3 Parabolic equations: alternative derivation of difference equations and miscellaneous topics

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This chapter is not necessary for any reader who would prefer to study, at this stage, the numerical solution of hyperbolic and/or elliptic equations.

Reduction to a system of ordinary differential equations

Consider the equation

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x^2}, \quad 0<x<X, \quad t>0, \tag{3.1}$$

where U satisfies the initial condition $U(x, 0)=g(x)$, $0 \leqslant x \leqslant X$, and has known boundary values at $x=0$ and X, $t>0$.

If the x derivative at (x, t) is replaced by

$$\frac{1}{h^2}\{U(x-h, t)-2U(x, t)+U(x+h, t)\}+O(h^2)$$

and x is considered as a constant, eqn (3.1) can be written as the ordinary differential equation

$$\frac{dU(t)}{dt}=\frac{1}{h^2}\{U(x-h, t)-2U(x, t)+U(x+h, t)\}+O(h^2). \tag{3.2}$$

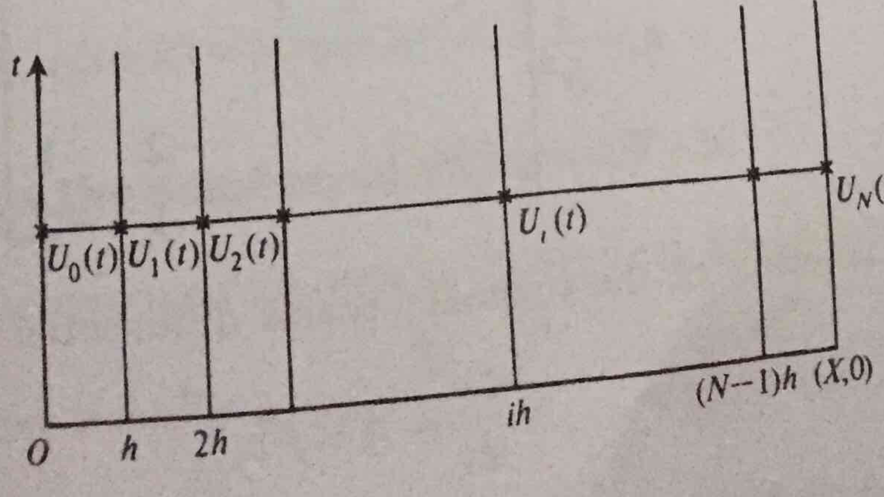

Fig. 3.1

Subdivide the interval $0 \leqslant x \leqslant X$ into N equal subintervals by the grid lines $x_i = ih$, $i = 0(1)N$, where $Nh = X$, and write down eqn (3.2) at every mesh point $x_i = ih$, $i = 1(1)N-1$, along time-level t. It then follows that the values $V_i(t)$ approximating $U_i(t)$ will be the exact solution values of the system of $(N-1)$ ordinary differential equations

$$\frac{dV_1(t)}{dt} = \frac{1}{h^2}(V_0 - 2V_1 + V_2)$$

$$\frac{dV_2(t)}{dt} = \frac{1}{h^2}(V_1 - 2V_2 + V_3)$$

$$\vdots$$

$$\frac{dV_{N-1}}{dt} = \frac{1}{h^2}(V_{N-2} - 2V_{N-1} + V_N),$$

where V_0 and V_N are known boundary-values. These can be written in matrix form as

$$\frac{d}{dt}\begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-2} \\ V_{N-1} \end{bmatrix} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & \cdot & \vdots & \vdots & . & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}\begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-2} \\ V_{N-1} \end{bmatrix} + \frac{1}{h^2}\begin{bmatrix} V_0 \\ 0 \\ \vdots \\ 0 \\ V_N \end{bmatrix},$$

i.e. as

$$\frac{d\mathbf{V}(t)}{dt} = \mathbf{A}\mathbf{V}(t) + \mathbf{b}, \tag{3.3}$$

where $\mathbf{V}(t) = [V_1, V_2, \ldots, V_{N-1}]^T$, $\mathbf{b}$ is a column vector of zeros and known boundary-values and matrix $\mathbf{A}$ of order $(N-1)$ is given by

$$\mathbf{A} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}. \tag{3.4}$$

The solution of the ordinary scalar differential equation

$$\frac{dV}{dt} = AV + b,$$

where A and b are independent of t and $V(t)$ satisfies the initial condition $V(0) = g$, is easily shown, by the method of separation of the variables, to be

$$V(t) = -\frac{b}{A} + \left(g + \frac{b}{A}\right)\exp(At).$$

At the end of this section it is shown that the solution of (3.3) satisfying the initial condition $\mathbf{V}(0) = [g_1, g_2, \ldots, g_{N-1}]^T = \mathbf{g}$, and where $\mathbf{b}$ is independent of t, is

$$\mathbf{V}(t) = -\mathbf{A}^{-1}\mathbf{b} + \{\exp(t\mathbf{A})\}(\mathbf{g} + \mathbf{A}^{-1}\mathbf{b}). \tag{3.5}$$

Hence,

$$\begin{aligned}\mathbf{V}(t+k) &= -\mathbf{A}^{-1}\mathbf{b} + \{\exp(t+k)\mathbf{A}\}(\mathbf{g} + \mathbf{A}^{-1}\mathbf{b}) \\ &= -\mathbf{A}^{-1}\mathbf{b} + \{\exp(k\mathbf{A})\}\{\exp(t\mathbf{A})\}(\mathbf{g} + \mathbf{A}^{-1}\mathbf{b}).\end{aligned}$$

By eqn (3.5) this leads to

$$\mathbf{V}(t+k) = -\mathbf{A}^{-1}\mathbf{b} + \{\exp(k\mathbf{A})\}(\mathbf{V}(t) + \mathbf{A}^{-1}\mathbf{b}). \tag{3.6}$$

If all boundary values are zero,

$$\mathbf{V}(t+k) = \{\exp(k\mathbf{A})\}\mathbf{V}(t). \tag{3.7}$$

The boundary values can always be eliminated if we are concerned more, say, with stability than with a particular numerical solution. Perturb the vector of initial values from $\mathbf{g}$ to $\mathbf{g}^*$. By eqn (3.5), the solution $\mathbf{V}^*(t)$ is

$$\mathbf{V}^*(t) = -\mathbf{A}^{-1}\mathbf{b} + \{\exp(t\mathbf{A})\}(\mathbf{g}^* + \mathbf{A}^{-1}\mathbf{b}). \tag{3.8}$$

Equations (3.5) and (3.8) then show that

$$\mathbf{V}^*(t) - \mathbf{V}(t) = \{\exp(t\mathbf{A})\}(\mathbf{g}^* - \mathbf{g}).$$

Hence the perturbation vector $\mathbf{e}(t) = \mathbf{V}^*(t) - \mathbf{V}(t)$ at time t is related to the initial perturbation vector $\mathbf{e}(0) = \mathbf{g}^* - \mathbf{g}$ by

$$\mathbf{e}(t) = \{\exp(t\mathbf{A})\}\mathbf{e}(0).$$

As before, $\mathbf{e}(t+k) = \{\exp(k\mathbf{A})\}\mathbf{e}(t)$.

A note on the solution of $\mathrm{d}\mathbf{V}/\mathrm{d}t = \mathbf{A}\mathbf{V} + \mathbf{b}$

Define the exponential matrix of the real $n \times n$ matrix $\mathbf{P}$ by

$$\exp \mathbf{P} = e^{\mathbf{P}} = \mathbf{I}_n + \mathbf{P} + \frac{\mathbf{P}^2}{2!} + \frac{\mathbf{P}^3}{3!} + \cdots \sum_{m=0}^{\infty} \frac{\mathbf{P}^m}{m!}, \tag{3.9}$$

where $\mathbf{P}^0 = \mathbf{I}_n$ is the unit matrix of order n.

If $\mathbf{Q}$ is a real $n \times n$ matrix such that $\mathbf{PQ}=\mathbf{QP}$, it can be proved by (3.9) that

$$e^{\mathbf{P}}e^{\mathbf{Q}}=e^{\mathbf{Q}}e^{\mathbf{P}}=e^{\mathbf{P}+\mathbf{Q}}.$$

Hence

$$e^{\mathbf{P}}e^{-\mathbf{P}}=e^{-\mathbf{P}}e^{\mathbf{P}}=e^{\mathbf{O}}.$$

But, by (3.9),

$$e^{\mathbf{O}}=\mathbf{I}_n.$$

Therefore

$$e^{\mathbf{P}}e^{-\mathbf{P}}=\mathbf{I}_n. \tag{3.10}$$

Premultiplication of both sides of (3.10) by the inverse $(e^{\mathbf{P}})^{-1}$ of $e^{\mathbf{P}}$, defined by $(e^{\mathbf{P}})^{-1}e^{\mathbf{P}}=\mathbf{I}_n$, then shows

$$e^{-\mathbf{P}}=(e^{\mathbf{P}})^{-1}.$$

On putting $\mathbf{P}=\mathbf{A}t$ into (3.9), where matrix $\mathbf{A}$ is independent of t, and differentiating with respect to t, it follows that

$$\frac{d}{dt}(e^{\mathbf{A}t})=\mathbf{A}e^{\mathbf{A}t}=e^{\mathbf{A}t}\mathbf{A}.$$

Now consider $\mathbf{V}(t)=e^{\mathbf{A}t}\mathbf{g}$, where $\mathbf{g}$ is independent of t. This clearly satisfies the initial condition $\mathbf{V}(0)=\mathbf{g}$. Differentiation with respect to t gives that

$$\frac{d\mathbf{V}}{dt}=\mathbf{A}e^{\mathbf{A}t}\mathbf{g}=\mathbf{AV}.$$

In other words, the solution of

$$\frac{d\mathbf{V}}{dt}=\mathbf{AV} \tag{3.11}$$

which satisfies $\mathbf{V}(0)=\mathbf{g}$, is

$$\mathbf{V}(t)=e^{\mathbf{A}t}\mathbf{g}.$$

Similarly, the vector function

$$\mathbf{V}(t)=-\mathbf{A}^{-1}\mathbf{b}+e^{t\mathbf{A}}(\mathbf{g}+\mathbf{A}^{-1}\mathbf{b}),$$

which obviously satisfies the initial condition $\mathbf{V}(0)=\mathbf{g}$, is the solution of

$$\frac{d\mathbf{V}}{dt}=\mathbf{AV}+\mathbf{b},$$

provided vector $\mathbf{b}$ and matrix $\mathbf{A}$ are independent of t. The analytical solution of (3.11) in terms of the eigenvalues and eigenvectors of matrix $\mathbf{A}$ is given later.

Finite difference approximation via the ordinary differential equations

For simplicity, assume that the boundary values associated with

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x^2}, \quad 0<x<X, \quad t>0,$$

are zero. By eqn (3.7) the recurrence relationship satisfied by the vector of values $\mathbf{V}(t)$ approximating $U(t)$ at the mesh points $x_i = ih$, $i = 1(1)N-1$, along time-level t, is

$$\mathbf{V}(t+k)=\{\exp(k\mathbf{A})\}\mathbf{V}(t), \quad t=0, k, 2k, \ldots, \tag{3.12}$$

where matrix $\mathbf{A}$ is defined by eqn (3.4).

In order to derive a set of finite difference equations from this it is necessary to approximate the exponential of $k\mathbf{A}$ by a finite algebraic function of $k\mathbf{A}$. Since $\exp(k\mathbf{A})$, by definition, is

$$\mathbf{I}+k\mathbf{A}+\tfrac{1}{2}k^2\mathbf{A}^2+\tfrac{1}{6}k^3\mathbf{A}^3+\ldots,$$

one obvious approximation is $\mathbf{I}+k\mathbf{A}$, with a leading error term of order k^2. The vector of values $\mathbf{u}=[u_1, u_2, \ldots, u_{N-1}]^T$ approximating $\mathbf{V}$ in eqn (3.12) will then be the solution of the finite-difference equations

$$\mathbf{u}(t+k)=(\mathbf{I}+k\mathbf{A})\mathbf{u}(t). \tag{3.13}$$

If $t=t_j=jk$ and $r=k/h^2$, these equations in detail, for zero boundary-values, are

$$\begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ u_{N-2,j+1} \\ u_{N-1,j+1} \end{bmatrix} = \begin{bmatrix} (1-2r) & r & & & \\ r & (1-2r) & r & & \\ & \ddots & \ddots & \ddots & \\ & & r & (1-2r) & r \\ & & & r & (1-2r) \end{bmatrix} \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{N-2,j} \\ u_{N-1,j} \end{bmatrix}$$

The ith equation is the classical explicit approximation

$$u_{i,j+1} = ru_{i-1,j}+(1-2r)u_{i,j}+ru_{i+1,j}, \quad i=1(1)N-1.$$

TABLE 3.1

(S, T)	$R_{S,T}(\theta)$	Principal error term
(0, 1)	$1+\theta$	$\frac{1}{2}\theta^2$
(0, 2)	$1+\theta+\frac{1}{2}\theta^2$	$\frac{1}{6}\theta^3$
(1, 0)	$\dfrac{1}{1-\theta}$	$-\frac{1}{2}\theta^2$
(1, 1)	$\dfrac{1+\frac{1}{2}\theta}{1-\frac{1}{2}\theta}$	$-\frac{1}{12}\theta^3$
(1, 2)	$\dfrac{1+\frac{2}{3}\theta+\frac{1}{6}\theta^2}{1-\frac{1}{3}\theta}$	$-\frac{1}{72}\theta^4$
(2, 0)	$\dfrac{1}{1-\theta+\frac{1}{2}\theta^2}$	$\frac{1}{6}\theta^3$
(2, 1)	$\dfrac{1+\frac{1}{3}\theta}{1-\frac{2}{3}\theta+\frac{1}{6}\theta^2}$	$\frac{1}{72}\theta^4$
(2, 2)	$\dfrac{1+\frac{1}{2}\theta+\frac{1}{12}\theta^2}{1-\frac{1}{2}\theta+\frac{1}{12}\theta^2}$	$\frac{1}{720}\theta^5$

Standard finite difference equations via the Padé approximants

The classical explicit approximation

It is seen by Table 3.1 and eqn (3.13) that the classical explicit approximation to $\partial U/\partial t = \partial^2 U/\partial x^2$ is given by approximating $\exp(k\mathbf{A})$ by its (0, 1) Padé approximant.

The classical implicit approximation

The (1, 0) Padé approximant approximates

$$\mathbf{V}(t+k) = \{\exp(k\mathbf{A})\}\mathbf{V}(t)$$

by

$$\mathbf{u}(t+k)=(\mathbf{I}-k\mathbf{A})^{-1}\mathbf{u}(t).$$

Premultiplication of both sides by the matrix $(\mathbf{I}-k\mathbf{A})$ yields

$$(\mathbf{I}-k\mathbf{A})\mathbf{u}(t_j+k)=\mathbf{u}(t_j),\quad j=0,1,2,\ldots,$$

where $\mathbf{u}(t_j+k)=[u_{1,j+1},u_{2,j+1},\ldots,u_{N-1,j+1}]^T$ and matrix $\mathbf{A}$ is defined by (3.4). In detail, for zero boundary-conditions,

$$\begin{bmatrix}(1+2r) & -r & & & \\ -r & (1+2r) & -r & & \\ & & \ddots & & \\ & & -r & (1+2r) & -r \\ & & & -r & (1+2r)\end{bmatrix}$$

$$\times\begin{bmatrix}u_{1,j+1}\\ u_{2,j+1}\\ \vdots\\ u_{N-2,j+1}\\ u_{N-1,j+1}\end{bmatrix}=\begin{bmatrix}u_{1,j}\\ u_{2,j}\\ \vdots\\ u_{N-2,j}\\ u_{N-1,j}\end{bmatrix}.$$

The ith equation gives the implicit or backward-difference scheme

$$-ru_{i-1,j+1}+(1-2r)u_{i,j+1}-ru_{i+1,j+1}=u_{i,j},\quad i=1(1)N-1.$$

This is unconditionally stable for all $r=k/h^2>0$. The leading error terms are of order h^2 in x because of the central-difference approximation to $\partial^2U/\partial x^2$ and of order k in t. (The leading error term of the (1, 0) Padé approximant to $\exp(k\mathbf{A})$ is $O(k^2)$ but eqn (3.12) was derived by integrating the ordinary differential for $\mathbf{V}(t)$ with respect to t.) The method is said to be first order accurate in t.

The Crank–Nicolson equations

Table 3.1 shows that the (1, 1) Padé approximant replaces

$$\mathbf{V}(t+k)=\{\exp(k\mathbf{A})\}\mathbf{V}(t)$$

by

$$\mathbf{u}(t+k)=(\mathbf{I}-\tfrac{1}{2}k\mathbf{A})^{-1}(\mathbf{I}+\tfrac{1}{2}k\mathbf{A})\mathbf{u}(t).$$

For numerical calculations this needs to be written as

$$(\mathbf{I}-\tfrac{1}{2}k\,\mathbf{A})\mathbf{u}(t+k)=(\mathbf{I}+\tfrac{1}{2}k\,\mathbf{A})\mathbf{u}(t).$$

This gives the Crank–Nicolson scheme

$$\begin{aligned}-ru_{i-1,j+1}&+2(1+r)u_{i,j+1}-ru_{i+1,j+1}\\&=ru_{i-1,j}+2(1-r)u_{i,j}+ru_{i+1,j},\quad i=1(1)N-1.\end{aligned}$$

It is second-order accurate in t, having an error term via its Padé approximant of order k^3, and may be used with larger time-intervals than the backward difference method. As shown later, it can, however, produce unwanted finite oscillations near points of discontinuity if $k/h>X/\pi$. (See Fig. 3.2.)

A_0-stability, L_0-stability and the symbol of the method

Assume that the boundary values associated with the equation

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x^2},\quad 0<x<X,\quad t>0,$$

are zero and that the vector of initial values is

$$\mathbf{U}(0)=\mathbf{g}=[g_1,g_2,\ldots,g_{N-1}]^T,\quad Nh=X.$$

Then the vector of values $\mathbf{V}(t)$ approximating $\mathbf{U}(t)$ at the mesh points $x_i=ih$, $i=1(1)N-1$, along time-level $t_j=jk$ satisfies the recurrence relationship

$$\mathbf{V}(t_j+k)=\{\exp(k\mathbf{A})\}\mathbf{V}(t_j),\quad j=0,1,2,\ldots.$$

If the exponential of $k\mathbf{A}$ is approximated by its (S,T) Padé approximant $R_{S,T}(k\mathbf{A})$, the resulting set of finite difference equations is

$$\mathbf{u}(t_j+k)=R_{S,T}(k\mathbf{A})\mathbf{u}(t_j),$$

which can be written equivalently as

$$\mathbf{u}(t_j)=R_{S,T}(k\mathbf{A})\mathbf{u}(t_{j-1}).$$

Applied recursively this leads to

$$\mathbf{u}(t_j)=[R_{S,T}(k\mathbf{A})]^j\mathbf{u}(0),\tag{3.14}$$