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'HALF-BREED' METHOD APPLIED TO PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

BY

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Introduction

Partial differential equations (p.d.e's) are frequently solved numerically by methods that replace the partial derivatives in the p.d.e and its boundary conditions by their finite differences and then solve the resulting (often linear) equations. The original 'finite difference' method was simple in principle and as a result was applicable to a variety of p.d.e's, see SMITH[3]. Boundary conditions were readily incorporated and the stability of the method was studied and understood. An early refinement was the well known Crank-Nicolson method which is often very effective. More recently variations based on rational approximations to the matrix exponential function have been investigated by Lawson & Morris[2],Gourlay & Morris[1], Twizell & Khaliq[4]. However,the more refinements that are introduced the less simple becomes the method, and as a result the ease with which the method can be applied and the flexibility for incorporating the boundary conditions suffer. Finite difference methods consume considerable computer time, although this is often not considered a draw back, but more seriously they do not indicate the analytic basis of the solution. This frequently inhibits further analytic development. An analytic solution, on the other hand, can often be obtained by separating the variables and solving the resulting Sturm-Liouville problem. The convergence of such solutions should be established, then this analytic solution is readily computed for any particular values of the variables. However, the eigenvalues may be difficult to locate accurately and often the fitting of the boundary conditions requires treatment particular to the problem under consideration. In order to fit the boundary conditions it may be necessary to calculate the coefficients in the Fourier series numerically.

In this paper we will show that the 'finite difference' method is related to the 'separating the variables' method and that there is a way of combining the advantages of both. Finite difference techniques will be used to incorporate the boundary conditions, and yet the final solution of the p.d.e will have an analytic character. The method we develop treats one variable analytically while applying the finite difference techniques to the other variables. In our problems the time variable is treated analytically, while the space derivatives are replaced by finite differences. The solutions obtained, in the limit, tend to the solutions that would be obtained by separating the variables. Further they throw light on the nature of solutions obtained by the finite difference method.

One Dimensional Parabolic Equation.

The parabolic equation for conduction in one space variable is

$$\frac{\partial t}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad 0 < x < 1, \quad t > 0 \tag{1}$$

Dividing the interval $0 \le x \le 1$ into $N + 1$ steps of length h, we replace the space derivative in (1) by the finite difference approximation

$$\frac{\partial^2 u}{\partial x^2} \simeq \frac{1}{h^2}\left\{u(x-h,t) - 2u(x,t) + u(x+h,t)\right\}, \tag{2}$$

and apply the resulting equation to all interior mesh points at time t

With appropriate boundary conditions, the problem then reduces to solving the set of linear differential equations

$$\frac{du(t)}{dt} = A\underline{u}(t) \tag{3}$$

where A is a $N \times N$ square matrix and $\underline{u}(t)$ gives the values of the temperature u_{ih} at time t at the discretised value ih of x

This equation (3) has solution

$$\underline{u}(t) = e^{tA}\underline{u}(0) \tag{4}$$

where $e^{tA} = I + tA + \frac{t^2}{2!}A^2 \ldots + \frac{t^n}{n!}A^n + \ldots$.

Set $\underline{u}(t) - Lv(t)$, where L is composed of the eigenvectors of A

$$L\underline{v}(t) = e^{tA} L\underline{V}(0)$$

$$\underline{v}(t) = L^{-1} e^{tA} L\underline{V}(0)$$

Writing $L^{-1}AL = B \equiv \begin{bmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_N \end{bmatrix}$, $L^{-1} e^{tA} L = e^{tB}$

so that $$\underline{v}(t) = e^{tB}\,\underline{V}(0)$$

$$= \begin{bmatrix} e^{t\lambda_1} & & & 0 \\ & e^{t\lambda_2} & & \\ & & \ddots & \\ 0 & & & e^{t\lambda_N} \end{bmatrix} \cdot \underline{v}(0) \qquad (5)$$

where all the eigenvalues λ_r will in fact be negative, and

$|\lambda_1| < |\lambda_2| \; . \; . \; . < |\lambda_N|$.

From (5) $$v_r(t) = e^{t\lambda_r} v_r(0) \qquad r = 1 \; .. \; N \; .$$

and hence $$\underline{u}(t) = L \begin{bmatrix} e^{t\lambda_1} v_1(0) \\ e^{t\lambda_2} v_2(0) \\ - \; - \; - \\ e^{t\lambda_N} v_N(0) \end{bmatrix} \qquad (6)$$

In particular with boundary values u = 0 at x = 0 and x = 1, A is the

symmetric matrix $$\frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & & 1 & \\ & & & \ddots & & \\ & & & & & \\ & & & 1 & & -2 \end{bmatrix} \qquad (7)$$

the eigenvalues are $\lambda_r = -\frac{4}{h^2}\sin^2\frac{\pi r h}{2}$, and the eigenfunctions are

$\sin(\pi r h)i$ (8)

With h = 0.1 so that N = 9,

$$\lambda_1 = -\frac{4}{.01}\sin^2\frac{\pi}{20} \simeq -9.8, \text{ while } \lambda_2 \simeq -38.2$$

hence $$\underline{u}(t) \simeq L \begin{bmatrix} e^{t\lambda_1} v_1(0) \\ 0 \\ - \; - \; - \; - \\ 0 \end{bmatrix} = e^{t\lambda_1} \frac{v_2(0)}{|\underline{\ell}_2|} \begin{bmatrix} \ell_{11} \\ \ell_{21} \\ \\ \ell_{N1} \end{bmatrix}$$

certainly for $t > 0.25$. $\underline{\ell}_1$ is the eigenvector corresponding to λ_1, and consequently the first column of L is the normalised vector $\frac{\underline{\ell}_1}{|\underline{\ell}_1|}$.

Since $\underline{v}(t) = L^T\underline{u}(t)$,

$$v_1(0) = \frac{1}{|\underline{\ell}_1|} \sum \ell_{i1} u_i(0)$$

And

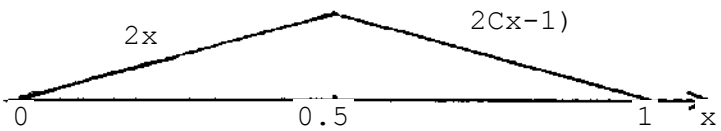
$$\underline{u}(t) \simeq e^{t\lambda_1} \frac{1}{|\underline{\ell}_1|^2} \sum \ell_{i1} u_i(0) \underline{\ell}_1 \qquad (9)$$

This clearly demonstrates the asymptotic behaviour of the solution, not only does it decay exponentially with time t in a manner determined by the eigenvalue λ_1 , but also along a time row it is proportional to the eigenvector $\underline{\ell}_1$. corresponding to λ_1.

When applied to the problem of computing the solution of the p.d.e.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

given u = 0 on x = 0 and x - 1 , and the initial condition



This solution (9) gave similar values to those obtained using the Crank-Nicolson Method (see example 2.2, p.21 Smith [3]) even at t = 0.1. The solution is considerably improved by halving h.

The advantages of the solution (6) given by this 'half-breed' method when it is compared to:

a) the original 'finite difference' method, is that it retains the analytic character of the solution and it can be readily computed at any time t.

b) the 'separation of variables' method, is that the eigenvalues of A can be computed by standard computer packages.

It however remains to be seen how easy It Is to incorporate the boundary conditions . Many methods of solving p.d.e's that have been proposed in the literature do not explain how to extend chem to deal with awkward boundary conditions. Yet the ease with which the boundary conditions are incorporated is a major test of the flexibility of a method.

Here the boundary conditions will be replaced, where appropriate, by finite difference approximations. We indicate the method by extending the above analysis to incorporate boundary conditions of the form $\frac{\partial u}{\partial x} = bu$ at both $x = 0$ and $x = 1$.

<u>Boundary Conditions of the form</u> $\frac{\partial u}{\partial x} = bu$

The boundary condition at x = 0, using a central difference approximation, Is

$$\frac{u_h(t) - u_{-h}(t)}{2h} = b_0 u_0(t) \quad \text{or} \quad u_{-h} = u_{-h} - 2hb_0 u_0 \quad .$$

This relation can be used to rewrite the equation

$$\frac{du_0}{dt} = \frac{1}{h^2}\left[u_{-h} - 2u_0 + u_h\right]$$

as

$$\frac{du_0}{dt} = \frac{1}{h^2}\left[-2(1+hb_0)\,u_0 + 2u_h\right] \quad . \tag{10}$$

Similarly the boundary condition at x — 1 gives $u_{1+h} = u_{1-h} + 2hb_1u_1$

$$\frac{du_1}{dt} = \frac{1}{h^2}\left[u_{1-h} - 2u_1 + u_{1+h}\right]$$

$$= \frac{1}{h^2}\left[2u_{1-h} - 2(1-hb_1)\,u_1\right]. \tag{11}$$

The heat equation written as a set of simultaneous differential equations

$$\frac{du_{ih}}{dt} = \frac{1}{h^2}\left[u_{(i-1)h} - 2u_{ih} + u_{(i+1)h}\right]$$

then becomes

$$\frac{d\underline{u}(t)}{dt} = \frac{1}{h^2}\begin{bmatrix} -2(1+hb_0) & 2 & & & \\ 1 & -2 & 1 & & \\ & & \ddots & & \\ & & 1 & -2 & 1 \\ & & & 2 & -2(1-hb_1) \end{bmatrix}\begin{bmatrix} u_0(t) \\ u_h(t) \\ \vdots \\ u_{1-h}(t) \\ u_1(t) \end{bmatrix}$$

$$\text{or}\ \frac{d\underline{u}(t)}{dt} = \frac{1}{h_2} A\ \underline{u}(t) \tag{12}$$

The matrix A can be made symmetric by a similarity transformation with a diagonal matrix D

$$D^{-1}AD = \begin{bmatrix} \frac{1}{\sqrt{2}} & & & & 0 \\ & 1 & & & \\ & & \cdot & & \\ & & & 1 & \\ 0 & & & & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} -2(1+hb_0) & 2 & & & \\ 1 & -2 & 1 & & \\ & \cdot & \cdot & \cdot & \\ & & -2 & 1 & \\ & & 2 & -2(+-hb_1) & \end{bmatrix} \begin{bmatrix} \sqrt{2} & & & & 0 \\ & 1 & & & \\ & & \cdot & & \\ & & & 1 & \\ 0 & & & & \sqrt{2} \end{bmatrix}$$

$$\begin{bmatrix} -2(1+hb_0) & \sqrt{2} & & & \\ \sqrt{2} & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \cdot & \cdot & \\ & 1 & -2 & \sqrt{2} & \\ & & \sqrt{2} & -2(1-hb_1) & \end{bmatrix} \tag{13}$$

Hence setting u(t)= DL*v(t) =Lv(t)

$$DL^{*}\frac{d\underline{v}(t)}{dt} = \frac{1}{h^2}ADL^{*}\underline{v}(t)$$

$$\frac{d\underline{v}(t)}{dt} = L^{*T}\frac{1}{h^2}(D^{-1}AD)L^{*}\underline{v}(t) \tag{14}$$

Forming L^{*} from the normalized eigenvectors of the symmetric matrix

$\frac{1}{h^2}D^{-1}AD$.

$$\frac{D\underline{v}(t)}{dt} = \begin{bmatrix} \lambda_1 & & & & & & 0 \\ & \lambda_2 & & & & & \\ & & \lambda_3 & & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ 0 & & & & & & \lambda_n \end{bmatrix} \underline{v}(t) \tag{15}$$

where n=N+2 .

All the eigenvalues λ_r are still nagative and ordered, λ_1 being the Smallest in magnitude . Thus

$$v_r(t) = e^{t\lambda_r} v_r^{(0)} \quad r = 1,\ldots,n.$$

Hence

$$u(t) = DL^{*} \begin{bmatrix} e^{t\lambda_1} v_2(0) \\ e^{t\lambda_2} v_2(0) \\ \cdot \quad \cdot \\ e^{t\lambda_n} v_n(0) \end{bmatrix} \underline{\sim} DL^{*} \begin{bmatrix} e^{t\lambda_1} v_1(0) \\ 0 \\ \cdot \quad \cdot \\ (0) \end{bmatrix} \tag{16}$$

for sufficiently large values of t.

The eigenvalues of A and D^{-1} AD are the same, while the eigenvectors are different but closely related. In fact if $\underline{\ell}_r$ is an eigenvector of A

$$\underline{\ell}_r^{*} = D^{-1} \underline{\ell}_r \tag{17}$$

is an eigenvector of D^{-1} AD. The columns of L^{*} are the vectors $\dfrac{\underline{\ell}_r^{*}}{|\underline{\ell}_r^{*}|}$

With the vectors $\underline{\ell}_r^{*}$, rather than $\underline{\ell}_r$, normalised we find

$$\underline{v}(t) = L^{*T} D^{-1} \underline{u}(t) = L^{*T} \begin{bmatrix} \frac{1}{\sqrt{2}} u_0 \\ u_h \\ \cdot \quad \cdot \quad \cdot \\ u_{1-h} \\ \frac{1}{\sqrt{2}} u_1 \end{bmatrix} \tag{18}$$

In particular $v_1(0) = \dfrac{1}{|\underline{\ell}_1^{*}|}\left[\dfrac{1}{2}(\ell_{11} u_0(0) + \ell_{n1} u_1(0)) \sum_{i=2}^{n-1} \ell_{i1} u(i-1)h(0)\right]$

and thus for sufficiently large values of t

$$\underline{u}(t) \underline{\sim} e^{t\lambda_1} v_1(0)\, D \frac{\underline{\ell}_1^{*}}{|\underline{\ell}_1^{*}|}$$

$$= e^{t\lambda_1} \frac{1}{|\underline{\ell}_1^{*}|^2} \left[\frac{1}{2}(\ell_{11} u_0(0) + \ell_{n1} u_1(0)) + \sum_{i=2}^{n-1} \ell_{i1} u(i-1)h(0)\right] \underline{\ell}_1 \quad . \tag{19}$$

For some numerical problems this solution will be adequate. Its analytic nature for large t is a bonus. To calculate this solution we require the eigenvalue λ_l and the corresponding eigenvector $\underline{\ell}_1$ of A, or alternatively $\underline{\ell}_l^*$ of D^{-1} AD. λ_l can be found either (a) from the boundary conditions, as in the following example, and $\underline{\ell}_1$ can be deduced analytically, or (b) λ_l and $\underline{\ell}_l^*$ can be calculated numerically from D^{-1} AD.

In general to obtain a solution with sufficient accuracy a number of eigenvalues and their corresponding eigenvectors must be calculated, and this will usually be most simply performed using matrix routines on the symmetric matrix D^{-1} AD.

The following problem is used to illustrate finite difference methods in Example 2.3, p.30 Smith [3]. We have calculated the approximate solution (19) for this problem and find that it gives comparable accuracy to the Crank—Nicolson method for $t \geq \frac{1}{4}$.

$$\left.\begin{array}{lll} \text{Solve} & \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} & \\ \text{initial conditions} & u = 1 \text{ for } 0 \leq x \leq 1 & \text{when } t = 0 \\ \text{boundary conditions} & \dfrac{\partial u}{\partial x} = u & \text{at } x = 0 \text{ for all } t \\ & \dfrac{\partial u}{\partial x} = -u & \text{at } x = 1 \text{ for all } t. \end{array}\right\} \qquad (20)$$

The eigenvectors of A are the solutions of the system of equations

$$v_{i-1} - (2 + \lambda) v_i + v_{i+1} = 0 \qquad i = 0(1)N+1$$

with the boundary conditions

$$v_{-1} = v_1 - 2hv_0 \qquad (21)$$
$$v_{N+2} = v_N - 2hv_{N+1} \qquad (22)$$

There is symmetry about $x = \frac{1}{2}$, so we put $2 + \lambda = 2\cos\alpha h$ and

$$v. \propto \cos\alpha(ih - \frac{1}{2})$$

The boundary conditions (21) and (22) are then satisfied if α is such that

$$\tan \frac{\alpha}{2} = \frac{h}{\sin\alpha i} \quad . \tag{23}$$

With $h = 0.1$ the value of α is 1.3081 $\ell_{i1} = \cos\alpha(ih - \frac{1}{2})$ and

$$\lambda_1 = \frac{2}{h_2}(\cos\alpha c - 1) = -\frac{4}{h_2}\sin^2\frac{\alpha h}{2} = -\frac{4}{(0.1)^2}\sin^2\frac{\alpha}{20} = -1.7088 \ .$$

This analysis establishes the character of the solution (19). When more than one eigenvalue is required it is usually best to calculate the eigenvalues and eigenvectors of A numerically.

We find in (19)

$$|\ell_2^*|^2 = 8.6701 \quad \text{and} \quad \frac{1}{2}(\ell_{01} + \ell_{10,1}) + \sum_{i=1}^{9} \ell_{i1} = 9.2888$$

and hence

$$u_i(\frac{1}{2}) = e^{\lambda_1/4}\ 1.0714\ell_{il} = 0.6989\ \ell_{il}$$

$$u_i(1) = e^{\lambda_1}\ 1.0714\ \ell_{il} = 0.1940\ \ell_{il} \ .$$

These solutions are now compared to the analytic solution of (20) for $i = 0(1)5$:

$u_i(\frac{1}{2})$	0.5547	0.6054	0.6457	0.6751	0.6929	0.6989
Analytic Soln.	0.5546	0.6052	0.6454	0.6747	0.6924	0.6984
$u_i(1)$	0.1540	0.1680	0.1792	0.1874	0.1924	0.1940
Analytic Soln.	0.1542	0.1682	0.1794	0. 1875	0.1925	0.1941

The first approximation (19) to the solution seems to be useful for $t \geq 1/4$ in this particular problem. Normally (19) is useful only at rather larger values of t. To deal with small values of t higher approximations to (16) must be calculated.

Conclusion

The half-breed method of solving p.d.e's developed in this paper

a) produces a sequence of approximations to the solution which is essentially analytic but readily suited to the use of standard numerical procedures for calculating the eigenvalues and eigenvectors.

b) expresses the asymptotic behaviour for large t in terms of the largest eigenvalue λ_1 and its eigenvector $\underline{\ell}_1$.

Many extensions of the method are possible, some of which are under investigation. This paper simply establishes the basis.

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