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NOTE

A Technique for Treating Dirichlet Conditions at Infinity in Numerical Field Problems

The simplest numerical treatment of Dirichlet boundary conditions at infinity is to assume that the solution takes a sufficiently accurate approximation to its asymptotic value on the boundary of a finite domain which is covered by a suitable grid. Probably only a small part of the domain is of primary interest where the solution is varying quite rapidly and, therefore, the mesh size must be small here. The rest of the domain may be covered by a coarser grid. In the technique described here, this latter part of the domain is transformed. The resulting transformed region is covered by a uniform grid which gives a graded grid in the original region. The remaining part of the domain, which is of primary interest, is covered by a uniform grid. By a suitable choice of transformation and grid sizes it is possible to match the two parts of the domain by a simple overlap method if the equations involve only first and second differences. The truncation error of the method is smaller than that obtained using a graded mesh from the start and setting up suitable difference equations and, unlike mesh doubling techniques, the method gives tridiagonal matrices.

As a simple example, we describe the technique for the parabolic equation

$$\frac{\partial u}{\partial t} = a\,\frac{\partial^2 u}{\partial x^2} + b\,\frac{\partial u}{\partial x} \tag{1}$$

for the domain $\infty > x \geqslant 0$, $t \geqslant 0$. $a(>0)$ and $b(>0)$ are constants and the boundary conditions are: $u(x, 0)$ known for $x \geqslant 0$, $u(0, t)$ known for $t > 0$ and $u(\infty, t) = 0$ for $t \geqslant 0$.

We divide the semi-infinite line $x \geqslant 0$ into two parts, $0 \leqslant x < 1$ and $x \geqslant 1$. For $x \geqslant 1$, we change the independent variable using the transformation $z = z(x)$, where $z(x)$ is a real differentiable monotonic increasing function of x with a unique inverse $x = x(z)$ for all $x \geqslant 1$. We also assume that $z(x) \to z_\infty$ as $x \to \infty$ where z_∞ is finite. $dz(x)/dx$ may be considered as a function of z. We write

$$f(z(x)) = \frac{dz(x)}{dx} \tag{2}$$

when, for $x \geqslant 1$, we have $f(z(x)) > 0$.

Equation (1) thus becomes

$$\frac{\partial u}{\partial t} = af(z)\frac{\partial}{\partial z}\left(f(z)\frac{\partial u}{\partial z}\right) + bf(z)\frac{\partial u}{\partial z}. \tag{3}$$

We first replace equations (1) and (3) by a partial discretization leaving time as a continuous variable. For $0 \leqslant x \leqslant 1$, we approximate to (1) using a mesh length h with $Nh = 1$ for some integer N. The grid points are $x_i = ih$, $i = 0, 1 \ldots N$ and the partial difference approximation to (1) is

$$\frac{du_i}{dt} = \frac{a}{h^2}(u_{i+1} - 2u_i + u_{i-1}) + \frac{b}{2h}(u_{i+1} - u_{i-1}), \qquad i = 1, 2\ldots(N-1), \tag{4}$$

where $u_i(t)$ is the approximation to $u(x_i, t)$ and $u_0(t) \equiv u(0, t)$.

For $x \geqslant 1$ we approximate to (3). On the z line we use a mesh length k defined by

$$k = z(x_N) - z(x_{N-1}). \tag{5}$$

The grid points on the z line are

$$z_i = z(x_N) + (i - N)k, \qquad N - 1 \leqslant i \leqslant M, \tag{6}$$

where M is the largest integer satisfying

$$M \leqslant \frac{z_\infty - z(x_N)}{k} + N. \tag{7}$$

From (5) and (6), it follows that $x_{N-1} = x(z_{N-1})$ and $x_N = x(z_N)$ and thus the two grids overlap. On the x line, we further define $x_i = x(z_i)$ for $N + 1 \leqslant i \leqslant M$, unless equality is satisfied in (7) when x_M is not defined.

Equation (3) is replaced by

$$\frac{du_i}{dt} = \frac{a}{k^2}f_i(f_{i+1/2}(u_{i+1} - u_i) - f_{i-1/2}(u_i - u_{i-1})) + \frac{bf_i}{2k}(u_{i+1} - u_{i-1}), \tag{8}$$

$$i = N, (N+1), \ldots (M-1),$$

where again $u_i(t)$ is the approximation to $u(x_i, t)$ and $f_i = f(z_i)$. The boundary condition is taken as $u_M = 0$. If equality is satisfied in (7) this is the exact infinity boundary condition of the problem, alternatively x_M must be sufficiently large to ensure that the approximation $u_M = 0$ to the condition $u(\infty, t) = 0$ is adequate.

Equations (4) and (8) form a set of $M - 1$ ordinary differential equations and can be integrated by one of the usual methods for parabolic equations.

Truncation Error

The truncation error introduced by replacing (1) by (4) is $O(h^2)$. By the Mean Value Theorem, it follows from (5) that

$$k = hf(z_\theta) \qquad \text{where} \quad z_{N-1} < z_\theta < z_N \tag{9}$$

The truncation error, involved in replacing (3) by (8), which can be found by Taylor series, is

$$-k^2 \cdot \left\{ \frac{af}{24} \cdot \left[\frac{\partial^3}{\partial z^3} \left(f \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial z} \left(f \frac{\partial^3 u}{\partial z^3} \right) \right] + \frac{bf}{6} \cdot \frac{\partial^3 u}{\partial z^3} \right\}_{z=z_i} + O(k^4) = O(h^2) \tag{10}$$

In the usual method of dealing with a graded mesh we replace (1) by

$$\frac{\partial u_i}{\partial t} = \frac{2a}{h_i + h_{i-1}} \left(\frac{u_{i+1} - u_i}{h_i} - \frac{u_i - u_{i-1}}{h_{i-1}} \right) + b \left(\frac{u_{i+1} - u_{i-1}}{h_i + h_{i-1}} \right) \tag{11}$$

where the grid points are x_i , $i = 0, 1, \ldots$ and $h_i = x_{i+1} - x_i$. The truncation error is

$$-\frac{a}{3} \cdot (h_i - h_{i-1}) \left(\frac{\partial^3 u}{\partial x^3} \right)_{x_i} - \frac{b}{2} \cdot (h_i - h_{i-1}) \left(\frac{\partial^2 u}{\partial x^2} \right)_{x_i} + O(h^2) \tag{12}$$

where $h = \max(h_{i-1}, h_i)$. This is considerably larger than (10), h_i may be quite large and $f(z)$ is a well behaved function. Brown [1] shows that if the changes in mesh size in (11) are gradual then the truncation error is $O(h^2)$. From (12) we can see that this requires $h_i - h_{i-1} = O(h^2)$ which is not satisfied for the grid points occuring in the following numerical cases.

Numerical Cases

If $u(x, 0) = 0$ for $x \geqslant 0$, $u(0, t) = 1$ for $t > 0$ and $a = 1$, $b = 0.5$, the solution of (1) is

$$u(x, t) = \frac{1}{2} \cdot \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} + \frac{\sqrt{t}}{4} \right) + \frac{1}{2} e^{-\frac{1}{2}x} \operatorname{erfc} \left(\frac{x}{2\sqrt{t}} - \frac{\sqrt{t}}{4} \right)$$

where

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-x^2} \, dx$$

The technique was tested with $h = 0.1$ using the Crank–Nicholson method with time step 0.005. In Table I we illustrate three different choices of $z(x)$. In all cases

TABLE I

$z(x)$	$-1/x$	$-1/(1+x)^2$	$-e^{-x}$
k	0.11111	0.02701	0.03869
x_M	∞	11.01	3.929
E_1	18	4	9
E_2	69	47	194

$M = 19$. $E_1 \times 10^{-5}$ and $E_2 \times 10^{-5}$ are the maximum absolute errors at time $t = 1.0$ for $x < 1$ and $x \geqslant 1$ respectively. If a constant mesh size $h = 0.1$ is used and $u(2.0, t) = 0$ is taken as the boundary condition, $E_1 = 1800$.

Extension to Higher Dimensions and Orders

There is no difficulty in extending the method to problems in two or more dimensions. For example, the author has applied it to an elliptic problem in the (x, y) plane using the transformations $z = z(x)$ for $x \geqslant 1$ and $w = w(y)$ for $y \geqslant 1$. This does not give a conformal transformation but is useful in providing closely spaced points in the x-direction near $y = 0$, and in the y-direction near $x = 0$.

If differences of higher order than two are used (so that more than three points in each space direction are involved in the difference equations) the simple matching technique used here is not applicable and it is necessary to use special difference formulae near the change in grids.

Reference

1. R. R. Brown, *J. Soc. Indust. Appl. Math.* **10**, 475 (1962).

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