A Comparison of Approximation Methods for the Convection-Diffusion Equation

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Abstract

The solutions to partial differential equations can be modeled in several ways. As an example, we will investigate the solution of the convection-diffusion equation. Unfortunately, the approximations used to study these often yield highly non-normal matrices. Consequently, we will look at the eigenvalues of the continuous problem and compare them to those of the matrix approximations based on the method of finite differences. Next, we present numerical evidence to show that the forward approximation provides a better model for computer based calculation than the continuous solution.

The problem

Imagine that a uniformly dense rod of length 1 is placed on the x-axis at the origin. Further imagine that an initial temperature distribution is placed on the rod and that the ends are kept at 0°. The diffusion of the heat through the rod is modeled by the equation

$$u_t = u_{xx}$$
$$u(0,t) = u(1,t) = 0\,, \qquad u(x,0) = f(x)$$

which has solutions of the form

$$u(x,t) = \sum_{n=1}^{\infty} c_n e^{-n^2\pi^2\,t}\sin(n\,\pi\,x)$$

where c_n is given by $2\int_0^1 f(x)\sin(n\,\pi\,x)dx$; see Braun[4].

The situation becomes more complicated when the possibility of convection is taken into account. The equation for this problem is

$$u_t = u_{xx} + Cu_x \qquad \text{for} \quad C \in I\!R$$
$$u(0,t) = u(1,t) = 0\ , \qquad u(x,0) = f(x).$$

We solve this problem by using the method of separation of variables, which assumes that the solution can be written as the product of two functions

$$u(x,t) = X(x)T(t).$$

The derivatives become $u_x = X'(x)T(t)$,$u_{xx} = X''(x)T(t)$ and $u_t = X(x)T'(t)$. This leads to the reformulation of the above differential equation as

$$XT' = X''T + CX'T$$

or, equivalently

$$\frac{T'}{T} = \frac{X'' + CX'}{X}.$$

Since the left hand side is a function of t alone and the right hand side is a function of x alone, we have that these functions are equal to a constant,

$$\frac{T}{T'} = \lambda = \frac{X'' + CX'}{X},$$

which allows us to write them as two ordinary differential equations

$$T' = \lambda T \quad \text{and} \quad X'' + CX' - \lambda X = 0.$$

The solutions of these equations are of the form

$$T = e^{\lambda t} \quad \text{and} \quad X = \alpha e^{r_1 x} + \beta e^{r_2 x}$$

where r_1,r_2 are the roots of the characteristic equation $R^2 + CR - \lambda = 0$ and α, β are constants. The roots r_1 and r_2 satisfy

$$r_1 + r_2 = -C \tag{1}$$

$$r_1 r_2 = -\lambda \tag{2}$$

Imposing the boundary conditions $X(0) = X(1) = 0$ gives

$$\alpha + \beta = 0$$

$$\alpha e^{r_1} + \beta e^{r_2} = 0.$$

Therefore, $e^{r_1} = e^{r_2}$ and so $r_1 - r_2 = 2\pi i n$ for n an integer. Squaring this yields

$$r_1^2 - 2r_1 r_2 + r_2^2 = -4\pi^2 n^2.$$

On the other hand, squaring (1) gives

$$r_1^2 + 2r_1r_2 + r_2^2 = C^2.$$

Upon subtraction we get

$$4r_1r_2 = C^2 + 4\pi^2 n^2,$$

and from (2) we conclude that

$$\lambda_n = -C^2/4 - \pi^2 n^2, \tag{3}$$

are the eigenvalues of $X'' + CX' - \lambda X = 0, X(0) = X(1) = 0$. To obtain the corresponding eigenfunctions, we recall from the equation $R^2 + CR - \lambda = 0$ that

$$r_1 = \frac{-C - \sqrt{C^2 + 4\lambda}}{2}, \qquad r_2 = \frac{-C + \sqrt{C^2 + 4\lambda}}{2}$$

or after using (3),

$$r_1 = -\frac{C}{2} + \pi i n, \qquad r_2 = -\frac{C}{2} - \pi i n.$$

Thus

$$X(x) = \alpha e^{r_1 x} + \beta e^{r_2 x} = \gamma e^{Cx/2} \sin(n\pi x)$$

for any constant γ. Therefore, a solution of the convection-diffusion equation has the form

$$U_n(x,t) = X_n(x)T_n(t) = c_n e^{\lambda_n t} e^{-Cx/2} \sin(n\pi x) \quad \text{for} \quad n \in I\!N.$$

By taking linear combinations of these, we arrive at the following series solution,

$$u(x,t) = X(x)T(t) = \sum_{n=1}^{\infty} c_n e^{\lambda_n t} e^{-Cx/2} \sin(n\pi x)$$

where the c_n's are obtained from the initial condition. By setting t=0 we have

$$f(x) = \sum_{n=1}^{\infty} c_n e^{-Cx/2} \sin(n\pi x).$$

Proceeding as in Braun [p. 457] we conclude that

$$c_n = 2 \int_0^1 f(x) e^{-Cx/2} \sin(n\,\pi\,x) dx.$$

Unfortunately, for large values of C, the eigenfunctions are close to being dependent as figure 1 shows below. Consequently, the coefficients c_n may be large for large values of C, making it difficult to represent the solutions accurately on a computer.

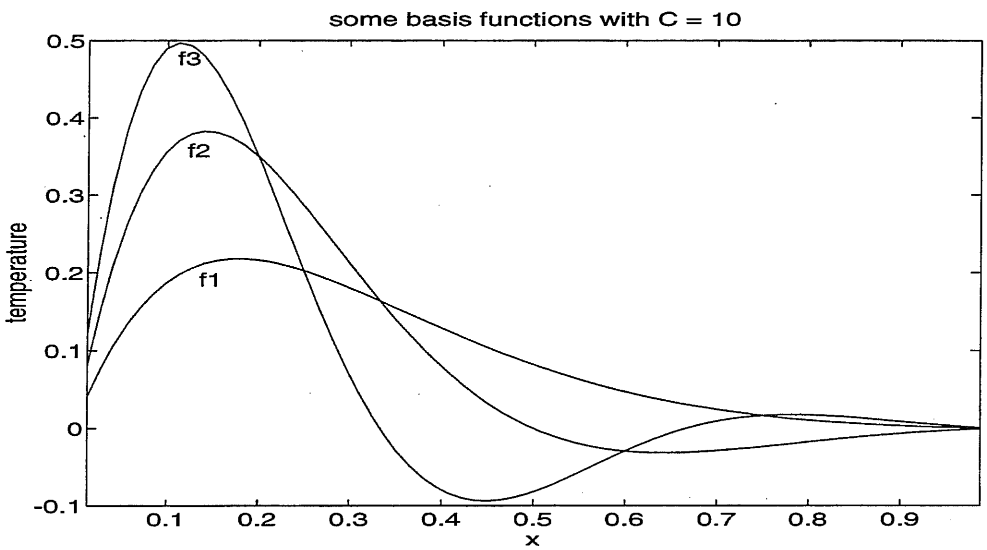

figure 1

For example, with initial heat distribution given by $f(x) = x(1-x)$ and convection coefficient $C = 75$, the continuous problem requires 80 basis eigenfunctions to produce the 3-D surface shown in figure 2.

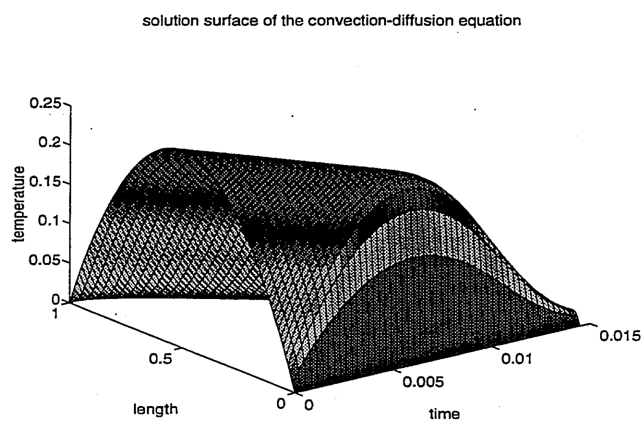

figure 2

Therefore, we look for numerical approximations to the above equations that may provide a better basis for representing the solutions of these equations. In particular, we will implement the method of finite differences which gives three separate estimates to the first derivative. To facilitate our study of these approximations, we will first calculate the eigenvalues of each and then compare them to those of the continuous equation.

The matrix eigenvalues

The method of finite differences first requires us to subdivide the interval (0,1) into $n+1$ equally spaced intervals of length h. The forward approximation to the derivative at each point $x_j \in (0,1)$ is given by

$$u'_+ = \frac{1}{h}(u(x_{j+1}) - u(x_j)) = \frac{1}{h}(u_{j+1} - u_j)$$

The backward and central approximations are

$$u'_- = \frac{1}{h}(u_j - u_{j-1}) \quad \text{and} \quad u'_c = \frac{1}{2h}(u_{j+1} - u_{j-1})$$

respectively. To compute the second derivative we will use the forward and backward approximations giving

$$u'' \approx \frac{u'_+ - u'_-}{h} = \frac{\frac{1}{h}(u_{j+1} - u_j) - \frac{1}{h}(u_j - u_{j-1})}{h} = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}.$$

These approximations combine to give three estimates

$$u_{xx} + Cu_x \approx u'' + Cu'_+$$
$$u_{xx} + Cu_x \approx u'' + Cu'_c$$
$$u_{xx} + Cu_x \approx u'' + Cu'_-$$

to the above differential equation. The eigenvalues of the forward or upwind estimate are computed by setting

$$u'' + Cu'_+ = \lambda u$$

so,

$$\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + \frac{C}{h}(u_{j+1} - u_j) = \lambda u_j.$$

Multiplying by h^2 and collecting like terms leads to

$$u_{j+1}(1 + hC) - u_j(2 + hC + h^2\lambda) + u_{j-1} = 0.$$

The substitution $u_j = r^j$ leads to the equation

$$r^2(1 + hC) + r(2 + hC + h^2\lambda) + 1 = 0,$$

which has roots r_1, r_2 such that

$$r_1 r_2 = \frac{1}{1 + hC} \quad \text{and} \quad r_1 + r_2 = \frac{2 + hC + h^2\lambda}{1 + hC}.$$

Consequently, by taking linear combinations of these roots, we get that

$$u_j = \alpha r_1^j + \beta r_2^j \qquad \alpha, \beta \in I\!R$$

$$u_0 = \alpha + \beta = 0$$

which implies that

$$u_{n+1} = \alpha(r_1^{(n+1)} - r_2^{(n+1)}) = 0$$

$$\left(\frac{r_1}{r_2}\right)^{n+1} = r_1^{2(n+1)}(1+hC)^{n+1} = 1$$

which, by finding the $2(n+1)^{st}$ roots of unity, give

$$r_1 = (1+hC)^{-\frac{1}{2}}\left(\cos\left(\frac{k\pi}{n+1}\right) + i\sin\left(\frac{k\pi}{n+1}\right)\right) \qquad k = 1, 2, 3 \ldots n$$

and

$$r_2 = (1+hC)^{-\frac{1}{2}}\left(\cos\left(\frac{k\pi}{n+1}\right) - i\sin\left(\frac{k\pi}{n+1}\right)\right) \qquad k = 1, 2, 3 \ldots n.$$

However, the conditions above imply that

$$r_1 + r_2 = 2(1+hC)^{-\frac{1}{2}}\left(\cos\left(\frac{k\pi}{n+1}\right)\right) = \frac{2 + hC + h^2\lambda}{1+hC}.$$

This equation when solved for λ yields

$$\lambda_{k+} = \frac{2\sqrt{1+hC}\cos\left(\frac{k\pi}{n+1}\right) - (2+hC)}{h^2} \qquad k = 1, 2, 3 \ldots n$$

as the finite difference approximation to the eigenvalues using the forward estimate for the first derivative. Similar calculations for the center and backward difference approximations give

$$\lambda_{kC} = \frac{\sqrt{2-hC}\sqrt{2+hC}\cos\left(\frac{k\pi}{n+1}\right) - 2}{h^2} \qquad k = 1, 2, 3 \ldots n$$

and

$$\lambda_{k-} = \frac{2\sqrt{1-hC}\cos\left(\frac{k\pi}{n+1}\right) - (2-hC)}{h^2} \qquad k = 1, 2, 3 \ldots n$$

respectively.

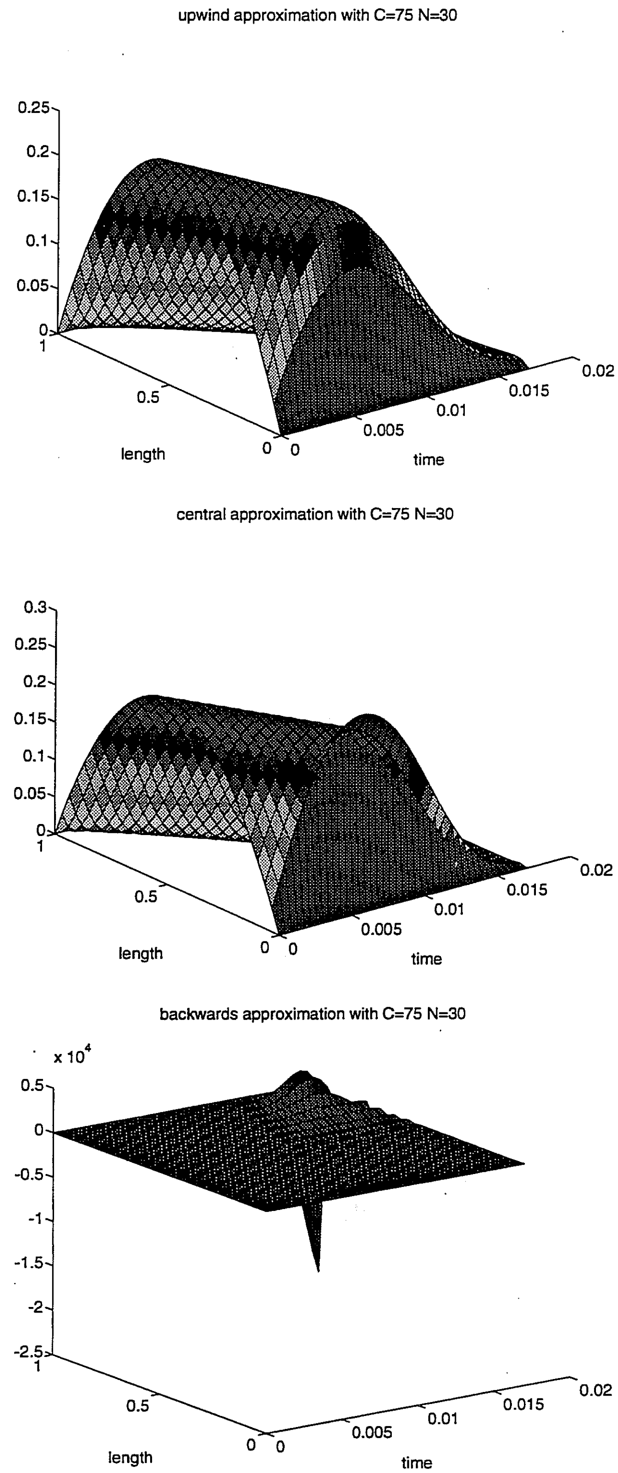

figure 3

Upon examination of these values we notice that the central and backwards approximations will give complex eigenvalues for large C. This is unfortunate since the true eigenvalues are never complex. The effect is noticeable when these different approximations are implemented on a computer. For example, consider the matrix approximations with convection term C equal to 75. Then, as the graphs in figure 3 demonstrate, both the backwards and central approximations are inaccurate for matrices of size 30×30.

On the other hand, the forward approximation does quite well when compared to the actual solution in figure 1. To understand this, we compare the coefficients of the approximation to those of the actual solution.

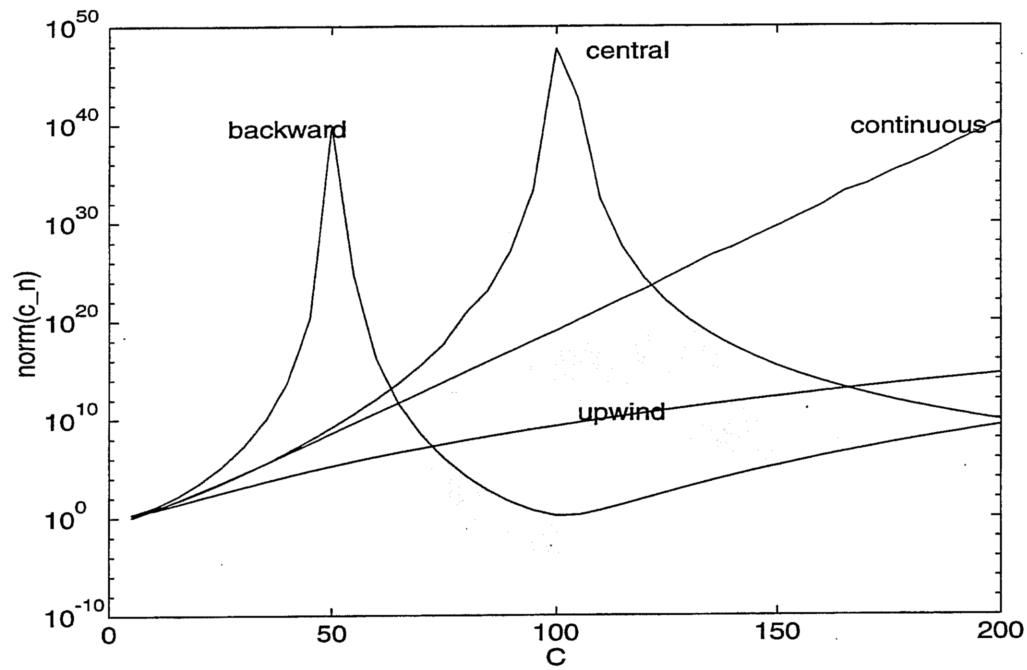

figure 4

Examination of the basis coefficients

When evaluating the series solution of this differential equation it is necessary to compute the coefficients c_n in the expansion

$$f(x) = \sum_{n=1}^{\infty} c_n e^{-Cx/2} \sin(n\pi x). \tag{4}$$

Similarly, the discrete case corresponds to expansions of the form

$$\vec{f} = \sum_{n=1}^{N} c_n \vec{V}_n \tag{5}$$

where $\vec{V}_n$ are the eigenvectors of the discrete approximation. In this section we demonstrate numerically that the coefficients ,c_n, corresponding to the continuous solution (4) are in general larger than the coefficients of the upwind approximation (5). This leads us to believe that upwind discretization provides a better conditioned basis for numerical work than does the analytic solution.

In figure 4 we show the norms of the coefficient vectors as a function of C for $N = 50$. As the figure demonstrates, the central and backwards approximation have coefficients that grow even faster than the continuous case and become infinite at the point where the eigenvalues become complex. This causes their coefficients to become complex as well. Consequently, these approximations are no good for computational use and we will focus our attention to the upwind estimate from now on.

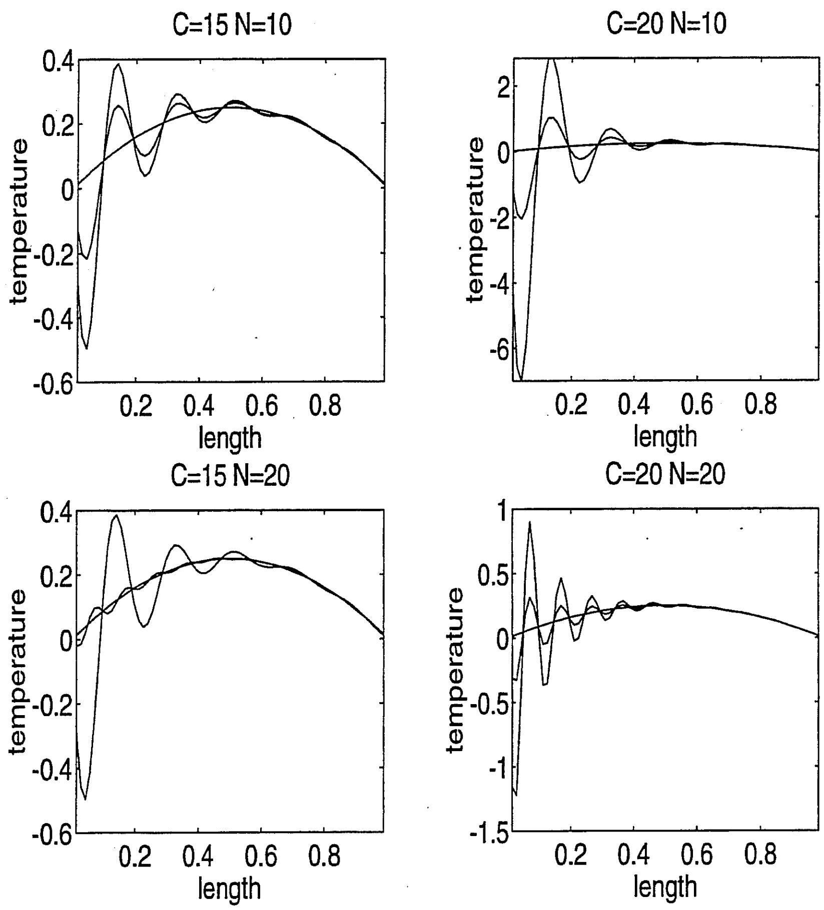

figure 5

The striking behavior in figure 4 of the upwind approximation is representative of the conditioning for this basis. This figure clearly shows the exponential growth of the coefficients and what looks like e^{C^m}, growth for the upwind approximation with $0 < m < 1$. This, in addition to the behavior of the upwind eigenvalues, leads us to believe that this method provides a better basis for modeling the solution. Confirmation of this is given empirically by figure 5 which show linear combinations of N basis functions and basis vectors to approximate the initial condition $f(x) = x(1-x)$.

In each of these pictures,the bigger oscillations correspond to the eigenfunctions of the continuous problem and the smaller oscillations to the eigenvectors of the upwind approximation. A better estimate of the initial condition is provided by the eigenvectors rather than the eigenfunctions, which is a direct consequence of the smaller coefficients necessary to represent the solution in the upwind case. We therefore conclude that because the degree of non-normality is much less severe in the discrete case than in the continuous case that the upwind numerical approximation gives a better representation for computational work.

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References

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[2] Satish C.Reddy, Lloyd N. Trefethen,Dimpy Pathria, Pseudospectra of the Convection-Diffusion Operator.