The numerical solution of the heat conduction equation subject to separated boundary conditions

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The stability of the Crank Nicolson scheme for the numerical solution of the heat conduction equation subject to separated boundary conditions is demonstrated. This result is extended to separable equations with variable coefficients and to the heat conduction equation in cylindrical geometry which has a singular coefficient. The solution of the difference approximation to the heat conduction equation is shown to reflect accurately the pattern of behaviour of the differential equation, and this result is applied to the phenomenon of 'persistent discretisation error' in the solution to the difference equation.

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1. Introduction

This note is occasioned by two recent papers concerned with the numerical solution by finite difference methods of the heat conduction equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x, t) \tag{1.1}$$

defined on $S(0, 1) = \{(x, t);\ 0 \leqslant \times \leqslant 1, t \geqslant 0\}$, and subject to an appropriate initial condition, and to separated boundary conditions of the form

$$\left.\begin{aligned} a_{11}u(0, t) + a_{12}\frac{\partial u}{\partial x}(0, t) &= A_1 \\ a_{21}u(1, t) + a_{22}\frac{\partial u}{\partial x}(1, t) &= A_2. \end{aligned}\right\} \tag{1.2}$$

In the first of these papers, Parker and Crank (1964) describe a phenomenon (also described by Radok and Merril (1960) and Phelps (1962)) which they call 'persistent discretisation error'. In the second paper, Keast and Mitchell (1966) identify this phenomenon as a weak case of an alleged serious instability.

It is the aim of this note to point out that the difference equations described by Keast and Mitchell as only 'apparently stable' are in fact stable in the usual sense (here only the Crank Nicolson formula will be considered), and that convergence as the mesh sizes are reduced can be demonstrated after the manner of the Lax equivalence theorem (Lax and Richtmyer (1956)) in any finite region $R = \{(x, t);\ 0 \leqslant x \leqslant 1, 0 \leqslant t \leqslant t_{max}\}$. The stability questions are considered in Sections 2 and 3. The approach given here can be generalised to separable equations with variable coefficients, and this is described in Section 4.

In our discussion of stability it is essential that t_{max} be finite because solution growth like e^{kt} is possible in equation (1.1). Other authors (for example Varga (1962), Gary (1966)) have attempted to relax this condition in cases where the solution of the differential equation is bounded as $t \to \infty$, and have adopted definitions of stability related to that used by Keast and Mitchell. Gary (his Theorem 4) claims that their condition for stability is necessary for stability in his sense, but an example will be given in Section 5 to show that this is not so. In Keast and Mitchell (1966) there is an apparent confusion between the spectral radius of a matrix and the concept of the spectrum of a family of operators used by Godunov and Ryabenki (1964). Keast and Mitchell allege a result not contained in the latter reference.

The problems discussed by Parker and Crank are characterised by discontinuous initial conditions. Keast and Mitchell are correct in pointing out that persistent discretisation error can occur with smooth initial conditions, and it may be noted that discretisation error is usually persistent. However, Parker and Crank do draw attention to a significant phenomenon, for it is often the case in the finite difference solution of equation (1.1) subject to equation (1.2) that the error due to discretisation tends to zero as t tends to ∞. The reason for this is that a solution to equation (1.1) with $f(x, t) = 0$ satisfying the conditions (1.2) can be found in the form

$$u = 2Ct + A + Bx + Cx^2 \tag{1.3}$$

where A, B, and C are suitably chosen constants, and this satisfies exactly the usual finite difference approximations to equations (1.1) and (1.2). This expression permits the part of the solution due to the inhomogeneity in the boundary conditions to be subtracted out, and in many practical cases the remaining part of the solution of both the differential equation and the difference approximation tends to zero as t tends to ∞. Often* the absolute contribution of the discretisation error also tends to zero as t tends to ∞, so that high absolute accuracy is obtained independent of the mesh size. This result is only valid for large enough values of t, and discretisation error is certainly a problem for small t.

2. Preliminary considerations

Let a finite difference grid be introduced on $S(0, 1)$ in the usual manner. Assuming that a_{12} and a_{22} are not

* An example that illustrates that this need not be the case is the following. It is readily verified that $u = \sin t^2(1 - x)x/t$ satisfies

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 2\cos t^2(1 - x) \times - \frac{\sin t^2}{t}\left\{\frac{(1 - x)x}{t} + 2\right\}.$$

The solution tends to zero as $t \to \infty$, and the right-hand side is bounded in $S(0, 1)$. However, the second and higher derivatives of u with respect to t are unbounded as $t \to \infty$.

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zero, then $v_{ij} = v((i-1)\Delta x, \; j\Delta t)$, $i = 1, 2, \ldots, n$, $j = 0, 1, 2, \ldots, p$, $pt < t_{max}$, $\Delta x = 1/(n-1)$, and $\sigma = \Delta t/\Delta x^2$. If $\boldsymbol{v}_j$ denotes the vector with components v_{ij}, $i = 1, 2, \ldots, n$, then the Crank Nicolson difference equation can be written

$$\boldsymbol{v}_{i+1} = \boldsymbol{v}_i + \sigma\{\theta M_i \boldsymbol{v}_{+1} + (1-\theta)M\boldsymbol{v}_i\} \tag{2.1}$$

where θ is a positive constant $\geqslant \frac{1}{2}$,

$$M = \begin{bmatrix} -2+2a_{11}\Delta x & 2 & & & \\ 1 & -2 & 1 & & \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ & & 1 & -2 & 1 \\ & & & 2 & -2-2a_{11}\Delta x \end{bmatrix} \tag{2.2}$$

and $a_{12} = a_{22} = 1$ for simplicity. If a_{12} and/or a_{22} equals zero then it is necessary to delete the row and column of (2.2) which contains a_{11} and/or a_{21} and to substitute $\Delta x = 1/(n+1)$ or $1/n$ as appropriate. If $a_{12} = 0$ then $v_{ij} = v(i\Delta x, j\Delta t)$.

Equation (2.1) can be put in the form

$$\boldsymbol{v}_{i+1} = C(\Delta t)\boldsymbol{v}_i + \{I - \sigma\theta M\}^{-1}\boldsymbol{f}_i \tag{2.3}$$

where

$$C(\Delta t) = \{I - \sigma\theta M\}^{-1}\{I + \sigma(1-\theta)M\} \tag{2.4}$$

and $\boldsymbol{f}_i$ takes account both of the inhomogeneous term $f(x, t)$ and the boundary conditions. Note that C depends on Δt through its dependence on σ, and also (in practice) through a functional relationship that ensures that $\Delta x \to 0$ when $\Delta t \to 0$.

Remark. The case $\Delta t \to 0$, $\Delta x =$ constant could be considered. It is simpler than the more general case, and convergence, if it can be proved, is to the solution of the system of ordinary differential equations obtained by finite difference approximation to equation (1.1) in the x direction only. Here it is assumed that

$$\Delta x = O(\Delta t).$$

To define stability it is necessary to define the norms used. Here we use the euclidean vector norm

$$||\boldsymbol{v}||_D = \Delta x^{1/2}\sqrt{(\boldsymbol{v}^T\boldsymbol{v})} \tag{2.5}$$

where $\Delta x \to 0$ as the dimension of $\boldsymbol{v}$ tends to ∞. The subordinate matrix norm is defined by

$$||A||_D = \max_x \left\{\frac{\boldsymbol{x}^T A^T A \boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}}\right\}^{1/2}. \tag{2.6}$$

The following Lemma is a consequence of this definition.

Lemma 2.1. Let the matrix A be symmetric, and let μ be the eigenvalue of largest modulus of A. Then

$$||A||_D = |\mu| \tag{2.7}$$

if D be a diagonal matrix then

$$||D||_D = \max_i |d_i|. \tag{2.8}$$

It is convenient to refer to the eigenvalue of largest modulus of an arbitrary square matrix A as the spectral radius of A, and to denote this by $\rho(A)$. If A is symmetric then Lemma 2.1 can be stated

$$||A||_D = |\mu| = \rho(A). \tag{2.9}$$

To measure solutions to the differential equation we use the L_2-norm

$$||u||_C = \left\{\int_0^1 u^2 dx\right\}^{1/2} \tag{2.10}$$

(The norm subscripts stand for Continuous and Discrete.) Let $u(x)$ be any bounded function. Then $||u||_C$ is bounded. Let $\boldsymbol{u}$ be the vector $\boldsymbol{u}^T = [u(x_1), \ldots u(x_n)]$, then $||\boldsymbol{u}||_D$ is also bounded. Further, with any vector $\boldsymbol{v}$ such that $||\boldsymbol{v}||_D$ is finite can be associated a function $v(x, \Delta)$ such that, for $x_{i-1} < x < x_{i+1}$,

$$v(x, \Delta) = v_i + (x - x_i)\frac{v_{i+1} - v_i}{\Delta x} \tag{2.11}$$

Lemma 2.2

$$||u(x, \Delta)||_C < K||\boldsymbol{u}||_D \tag{2.12}$$

Proof. We have

$$\begin{aligned} ||u(x, \Delta)||_C^2 &\leqslant \sum_{i=1}^{n-1}\left\{\frac{\Delta x}{2}(u_i^2 + {}_i^2u_{+1}) + \frac{\Delta x^3}{6}\left(\frac{u_{i+1} - u_i}{\Delta x}\right)^2\right\} \\ &\leqslant 2\Delta x \sum_{i=1}^{n} u_i^2 \end{aligned} \tag{2.13}$$

which gives the desired result with $K = \sqrt{2}$.

Definition 1. The family of operators $C(\Delta t)$ is *stable of order* α, if

$$||C(\Delta t)^i||_D \leqslant K_1 p^\alpha \tag{2.14}$$

for $i = 1, 2, \ldots, p$ as $\Delta t \to 0$, where K_1 is a constant.

Remark. If $\alpha = 0$ in (2.14), then the family of operators $C(\Delta t)^i$, $i = 1, 2, \ldots, p$ is uniformly bounded as $\Delta t \to 0$. In this case we speak of *stability*. In the above definition we follow Strang (1960).

Definition 2. Let u be a solution to the differential equation. The difference approximation is *consistent of order* β if

$$\begin{aligned} p^\beta||\boldsymbol{u}_{i+1} - C(\Delta t)\boldsymbol{u}_i - \{I - \sigma\theta M\}^{-1}\boldsymbol{f}_i||_D \\ = p^\beta||\boldsymbol{E}_i||_D \leqslant K_2 \end{aligned} \tag{2.15}$$

where K_2 is constant.

Theorem 2.1. If the difference approximation is stable of order α and consistent of order $\beta > \alpha + 1$, then $v_i(x, \Delta)$ converges to u in the L_2-norm.

Proof. We have

$$\boldsymbol{u}_{i+1} = C(\Delta t)\boldsymbol{u}_i + \{I - \sigma\theta M\}^{-1}\boldsymbol{f}_i + \boldsymbol{E}_i \tag{2.16}$$

so that, if $\boldsymbol{e}_i = \boldsymbol{u}_i - \boldsymbol{v}_i$,

$$\boldsymbol{e}_{i+1} = C(\Delta t)\boldsymbol{e}_i + \boldsymbol{E}_i = \boldsymbol{E}_i + C\boldsymbol{E}_{i-1} + \ldots + C^i\boldsymbol{E}_0 \tag{2.18}$$

We have

$$\begin{aligned} ||\boldsymbol{e}_{i+1}||_D &\leqslant (i+1)p^{\alpha-\beta}K_1K_2 \\ &\leqslant p^{\alpha+1-\beta}K_1K_2 \end{aligned} \tag{2.19}$$

so that

$$||e_i||_D \to 0, \Delta t \to 0, i = 1, 2, \ldots, p. \tag{2.20}$$

Now

$$\begin{aligned}||u(x, t_i) - v_i(x, \Delta)||_C &\leqslant ||u(x, t_i) - u_i(x, \Delta)||_C + ||u_i(x, \Delta) - v_i(x, \Delta)||_C \\ &\leqslant ||u(x, t_i) - u_i(x, \Delta)||_C + K||e_i||_D\end{aligned}$$

by Lemma 2.2, whence

$$\max_i ||u(x, t_i) - v_i(x, \Delta)||_C \to 0 \qquad i = 1, 2, \ldots, p, \Delta t \to 0 \tag{2.21}$$

Note. This result requires that

$$||u(x, t_i) - u_i(x, \Delta)||_C \to 0, i = 1, 2, \ldots, p$$

as $\Delta t \to 0$. This is obviously true if $u(x, t)$ is a solution to the differential equation in the ordinary sense.

3. The stability question

A detailed verification of the stability of the difference equation will now be given. We require certain preliminary results.

Theorem 3.1. Let $H(\Delta t)^i$ be such that

(i) H is similar to a symmetric matrix H^*,
(ii) the matrix T of the similarity transformation satisfies

$$||T|| \; ||T^{-1}|| \leqslant Kp^\alpha,$$

(iii) $\rho(H) \leqslant 1 + O(\Delta t)$,

then $H(\Delta t)$ is stable of order α.

Proof. We have

$$H^{*i} = TH^iT^{-1} \tag{3.1}$$

whence

$$\begin{aligned}||H^i||_D &\leqslant ||H^{*i}||_D||T||_D||T^{-1}||_D \\ &\leqslant \rho(H)^i||T||_D||T^{-1}||_D\end{aligned} \tag{3.2}$$

by Lemma 2.1. Thus

$$||H^i||_D \leqslant e^{Lt_{max}} Kp^\alpha \tag{3.3}$$

where L is an upper bound for $\{\rho(H) - 1\}/\Delta t$ and is finite by assumption (iii). This completes the proof.

Lemma 3.1. (Keast and Mitchell (1967)). Let W be a diagonal matrix with positive elements such that WH is symmetric then $W^{1/2}HW^{-1/2}$ is symmetric.

Corollary. Let $P(H)$ be a rational matrix function of H, then $W^{1/2}P(H)W^{-1/2}$ is symmetric.

Lemma 3.2. Let

$$W = \begin{bmatrix} 1/2 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1/2 \end{bmatrix} \tag{3.4}$$

then

(i) WM is symmetric, whence $W^{1/2}CW^{-1/2}$ is symmetric, and

(ii) $||W^{1/2}||_D||W^{-1/2}||_D = \max_{s,t} \sqrt{\frac{W_s}{W_t}} = \sqrt{2}$

Lemma 3.3. The spectral radius of C satisfies

$$\rho(C) = 1 + O(\Delta t) \tag{3.5}$$

Remark. For this result the following properties of the eigenproblem of M are required.

(i) The $\lambda_i(M)$ are bounded above.
(ii) Let $\lambda_1(M)$ be the algebraically largest eigenvalue, then $\Delta x^{-2}\lambda_1(M) \to K$ as $\Delta x \to 0$ (see, for example, Keller (1965)).
(iii) At most two eigenvalues can be positive, and $\Delta x^{-2}\lambda_n(M)$ is unbounded below as $\Delta x \to 0$ where $\lambda_n(M)$ is the algebraically smallest eigenvalue.

Proof. The eigenvalues of C are given by

$$\lambda_i(C) = \frac{1 + \sigma(1 - \theta)\lambda_i(M)}{1 - \sigma\theta\lambda_i(M)}. \tag{3.6}$$

The choice $\theta \geqslant 1/2$ ensures that $|\lambda_n(C)| < 1$ independent of θ. The properties of the eigenproblem of M summarised above show that Δt can be chosen small enough to ensure that $1 - \sigma\theta\lambda_i(M)$ is positive independent of Δx, and in this case all the eigenvalues of C lie on the branch of the curve $y = \dfrac{1 + (1 - \theta)x}{1 - \theta x}$ to the left of $x = 1/\theta$. On this branch y decreases monotonically as $x \to -\infty$. Thus we have either

$$\rho(C) \leqslant 1 \tag{3.7}$$

or

$$\rho(C) = |\lambda_1(C)| \tag{3.8}$$

so that the desired result follows as $\sigma\theta\lambda_1(M) = O(\Delta t)$.

Theorem 3.2. The difference scheme defined by equations (2.3) and (2.4) is stable.

Proof. This is a consequence of Theorem 3.1 and Lemmas 3.1 to 3.3 which show that stability of order zero obtains (that is the difference approximation is stable in the usual sense).

Note. The Crank Nicolson formula is clearly consistent of order $\beta = 3$ for sufficiently smooth initial and boundary conditions so that Theorem 2.1 provides a convergence result. Its scope includes all the cases called unstable by Keast and Mitchell.

4. A more general differential equation

The results of the previous section extend readily to the more general equation defined on $S(0, 1)$

$$\frac{\partial u}{\partial t} = \xi(t)\eta(x)\left\{\frac{\partial^2 u}{\partial x^2} + \alpha(x)\frac{\partial u}{\partial x} + \beta(x)u\right\} + f(x, t) \tag{4.1}$$

subject to an appropriate initial condition and the separated boundary conditions (1.2). It is assumed that $G > \xi(t)$, $\eta(x) > 0$ for some finite G and all x, t in $S(0, 1)$, and that $\alpha(x)$ and $\beta(x)$ are bounded. It is assumed that all functions are smooth enough for the solution u to satisfy appropriate consistency conditions in R.

In this case the Crank Nicolson difference scheme becomes

$$v_{i+1} = v_i + \sigma\{\theta\xi_{i+1}NMv_{i+1} + (1-\theta)\xi_i NMv_i\} \quad (4.2)$$

where $\xi_i = \xi(i\Delta t)$, N is a diagonal matrix with elements $N_j = \eta(x_j)$, and (assuming as before that $a_{12} = a_{22} = 1$) M is given by

$$M = \begin{bmatrix} M_1 & 2 & & & & \\ 1-\frac{\alpha_2\Delta x}{2} & -2+h^2\beta_2 & 1+\frac{\alpha_2\Delta x}{2} & & & \\ & \cdot & \cdot & \cdot & \cdot & \\ & & 1-\frac{\alpha_{n-1}\Delta x}{2} & -2+h^2\beta_{n-1} & 1+\frac{\alpha_{n-1}\Delta x}{2} \\ & & & 2 & M_n \end{bmatrix} \quad (4.3)$$

where

$$M_1 = -2 + \Delta x^2\beta_1 + 2\Delta x a_{11}\left(1 - \frac{\Delta x\alpha_1}{2}\right)$$

and

$$M_n = -2 + \Delta x^2\beta_n - 2\Delta x a_{21}\left(1 + \frac{\Delta x\alpha_n}{2}\right).$$

Let D be a diagonal matrix such that DM is symmetric. An appropriate form for D is

$$D_1 = 1/2,$$

$$D_2 = \frac{1}{1 - \frac{\alpha_2\Delta x}{2}}, \ldots$$

$$D_{i+1} = \frac{1 + \frac{\alpha_i\Delta x}{2}}{1 - \frac{\alpha_{i+1}\Delta x}{2}} D_i, \ldots$$

$$D_n = \frac{1}{2}\left(1 + \frac{\alpha_{n-1}\Delta x}{2}\right)D_{n-1}. \quad (4.4)$$

It will be seen that

$$D_i \to \exp\left\{\int_0^{x_i}\alpha(s)ds\right\} \quad (4.5)$$

as $\Delta x \to 0$.

From equation (4.2) we have

$$v_{i+1} = C_i(\Delta t)v_i + \{I - \sigma\theta\xi_{i+1}NM\}^{-1}f_i \quad (4.6)$$

where $C_i(\Delta t)$ is given by

$$C_i(\Delta t) = \{I - \sigma\theta\xi_{i+1}NM\}^{-1}\{I + \sigma(1-\theta)\xi_i NM\}$$
$$i = 1, 2, \ldots, p-1. \quad (4.7)$$

Let

$$W = N^{-1}D. \quad (4.8)$$

From the corollary to Lemma 3.1 it follows that

$$\bar{C}_i(\Delta t) = \prod_{j=1}^{i} C_j(\Delta t) \quad (4.9)$$

is similar to a symmetric matrix under transformation by $W^{1/2}$. Thus

$$||\bar{C}_i(\Delta t)||_D \leq \prod_{j=1} \rho(C_j) \max_{s,\,t} \sqrt{\left(\frac{W_s}{W_t}\right)}. \quad (4.10)$$

Lemma 3.3 applies also in this case, and we see (using equation (4.5)) that the difference equation is again stable of order zero (i.e. stable).

Thus there is essentially nothing new in the case when the coefficients α and β in the differential equation are bounded. A more interesting example is the heat conduction equation in cylindrical geometry. In this case the differential equation is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{1}{x}\frac{\partial u}{\partial x}. \quad (4.11)$$

M is the matrix (Albasiny (1960))

$$M = \begin{bmatrix} -4 & 4 & & & & \\ 1/2 & -2 & 3/2 & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & \frac{2n-5}{2n-4} & -2 & \frac{2n-3}{2n-4} \\ & & & & 2 & -2-2a_{21}\Delta x \end{bmatrix} \quad (4.12)$$

and an appropriate form for D is

$$D_1 = (\Delta x)^2/2,\ D_i = 4x_i\Delta x,\ i = 2, \ldots, n-1$$
$$D_n = 2\Delta x - \Delta x^2. \quad (4.13)$$

We have $W = D$, so that

$$||W^{\frac{1}{2}}||_D||W^{-\frac{1}{2}}||_D = \sqrt{[8(n-2)]} \quad (4.14)$$

giving *stability of order* 1/2 on our assumption that $\Delta x = O(\Delta t)$. It is not difficult to show that the difference approximation is consistent of order 2 (Albasiny (1960)), so that Theorem 2.1 again provides a convergence theorem.

5. The eigenfunction expansions

It is readily verified by separation of variables that equation (1.1) subject to homogeneous boundary conditions and the initial condition $u(x, 0) = f(x)$ has the solution

$$u(x, t) = \sum_{i=1}^{\infty} a_i\phi_i(x)e^{-\lambda_i t} \quad (5.1)$$

where the λ_i and ϕ_i, $i = 1, 2, \ldots$, are the eigenvalues and eigenfunctions of the problem

$$\frac{d^2\phi}{dx^2} + \lambda\phi = 0 \tag{5.2}$$

$$a_{11}\phi(0) + a_{12}\phi^{(1)}(0) = 0$$
$$a_{21}\phi(1) + a_{22}\phi^{(1)}(1) = 0 \tag{5.3}$$

and where

$$a_i = \int_0^1 f(x)\phi_i(x)dx \Big/ \int_0^1 \phi_i^2(x)dx \tag{5.4}$$

in particular

$$u(x, t) \to a_1\phi_1(x)e^{-\lambda_1 t} \tag{5.5}$$

as $t \to \infty$, where λ_1 is the algebraically least of the eigenvalues. Thus $u \to \pm\infty$, $a_1\phi_1(x)$, or 0 as $t \to \infty$, depending on whether $\lambda_1 < 0$, $= 0$, or > 0 respectively.

Note. In the case $\lambda_1 < 0$ it is possible to talk of the instability of the differential equation.

A corresponding expansion can be given for the difference equation. Setting

$$\boldsymbol{v}_0 = \begin{bmatrix} f(x_1) \\ \cdot \\ \cdot \\ \cdot \\ f(x_n) \end{bmatrix} \tag{5.6}$$

then

$$\begin{aligned} \boldsymbol{v}_i &= C^i\boldsymbol{v}_0 \\ &= C^iTT^{-1}\boldsymbol{v}_0 \\ &= T\Lambda(C)^iT^{-1}\boldsymbol{v}_0 \end{aligned} \tag{5.7}$$

where $\Lambda(C)$ is the diagonal matrix formed by the eigenvalues of C. Setting

$$\boldsymbol{a}^* = T^{-1}\boldsymbol{v}_0 \tag{5.8}$$

equation (5.7) can be written

$$\boldsymbol{v}_i = \sum_{j=1}^{n} a_j^*\lambda_j(C)^i\kappa_j(T) \tag{5.9}$$

where $\kappa_j(T)$ denotes the jth column of T.

Let

$$t_n(g) = \Delta x\{\tfrac{1}{2}g(x_1) + g(x_2) + \ldots + g(x_{n-1}) + \tfrac{1}{2}g(x_n)\} \tag{5.10}$$

then

$$a_j^* = t_n(fX_j)/t_n(X_j^2) \tag{5.11}$$

where

$$\boldsymbol{\chi}_j = \kappa_j(T)$$

and χ_j can be thought of as a function of x which interpolates the components of $\boldsymbol{\chi}_j$.

In this case it will be seen (using equation (3.5)) that $\boldsymbol{v}_i \to \pm\infty$, $a_1^*\kappa_1(T)$, or 0 as $i \to \infty$ depending on whether $\lambda_1(M) > 0$, $= 0$, or < 0 respectively. It will now be shown that as $i \to \infty$, $u(x, t_i)$ and $\boldsymbol{v}_i$ both either diverge or tend to a finite limit or to zero together independent of the mesh chosen (as the mesh is refined this is a consequence of the convergence theorem). It is required to show that $\lambda_1 < 0, = 0, > 0 \Rightarrow \lambda_1(M) > 0$, $= 0$, < 0 respectively, independent of Δx.

Remark. It is easy to show that $\lambda_1 = 0$ implies that M has a zero eigenvalue for in this case the solution to equation (3.2) must have the form $\phi_1(x) = A + Bx$, and this satisfies the difference equations exactly.

Consider now the principal minors of $\mu I - M$. These form a Sturm sequence. Therefore the number of changes in sign in this sequence for $\mu = 0$ gives the number of positive eigenvalues of M. The sequence is

$$\begin{aligned} P_0 &= 1 \\ P_1 &= 2 - 2a_{11}\Delta x \\ P_2 &= 2(2 - 2a_{11}\Delta x) - 2 = 2 - 4a_{11}\Delta x \\ &\cdots\cdots\cdots \\ P_{n-1} &= 2 - 2(n-1)a_{11}\Delta x \\ P_n &= 4a_{21}\Delta x - 4a_{11}\Delta x - 4a_{21}a_{11}(n-1)\Delta x^2. \end{aligned}$$

Using $\Delta x = 1/(n-1)$, the conditions that M has no positive eigenvalues are that

$$\begin{aligned} &\text{(i) } 1 - a_{11} > 0, \text{ and} \\ &\text{(ii) } a_{21} - a_{11} - a_{21}a_{11} > 0 \end{aligned} \tag{5.13}$$

The striking feature of these conditions is that they are independent of Δx. Now, because $-\Delta x^{-2}\lambda_1(M) \to \lambda_1$ as $\Delta x \to 0$ (Keller (1965)), they apply also to the differential equation eigenvalue problem (5.2), (5.3), and the stated result follows from this.

Remarks

(i) I am indebted to Dr. P. Keast for pointing out that a result equivalent to (5.13) is given for the difference approximation in Keast and Mitchell (1967), and for the differential equation in Copson and Keast (1966). Keast and Mitchell use these results to discuss the stability (in their terminology) of both systems. Although their results are similar to those obtained here, the emphasis is somewhat different. The above derivation of equation (5.13) is more direct.

(ii) The result on the equivalent behaviour of the difference approximation and the differential equation cannot be expected to hold for the more general equation (4.1). In this case the equivalence need only obtain as $\Delta x \to 0$, so that finite difference computations with finite Δx could produce misleading results. Campbell and Keast (1968) have given formulae generalising equation (5.13) in this case.

For the heat conduction equation it is unlikely that $\lambda_1 < 0$ in practice. The examples of Parker and Crank correspond to the case $\lambda_1 = 0$ so that $\phi_1(x) = A + Bx \Rightarrow X_1(x)$, and a^* is obtained by evaluating the integrals defining a_1 (equation (5.4)) using the trapezoidal rule. If f is sufficiently smooth, or if f has only jump discontinuities and these occur at mesh points, then the persistent discretisation error is $O(\Delta x^2)$. However, if f has a discontinuity at a non-mesh point then the persistent discretisation error is $O(\Delta x)$.

It can be expected that the requirement for the discontinuity to be at a mesh point could be difficult to satisfy unless formulae permitting the use of graded meshes in the x direction are available. Appropriate formulae have been derived by Dr. R. S. Anderssen and the author and will be the subject of a future paper.

It may be noted that we have shown that for the heat conduction equation subject to homogeneous boundary conditions such that $\lambda_1 = 0$.

(i) the solution is bounded as $t \to \infty$, and

(ii) the solution is approached *for all t* by the solution of the Crank Nicolson scheme as $\Delta t \to 0 (=\rangle\ \Delta x \to 0)$.

In this case $\rho(C) = 1$ independent of Δt, in contradiction of the stated necessary condition of Gary (1966).

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