxed{r \leq \frac{1}{2}}$

so $r = \frac{k}{h^2} \leq \frac{1}{2}$ for numerical stability

of Euler

In general, $\rho(A) \leqslant \|A\|$ $\left[\|A\| = \max_{\|x\|=1} \|Ax\| \right]$

↑ spectral radius of A.

If A is real + symmetric

$$\|A\|_2 = \sqrt{\rho(A^T A)} = \sqrt{\rho(A^2)} = \sqrt{[\rho(A)]^2} = \rho(A)$$

So for real + symmetric A, we require $\rho(A) \leq 1$ for (Lax) stability.

Euler: $\vec{\Phi}^{i+1} = A \vec{\Phi}^{i}$ $\qquad A = I + rT_{N-1}$

$$A = \begin{bmatrix} 1-2r & r & & 0 \\ r & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}$$

A is real + symmetric

$$\text{eig}(A) = \text{eig}(I + rT_{N-1}) = 1 + r\,\text{eig}(T_{N-1})$$

$$= 1 - 4r\sin^2 \frac{s\pi}{2N} \qquad s = 1, \ldots, N-1$$

$\left\{ \begin{array}{l} \text{from before...} \\ \text{eig}(T_{N-1}) = -4\sin^2 \frac{s\pi}{2N} \\ \qquad s = 1, \ldots, N-1 \end{array} \right\}$

Backward Euler

Here $A = (I - rT_{N-1})^{-1}$

Since $I - rT_{N-1}$ is real + symmetric then $(I - rT_{N-1})^{-1}$ is real + symmetric

Again, examine $\rho(A)$ and require $\rho(A) \leq 1$ for numerical stability

$$\rho(A) = \max_s \left(\frac{1}{1 + 4r\sin^2 \frac{s\pi}{2N}} \right) \qquad s = 1, \ldots, N-1$$

but $\max_s \left(\dfrac{1}{1 + 4r\sin^2 \frac{s\pi}{2N}} \right) < 1 \quad \forall r > 0$

so $\rho(A) < 1$ $\therefore$ Backward Euler is unconditionally stable.

Crank-Nicolson (see section 2.7)

Here $\vec{\Phi}^{i+1} = A\vec{\Phi}^{i}$ where

$$A = (2I - rT_{N-1})^{-1}(2I + rT_{N-1})$$

$$\rho(A) = \max_{s} \left| \frac{2 - 4r\sin^2\left(\frac{s\pi}{2N}\right)}{2 + 4r\sin^2\left(\frac{s\pi}{2N}\right)} \right| \qquad s = 1, 2, \ldots, N-1$$

Here $\rho(A) < 1 \quad \forall r > 0$ so C-N is also unconditionally stable.