Numerical Methods for PDEs

Local Truncation Error, Consistency, and Matrix Version of the FTCS Scheme

(Lecture 4, Week 2)

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Outline

1. Local Truncation Error (LTE) analysis
2. Example: Heat equation
3. Matrix formulation of the FTCS scheme
4. Matlab specific notation

Quality of a numerical approximation

First examination: The Local Truncation Error (LTE)

Preparatory work:

1. Rewrite the PDE (heat equation) in operator form

$$Lu = 0\,, \qquad \text{with } L = \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}$$

2. **FD approximation of L:** For the FTCS scheme we have

$$L_{k,h} = D_t^+ - D_x^2\,.$$

Recall that the numerical solution solves

$$0 = L_{k,h} w_j^n = \frac{w_j^{n+1} - w_j^n}{k} - \frac{w_{j-1}^n - 2w_j^n + w_{j+1}^n}{h^2}\,.$$

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Definition. *Let $L_{k,h}$ be the difference operator approximating L. The local truncation error (LTE) is given by the leading terms of the Taylor expansion of $L_{k,h}u(x_j, t_n) = 0$, where u satisfies $Lu = 0$.*

In other words: Apply the finite difference operator $L_{k,h}$ of the PDE on the exact solution u, then Taylor expand and cancel as many terms as possible by using $Lu = 0$ for instance. That means $\mathrm{LTE} = \mathrm{LOT}\left[L_{k,h}u\right](x_j, t_n)$, where $\mathrm{LOT}[\cdot]$ denotes leading order Taylor expansion.

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Example: LTE of the FTCS scheme

Calculate the LTE of the FTCS scheme of the heat equation:

$$\begin{aligned} \mathrm{LTE} &= L_{k,h}u(x_j, t_n) \\ &= \frac{u(x_j, t_n + k) - u(x_j, t_n)}{k} \\ &\quad - \frac{u(x_j - h, t_n) - 2u(x_j, t_n) + u(x_j + h, t_n)}{h^2} \end{aligned}$$

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&= \frac{1}{k}\left(u + ku_t + \frac{1}{2}k^2 u_{tt} + \cdots - u\right)\bigg|_{x_j, t_n} \\
&\quad - \frac{1}{h^2}\left(u - hu_x + \frac{1}{2}h^2 u_{xx} - \frac{1}{3!}h^3 u_{xxx} + \frac{1}{4!}h^4 u_{xxxx} - 2u + \right. \\
&\qquad \left. + u + hu_x + \frac{1}{2}h^2 u_{xx} + \frac{1}{3!}h^3 u_{xxx} + \frac{1}{4!}h^4 u_{xxxx}\right)\bigg|_{x_j, t_n}
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&= u_t(x_j,t_n)+\frac{1}{2}ku_{tt}(x_j,t_n)-u_{xx}(x_j,t_n)-\frac{1}{12}h^2u_{xxxx}(x_j,t_n)+\ldots\,.
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Since u satisfies the heat equation $u_t - u_{xx} = 0$, we are left with

$$\mathrm{LTE} = \frac{k}{2} u_{tt} - \frac{h^2}{12} u_{xxxx} + \mathcal{O}(k^2, h^4)\,.$$

By using again the assumption on smoothness and the heat equation, that is,

$$u_{tt} = \frac{\partial}{\partial t} u_t = \frac{\partial}{\partial t} u_{xx} = \frac{\partial^2}{\partial x^2} u_t = \frac{\partial^2}{\partial x^2} u_{xx} = u_{xxxx}\,,$$

we can rewrite the LTE as

$$\mathrm{LTE} = \left(\frac{k}{2} - \frac{h^2}{12}\right) u_{xxxx} + \mathcal{O}(k^2, h^4) = \frac{h^2}{2}\left(r - \frac{1}{6}\right) u_{xxxx} + \mathcal{O}(k^2, h^4)\,,$$

where $r = k/h^2$. Hence, if $r = 1/6$, then the $\mathcal{O}(h^2)$ terms vanish and the LTE becomes $\mathcal{O}(k^2, h^4)$. The *leading term* of the LTE (in green above) is *first order accurate in time* and *2nd order accurate in space*.

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Consistency and order of a scheme

Definition. *Let* LTE *be the local truncation error of a scheme. A scheme is said to be consistent, if* $\mathrm{LTE} \to 0$ *as* $h, k \to 0$.
Moreover, a scheme is said to be of order p *in space and* q *in time, if the* LTE *is of order* $\mathcal{O}(h^p, k^q)$.

Remark. *If* r *is a fixed value, then we can rewrite the* LTE *as* $\mathcal{O}(h^p)$ *as shown above, i.e., the FTCS scheme is 2nd order if* $r \neq 1/6$ *and 4th order if* $r = 1/6$.

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FTCS scheme in matrix form

Basic definitions:

- Vector containing numerical solutions w_j^n at internal grid points $j = 1, 2, \ldots, J-1$ at time t_n

$$\mathbf{w}^n = \begin{pmatrix} w_1^n \\ w_2^n \\ \vdots \\ w_{J-1}^n \end{pmatrix}$$

- Vector of initial values (known)

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These definitions allow us to rewrite the FTCS scheme

$$w_j^{n+1} = r w_{j-1}^n + (1-2r) w_j^n + r w_{j+1}^n, \quad j = 1, \ldots, J-1,$$

as follows

$$\mathbf{w}^{n+1} = S\mathbf{w}^n + \mathbf{b}^n,$$

where

$$S = \begin{pmatrix} 1-2r & r & 0 & \ldots & \ldots & 0 \\ r & 1-2r & r & 0 & \ddots & \ddots \\ 0 & r & 1-2r & r & 0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & 0 & r & 1-2r & r \\ 0 & \ddots & \ddots & 0 & r & 1-2r \end{pmatrix}, \quad \mathbf{b}^n = \begin{pmatrix} r\alpha(t_n) \\ 0 \\ \vdots \\ \vdots \\ 0 \\ r\beta(t_n) \end{pmatrix}.$$

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Applying now recursively the matrix FTCS scheme

$$\begin{aligned}\mathbf{w}^{n+1} &= S\mathbf{w}^n + \mathbf{b}^n \\ &= S(S\mathbf{w}^{n-1} + \mathbf{b}^{n-1}) + \mathbf{b}^n \\ &= S^2\mathbf{w}^{n-1} + S\mathbf{b}^{n-1} + \mathbf{b}^n\,,\end{aligned}$$

gives by repeating back to $\mathbf{w}^0$ (or by induction)

$$\mathbf{w}^{n+1} = S^{n+1}\mathbf{w}^0 + S^n\mathbf{b}^0 + S^{n-1}\mathbf{b}^1 + \cdots + S\mathbf{b}^{n-1} + \mathbf{b}^n\,,$$

where $S^n := \underbrace{S \times S \times S \times \cdots \times S}_{n \text{ times}}$.

Remark. If we have homogeneous Dirichlet BC, i.e., $\alpha(t) = \beta(t) = 0$, then $\mathbf{b}^n = \mathbf{0}$ for all n and hence

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Notation in matlab

Mathematical (analytical) notation:
The spatial index j goes over the spatial grid points $0, 2, \ldots, J$ (including boundary points).

Notation adapted to matlab:
The spatial index j goes over the spatial grid points $1, 2, \ldots, J+1$ (including boundary points).

Sparse matrix:
Declare the matrix S as sparse in matlab (as most elements are zero)

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S = sparse( diag((1-2*r)*ones(J-1,1)) ...
    +diag(r*ones(J-2,1),1)+diag(r*ones(J-2,1),-1) );
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"sparse" squeezes out any zero elements (type "help sparse" in matlab shell for more information)

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1. What means LTE and how can it be obtained for a finite difference scheme?

2. How does the finite difference operator for the FTCS scheme with respect to all internal grid points look like? Does it show a special structure?

3. Can you define diagonal matrices in matlab? How can one prevent the storage of zeros?

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