Numerical Solutions to Partial Differential Equations

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1-D Initial Boundary Value Problem of Heat Equation

2.2 ,P34

The standard model problem: Homogeneous heat equation with homogeneous Dirichlet boundary condition

$$u_t = u_{xx}, \qquad 0 < x < 1, \;\; t > 0, \qquad (2.2.1)$$

$$u(x,0) = u^0(x), \qquad 0 \le x \le 1, \qquad (2.2.2)$$

$$u(0,t) = u(1,t) = 0, \qquad t > 0. \qquad (2.2.3)$$

1 A sequence of independent nontrivial special solutions:

$$u_k(x,t) = e^{-k^2\pi^2 t} \sin k\pi x, \qquad k = 1, 2, \cdots. \qquad (2.2.4)$$

Analytical Solutions of the Homogeneous Heat Equation

❷ If the initial data u^0 has a Fourier sine expansion

$$u^0(x) = \sum_{k=1}^{\infty} a_k \sin k\pi x, \qquad (2.2.5)$$

where
$$a_k = 2 \int_0^1 u^0(x) \sin k\pi x \, \mathrm{d}x, \qquad k = 1, 2, \cdots, \qquad (2.2.6)$$

❸ then, the solution to the model problem (1)-(3) can be written as

$$u(x, t) = \sum_{k=1}^{\infty} a_k e^{-k^2 \pi^2 t} \sin k\pi x. \qquad (2.2.7)$$

Grid and Grid Function

1. <u>Spatial grid:</u> $h = h_N = \triangle x = 1/N$, and $x_j = j\,h$, $j = 0, 1, \cdots, N$;

2. <u>Temporal grid:</u> $\tau = \triangle t$, and $t_m = m\,\tau$, $m = 0, 1, \cdots$;

3. <u>Grid function</u>:
   $U = U_{(h,\tau)} = \{U_j^m : j = 0, 1, \cdots, N;\ m = 0, 1, \cdots\}$;

Next, we are going to discuss finite difference schemes of heat equations and their analytical properties.

Finite Difference Methods for Parabolic Equations
└─ The Explicit Scheme and Its Stability and Convergence
  └─ The Explicit Scheme for the Heat Equation

An Explicit Scheme of the Heat Equation

- Substituting $\partial/\partial t$ by $\triangle_{+t}/\triangle t$;
- Substituting $\partial^2/\partial x^2$ by $\delta_x^2/(\triangle x)^2$; (j,m)

leads to the explicit difference scheme

$$\frac{U_j^{m+1} - U_j^m}{\tau} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \quad 1 \leq j \leq N-1; \ m \geq 0; \quad (2.2.8)$$

$$U_j^0 = u_j^0, \qquad 0 \leq j \leq N; \qquad (2.2.9)$$

$$U_0^m = U_N^m = 0, \qquad m \geq 1. \qquad (2.2.10)$$

The explicit scheme (4) can be equivalently written as

$$\left[\frac{\triangle_{+t}}{\tau} - \frac{\delta_x^2}{h^2} \right] U_j^m = 0. \qquad (2.2.8b)$$

The Stencil of the Explicit Scheme of the Heat Equation

The scheme (4) is called an explicit scheme, since

$$U_j^{m+1} = (1 - 2\mu)U_j^m + \mu\left(U_{j-1}^m + U_{j+1}^m\right), \quad \forall j, \qquad (2.2.8c)$$

where $\mu = \tau/h^2$ is called the grid ratio of the heat equation, thus, U_j^{m+1} can be explicitly calculated from U^m node by node.
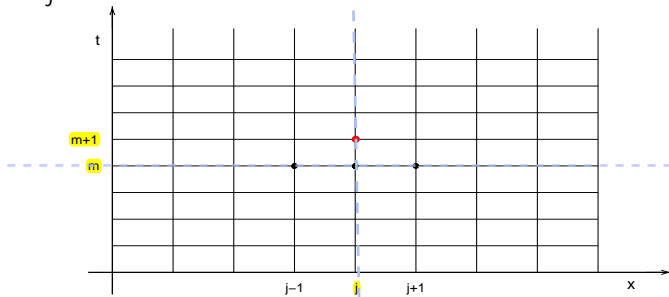

Fig. 2.1

Truncation Error of the Explicit Scheme

By comparing the explicit scheme and the heat equation

$$\left[\frac{\triangle_{+t}}{\tau} - \frac{\delta_x^2}{h^2}\right] U_j^m = 0, \quad \left[\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right] u = 0,$$

we introduce the truncation operator

$$T = T_{(h,\tau)} := \left[\frac{\triangle_{+t}}{\tau} - \frac{\delta_x^2}{h^2}\right] - \left[\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right]. \qquad (2.2.11)$$

For sufficiently smooth u, by Taylor series expansion,

$$\triangle_{+t} u(x,t) = \underline{u_t(x,t)\triangle t} + \frac{1}{2}u_{tt}(x,t)(\triangle t)^2 + \frac{1}{6}u_{ttt}(x,t)(\triangle t)^3 + \cdots \quad (2.2.12)$$

$$\delta_x^2 u(x,t) = \underline{u_{xx}(x,t)(\triangle x)^2} + \frac{1}{12}u_{xxxx}(x,t)(\triangle x)^4 + \cdots . \qquad (2.2.13)$$

Hence the truncation error can be written as $\overset{u}{\underset{\text{PDE}}{\downarrow}}$

$$Tu(x,t) = \frac{1}{2}u_{tt}(x,t)\tau - \frac{1}{12}u_{xxxx}(x,t)h^2 + O(\tau^2 + h^4). \qquad (2.2.14)$$

Truncation Error of the Explicit Scheme

We can also use another form of the Taylor expansion of u at (x, t)

$$\triangle_{+t} u(x, t) = u_t(x, t)\triangle t + \frac{1}{2} u_{tt}(x, \eta)(\triangle t)^2, \quad (2.2.15)$$

$$\delta_x^2 u(x, t) = u_{xx}(x, t)(\triangle x)^2 + \frac{1}{12} u_{xxxx}(\xi, t)(\triangle x)^4, \quad (2.2.16)$$

where $\eta \in (t, t + \tau)$, $\xi \in (x - h, x + h)$, to express the truncation error in the form

$$Tu(x, t) = \frac{1}{2} u_{tt}(x, \eta)\tau - \frac{1}{12} u_{xxxx}(\xi, t)h^2. \quad (2.2.17)$$

Consistency and Order of Accuracy of the Explicit Scheme

Since, for smooth u, the truncation error satisfy

$$Tu(x, t) = \frac{1}{2} u_{tt}(x, \eta)\tau - \frac{1}{12} u_{xxxx}(\xi, t)h^2, \qquad (2.2.17)$$

1. $[\tau^{-1}\triangle_{+t} - h^{-2}\delta_x^2]$ is <mark>consistent</mark> with $[\partial_t - \partial_x^2]$, since

$$Tu(x, t) \to 0, \quad \text{as } h \to 0, \ \tau \to 0, \ \forall(x, t) \in (0, 1) \times \mathbb{R}_+. \quad (2.2.18)$$

2. The explicit scheme is of <mark>first</mark> and <mark>second order accurate</mark> with respect to time and space, since $Tu(x, t) = O(\tau) + O(h^2)$.

3. $|Tu(x, t)| \leq \frac{1}{2} M_{tt} \tau + \frac{1}{12} M_{xxxx} h^2, \quad \forall(x, t) \in \Omega_{t_{\max}}, \qquad (2.2.19)$

where $\Omega_{t_{\max}} \triangleq (0, 1) \times (0, t_{\max})$, $M_{tt} = \sup_{(x,t)\in\Omega_{t_{\max}}} |u_{tt}(x, t)|$ and $M_{xxxx} = \sup_{(x,t)\in\Omega_{t_{\max}}} |u_{xxxx}(x, t)|$.

$\mathbb{L}^\infty$ Stability and Convergence of the Explicit Scheme

① Error: $e_j^m = U_j^m - u_j^m$, $j = 0, 1, \cdots, N$, $m = 0, 1, \cdots$.

② The error equation (compare $\tau^{-1} \triangle_{+t} U_j^m = h^{-2} \delta_x^2 U_j^m + f_j^m$):

$$\frac{e_j^{m+1} - e_j^m}{\tau} = \frac{e_{j+1}^m - 2e_j^m + e_{j-1}^m}{h^2} - T_j^m, \quad 1 \leq j \leq N-1; \ m \geq 0; \quad (2.2.21)$$

$$e_j^0 = 0, \quad 0 \leq j \leq N; \quad (2.2.22)$$

$$e_0^m = e_N^m = 0, \quad m \geq 1, \quad (2.2.23)$$

③ Stability (uniformly well-posedness of (7)-(9), to be proved):

$$\|e\|_{\infty, \Omega_{t_{\max}}} \leq C_1 \left(\max_{0 \leq j \leq N} |e_j^0| + \max_{0 < m\tau \leq t_{\max}} (|e_0^m| + |e_N^m|) \right) + C_2 \|T\|_{\infty, \Omega_{t_{\max}}} \quad (2.2.24)$$

④ A priori error estimate $\|e\|_{\infty, \Omega_{t_{\max}}} \leq C(M_{tt} \tau + M_{xxxx} h^2)$. $\quad (2.2.25)$

What remains to show is the stability.

Finite Difference Methods for Parabolic Equations
└─ The Explicit Scheme and Its Stability and Convergence
   └─ Stability and Convergence of the Explicit Scheme

$\mathbb{L}^\infty$ Stability of the Explicit Scheme

1 Define $\Omega = \Omega_{t_{\max}}$, $\partial\Omega_D = \{(x, t) \in \partial\Omega_{t_{\max}} : t = 0, \text{ or } x = 0, 1\}$,

(2.2.28) $L_{(h,\tau)} U_j^{m+1} = \left(\dfrac{\delta_x^2}{(\Delta x)^2} - \dfrac{\Delta_{+t}}{\Delta t} \right) U_j^m$, then the conditions (1). (2)

of the maximum principle are satisfied, if $0 < \mu \le 1/2$, P20

(Exercises 2.4).
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2 Proper comparison function can also be found (Exercises 2.5).
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3 The explicit scheme and its error equation:
$-L_{(h,\tau)} U_j^{m+1} = f_j^m, \qquad -L_{(h,\tau)} e_j^{m+1} = -T_j^m;$ (2.2.26)
    (2.2.27)

4 The stability then follows from the maximum principle.

$\mathbb{L}^\infty$ Stability of the Explicit Scheme

For parabolic problems, we have an alternative approach.

- The explicit scheme and its error equation ($\mu = \tau/h^2$):

$$
\begin{aligned}
U_j^{m+1} &= (1-2\mu)U_j^m + \mu\left(U_{j-1}^m + U_{j+1}^m\right) + \tau f_j^m, & (2.2.26)\\
e_j^{m+1} &= (1-2\mu)e_j^m + \mu\left(e_{j-1}^m + e_{j+1}^m\right) - \tau\, T_j^m. & (2.2.27)
\end{aligned}
$$

- If $\mu \leq \frac{1}{2}$, $|e_j^{m+1}| \leq \max\limits_{0\leq j\leq N}|e_j^m| + \tau\, T^m$, $\forall j = 1, 2, \cdots, N-1$;

$$(2.2.29)$$

where $T^m = \max\limits_{1\leq j\leq N-1}|T_j^m|$. Therefore, for all $m \geq 0$, we have

$$
\max_{1\leq j\leq N-1}|e_j^{m+1}| \leq \max\left\{\max_{0\leq j\leq N}|e_j^0|, \max_{1\leq l\leq m}\max\left(|e_0^l|, |e_N^l|\right)\right\} + \tau\sum_{l=0}^{m}T^l.
$$

$$(2.2.30)$$

Finite Difference Methods for Parabolic Equations
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$\mathbb{L}^\infty$ Stability Condition of the Explicit Scheme

If the grid ratio satisfies $\mu \triangleq \triangle t/(\triangle x)^2 \leq 1/2$, then, the explicit scheme has the following properties

2.1 stability: for all $m \geq 0$,

$$\max_{1 \leq j \leq N-1} |U_j^{m+1}| \leq \max\left\{\max_{0 \leq j \leq N} |U_j^0|, \max_{1 \leq l \leq m} \max\left(|U_0^l|, |U_N^l|\right)\right\} + t_{\max}\|f\|_{\infty, \Omega_{t_{\max}}},$$
(2.2.31)

$$\|e\|_{\infty, \Omega_{t_{\max}}} \leq \max_{0 \leq j \leq N} |e_j^0| + \max_{0 < m\tau \leq t_{\max}} \max\left(|e_0^m|, |e_N^m|\right) + t_{\max}\|T\|_{\infty, \Omega_{t_{\max}}};$$
(2.2.32)

$\mathbb{L}^\infty$ Stability Condition of the Explicit Scheme

2.2 convergence rate is $O(\tau)$ (or $O(h^2)$), more precisely

$$\|e\|_{\infty,\Omega_{t_{\max}}} \le \tau \left(\frac{1}{2} + \frac{1}{12\mu} \right) M_{xxxx}\, t_{\max}. \tag{2.2.33}$$

(Recall $|Tu(x,t)| \le \frac{1}{2} M_{tt}\, \tau + \frac{1}{12} M_{xxxx}\, h^2$, $\mu = \frac{\tau}{h^2}$ and $u_t = u_{xx}$)

Refinement Path and Condition of $\mathbb{L}^\infty$ Stability

$\tau = r(h)$ is said to give a refinement path, if r is a strictly increasing function and $r(0) = 0$. `2.2` can be rewritten as

`2.3` Let $\{h_i\}_{i=1}^\infty$ satisfy $\lim_{i \to 0} h_i = 0$. Let the refinement path $\tau = r(h)$ satisfy $\mu_i = r(h_i)/h_i^2 \leq 1/2$. Suppose the solution u of (2.2.1-3) satisfies that $|u_{xxxx}| \leq C$ on $(0,1) \times (0, t_{\max})$. Then the solution sequence $U^{(i)}$ of (2.2.8-10), with grid sizes $(h_i, \tau_i = r(h_i))$, converge uniformly on $[0,1] \times [0, t_{\max}]$ to u, and the convergence rate is $O(h_i^2)$.

Refinement Path and Condition of $\mathbb{L}^\infty$ Stability

The convergence rate is optimal. However, for any fixed grid spacing, as $t_{\max} \to \infty$, we lost control on the error.

Recall that, if $f = 0$, the exact solution $u(x, t) \to 0$, as $t \to \infty$, $\|e\|_{\infty, \Omega_{t_{\max}}} \leq \tau \left(\frac{1}{2} + \frac{1}{12\mu} \right) M_{xxxx} \, t_{\max}$ is certainly not a satisfactory error estimate for large $t_{\max}$.

Better results on error estimates can be obtained by applying the maximum principle and choosing proper comparison functions (Exercises 2.5 and 2.6).

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Fourier Analysis and $\mathbb{L}^2$ Stability of the Explicit Scheme

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Similar as the model problem (1)-(3), the difference problem

$$\frac{U_j^{m+1} - U_j^m}{\tau} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \qquad 1 \le j \le N-1; \ m \ge 0,$$

$$U_j^0 = u_j^0, \qquad 0 \le j \le N,$$

$$U_0^m = U_N^m = 0, \qquad m \ge 1,$$

can also be solved by the method of separation of variables.

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Fourier Analysis and $\mathbb{L}^2$ Stability of the Explicit Scheme

In fact, any given general constant-coefficient linear homogeneous difference equation defined on a uniform grid on $[-1, 1] \times [0, \infty)$ admits a complete set of Fourier modes solutions:

$$U_j^{(k)m} = \lambda_k^m e^{ik\pi j \triangle x}, \qquad -N+1 \leq j \leq N, \ -N+1 \leq k \leq N,$$
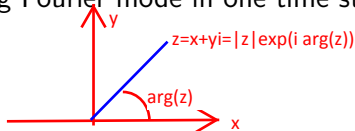(2.2.34)

$\triangle x = 1/N$:   the spatial grid size,

$\lambda_k = |\lambda_k| e^{i \arg \lambda_k}$:   the amplification factor,

     $|\lambda_k|$:   relative change in the modulus

     $\arg \lambda_k$:   the change in the phase angle

of the corresponding Fourier mode in one time step.

Fourier Modes and Characteristic Equations

Substituting the Fourier mode $U_j^m = \lambda_k^m e^{ik\pi \frac{j}{N}}$ into the homogeneous explicit difference scheme

$$U_j^{m+1} = U_j^m + \mu \left(U_{j-1}^m - 2U_j^m + U_{j+1}^m \right),$$

yields the <mark>characteristic equation</mark> of the explicit scheme

$$\lambda_k^{m+1} e^{ik\pi \frac{j}{N}} = \lambda_k^m e^{ik\pi \frac{j}{N}} \left[1 + \mu \left(e^{ik\pi \frac{1}{N}} + e^{-ik\pi \frac{1}{N}} - 2 \right) \right],$$

which has a unique solution

$$\lambda_k = 1 - 4\,\mu\, \sin^2 \frac{k\pi \triangle x}{2}. \qquad (2.2.35)$$

The stability of the computation requires that all Fourier modes should be uniformly bounded, *i.e.* there exist a constant C independent of N and k such that

$$|\lambda_k^m| \leq C, \qquad \forall\, m\tau \leq t_{\max},\ -N+1 \leq k \leq N.$$

Assume $C > 1$, $2\tau \leq t_{\max}$, and set $\tilde{m} = [t_{\max}/\tau]$, hence $\tilde{m} \geq t_{\max}/\tau - 1 \geq t_{\max}/2\tau$. Since C^s is a concave function of C if $0 < s < 1$, the above condition implies

$$|\lambda_k| \leq C^{1/\tilde{m}} \leq 1 + (C-1)/\tilde{m} \leq 1 + 2\tau(C-1)/t_{\max},$$

which leads to the following necessary condition, usually called the von Neumann condition, for the $\mathbb{L}^2$ stability: there exists a constant K independent of N and k such that

$$|\lambda_k| \leq 1 + K\tau, \qquad -N+1 \leq k \leq N. \tag{2.2.36}$$

A Necessary $\mathbb{L}^2$ Stability Condition of the Explicit Scheme

Take $k = N$, since $\lambda_N = 1 - 4\mu$, it follows from the von Neumann condition for the $\mathbb{L}^2$ stability:

$$|\lambda_k| \leq 1 + K\,\tau, \qquad -N + 1 \leq k \leq N,$$

we obtain a necessary condition for the $\mathbb{L}^2$ stability of the explicit scheme: $-1 \leq 1 - 4\mu \leq 1$, or more concisely (since $\mu > 0$)

$$\mu \leq \frac{1}{2}. \tag{2.2.37}$$

In fact, if $\mu > 1/2$, it follows from $\lambda_N = 1 - 4\mu < -1$ that the modulus of $\lambda_N^m e^{i\pi j}$ will grow exponentially fast as m increases. Thus the scheme is unstable for $\mu > 1/2$.

A Sufficient $\mathbb{L}^2$ Stability Condition of the Explicit Scheme

On the other hand, if $\mu \leq \frac{1}{2}$, then $0 \leq 4\mu \sin^2 \frac{k\pi}{2N} \leq 2$, thus

$$|\lambda_k| \leq 1, \quad -N+1 \leq k \leq N.$$

2.4 $\mu \leq \frac{1}{2} \quad \Rightarrow \quad$ the $\mathbb{L}^2$ stability of the explicit scheme.

Proof: Let $U_j^0 = \frac{1}{\sqrt{2}} \sum_{k=-N+1}^{N} \widehat{(U^0)}_k \, e^{\mathrm{i}k\pi \frac{j}{N}}$. Then,
(2.2.40)

$$U_j^m = \frac{1}{\sqrt{2}} \sum_{k=-N+1}^{N} \lambda_k^m \widehat{(U^0)}_k \, e^{\mathrm{i}k\pi \frac{j}{N}}.$$

(2.2.38)

Thus, it follows from $|\lambda_k| \leq 1$, $\forall k$ and the Parseval relation that

$$\|U^m\|_2^2 = \|\widehat{(U^m)}\|_2^2 = \sum_{k=-N+1}^{N} \left|\lambda_k^m \widehat{(U^0)}_k\right|^2 \leq \sum_{k=-N+1}^{N} \left|\widehat{(U^0)}_k\right|^2 = \|U^0\|_2^2.$$

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A Sufficient $\mathbb{L}^2$ Stability Condition of the Explicit Scheme

Rewrite the explicit scheme as $U^{m+1} = \mathcal{N}(U^m)$, then, we have shown that, for $\mu \leq 1/2$, $\|\mathcal{N}(U^m)\|_2 \leq \|U^m\|_2 \leq \|U^0\|_2$.

The corresponding error equation is $e^{m+1} = \mathcal{N}(e^m) - \tau T^m$, thus we have
$$\|e^{m+1}\|_2 = \|\mathcal{N}(e^m) - \tau T^m\|_2 \leq \|e^m\|_2 + \tau \|T^m\|_2$$

$$\leq \|e^0\|_2 + \tau \sum_{l=0}^{m} \|T^l\|_2. \qquad (2.2.41)$$

This shows that the dependence of the solution of the explicit scheme on the right hand side as well as the initial data is uniformly continuous in the $\mathbb{L}^2$ norm, therefore is $\mathbb{L}^2$ stable. $\qquad \square$

$\mathbb{L}^2$ Convergence of the Explicit Scheme

Since, for $\mu \leq 1/2$, the error of the explicit scheme satisfies

$$\|e^{m+1}\|_2 \leq \|e^0\|_2 + \tau \sum_{l=0}^{m} \|T^l\|_2,$$

if the corresponding consistency holds, say $\lim_{h \to 0} \|e^0\|_2 = 0$ and

$$\lim_{\tau \to 0} \tau \sum_{l=0}^{m} \|T^l\|_2 = 0, \ \ \forall m \leq t_{max}/\tau,$$

then the difference solution is convergent. Note, if $\|Tu(\cdot, t)\|_2$ is a uniformly continuous function of t, then

$$\lim_{\tau \to 0} \tau \sum_{l=0}^{[t_{max}/\tau]} \|T^l\|_2 = 0 \ \Leftrightarrow \ \lim_{\tau \to 0} \int_0^{t_{max}} \|Tu(\cdot, t)\|_2 \, dt = 0.$$

： （   ）   （   ） Riemann   .

2.5(P45).

Finite Difference Methods for Parabolic Equations
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$\mathbb{L}^2$ Convergence of the Explicit Scheme

　 2.5 Suppose

1. $\{h_i\}_{i=1}^{\infty}$ satisfies $\lim_{i \to 0} h_i = 0$;

2. the refinement path r satisfies $\mu_i = r(h_i)/h_i^2 \leq 1/2$;

3. the solution u satisfies $u_{xxxx} \in \mathbb{C}((-1,1) \times R_+)$ and $\int_0^{t_{max}} \|u_{xxxx}(\cdot, t)\|_2 \, dt < \infty$.

Then, $$\max_{0 < m\tau_i \leq t_{max}} \|e^{(i)m}\|_2 = O(h_i^2).$$

Remark: Here it is assumed that $\|e^{(i)0}\|_2 = O(h_i^2)$, i.e. the initial data is approximated with second order accuracy.

2.5   ,   2.6(P45).

Summary of the 1st Order Forward Explicit Scheme

1. A sufficient and necessary condition for L^2 stability, also a sufficient condition for L^∞ stability: $\mu = \tau/h^2 \leq 1/2$, a rather strict restriction on the time step;

2. Convergence rate $O(\tau + h^2)$.

3. Easy to solve, and the computational cost is low.

Question: is it possible to develop an explicit scheme so that the stability condition is relaxed to say $\tau = O(h)$, and the convergence rate is $O(\tau^2 + h^2)$.

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The Richardson scheme

The Richardson scheme (with truncation error $O(\tau^2 + h^2)$):
$$\frac{U_j^{m+1} - U_j^{m-1}}{2\tau} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}. \tag{2.2.42}$$

Substitute the Fourier mode $U_j^m = \lambda_k^m e^{ik\pi j \triangle x}$ into the scheme, we are led to the characteristic equation of the Richardson scheme:
$$\lambda_k^2 + 8\lambda_k \mu \sin^2 \frac{k\pi \triangle x}{2} - 1 = 0.$$

The equation has two distinct real roots $\lambda_k^\pm$, and for all $k \neq 0$,
$$\lambda_k^+ + \lambda_k^- = -8\mu \sin^2 \frac{k\pi \triangle x}{2} < 0, \quad \lambda_k^+ \lambda_k^- = -1, \Rightarrow \lambda_k^- < -1.$$

Hence, the Richardson scheme is unconditionally unstable.

The Du Fort-Frankel scheme

The Du Fort-Frankel scheme:

$$\frac{U_j^{m+1} - U_j^{m-1}}{2\tau} = \frac{U_{j+1}^m - (U_j^{m+1} + U_j^{m-1}) + U_{j-1}^m}{h^2}. \qquad (2.2.43)$$

The characteristic equation of the Du Fort-Frankel scheme:
$(1 + 2\mu)\lambda_k^2 - 4\lambda_k\mu \cos(k\pi\triangle x) - (1 - 2\mu) = 0$, which has roots
$\lambda_k^{\pm} = \frac{2\mu \cos(k\pi\triangle x) \pm \sqrt{1 - 4\mu^2 \sin^2(k\pi\triangle x)}}{1 + 2\mu}$.

If $4\mu^2 \sin^2(k\pi\triangle x) > 1$, $\lambda_k^{\pm}$ are conjugate complex roots, hence
$|\lambda_k^{\pm}| = |\lambda_k^+ \lambda_k^-| = |(1 - 2\mu)/(1 + 2\mu)| < 1$;

If $4\mu^2 \sin^2(k\pi\triangle x) \leq 1$, $|\lambda_k^{\pm}| \leq (2\mu|\cos(k\pi\triangle x)| + 1)/(1 + 2\mu) \leq 1$.

Consequently Du Fort-Frankel scheme is unconditionally $\mathbb{L}^2$ stable.

The truncation error is $T_j^m = O((\frac{\tau}{h})^2) + O(\tau^2 + h^2) + O(\frac{\tau^4}{h^2})$.

consistent if $\tau = o(h)$; convergence rate $O(h^2)$ only if $\tau = O(h^2)$.

Finite Difference Methods for Parabolic Equations
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No Explicit Scheme Can Unconditionally Converge

Since the solution of the heat equation picks up information globally on the initial and the boundary data, it is impossible to develop an explicit scheme which is unconditionally stable and at the same time unconditionally consistent.

In fact, to guarantee an explicit scheme to converge, $\tau = o(h)$ must hold on the refinement path.

Therefore, it is necessary to develop implicit finite difference schemes for the parabolic partial differential equations.

The 1st Order Backward Implicit Finite Difference Scheme

The initial-boundary value problem of the <mark>simplest implicit</mark> finite difference scheme for the model problem (2.2.1)-(2.2.3):

$$\frac{U_j^{m+1} - U_j^m}{\tau} = \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2}, \ 1 \le j \le N-1; \ m \ge 0; \quad (2.2.44)$$

$$U_j^0 = u_j^0, \ 0 \le j \le N; \quad (2.2.45)$$

$$U_0^m = U_N^m = 0, \quad m \ge 1. \quad (2.2.46)$$

The scheme can be equivalently rewritten as

$$\boxed{(1 + 2\mu)U_j^{m+1} = \mu U_{j-1}^{m+1} + U_j^m + \mu U_{j+1}^{m+1}.} \quad (2.2.47)$$
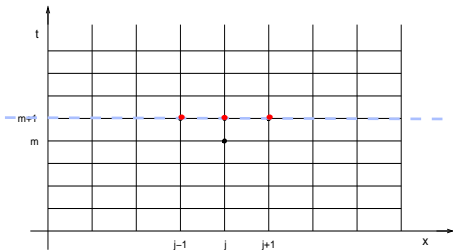
The <mark>truncation operator</mark>

$$T_{(h,\tau)} := \left[\frac{\triangle_{-t}}{\tau} - \frac{\delta_x^2}{h^2} \right] - \left[\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2} \right]. \quad (2.2.48)$$

$$L_{(h,\tau)} = \frac{\delta_x^2}{(\triangle x)^2} - \frac{\triangle_{-t}}{\triangle t}. \quad (2.2.54)$$

<mark>Maximum principle</mark> holds for $\Omega = \Omega_{t_{\max}}, \ \partial \Omega_D = \{(x,t) \in \partial \Omega_{t_{\max}} : x = 0, 1 \ \text{or} \ t = 0\}.$

Truncation Error and Order of Accuracy

The truncation operator $T_{(h,\tau)} := \left[\frac{\triangle_{-t}}{\tau} - \frac{\delta_x^2}{h^2} \right] - \left[\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2} \right]$.

By the Taylor series expansion, the truncation error of the 1st order backward implicit scheme is

$$Tu(x,t) = -\frac{1}{2}u_{tt}(x,t)\tau - \frac{1}{12}u_{xxxx}(x,t)h^2 + O(\tau^2 + h^4), \quad \text{(2.2.49)}$$

$$Tu(x,t) = -\frac{1}{2}u_{tt}(x,\eta)\tau - \frac{1}{12}u_{xxxx}(\xi,t)h^2. \quad \text{(2.2.50)}$$

Thus the 1st order backward implicit scheme is consistent with the heat equation, and is of first and second order accurate with respect to time and space respectively, *i.e.* $Tu(x,t) = O(\tau + h^2)$.

$\mathbb{L}^\infty$ Stability of the 1st Order Backward Implicit Scheme

The 1st order backward implicit scheme and its error equation can be equivalently written as

$$(1 + 2\mu)U_j^{m+1} = U_j^m + \mu\left(U_{j-1}^{m+1} + U_{j+1}^{m+1}\right) + \tau f_j^{m+1}, \quad \text{(2.2.51)}$$

$$(1 + 2\mu)e_j^{m+1} = e_j^m + \mu\left(e_{j-1}^{m+1} + e_{j+1}^{m+1}\right) - \tau T_j^{m+1}, \quad \text{(2.2.52)}$$

(or $(I + \mu A_{N-1})U^{m+1} = \mu U_b^{m+1} + U^m + \tau f^m$, eigenvalue$(I + \mu A_{N-1}) > 1$).

Thus, for any $\mu > 0$ and for all $m \geq 0$,

$$\max_{1 \leq j \leq N-1} |e_j^{m+1}| \leq \max\left\{\max_{0 \leq j \leq N} |e_j^0|, \max_{1 \leq l \leq m+1} \max\left(|e_0^l|, |e_N^l|\right)\right\} + \tau \sum_{l=1}^{m+1} T^l.$$

Hence, the 1st order backward implicit scheme is unconditionally (2.2.53) $\mathbb{L}^\infty$ stable and satisfies the maximum principle. Better estimate can be obtained by taking proper comparison functions.

$\mathbb{L}^2$ Stability of the 1st Order Backward Implicit Scheme

Substituting the Fourier mode $U_j^m = \lambda_k^m e^{ik\pi j \triangle x}$ into the homogeneous 1st order backward implicit scheme, yields the characteristic equations of the scheme

$$\lambda_k^{m+1} e^{ik\pi \frac{j}{N}} \left[1 - \mu \left(e^{ik\pi \frac{1}{N}} + e^{-ik\pi \frac{1}{N}} - 2 \right) \right] = \lambda_k^m e^{ik\pi \frac{j}{N}},$$

which has a unique solution

$$\lambda_k = \frac{1}{1 + 4\,\mu \, \sin^2 \frac{k\pi \triangle x}{2}}. \tag{2.2.55}$$

Hence, the 1st order backward implicit scheme is unconditionally $\mathbb{L}^2$ stable.

Efficiency of the 1st Order Backward Implicit Scheme

1. Unconditionally $\mathbb{L}^2$ and $\mathbb{L}^\infty$ stable, can use larger τ;

2. Convergence rate $O(\tau + h^2)$, $\tau = O(h^2)$, for efficiency.

3. Need to solve a tridiagonal and diagonally dominant linear system, and the computational cost is about twice that of the 1st order forward explicit scheme if solved by the Thompson method (forward elimination and backward substitution).

4. More efficient only if $\mu > 1$, the computational cost is about $1/\mu$ of that of the 1st order forward explicit scheme.

Better, but not good enough.

The Crank-Nicolson scheme

The well known Crank-Nicolson scheme:

$$\frac{U_j^{m+1} - U_j^m}{\tau} = \frac{1}{2}\left[\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} + \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2}\right];$$

(2.2.56)

$$(1+\mu)U_j^{m+1} = (1-\mu)U_j^m + \frac{\mu}{2}\left(U_{j-1}^m + U_{j+1}^m + U_{j-1}^{m+1} + U_{j+1}^{m+1}\right)$$

(2.2.60)

1. $T_j^{m+\frac{1}{2}} = \frac{-1}{12}\left[u_{ttt}(x_j, t_{m+\frac{1}{2}})\tau^2 + u_{xxxx}(x_j, t_{m+\frac{1}{2}})h^2\right] + O(\tau^4 + h^4);$

   (2.2.57)

2. $\lambda_k = \left[1 - 2\mu\sin^2\frac{k\pi\triangle x}{2}\right] / \left[1 + 2\mu\sin^2\frac{k\pi\triangle x}{2}\right]$, thus
   unconditionally $\mathbb{L}^2$ stable.

   (2.2.59)

3. The computational cost is about twice that of the explicit scheme if solved by the Thompson method.

4. The maximum principle holds for $\mu \leq 1$.

5. Convergence rate is $O(\tau^2 + h^2)$, efficient if $\tau = O(h)$.

The θ-scheme ($0 < \theta < 1$, $\theta \neq 1/2$)

$$\frac{U_j^{m+1} - U_j^m}{\tau} = (1-\theta)\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} + \theta\frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{h^2};$$
(2.2.61)

$$(1+2\mu\theta)U_j^{m+1} = (1-2\mu(1-\theta))U_j^m + \mu(1-\theta)\left(U_{j-1}^m + U_{j+1}^m\right) + \mu\theta\left(U_{j-1}^{m+1} + U_{j+1}^{m+1}\right).$$

1. $T_j^{m+\frac{1}{2}} = O(\tau^2 + h^4)$, if $\theta = \frac{1}{2} - \frac{1}{12\mu}$; $= O(\tau + h^2)$, otherwise.

2. $\lambda_k = \left[1 - 4(1-\theta)\,\mu\,\sin^2\frac{k\pi\triangle x}{2}\right] / \left[1 + 4\theta\,\mu\,\sin^2\frac{k\pi\triangle x}{2}\right]$, thus (2.2.62) $\mathbb{L}^2$ stable for $2\mu(1-2\theta) \leq 1$ (unconditional for $\theta \geq 1/2$).

3. The maximum principle holds for $2\mu(1-\theta) \leq 1$.

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Thank You!