Numerical Solutions to Partial Differential Equations

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The Maximum Principle

Theorem

Suppose $L_h U_{\mathbf{j}} = \sum_{\mathbf{i} \in J \setminus \{\mathbf{j}\}} c_{\mathbf{ij}} U_{\mathbf{i}} - c_{\mathbf{j}} U_{\mathbf{j}},\ \forall \mathbf{j} \in J_\Omega$; *$J$ and L_h satisfy*

(1) $J_D \neq \emptyset$, *and J is J_D connected with respect to L_h;*

(2) $c_{\mathbf{j}} > 0,\ c_{\mathbf{ij}} > 0,\ \forall \mathbf{i} \in D_{L_h}(\mathbf{j})$, *and* $c_{\mathbf{j}} \geq \sum_{\mathbf{i} \in D_{L_h}(\mathbf{j})} c_{\mathbf{ij}}$.

Suppose the grid function U satisfies $L_h U_{\mathbf{j}} \geq 0,\ \forall \mathbf{j} \in J_\Omega$. *Then,*

$$M_\Omega \triangleq \max_{\mathbf{i} \in J_\Omega} U_{\mathbf{i}} \leq \max \left\{ \max_{\mathbf{i} \in J_D} U_{\mathbf{i}},\ 0 \right\}.$$

Furthermore, if J and L_h satisfy (3): *J is connected with respect to L_h; and there exists interior node $\mathbf{j} \in J_\Omega$ such that*

$$U_{\mathbf{j}} = \max_{\mathbf{i} \in J} U_{\mathbf{i}} \geq 0.$$

Then, U must be a constant on J.

The Existence Theorem

Theorem

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Then, the difference equation

$$\begin{cases} -L_h U_{\mathbf{j}} = f_{\mathbf{j}}, & \forall \mathbf{j} \in J_\Omega, \\ U_{\mathbf{j}} = g_{\mathbf{j}}, & \forall \mathbf{j} \in J_D, \end{cases}$$

has a unique solution.

proof: We only need to show that

$$L_h U_{\mathbf{j}} = 0,\ \forall \mathbf{j} \in J_\Omega; \quad U_{\mathbf{j}} = 0,\ \forall \mathbf{j} \in J_D \quad \Rightarrow \quad U_{\mathbf{j}} = 0,\ \forall \mathbf{j} \in J.$$

In fact, by the maximum principle $L_h U \geq 0$ implies $U \leq 0$, and by the corollary of the maximum principle, $L_h U \leq 0$ implies $U \geq 0$, thus $U \equiv 0$ on J . □

$(-L_h)^{-1}$ is a Positive Operator

Corollary

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Then,

$$f_{\mathbf{j}} \geq 0, \forall \mathbf{j} \in J_\Omega, \; g_{\mathbf{j}} \geq 0, \forall \mathbf{j} \in J_D, \quad \Rightarrow \quad U_{\mathbf{j}} \geq 0, \forall \mathbf{j} \in J;$$

and

$$f_{\mathbf{j}} \leq 0, \forall \mathbf{j} \in J_\Omega, \; g_{\mathbf{j}} \leq 0, \forall \mathbf{j} \in J_D, \quad \Rightarrow \quad U_{\mathbf{j}} \leq 0, \forall \mathbf{j} \in J;$$

The corollary says that $(-L_h)^{-1}$ is a positive operator, *i.e.* $(-L_h)^{-1} \geq 0$. In other words, every element of the matrix $(-L_h)^{-1}$ is nonnegative.

In fact, the matrix $-L_h$ is a M matrix, *i.e.* the diagonal elements of A are all positive, the off-diagonal elements are all nonpositive, and elements of A^{-1} are all nonnegative.

The Comparison Theorem and the Stability

Theorem

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Let the grid function U be the solution to the linear difference equation

$$\begin{cases} -L_h U_{\mathbf{j}} = f_{\mathbf{j}}, & \forall \mathbf{j} \in J_\Omega, \\ U_{\mathbf{j}} = g_{\mathbf{j}}, & \forall \mathbf{j} \in J_D. \end{cases}$$

Let Φ be a nonnegative grid function defined on J satisfying

$$L_h \Phi_{\mathbf{j}} \geq 1, \qquad \forall \mathbf{j} \in J_\Omega.$$

Then, we have $\max_{\mathbf{j}\in J_\Omega} |U_{\mathbf{j}}| \leq \max_{\mathbf{j}\in J_D} |U_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max_{\mathbf{j}\in J_\Omega} |f_{\mathbf{j}}|.$

The Proof of the Comparison Theorem

Proof: Firstly, it follows from the maximum principle that

$$0 \le \max_{\mathbf{j}\in J_\Omega} \Phi_{\mathbf{j}} \le \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}}.$$

Next, define

$$\Psi_{\mathbf{j}}^{\pm} = \pm U_{\mathbf{j}} + \left[\max_{\mathbf{i}\in J_\Omega} |f_{\mathbf{i}}|\right] \Phi_{\mathbf{j}}, \qquad \forall \mathbf{j} \in J.$$

It is easily verified that $L_h \Psi_{\mathbf{j}}^{\pm} \ge 0$ on J_Ω, thus by the maximum principle

$$\pm U_{\mathbf{j}} \le \Psi_{\mathbf{j}}^{\pm} \le \max_{\mathbf{j}\in J_D} |U_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max_{\mathbf{j}\in J_\Omega} |f_{\mathbf{j}}|, \ \ \forall \mathbf{j} \in J_\Omega,$$

since Φ is nonnegative. □

The Comparison Theorem and the Stability

If the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Let the grid function U be the solution to the linear difference equation

$$\begin{cases} -L_h U_{\mathbf{j}} = f_{\mathbf{j}}, & \forall \mathbf{j} \in J_\Omega, \\ U_{\mathbf{j}} = g_{\mathbf{j}}, & \forall \mathbf{j} \in J_D. \end{cases}$$

Then, the comparison theorem says that

$$\max_{\mathbf{j}\in J_\Omega} |U_{\mathbf{j}}| \le \max_{\mathbf{j}\in J_D} |g_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max_{\mathbf{j}\in J_\Omega} |f_{\mathbf{j}}|,$$

in other words, the finite difference scheme is stable in the $\mathbb{L}^\infty$ norm $\|\cdot\|_\infty$, as long as there is a nonnegative Φ s.t. $L_h\Phi \ge 1$, and $\max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}}$ is uniformly bounded with respect to J.

A Priori Error Estimate

Theorem

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Let Φ be a nonnegative grid function defined on J satisfying

$$L_h \Phi_{\mathbf{j}} \geq 1, \qquad \forall \mathbf{j} \in J_\Omega.$$

Then, the error of the finite difference approximation equation $e_h = \{U_{\mathbf{j}} - u_{\mathbf{j}}\}_{\mathbf{j} \in J_\Omega}$ can be bounded by the error on the Dirichlet boundary and the local truncation error $T_h = \{L_h(U_{\mathbf{j}} - u_{\mathbf{j}})\}_{\mathbf{j} \in J_\Omega}$ in the sense that

$$\max_{\mathbf{j} \in J_\Omega} |e_{\mathbf{j}}| \leq \max_{\mathbf{j} \in J_D} |e_{\mathbf{j}}| + \max_{\mathbf{j} \in J_D} \Phi_{\mathbf{j}} \max_{\mathbf{j} \in J_\Omega} |T_{\mathbf{j}}|.$$

$T_{\mathbf{j}}$ can be of different order on the regular and irregular interior nodes. Is it possible for us to choose different comparison functions for them, so that better error estimates can be obtained?

A Generalized version of the Comparison Theorem

Theorem

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Let the grid function U be the solution to the linear difference equation

$$\begin{cases} -L_h U_{\mathbf{j}} = f_{\mathbf{j}}, & \forall \mathbf{j} \in J_\Omega, \\ U_{\mathbf{j}} = g_{\mathbf{j}}, & \forall \mathbf{j} \in J_D. \end{cases}$$

Let Φ be a nonnegative grid function defined on J satisfying

$$\begin{cases} L_h \Phi_{\mathbf{j}} \geq C_1 > 0, & \forall \mathbf{j} \in J_{\Omega_1}, \\ L_h \Phi_{\mathbf{j}} \geq C_2 > 0, & \forall \mathbf{j} \in J_{\Omega_2}, \end{cases}$$

where $J_{\Omega_1} \cup J_{\Omega_2} = J_\Omega$, $J_{\Omega_1} \cap J_{\Omega_2} = \emptyset$. Then

$$\max_{\mathbf{j} \in J_\Omega} |U_{\mathbf{j}}| \leq \max_{\mathbf{j} \in J_D} |U_{\mathbf{j}}| + \max_{\mathbf{j} \in J_D} \Phi_{\mathbf{j}} \max \left\{ C_1^{-1} \max_{\mathbf{j} \in J_{\Omega_1}} |f_{\mathbf{j}}|, C_2^{-1} \max_{\mathbf{j} \in J_{\Omega_2}} |f_{\mathbf{j}}| \right\}.$$

Proof of the Generalized Comparison Theorem

Proof: Firstly, it follows from the maximum principle that

$$0 \le \max_{\mathbf{j}\in J_\Omega} \Phi_{\mathbf{j}} \le \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}}.$$

Next, define

$$\Psi^{\pm}_{\mathbf{j}} = \pm U_{\mathbf{j}} + \max\left\{ C_1^{-1} \max_{\mathbf{j}\in J_{\Omega_1}} |f_{\mathbf{j}}|, C_2^{-1} \max_{\mathbf{j}\in J_{\Omega_2}} |f_{\mathbf{j}}| \right\} \Phi_{\mathbf{j}}, \quad \forall \mathbf{j} \in J.$$

We have $L_h \Psi^{\pm}_{\mathbf{j}} \ge 0$ on J_Ω, thus, by the maximum principle,

$$\pm U_{\mathbf{j}} \le \Psi^{\pm}_{\mathbf{j}} \le \max_{\mathbf{j}\in J_D} |U_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max\left\{ C_1^{-1} \max_{\mathbf{j}\in J_{\Omega_1}} |f_{\mathbf{j}}|, C_2^{-1} \max_{\mathbf{j}\in J_{\Omega_2}} |f_{\mathbf{j}}| \right\},$$

since Φ is nonnegative. □

A Better a Priori Error Estimate

Theorem

Suppose the grid J and the linear operator L_h satisfy the conditions (1) and (2) of the maximum principle. Let Φ be a nonnegative grid function defined on J satisfying

$$\begin{cases} L_h\Phi_{\mathbf{j}} \geq C_1 > 0, & \forall \mathbf{j} \in J_{\Omega_1}, \\ L_h\Phi_{\mathbf{j}} \geq C_2 > 0, & \forall \mathbf{j} \in J_{\Omega_2}, \end{cases}$$

Then, the error of the finite difference approximation equation $e_h = \{U_{\mathbf{j}} - u_{\mathbf{j}}\}_{\mathbf{j}\in J_\Omega}$ satisfies

$$\max_{\mathbf{j}\in J_\Omega} |e_{\mathbf{j}}| \leq \max_{\mathbf{j}\in J_D} |e_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max\left\{ C_1^{-1} \max_{\mathbf{j}\in J_{\Omega_1}} |T_{\mathbf{j}}|, C_2^{-1} \max_{\mathbf{j}\in J_{\Omega_2}} |T_{\mathbf{j}}| \right\}.$$

We will see that, by defining proper Φ, this can actually produce "optimal" error estimate for Dirichlet boundary value problems of elliptic equations defined on domains with curved boundaries.

An Example of Optimal Error Estimate

1. Poisson equation defined on 2-D region with curved boundary;
2. Uniform grid with $h_x = h_y = h$;
3. On $\overset{\circ}{J}_\Omega =: J_{\Omega_1}$, L_h is the standard 5-point difference scheme;
4. On $J_\Omega \setminus \overset{\circ}{J}_\Omega =: J_{\Omega_2}$, L_h is a symmetric 5-point scheme on nonuniform grid, for example (see (1.3.24))

$$L_h U_P = \frac{1}{h_x}\left(\frac{U_{E^*} - U_P}{h_x^*} - \frac{U_P - U_W}{h_x}\right) + \frac{1}{h_y}\left(\frac{U_{N^*} - U_P}{h_y^*} - \frac{U_P - U_S}{h_y}\right).$$

5. Define $\tilde{J}_D = J_D \cap [\cup_{\mathbf{j} \in J_{\Omega_2}} D_{L_h}(\mathbf{j})]$.

An Example of Optimal Error Estimate

6. The local truncation error satisfies

$$\max_{\mathbf{j}\in J_{\Omega_1}} |T_{\mathbf{j}}| \le K_1 h^2, \qquad \max_{\mathbf{j}\in J_{\Omega_2}} |T_{\mathbf{j}}| \le K_2,$$

   where K_1 and K_2 are constants independent of h.

7. $(\bar{x}, \bar{y})$ is the circumcenter of Ω, R is the circumradius.

8. Take comparison functions of the following form

$$\begin{cases} \Phi(x,y) = E_1\left\{(x-\bar{x})^2 + (y-\bar{y})^2\right\}, & \forall\,(x,y) \notin \tilde{J}_D, \\ \Phi(x,y) = E_1\left\{(x-\bar{x})^2 + (y-\bar{y})^2\right\} + E_2, & \forall\,(x,y) \in \tilde{J}_D, \end{cases}$$

   where E_1 and E_2 are positive undetermined coefficients;

An Example of Optimal Error Estimate

9. Since $D_{L_h}(\mathbf{j}) \cap \tilde{J}_D \neq \emptyset$ if and only if $\mathbf{j} \in J_{\Omega_2}$, we have

$$\begin{cases} 0 \leq \Phi_{\mathbf{j}} \leq E_1 R^2 + E_2, & \forall \mathbf{j} \in J_D, \\ L_h \Phi_{\mathbf{j}} = 4\, E_1, & \forall \mathbf{j} \in J_{\Omega_1}, \\ L_h \Phi_{\mathbf{j}} \geq E_1 + E_2 h^{-2} \geq E_2 h^{-2}, & \forall \mathbf{j} \in J_{\Omega_2}. \end{cases}$$

The last inequality follows from $\dfrac{h_x^* + h_x}{2h_x} \geq \dfrac{1}{2}$, $\dfrac{1}{h_x h_x^*} \geq h^{-2}$ and $L_h(x - \bar{x})^2 = L_h(y - \bar{y})^2 = 2$.

An Example of Optimal Error Estimate

Thus, by taking $C_1 = 4E_1$ and $C_2 = E_2 h^{-2}$, it follow from the generalized comparison theorem

$$\max_{\mathbf{j}\in J_\Omega} |e_{\mathbf{j}}| \le \max_{\mathbf{j}\in J_D} |e_{\mathbf{j}}| + \max_{\mathbf{j}\in J_D} \Phi_{\mathbf{j}} \max\left\{ C_1^{-1} \max_{\mathbf{j}\in J_{\Omega_1}} |T_{\mathbf{j}}|, C_2^{-1} \max_{\mathbf{j}\in J_{\Omega_2}} |T_{\mathbf{j}}| \right\},$$

and $0 \le \Phi_{\mathbf{j}} \le E_1 R^2 + E_2$, $\forall \mathbf{j} \in J_D$ that

$$\max_{\mathbf{j}\in J_\Omega} |e_{\mathbf{j}}| \le \max_{\mathbf{j}\in J_D} |e_{\mathbf{j}}| + (E_1 R^2 + E_2) \max\left\{ \frac{K_1 h^2}{4E_1}, \frac{K_2 h^2}{E_2} \right\}.$$

An Example of Optimal Error Estimate

Notice that

$$\min_{E_2/E_1} \left\{ \left(R^2 + E_2/E_1 \right) \max \left\{ \frac{K_1 h^2}{4}, \frac{K_2 h^2}{E_2/E_1} \right\} \right\} = \left(\frac{1}{4} K_1 R^2 + K_2 \right) h^2$$

when $\dfrac{K_1 h^2}{4} = \dfrac{K_2 h^2}{E_2/E_1}$, we obtain an optimal error estimate

$$\max_{\mathbf{j} \in J_\Omega} |e_{\mathbf{j}}| \leq \max_{\mathbf{j} \in J_D} |e_{\mathbf{j}}| + \left(\frac{1}{4} K_1 R^2 + K_2 \right) h^2.$$

More General Extensions

1. The error estimates based on the maximum principle and the comparison theorem can be extended to cover more general problems.
2. The key to the maximum principle is the conditions (1), (2).
3. The key to the comparison theorem is the non-negative function Φ such that $L_h\Phi \geq 1$, which for the second order problem can always be realized by taking a proper second order polynomial.

Extensions to Parabolic Problems

The maximum principle and comparison theorem can also be applied to the stability analysis and error estimations for the finite difference approximation solutions to the initial-boundary value problems of parabolic partial differential equations (see Chapter 2).

The main difference is that the parabolic difference operators generally only have the J_D connection, which is the condition we actually use in applications.

Asymptotical Error Analysis

The upper bound of the error obtained above for the Dirichlet boundary value problems of elliptic equations is of the same order as the local truncation error on the regular interior nodes.

The questions are

1. Is this the best error estimate we can have in general?

2. Can we obtain better numerical approximation by some post procession?

The answers to both questions are positive.

Taylor Expanding the Error Equation

- For the poisson equation and 5-point scheme;
- Suppose the solution u is sufficiently smooth;
- Let $h_x = h_y = h$, let J_h be the corresponding set of grid nodes,

then the local truncation error can be Taylor expanded as

$$T_{\mathbf{j}} = \frac{1}{12} h^2 (\partial_x^4 u + \partial_y^4 u)_{\mathbf{j}} + \frac{1}{360} h^4 (\partial_x^6 u + \partial_y^6 u)_{\mathbf{j}} + \cdots, \quad \forall \mathbf{j} \in J_h.$$

Hence, the error $e_{\mathbf{j}} = U_{\mathbf{j}} - u_{\mathbf{j}}$ of the difference solution U satisfies

$$L_h e_{\mathbf{j}} = -T_{\mathbf{j}} = -\frac{1}{12} h^2 (\partial_x^4 u + \partial_y^4 u)_{\mathbf{j}} + O(h^4), \quad \forall \mathbf{j} \in J_h.$$

Find the Leading Term of the Error

Suppose the solution ψ to the problem

$$\begin{cases} -L\psi := -(\psi_{xx} + \psi_{yy}) = \frac{1}{12}(\partial_x^4 u + \partial_y^4 u), & x \in \Omega, \\ \psi = 0, & x \in \partial\Omega, \end{cases}$$

is sufficiently smooth. Let Ψ_h be the corresponding finite difference approximation solution. Then,

1. $L_h(\Psi - \psi)_{\mathbf{j}} = O(h^2) \quad \Rightarrow$
2. $L_h\psi_{\mathbf{j}} = L_h\Psi_{\mathbf{j}} + O(h^2) = -\frac{1}{12}(\partial_x^4 u + \partial_y^4 u)_{\mathbf{j}} + O(h^2) \ \Rightarrow$
3. $L_h e_{\mathbf{j}} = -\frac{1}{12}h^2(\partial_x^4 u + \partial_y^4 u)_{\mathbf{j}} + O(h^4) = h^2 L_h\psi_{\mathbf{j}} + O(h^4)$
4. $\Rightarrow \quad L_h(U - u - h^2\psi)_{\mathbf{j}} = L_h(e_h - h^2\psi)_{\mathbf{j}} = O(h^4).$

Thus, MaxP & CompTh $\Rightarrow U_{\mathbf{j}} = u_{\mathbf{j}} + h^2\psi_{\mathbf{j}} + O(h^4)$, $\forall \mathbf{j} \in J_h$. This says that $h^2\psi_{\mathbf{j}}$ is generally the leading term of the error $e_{\mathbf{j}}$.

The Optimal Order of Finite Difference Approximation

We see that the leading term of the error e_h is of second order in general, unless $\partial_x^4 u + \partial_y^4 u \equiv 0$, *i.e.* the solution u is a polynomial of degree no greater than 3 with respect to x and y.

Since by the maximum principle and the comparison theorem, we have $\|\Psi_h - \psi\|_\infty = O(h^2)$, we also have

$$U_{\mathbf{j}} - h^2\Psi_{\mathbf{j}} = u_{\mathbf{j}} + O(h^4), \quad \forall \mathbf{j} \in J_h.$$

Since $\partial_x^4 u + \partial_y^4 u$ is not known a priori, Ψ_h is not easily computationally available. However, the expression suggests a way to improve the approximation accuracy: the extrapolation.

Extrapolation Using Solutions on J_h and $J_{h/2}$

1. On the coarse mesh: $U_{h,\mathbf{j}} = u_{\mathbf{j}} + h^2\psi_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_h$;
2. On the fine mesh: $U_{h/2,\mathbf{j}} = u_{\mathbf{j}} + (h/2)^2\psi_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_{h/2}$,
3. Define $U^1_{h,\mathbf{j}} \triangleq \frac{4U_{h/2,\mathbf{j}} - U_{h,\mathbf{j}}}{3} = u_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_h$.

We see that the leading term of the error of $U^1_{h,\mathbf{j}}$ is $O(h^4)$.

4. Remember $U_{\mathbf{j}} = u_{\mathbf{j}} + h^2\psi_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_h$. Thus
5. iff $h << 1$ such that $O(h^4) << h^2\psi$, $h^2\psi$ is the leading term,
6. and $U^1_{h,\mathbf{j}} = u_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_h$ is really a better approximation.

Extrapolation Using Solutions on J_h, $J_{h/2}$ and $J_{h/4}$

If h is sufficiently small, by $U^1_{h,\mathbf{j}} = u_{\mathbf{j}} + O(h^4), \ \forall \mathbf{j} \in J_h$ and the corresponding extrapolation formula, we are lead to

$$U^2_{h,\mathbf{j}} \triangleq \frac{2^4 U^1_{h/2,\mathbf{j}} - U^1_{h,\mathbf{j}}}{2^4 - 1} = u_{\mathbf{j}} + O(h^6), \ \forall \mathbf{j} \in J_h.$$

The question is: How do we know whether a given grid size h is sufficiently small or not?

An a Posteriori Error Estimation for U_h

Another important application of the extrapolation method is the a posteriori error estimation. For example, if $U_{h,\mathbf{j}} = u_{\mathbf{j}} + h^2\psi_{\mathbf{j}} + O(h^4), \ \ \forall \mathbf{j} \in J_h$ for all $h > 0$, Then, it follows from $\frac{4U_{h/2,\mathbf{j}} - U_{h,\mathbf{j}}}{3} = u_{\mathbf{j}} + O(h^4)$ that

$$U_{h,\mathbf{j}} - u_{\mathbf{j}} = \frac{4}{3}\left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}}\right) + O(h^4), \ \ \forall \mathbf{j} \in J_h.$$

This implies that the leading term of the error e_h is approximately $\frac{4}{3}\left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}}\right)$, which is supposed to be of order $O(h^2)$.

Hence, if $\left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}}\right) / \left(U_{h/2,\mathbf{j}} - U_{h/4,\mathbf{j}}\right) \approx 2^2$, then we may view h as being sufficiently small and $e_{h,\mathbf{j}} \approx \frac{4}{3}\left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}}\right)$ (an asymptotically exact a posteriori error estimator).

An a Posteriori Error Estimation for U_h^1

Similarly, since

$$U_{h,\mathbf{j}}^1 - u_{\mathbf{j}} = \frac{2^4}{2^4-1}\left(U_{h,\mathbf{j}}^1 - U_{h/2,\mathbf{j}}^1\right) + O(h^6), \ \ \forall \mathbf{j} \in J_h.$$

This implies that the leading term of the error $U_{h,\mathbf{j}}^1 - u_{\mathbf{j}}$ is approximately $\frac{2^4}{2^4-1}\left(U_{h,\mathbf{j}}^1 - U_{h/2,\mathbf{j}}^1\right)$, which is supposed to be of order $O(h^4)$.

Hence, if $\left(U_{h,\mathbf{j}}^1 - U_{h/2,\mathbf{j}}^1\right) / \left(U_{h/2,\mathbf{j}}^1 - U_{h/4,\mathbf{j}}^1\right) \approx 2^4$, then we may view h as being sufficiently small for U_h^1 and $U_{h,\mathbf{j}}^1 - u_{\mathbf{j}} \approx \frac{2^4}{2^4-1}\left(U_{h,\mathbf{j}}^1 - U_{h/2,\mathbf{j}}^1\right)$ (an asymptotically exact a posteriori error estimator for U_h^1).

a Posteriori Error Estimation in General Case

Assume $U_{h,\mathbf{j}} = u_{\mathbf{j}} + C_{\mathbf{j}} h^{\alpha} + o(h^{\alpha})$, where $\alpha > 0$ is the undetermined order of the leading term of the error, then, we have

$$U_{h,\mathbf{j}} - u_{\mathbf{j}} = \frac{2^{\alpha}}{2^{\alpha} - 1} \left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}} \right) + o(h^{\alpha}),$$

and
$$U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}} = (1 - 2^{-\alpha}) C_{\mathbf{j}} h^{\alpha} + o(h^{\alpha}).$$

Thus, if h is sufficiently small, we have

$$\|U_h - u\| \approx Ch^{\alpha}, \qquad \|U_h - U_{h/2}\| \approx (1 - 2^{-\alpha}) Ch^{\alpha},$$

$$\Rightarrow \quad \log \|U_h - U_{h/2}\| \approx \log((1 - 2^{-\alpha})C) - \alpha \log(h^{-1}).$$

a Posteriori Error Estimation in General Case

This shows that theoretically, in the log-log coordinate system with $\log(h^{-1})$ as the abscissa and $\log \|U_h - U_{h/2}\|$ as the ordinate, $\log \|U_h - U_{h/2}\|$ asymptotically converges to a straight line with slope $-\alpha$.

Remark: Recall that

$$\|U - u\| = \|e_h\| \leq K\|L_h U - L_h u\| \leq K(\|L_h U - \bar{L}u\| + \|\bar{L}u - L_h u\|),$$

where $L_h U - \bar{L}u$ is the residual of the algebraic equation $L_h U = \bar{f}$, and $L_h u - \bar{L}u = T_h$ is the truncation error. In practical computation, there exist $h_0 > h_1 > h_2 > 0$, for $h_0 > h > h_1$, $\log \|U_h - U_{h/2}\|$ is close to a straight line with slope $-\alpha$, while for $h_2 > h > 0$, $\log \|U_h - U_{h/2}\|$ is a decreasing function of h.

Estimate the Convergence Rate and the Constant C

Since, for sufficiently small h, the error satisfies

$$\log \|U_h - U_{h/2}\| \approx \log((1 - 2^{-\alpha})C) - \alpha \log(h^{-1})$$

we can apply the least square method to estimate C and α.

To estimate α alone, we can make use of the formula

$$\left(U_{h,\mathbf{j}} - U_{h/2,\mathbf{j}}\right) / \left(U_{h/2,\mathbf{j}} - U_{h/4,\mathbf{j}}\right) \to 2^{\alpha}, \quad \text{as} \quad h \to 0.$$

For sufficiently small h, we have

$$U^1_{h,\mathbf{j}} \triangleq \frac{2^{\alpha} U_{h/2,\mathbf{j}} - U_{h,\mathbf{j}}}{2^{\alpha} - 1} = u_{\mathbf{j}} + o(h^{\alpha}), \;\; \forall \mathbf{j} \in J_h.$$

The Parabolic Partial Differential Equations

The parabolic partial differential equations are typical evolution equations. A general linear parabolic partial differential equation has the following form

$$\frac{\partial u}{\partial t} - L(u) = f,$$

1. $u(x, t)$: a unknown function of $x = (x_1, \cdots, x_n)$ and t;
2. L: a linear elliptic differential operator with respect to x;
3. The coefficients of L are functions of (x, t) in general;
4. The source term f is generally a real function of (x, t).
5. Steady state solution: if L and f are independent of t, then the solution to the elliptic equation $-L(u) = f$ also solves the parabolic equation.

An Example of the Parabolic Partial Differential Equations

Physics of heat conduction:

1. $x \in \Omega \subset \mathbb{R}^n$, $t > 0$;
2. κ: the heat capacity of the media on x;
3. $u(x, t)$: the temperature of the media on x at t;
4. $\kappa u(x, t)$: the heat density of the media on x at t;
5. $a(x) > 0$: the conduction parameter of the media on x;
6. $f(x)$: the density of the source or sink of heat;
7. J: the heat flux (measured by amount of heat per unit area per unit time)
8. Fourier's law: $J = -a(x)\nabla u(x)$.

The Change of Heat in the Media

For an arbitrary open subset $\omega \subset \Omega$ with piecewise smooth boundary $\partial\omega$, the Fourier's law says the heat brought into ω by the heat diffusion per unit time is given by

$$\int_{\partial\omega} J \cdot (-\nu(x))\, ds = \int_{\partial\omega} a(x)\nabla u(x) \cdot \nu(x)\, ds,$$

while the heat produced in ω by the source per unit time is

$$\int_{\omega} f(x)\, dx.$$

The Conservation of Heat and the Heat Equation

Therefore, the net change of the heat in ω per unit time is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\omega}\kappa(x)u(x,t)dx = \int_{\partial\omega} a(x)\nabla u(x,t)\cdot\nu(x)ds + \int_{\omega} f(x)dx.$$

By the divergence theorem (or Green's formula or Stokes formula), this leads to the heat equation in the integral form

$$\int_{\omega}\{\kappa(x)u_t(x,t) - \nabla\cdot(a(x)\nabla u(x,t))\}\,dx = \int_{\omega} f(x,t)\,dx, \quad \forall\omega$$

The Heat Equation

The term $-[a(x)\nabla u(x,t)]$ is called as the heat flux, since it represents the speed that the heat flows.

Assume that $\kappa(x)u_t(x,t) - \nabla \cdot (a(x)\nabla u(x,t)) - f$ is smooth, then, we obtain the the heat equation in the differential form

$$\kappa(x)u_t(x,t) - \nabla \cdot (a(x)\nabla u(x)) = f(x), \quad \forall x \in \Omega,$$

or equivalently

$$u_t(x,t) - \kappa^{-1}(x)\,\nabla \cdot (a(x)\nabla u(x,t)) = \kappa^{-1}(x)f(x,t), \quad \forall x \in \Omega.$$

In particular, if $\kappa = 1$ and $a = 1$, we have the classical heat equation $u_t - \triangle u = f$.

Initial and Boundary Conditions for the Heat Equation

For a complete heat conduction problem, we also need to impose the initial condition

$$u(x,0) = u_0(x), \ \forall x \in \Omega$$

as well as proper boundary conditions.

There are three types of most commonly used boundary conditions:

First type $$u(x,t) = u_D(x,t), \quad \forall x \in \partial\Omega, \ \ t > 0;$$

Second type $$\frac{\partial u}{\partial \nu}(x,t) = g(x,t), \quad \forall x \in \partial\Omega, \ \ t > 0;$$

Third type $$\left(\frac{\partial u}{\partial \nu} + \beta u\right)(x,t) = g(x,t), \quad \forall x \in \partial\Omega, \ \ t > 0;$$

where $\beta \geq 0$, and $\beta > 0$ at least on some part of the boundary (*physical meaning: higher temprature produces bigger outward heat flux*).

Boundary Conditions for the Heat Equation

1. 1st type boundary condition — Dirichlet boundary condition;
2. 2nd type boundary condition — Neumann boundary condition;
3. 3rd type boundary condition — Robin boundary condition;
4. Mixed-type boundary conditions — different types of boundary conditions imposed on different parts of the boundary.

General Issues on Finite Difference Methods

1. Discretize the domain $\Omega \times \mathbb{R}_+$ by introducing a grid, say a grid $\{(x_{\mathbf{j}}, t_m) : \mathbf{j} \in J,\ t_m = m\triangle t,\ m \geq 0\}$ produced by a grid J on Ω and a uniform temporal grid with a time spacing $\triangle t$;
2. Discretize the function space by introducing grid functions, say $U_{\mathbf{j}}^m$, for $\mathbf{j} \in J$ and $m \geq 0$;
3. Discretize the differential operators by properly defined difference operators, say L_h and $\triangle_{+t}$;
4. Solve the discretized problem to get a finite difference solution;
5. Analyze the approximate properties of the finite difference solution.

习题 1：11，12;　习题 2：1

Thank You!